



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 06:48 PM EDT

PDB ID : 4LT8
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-07-23
Resolution : 3.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

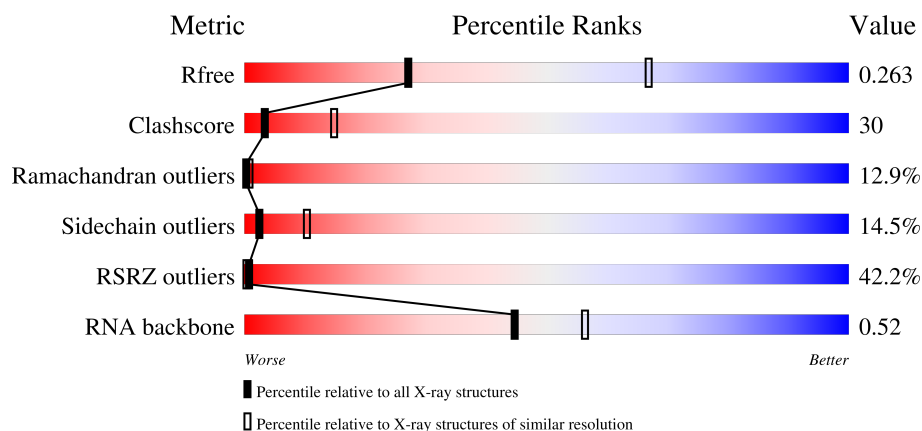
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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}	164625	2149 (3.18-3.10)
Clashscore	180529	2290 (3.18-3.10)
Ramachandran outliers	177936	2178 (3.18-3.10)
Sidechain outliers	177891	2178 (3.18-3.10)
RSRZ outliers	164620	2149 (3.18-3.10)
RNA backbone	3690	1020 (3.40-2.88)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div>29%</div> <div>50% 37% 10% ..</div> </div>
1	XA	1522	<div> <div>25%</div> <div>50% 37% 11% ..</div> </div>
2	QB	256	<div> <div>70%</div> <div>17% 58% 16% • 7%</div> </div>
2	XB	256	<div> <div>71%</div> <div>17% 59% 16% • 7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QY	17	
23	XY	17	
24	QX	25	
24	XX	25	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	Z8	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3222	-	-	-	X
57	MG	YA	3120	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called messenger RNA.

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

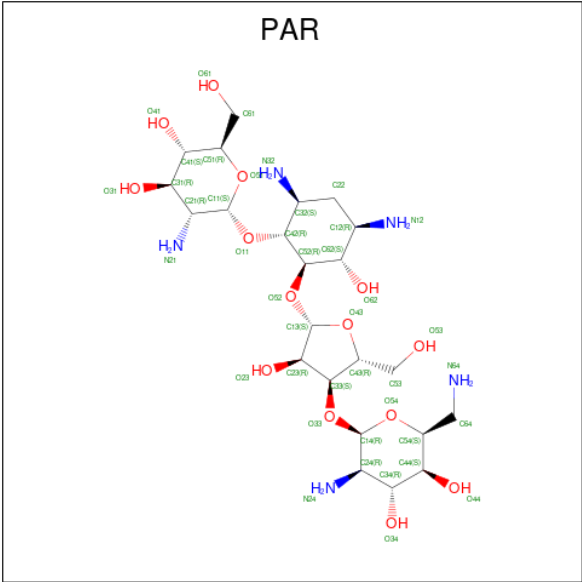
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	69	Total	Mg	0	0
			69	69		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RA	240	Total 240	Mg 240	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	XA	74	Total 74	Mg 74	0	0
57	XV	2	Total 2	Mg 2	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	265	Total 265	Mg 265	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YE	2	Total 2	Mg 2	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0

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



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

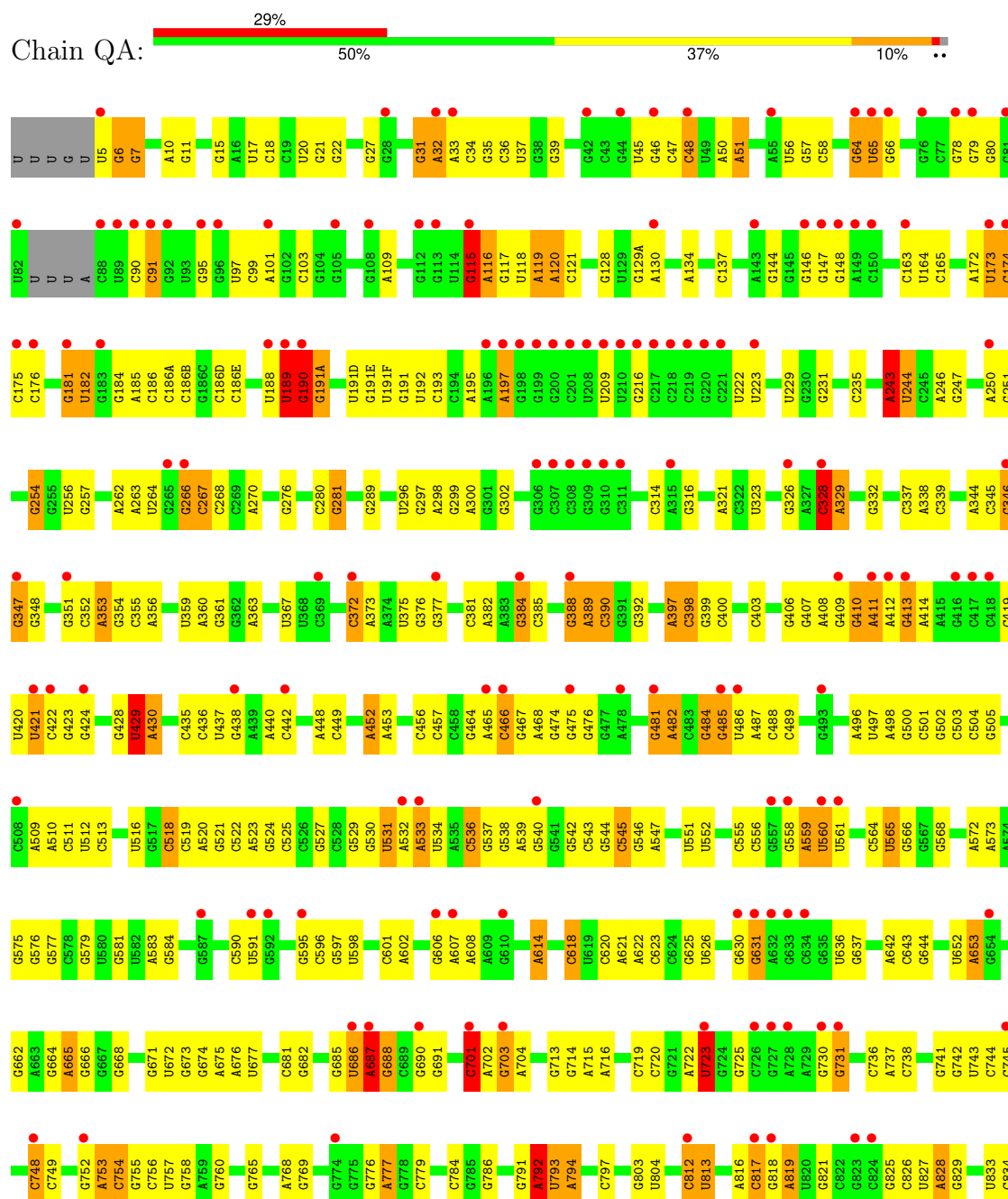
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

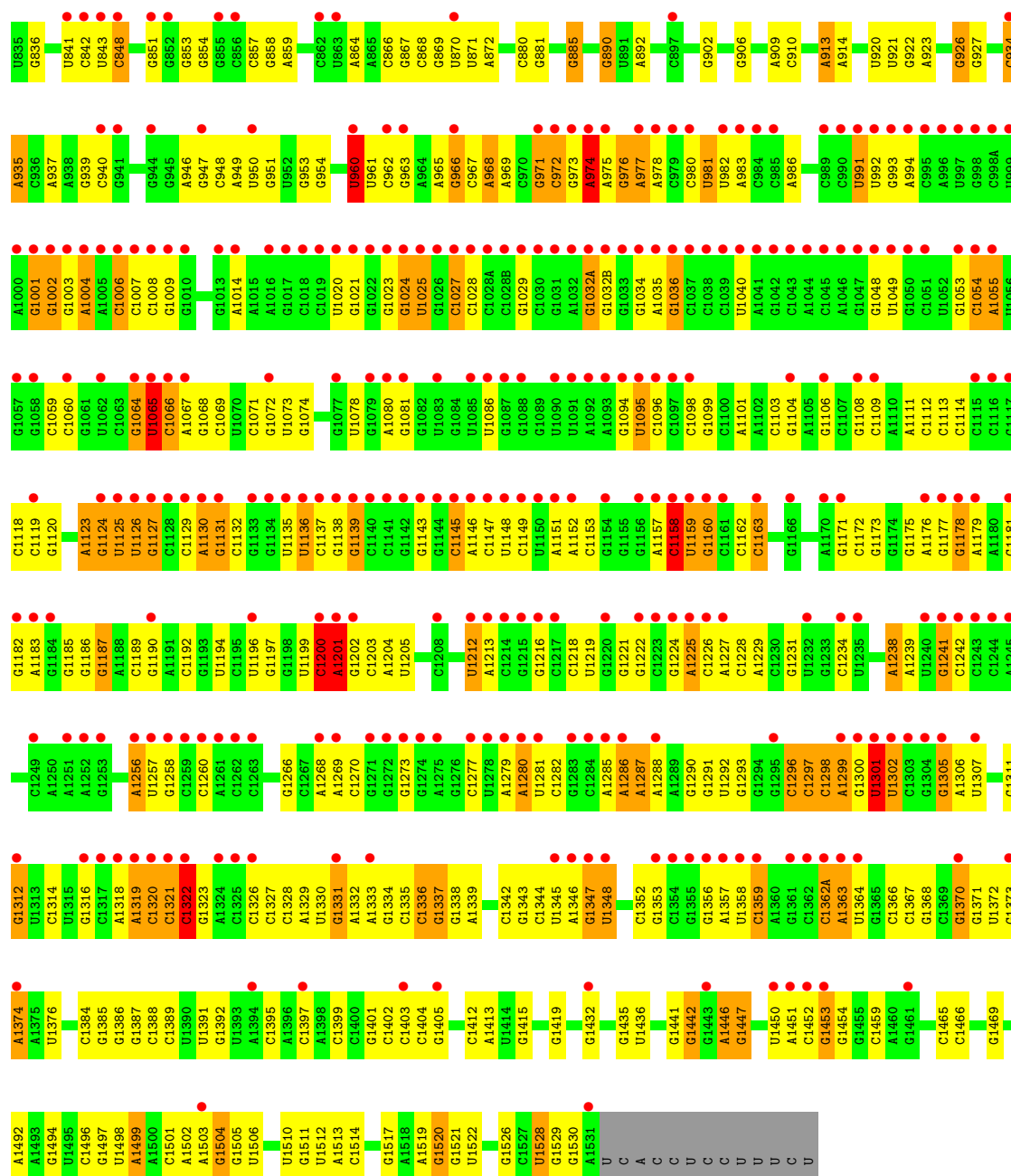
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QD	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XD	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

3 Residue-property plots [i](#)

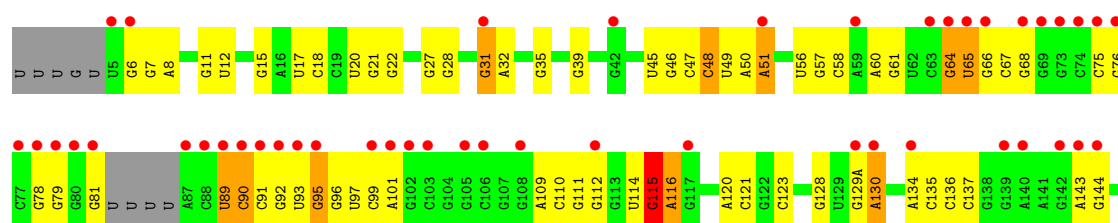
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

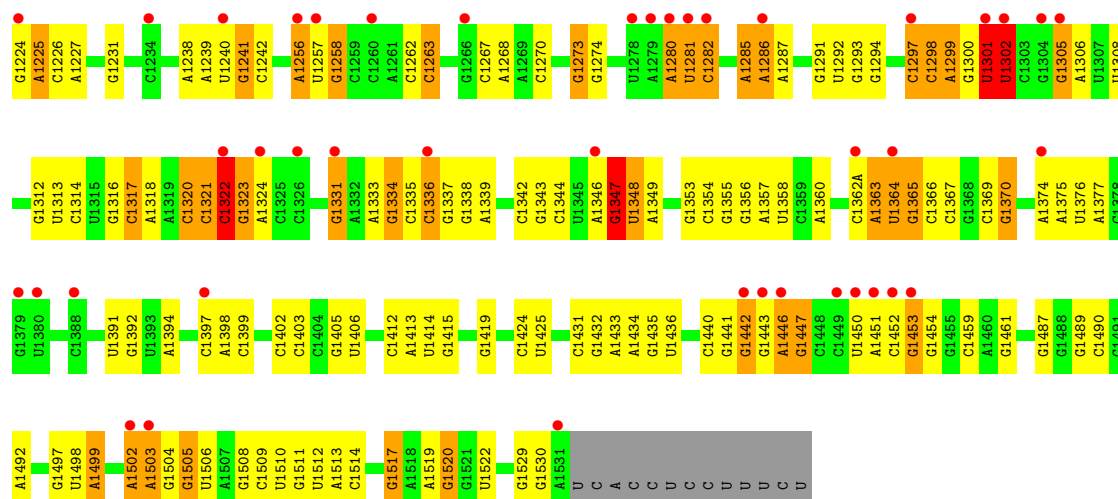


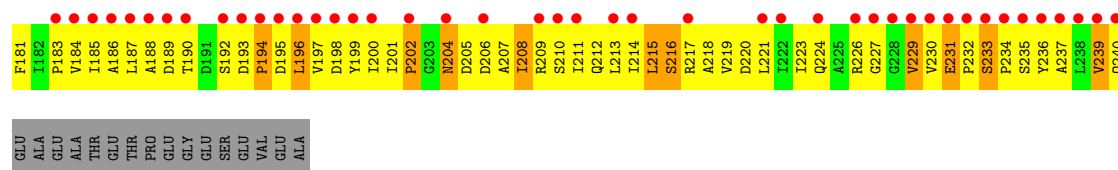


● Molecule 1: 16S rRNA

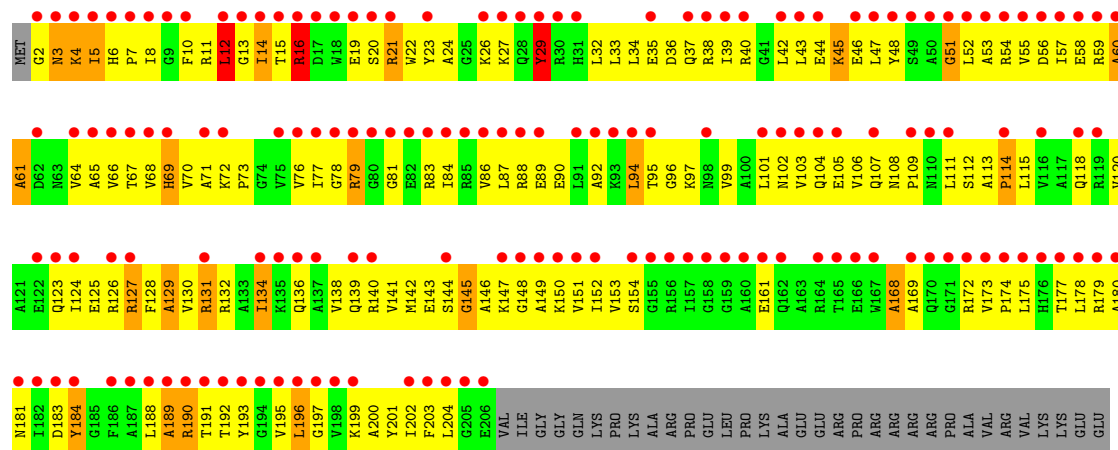




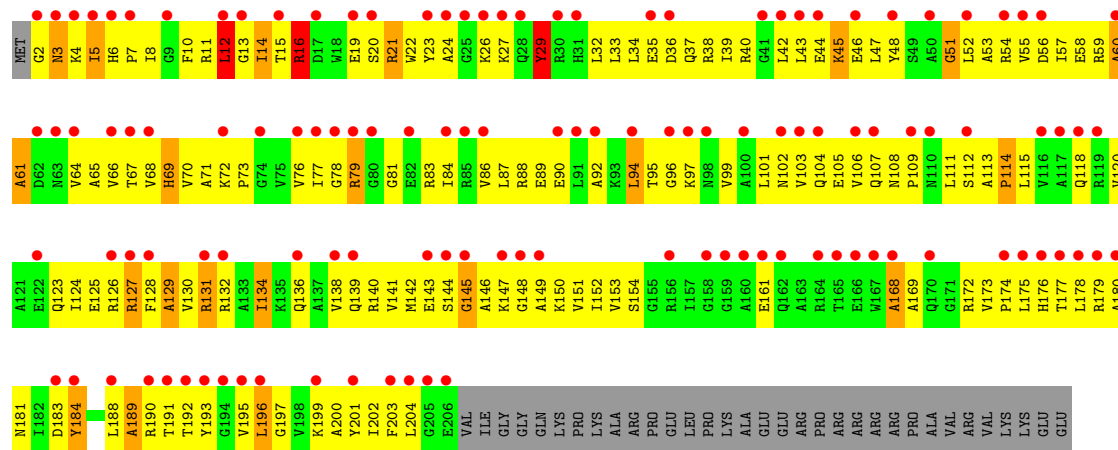




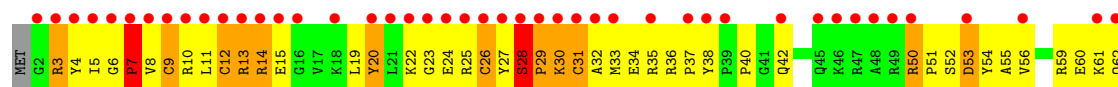
• Molecule 3: 30S ribosomal protein S3

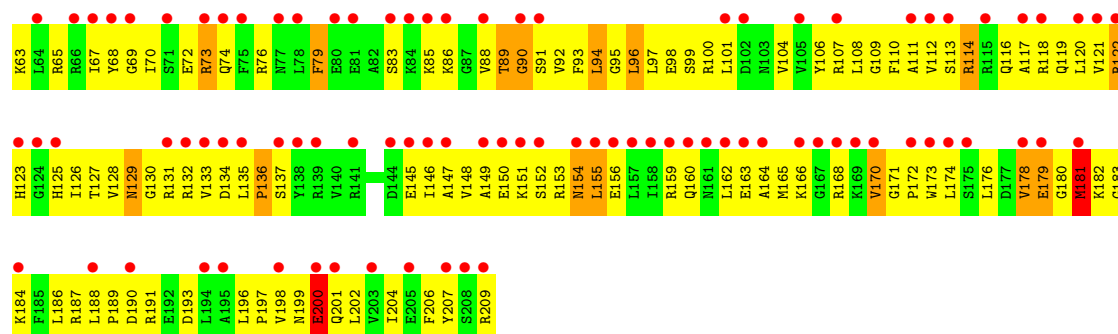


• Molecule 3: 30S ribosomal protein S3

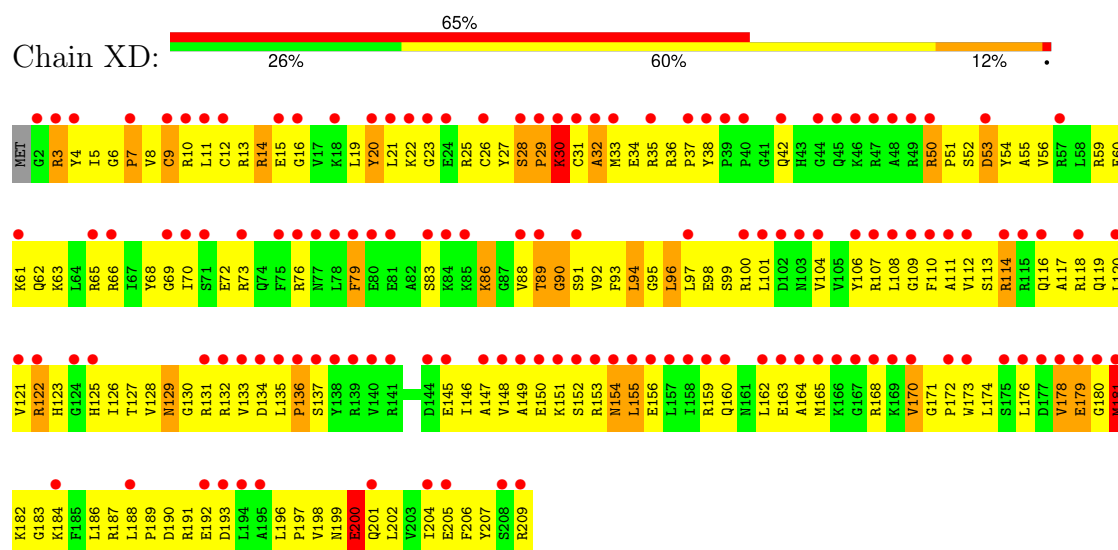


• Molecule 4: 30S ribosomal protein S4

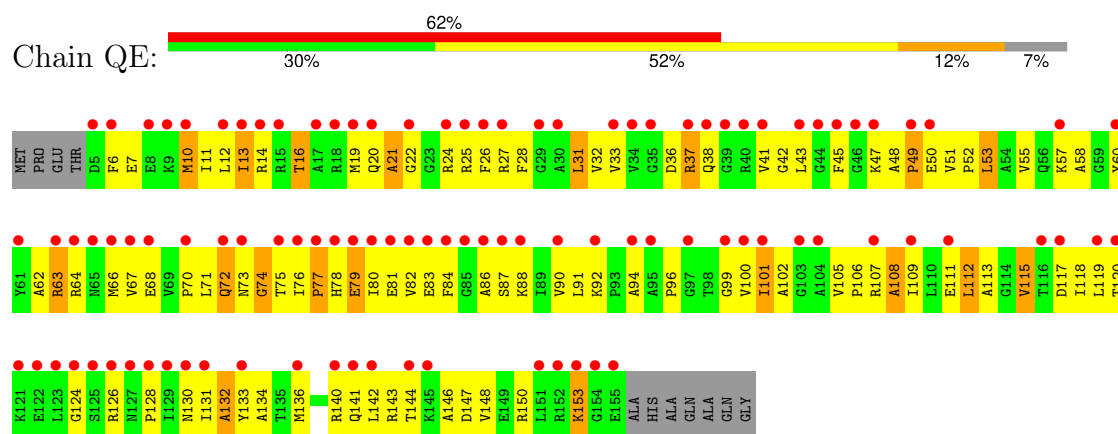




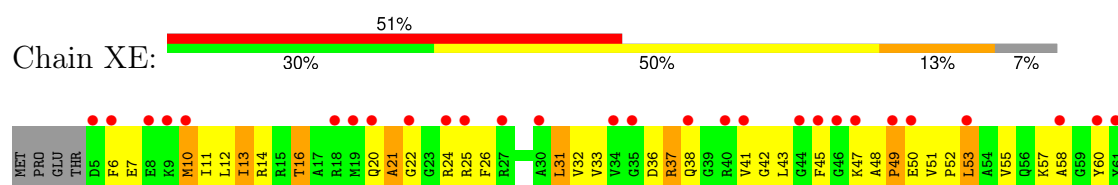
• Molecule 4: 30S ribosomal protein S4

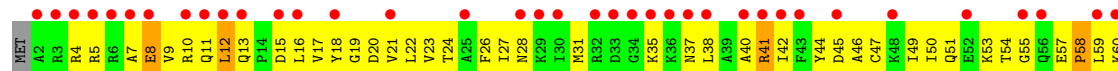


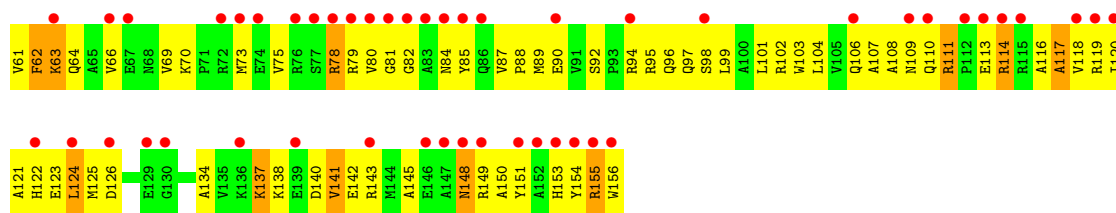
• Molecule 5: 30S ribosomal protein S5



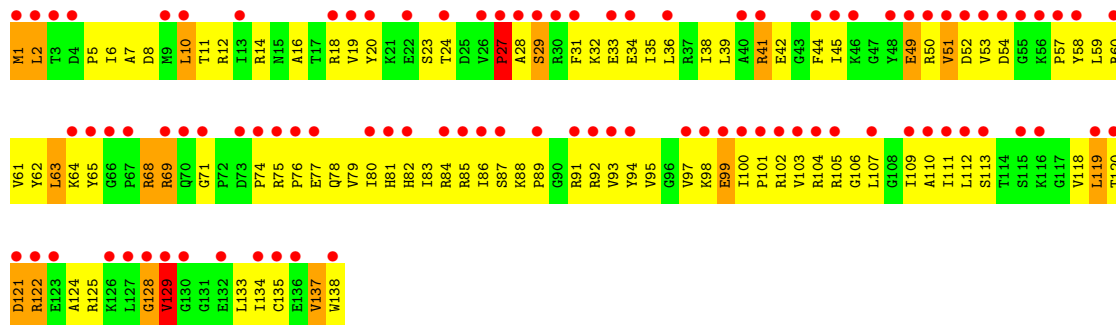
• Molecule 5: 30S ribosomal protein S5



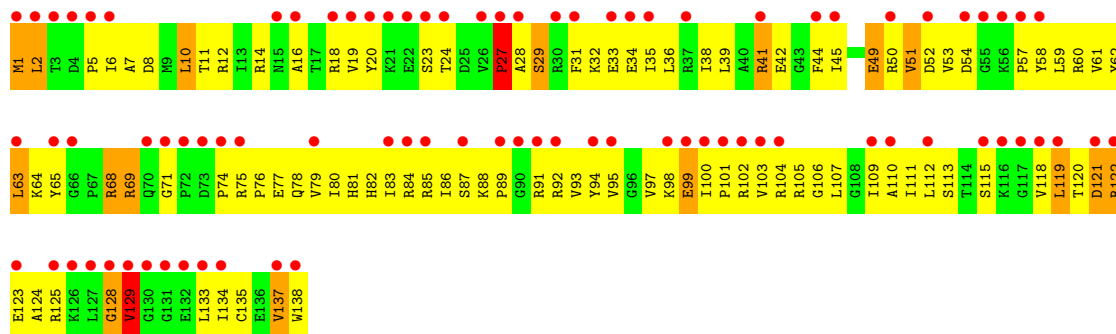




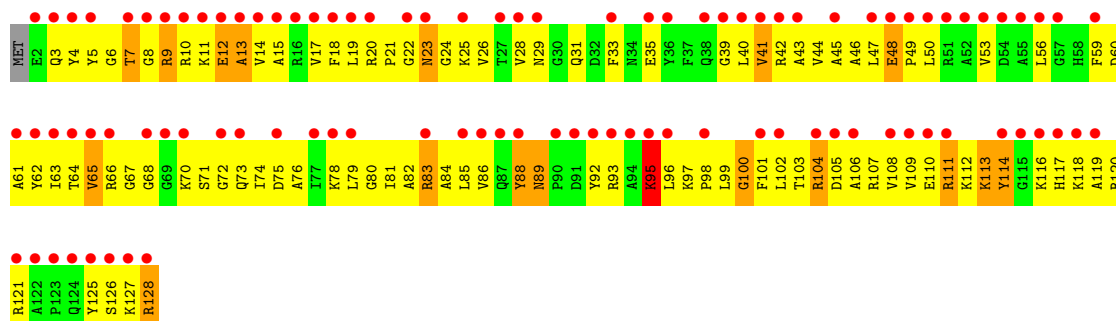
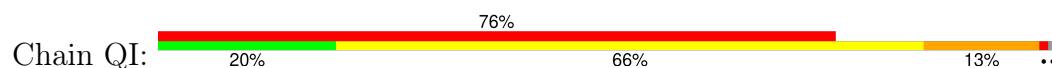
● Molecule 8: 30S ribosomal protein S8



● Molecule 8: 30S ribosomal protein S8

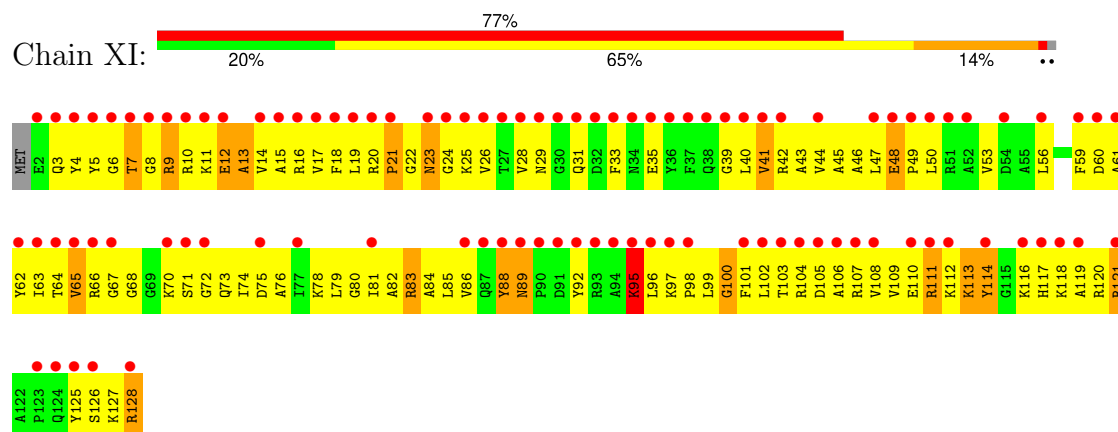


● Molecule 9: 30S ribosomal protein S9



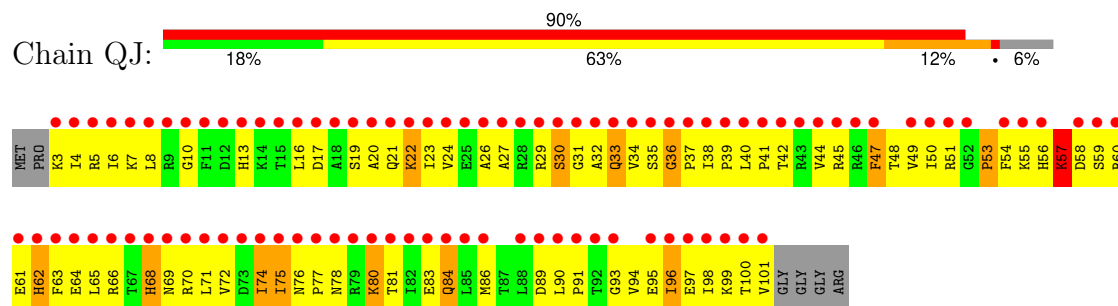
- Molecule 9: 30S ribosomal protein S9

Chain XI:



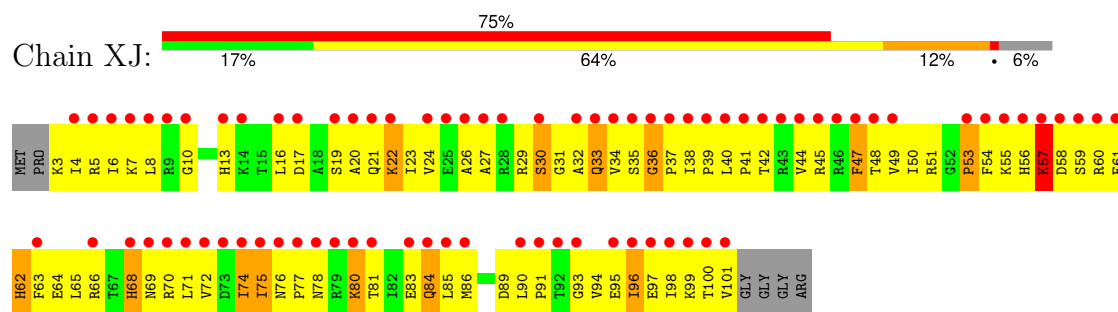
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



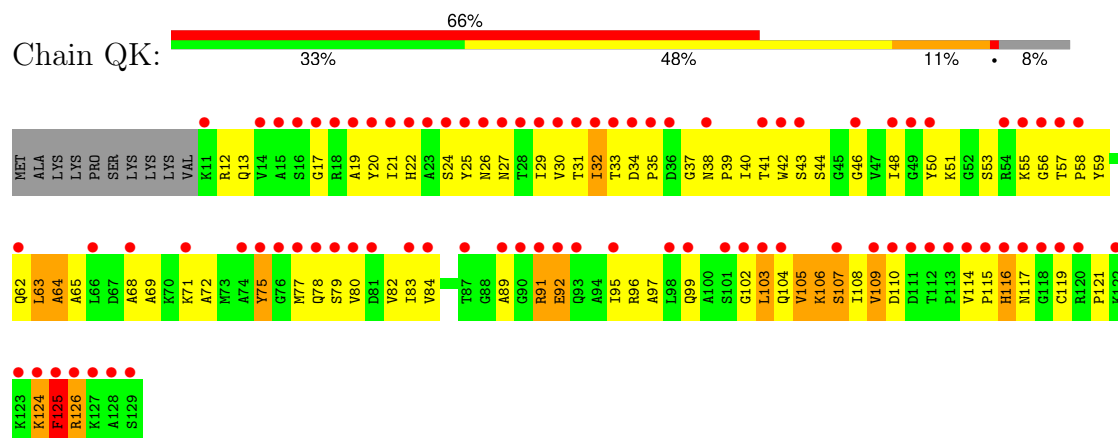
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



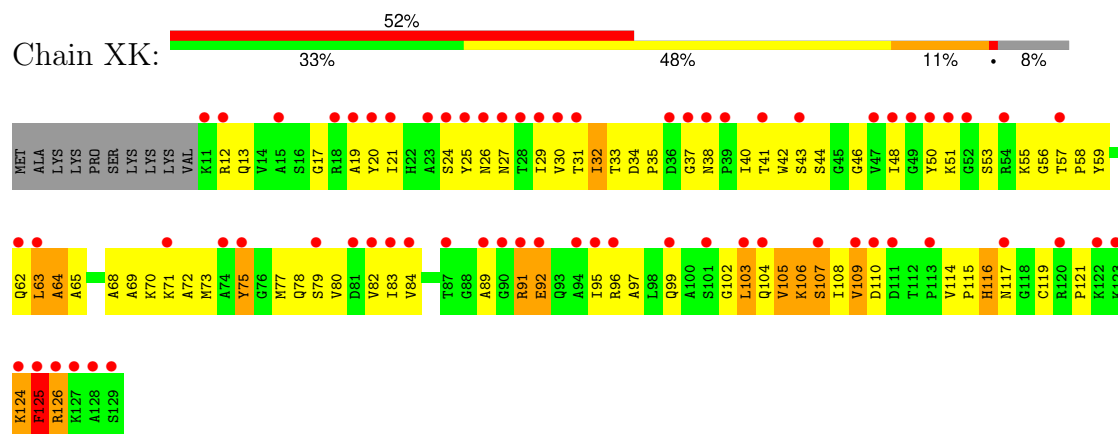
- Molecule 11: 30S ribosomal protein S11

Chain QK:



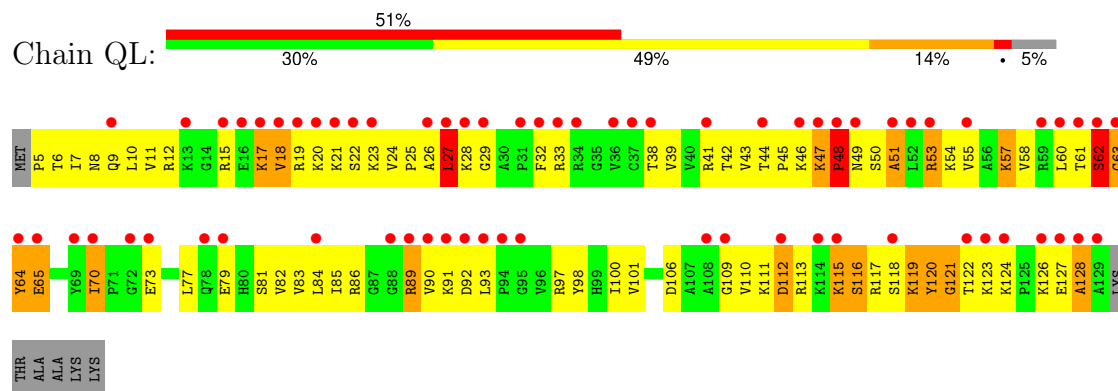
- Molecule 11: 30S ribosomal protein S11

Chain XK:



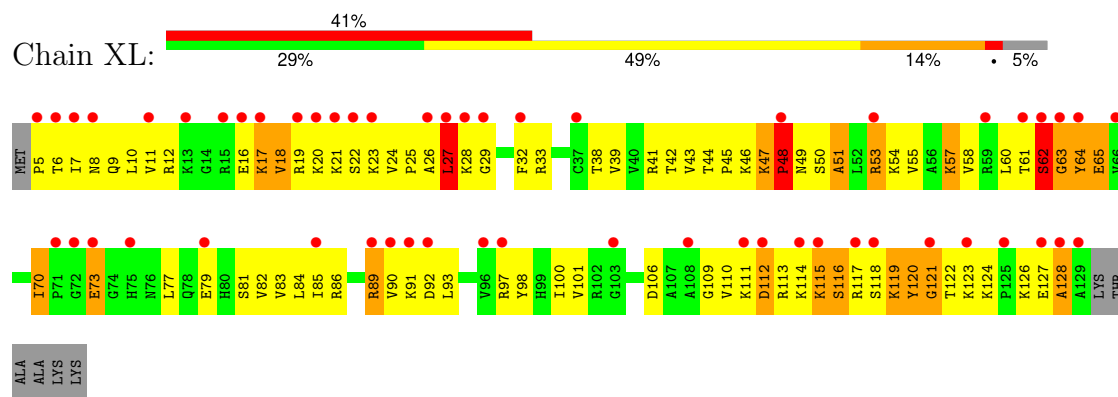
- Molecule 12: 30S ribosomal protein S12

Chain QL:



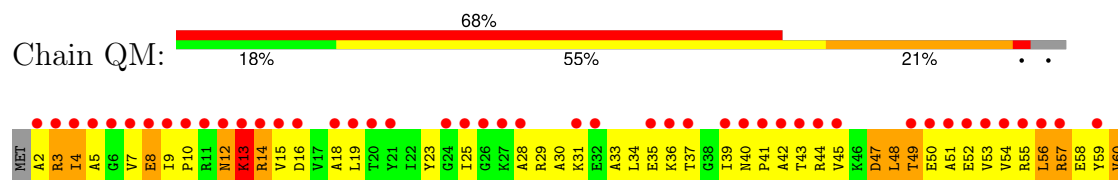
- Molecule 12: 30S ribosomal protein S12

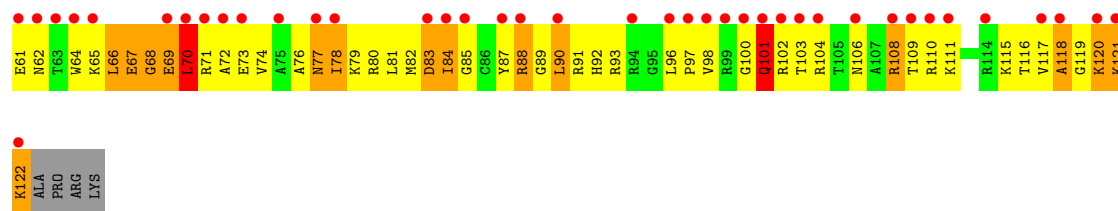
Chain XL:



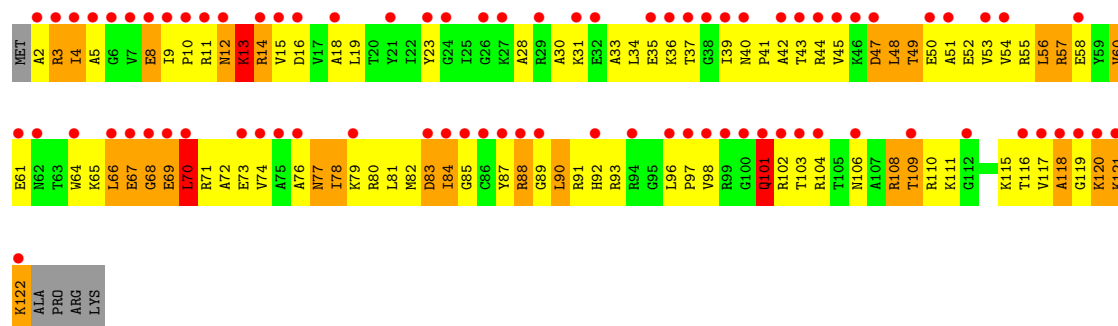
- Molecule 13: 30S ribosomal protein S13

Chain QM:

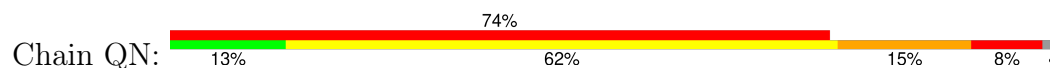




• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15

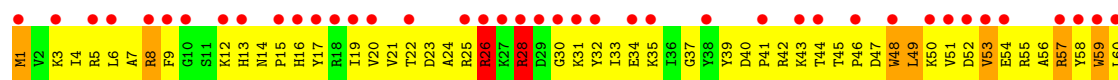




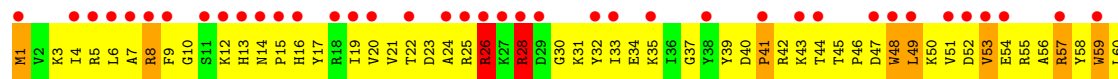
• Molecule 15: 30S ribosomal protein S15



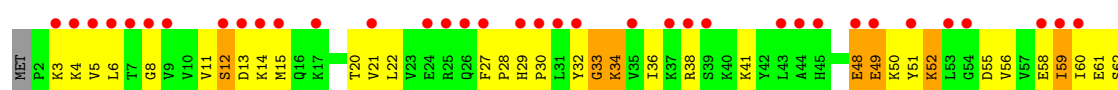
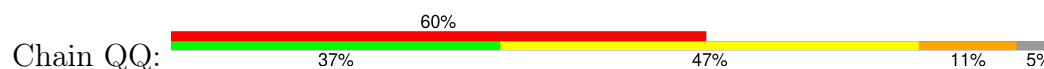
• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16

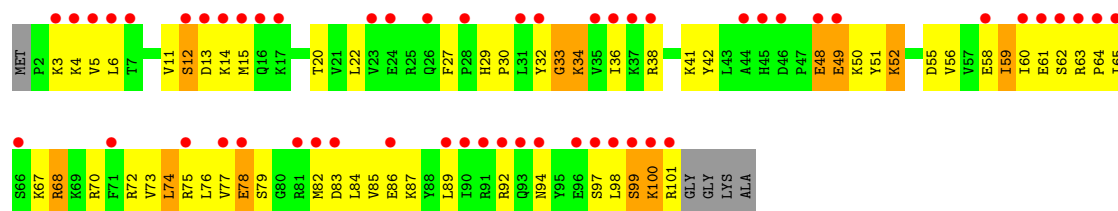


• Molecule 17: 30S ribosomal protein S17

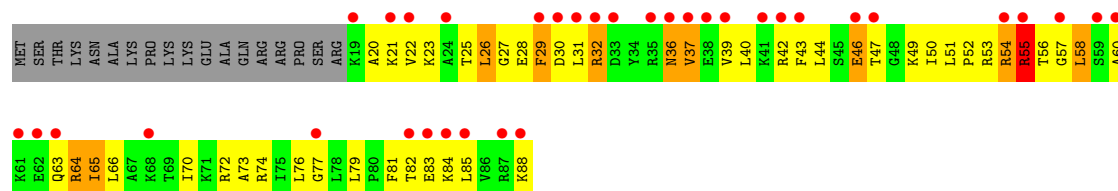
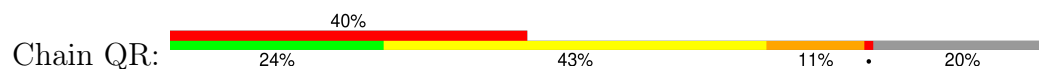


• Molecule 17: 30S ribosomal protein S17

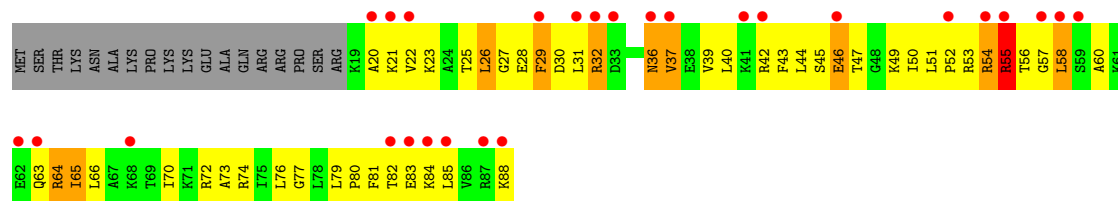




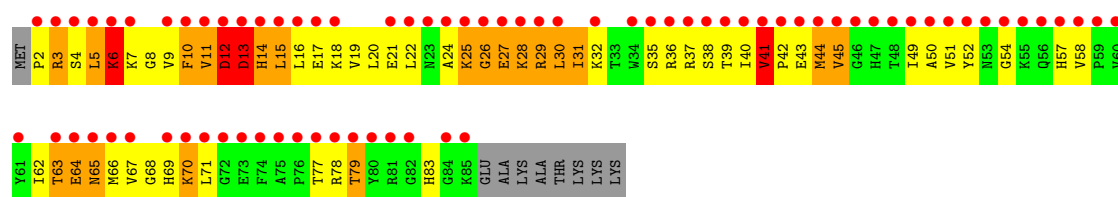
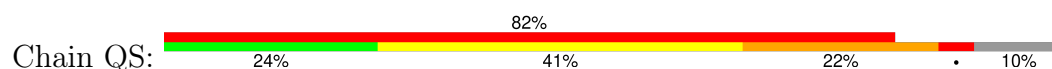
• Molecule 18: 30S ribosomal protein S18



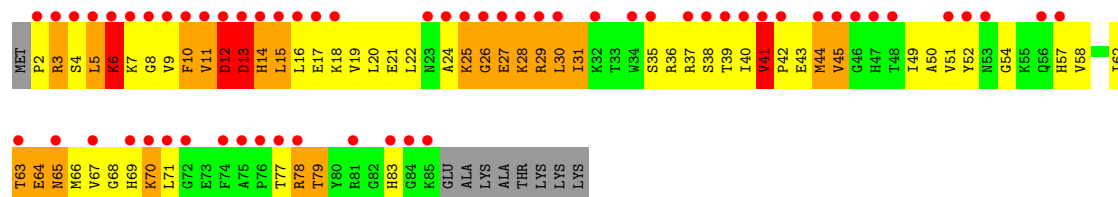
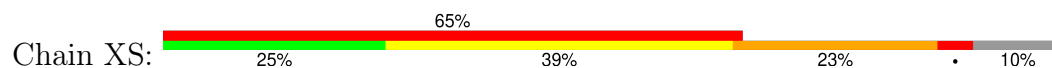
• Molecule 18: 30S ribosomal protein S18



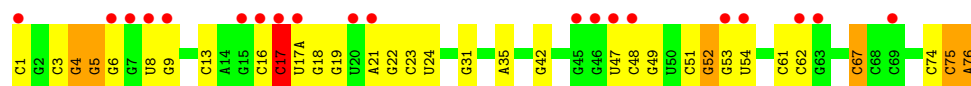
• Molecule 19: 30S ribosomal protein S19



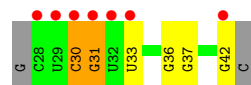
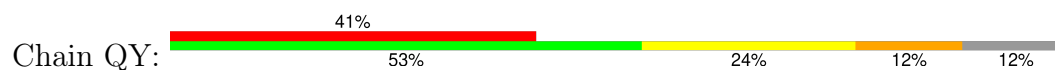
• Molecule 19: 30S ribosomal protein S19



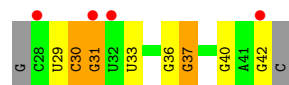
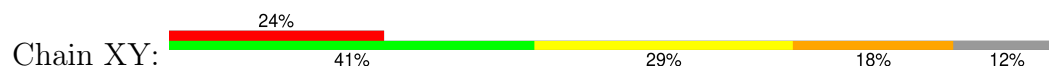
-
- | Frequency | Percentage |
|-----------|------------|
| Daily | 26% |
| Often | 57% |
| Sometimes | 34% |
| Never | 8% |



• Molecule 23: messenger RNA



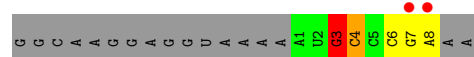
• Molecule 23: messenger RNA



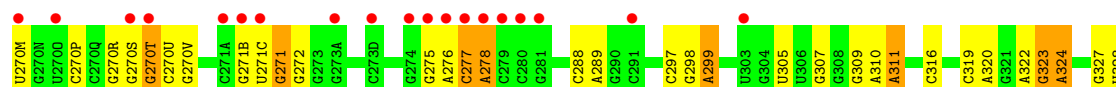
• Molecule 24: A-site ASL Pro

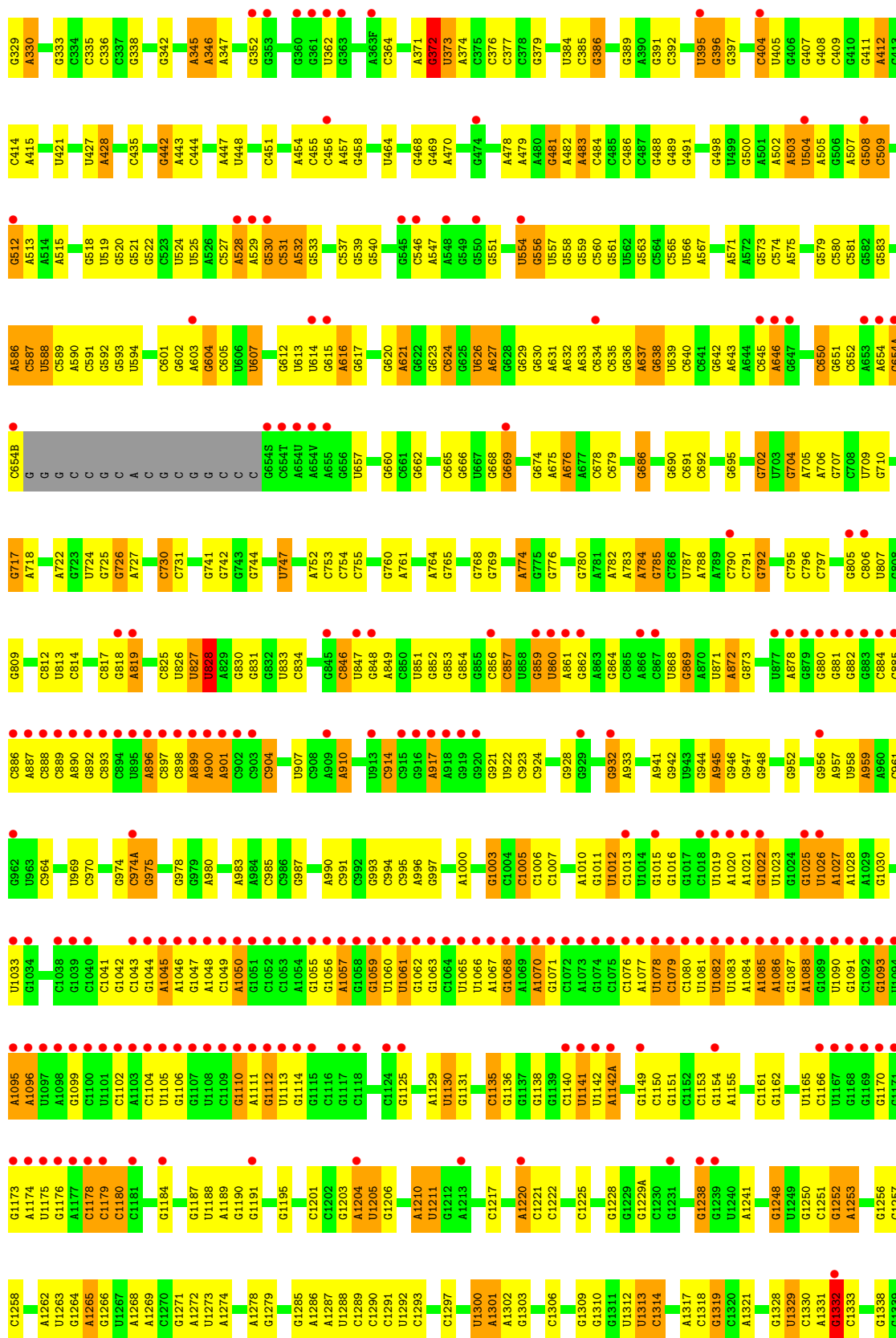


• Molecule 24: A-site ASL Pro

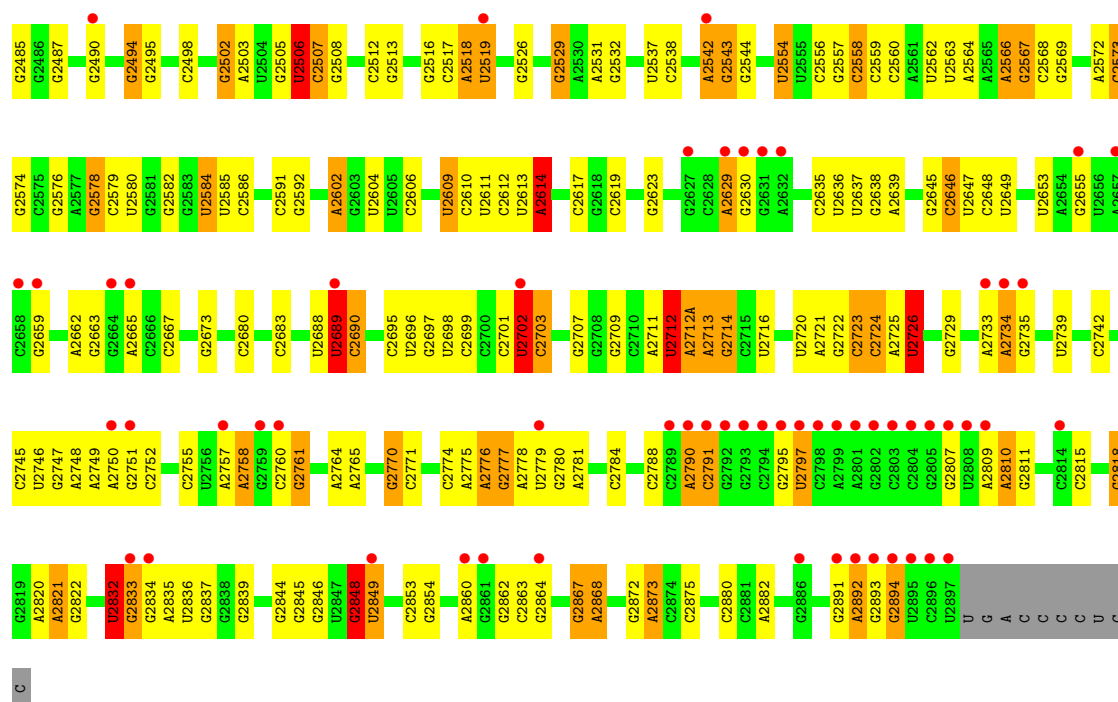


• Molecule 25: 23S rRNA

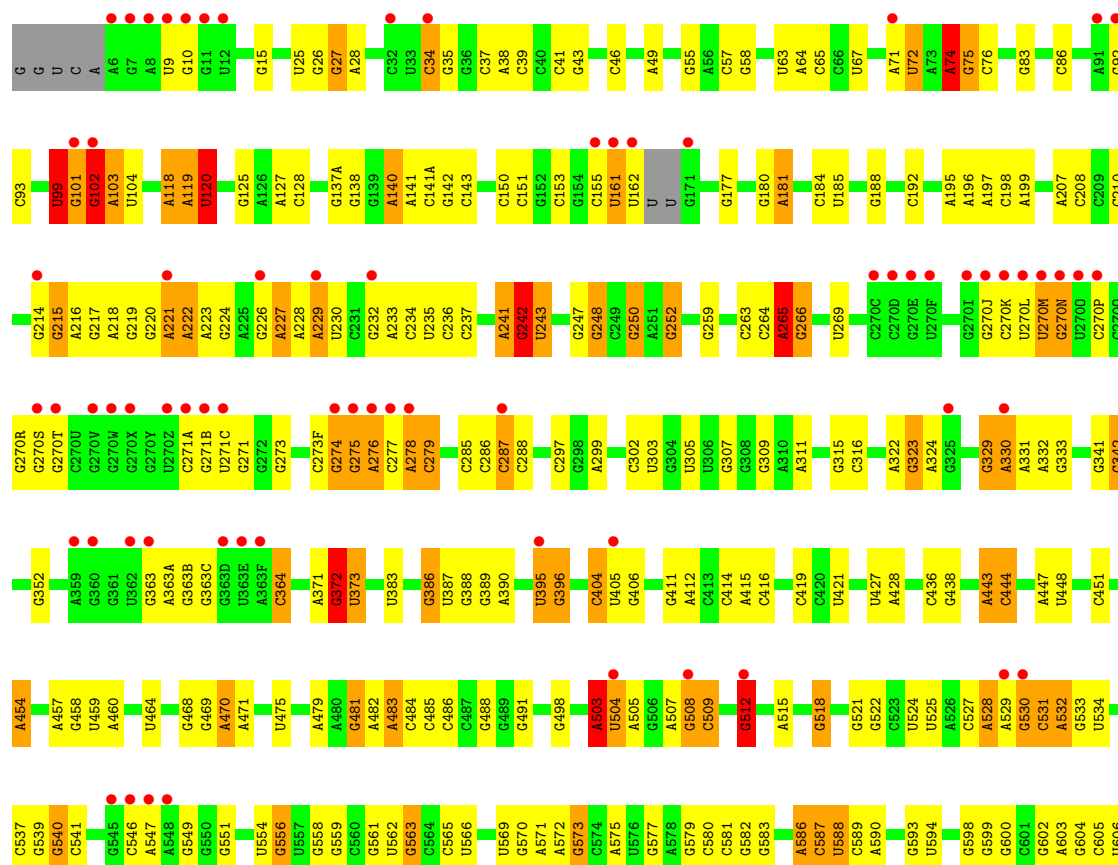


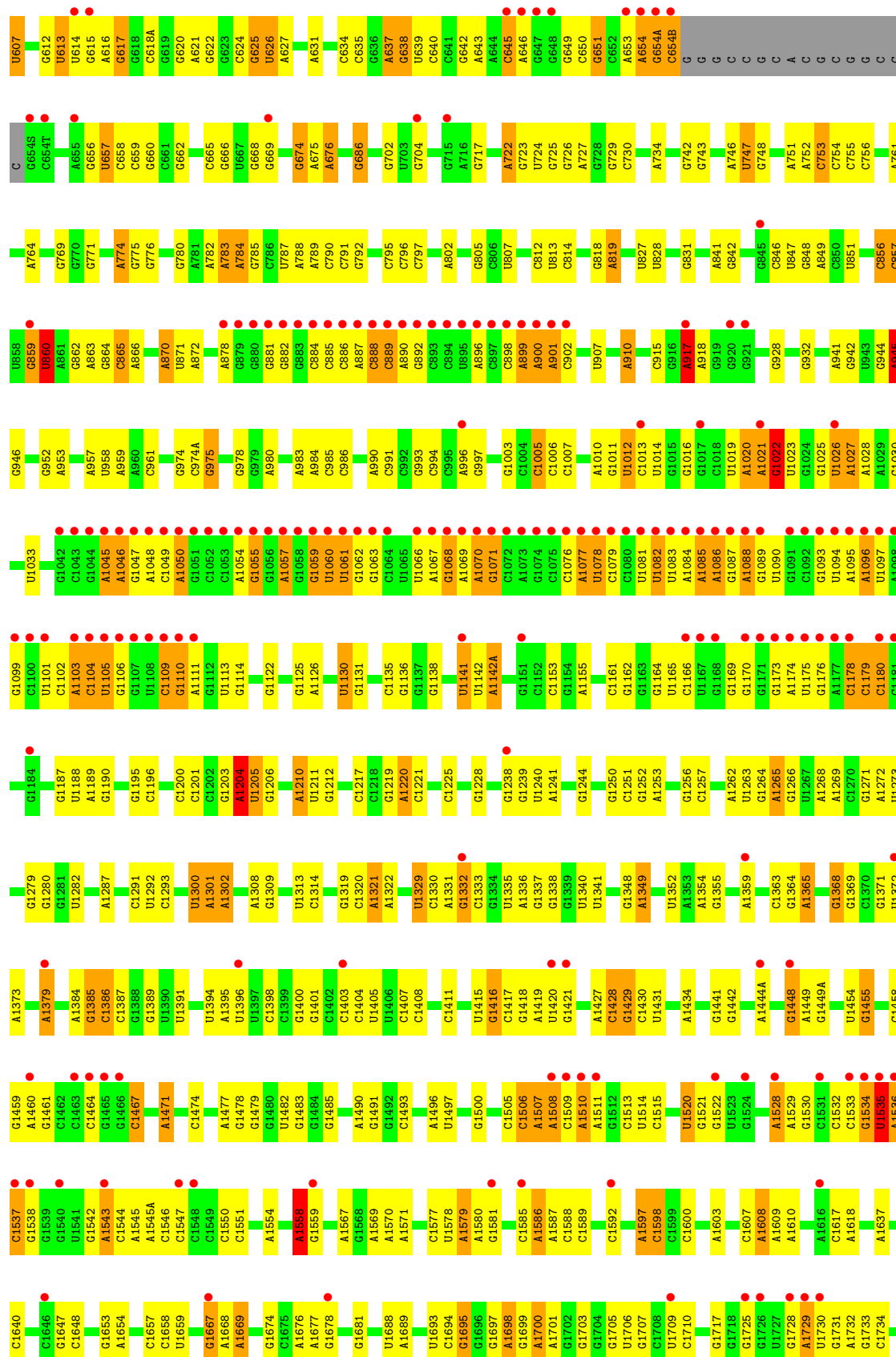


G2405	U2406	A2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	U2419	G2420	U2423	G2424	A2425	G2429	G2430	A2434	A2435	U2438	A2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	A2448	A2451	G2452	G2453	G2454	U2457	G2466	G2467	G2468	A2469	G2470	G2471	G2472	G2473	G2474	A2475	G2476	G2477	G2481	G2482	G2483	G2484								
G2318	G2319	A2320	G2325	G2326	A2327	A2328	G2329	G2330	G2331	A2335	A2336	G2340	G2341	G2342	G2343	G2344	G2345	A2346	G2347	G2350	G2351	G2356	A2361	A2366	G2367	G2368	A2369	G2372	G2373	G2374	A2377	A2378	A2398	G2399	G2400	G2384	G2385	A2392	A2393	G2394	G2395	G2396	G2397	U2398	U2401	G2402	G2403	G2404										
U2233	G2234	G2238	G2239	U2243	U2244	U2245	G2246	G2250	G2261	G2264	A2268	A2269	G2270	G2271	U2272	A2273	G2274	G2275	G2276	G2277	G2280	G2283	G2284	G2285	A2286	A2287	A2288	U2291	G2292	G2295	A2298	G2299	G2300	G2301	G2302	G2303	G2304	A2305	G2306	G2307	A2308	A2309	A2310	A2311	U2312	G2313	G2314											
A2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	A2169	A2170	A2171	U2172	G2173	G2174	A2175	G2176	G2177	G2178	U2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	U2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	U2197	A2198	G2199	G2200	U2208	G2209	G2210	G2211	A2212	U2213	G2215	G2219	G2224	A2225	G2226	A2227	G2231	U2232		
U2099	G2100	G2101	U2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	U2113	G2114	G2115	G2116	G2117	U2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	A2126	G2127	G2128	G2129	U2130	G2131	U2132	G2133	G2134	A2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	U2144	G2145	G2146	G2147	G2148	U2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157
G1998	G1999	G2008	G2009	G2012	A2013	A2014	A2015	G2018	A2019	A2020	G2021	U2022	G2023	G2024	G2025	A2030	A2031	G2032	A2033	G2037	G2038	A2042	G2043	A2051	G2052	G2053	A2054	G2055	G2056	A2059	A2060	G2061	A2062	U2068	G2069	G2070	A2071	G2072	G2073	U2074	U2075	U2086	G2087	G2093	G2096	U2096												
G1999	C1902	G1800	A1801	A1802	A1803	A1810	G1811	A1812	G1813	G1814	A1815	G1816	A1819	U1820	A1821	G1824	A1825	G1826	A1829	G1835	G1836	G1837	G1844	A1847	A1848	G1849	G1850	A1853	G1857	G1858	A1859	U1864	G1869	G1870	A1871	G1872	G1873	A1881	G1882	G1883	A1884	A1885	G1888	A1889	U1891	G1892	U1893	C1894	G1895	G1896	C1897							
G1903	G1904	G1905	G1906	A1913	G1914	A1918	A1919	G1920	C1925	U1926	G1927	A1928	G1929	G1930	U1931	A1936	A1937	A1938	U1939	G1948	G1949	G1950	U1951	A1952	U1955	U1956	G1957	G1958	U1963	G1964	G1967	G1968	A1969	A1970	A1971	A1972	G1973	C1974	G1980	A1981	C1982	G1989	C1990	U1991	G1992	U1993	U1994	G1995	G1996	C1997								
A1698	G1699	A1700	A1701	U1709	C1710	G1725	G1726	U1727	G1728	A1729	U1730	G1732	G1733	G1734	G1735	G1741	G1742	G1743	G1750	C1751	G1752	G1753	A1754	G1755	U1756	U1757	G1758	A1762	G1763	G1764	G1769	G1770	G1771	G1772	A1773	U1778	U1779	A1780	G1781	G1782	A1783	A1784	A1785	A1786	A1791	G1792	C1793	U1794	G1795	U1796	C1797							
G1594	G1595	A1596	A1597	G1598	G1599	C1600	C1607	A1608	A1609	A1610	A1616	C1617	A1618	G1622	U1629	G1630	C1636	A1637	G1638	U1639	C1640	G1647	G1648	G1651	A1652	G1653	A1654	C1657	C1658	G1667	A1668	A1669	C1672	U1673	G1674	C1675	A1676	A1677	G1678	C1686	G1687	U1688	A1689	U1693	C1694	G1695												
A1508	C1509	A1510	A1511	G1512	G1513	U1514	C1515	U1520	G1521	G1522	G1525	G1526	G1527	A1528	G1534	U1535	A1536	C1537	G1538	A1539	G1540	U1541	G1542	A1543	C1544	A1545	C1547	A1554	A1558	G1559	A1567	G1568	A1569	A1570	A1571	C1577	U1578	A1579	A1580	G1581	C1582	A1583	C1585	A1586	A1587	C1588	C1589	U1590	G1591	C1592	G1593							
G1434	G1435	A1436	A1427	G1428	G1429	C1430	U1431	A1434	G1435	G1436	A1444A	C1445	A1448	A1449	G1449A	G1449	C1450	A1451	U1453	U1454	G1455	C1458	G1459	A1460	G1461	G1462	C1463	G1464	G1465	G1466	C1467	C1468	A1469	G1470	A1471	A1477	G1480	U1482	G1483	G1484	G1485	A1490	C1493	A1496	U1497	U1503	C1504	C1505	C1506	U1507								
U1340	U1341	A1342	G1348	A1349	A1354	U1357	G1358	A1359	G1364	A1365	A1366	A1367	G1368	G1369	G1370	G1371	A1372	U1373	A1374	A1379	G1380	A1384	G1385	C1386	G1387	G1388	A1395	U1396	U1397	C1398	G1401	G1402	C1403	G1404	U1405	U1406	G1407	C1408	C1411	A1412	G1413	G1416	G1418	A1419	U1420	G1421	G1422	G1423										

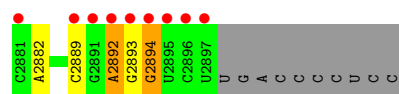


• Molecule 25: 23S rRNA

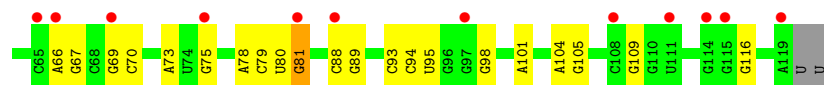
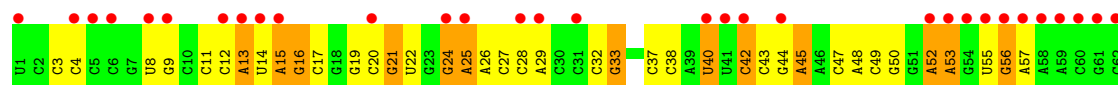




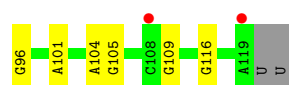
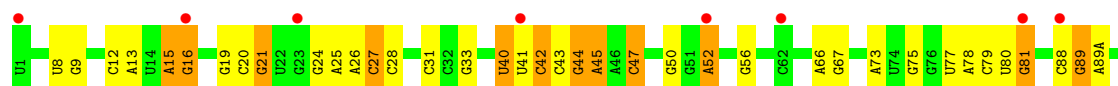




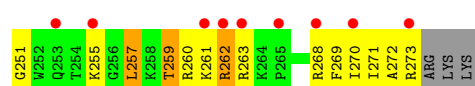
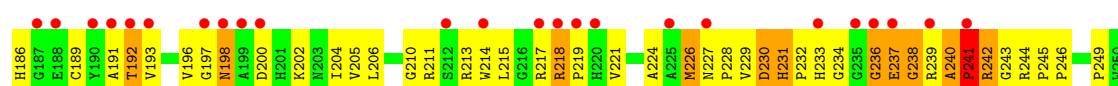
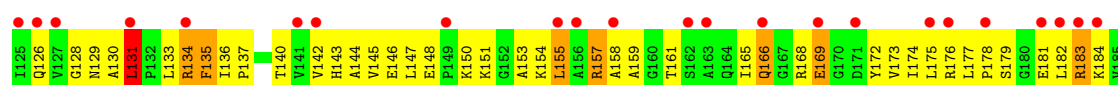
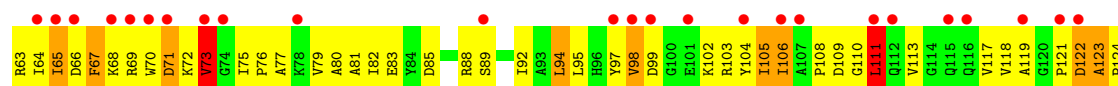
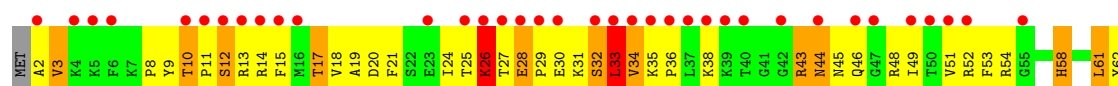
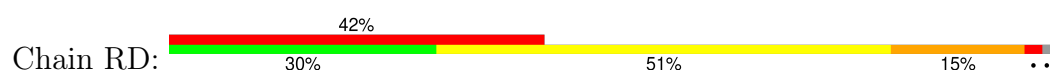
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA

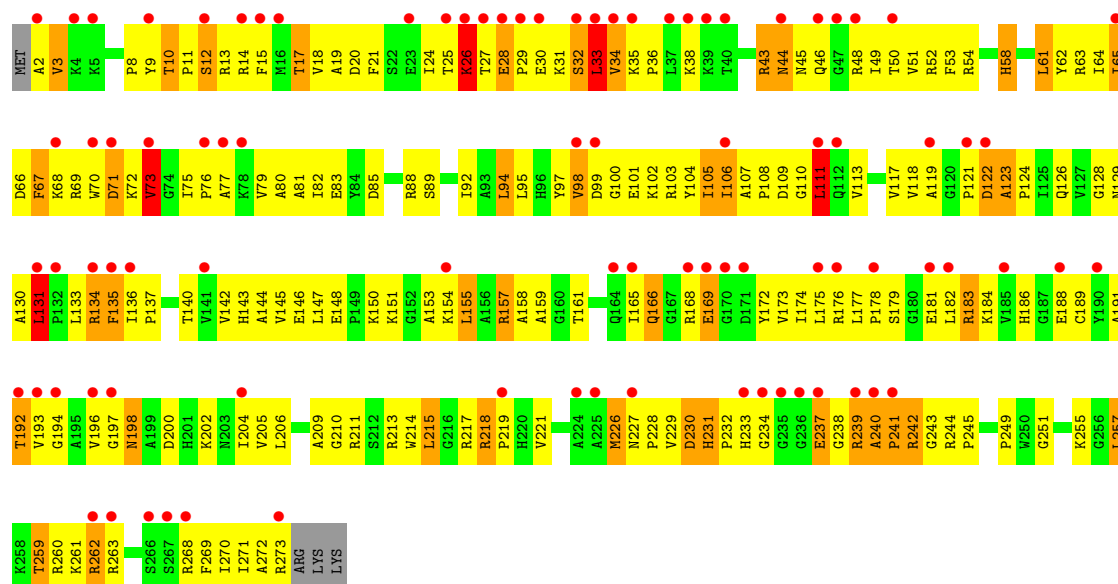


• Molecule 27: 50S ribosomal protein L2

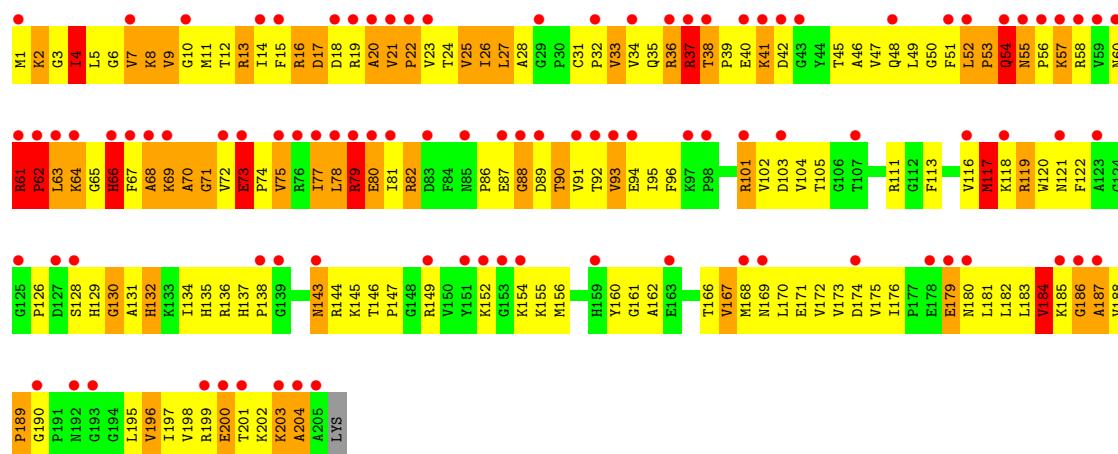


• Molecule 27: 50S ribosomal protein L2

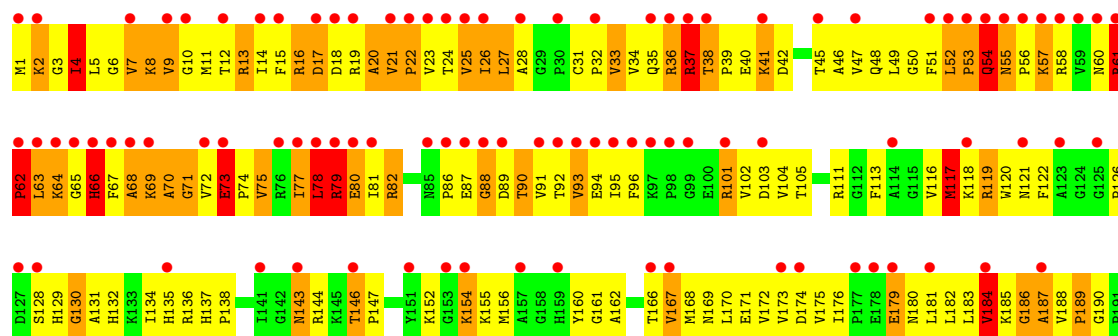




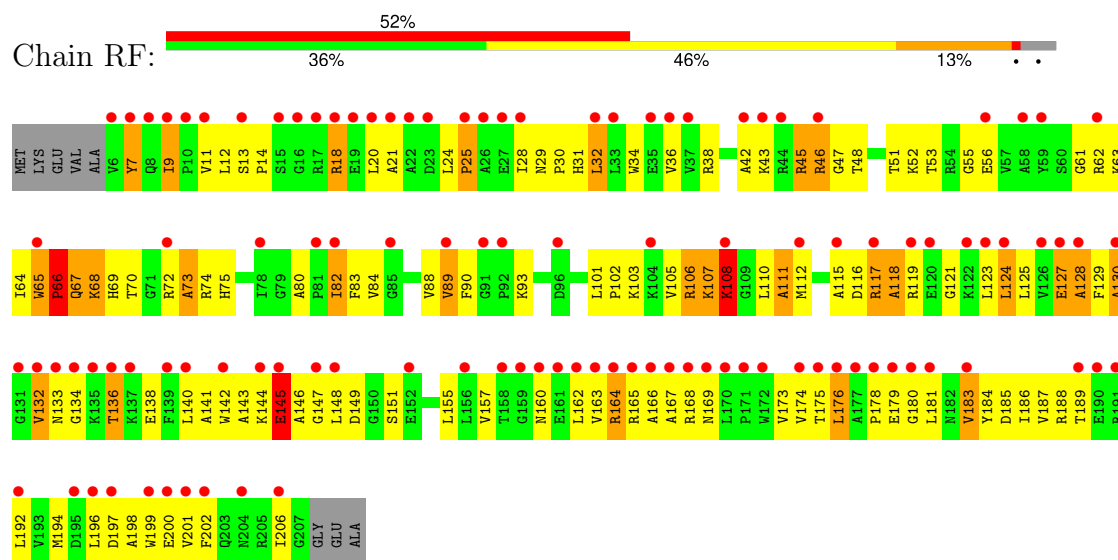
• Molecule 28: 50S ribosomal protein L3



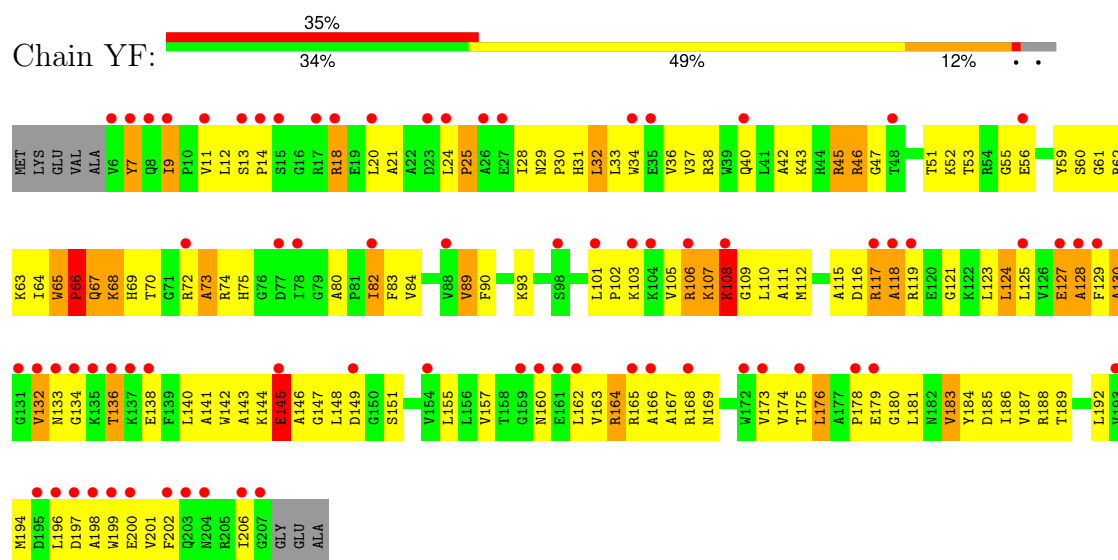
• Molecule 28: 50S ribosomal protein L3



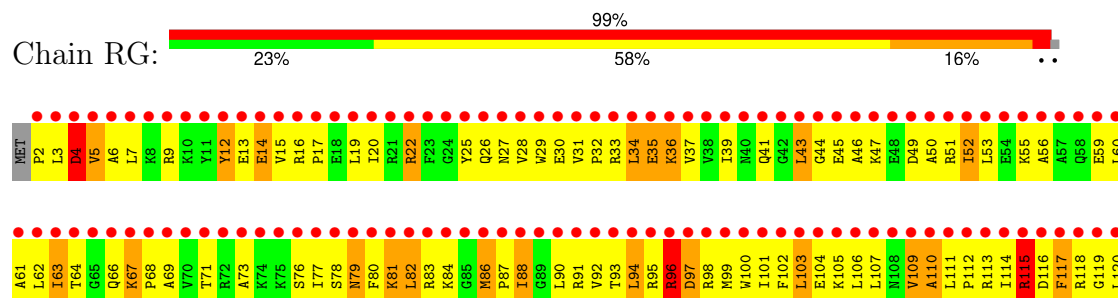
- Molecule 29: 50S ribosomal protein L4



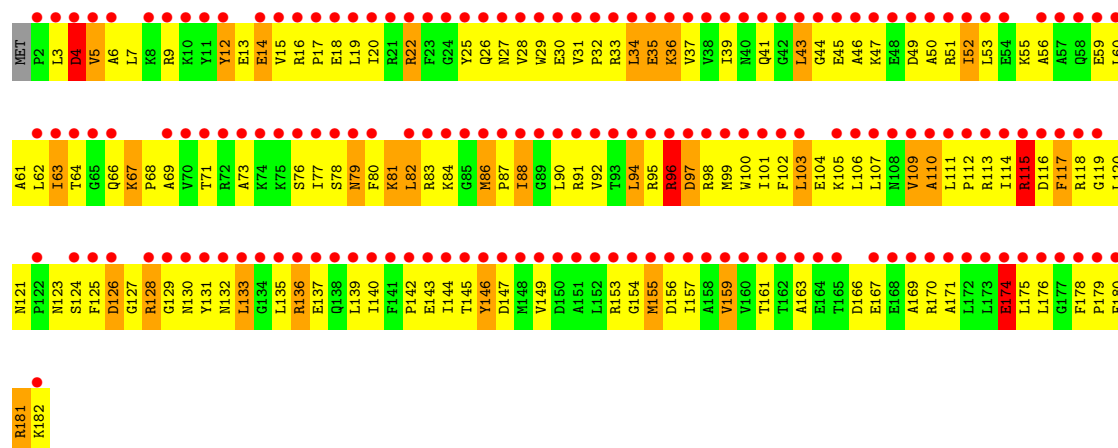
- Molecule 29: 50S ribosomal protein L4



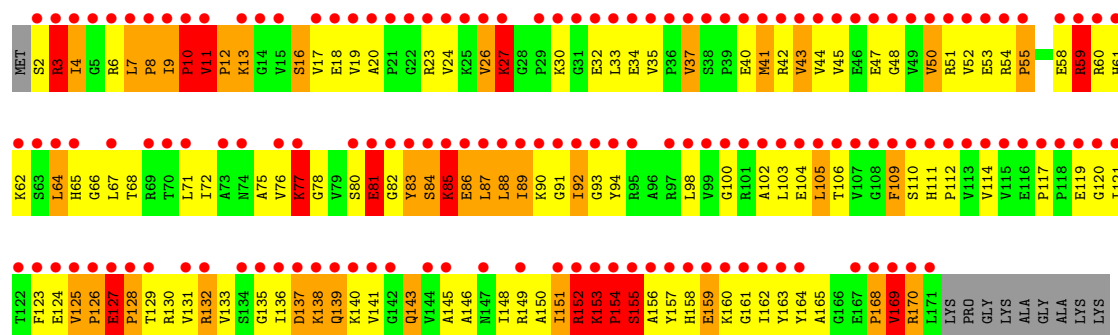
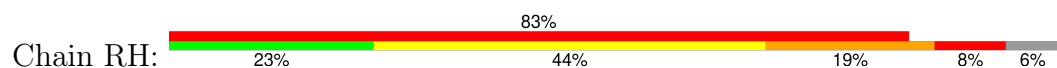
- Molecule 30: 50S ribosomal protein L5



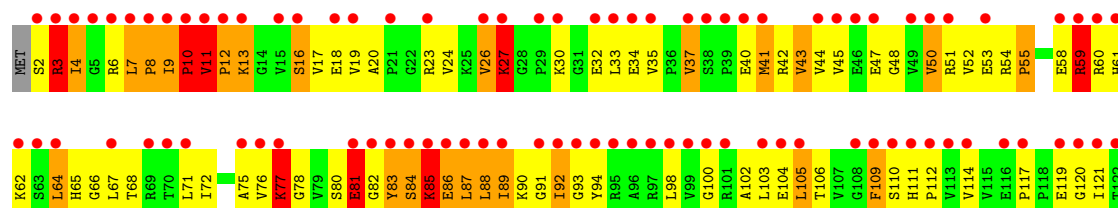
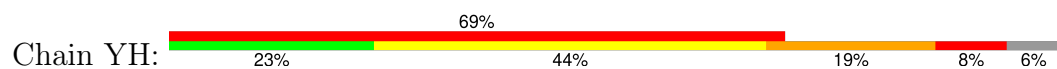
- Molecule 30: 50S ribosomal protein L5

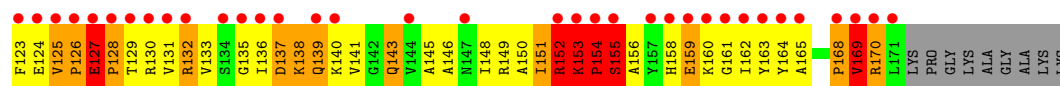


- Molecule 31: 50S ribosomal protein L6

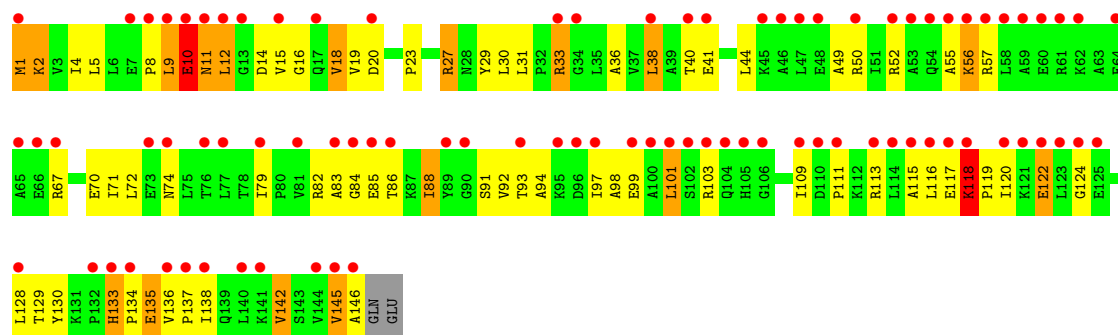


- Molecule 31: 50S ribosomal protein L6

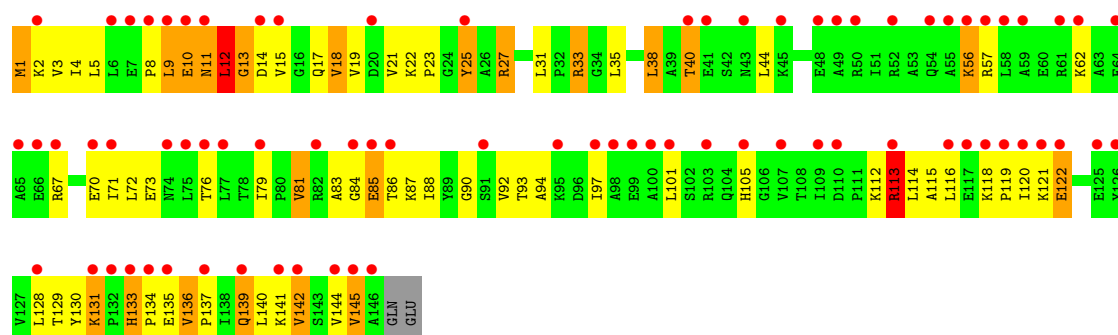




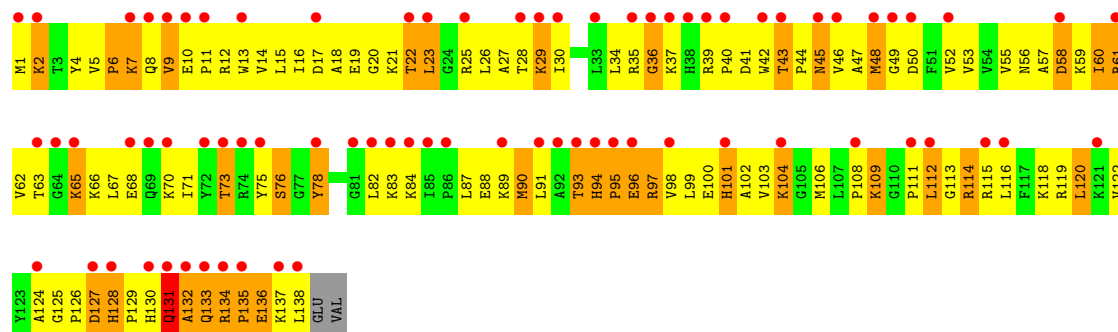
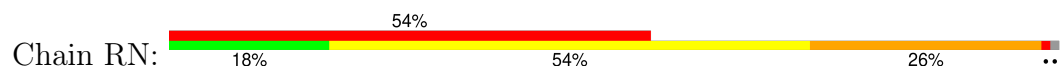
• Molecule 32: 50S ribosomal protein L9



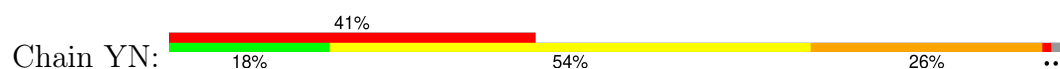
• Molecule 32: 50S ribosomal protein L9

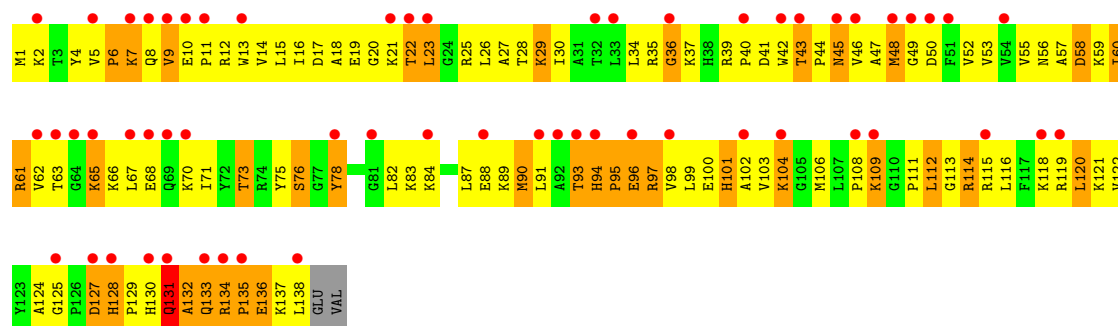


• Molecule 33: 50S ribosomal protein L11

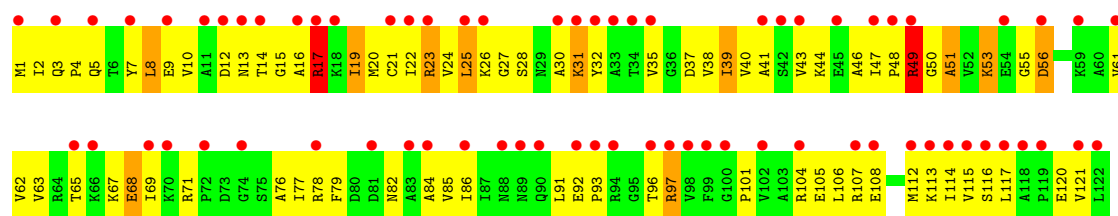


• Molecule 33: 50S ribosomal protein L11

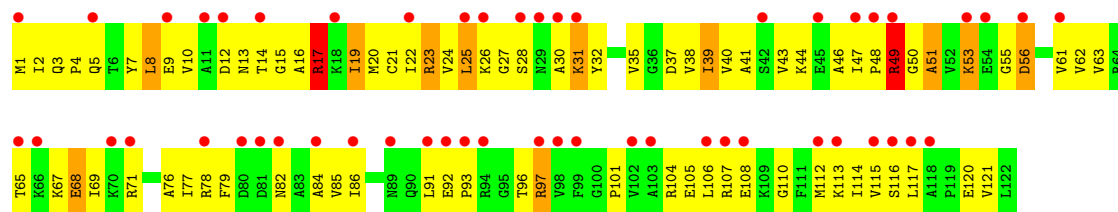




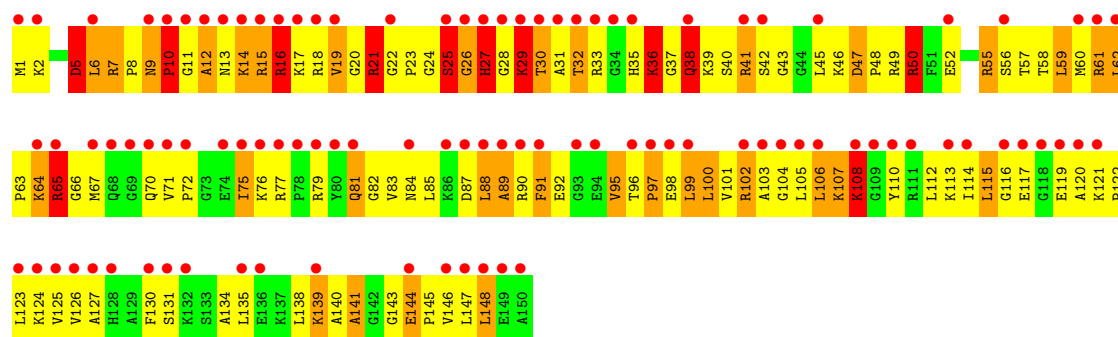
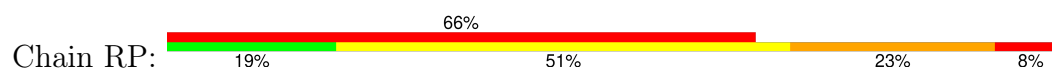
• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13

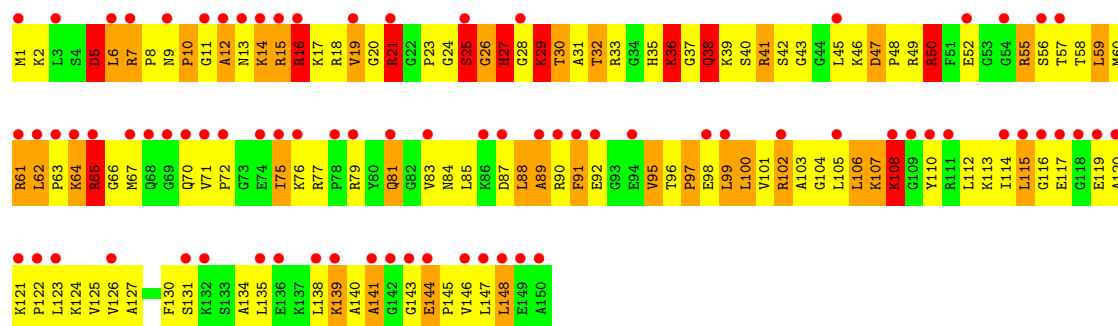


• Molecule 35: 50S ribosomal protein L14

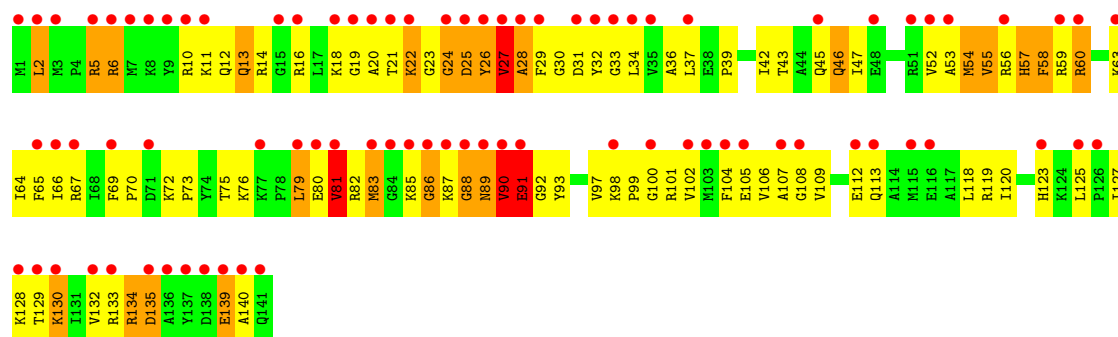


• Molecule 35: 50S ribosomal protein L14

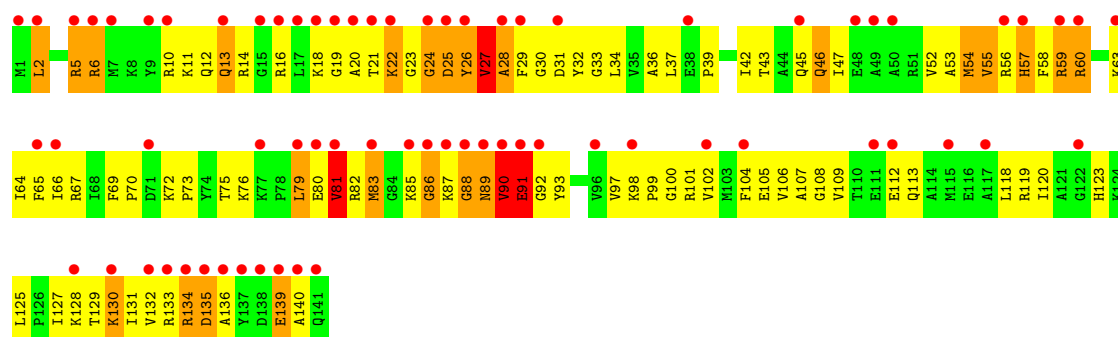




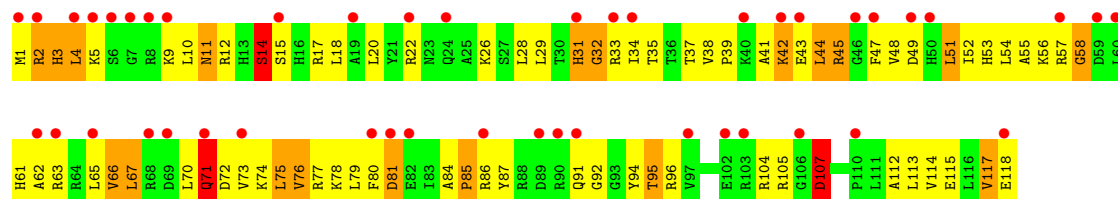
• Molecule 36: 50S ribosomal protein L15



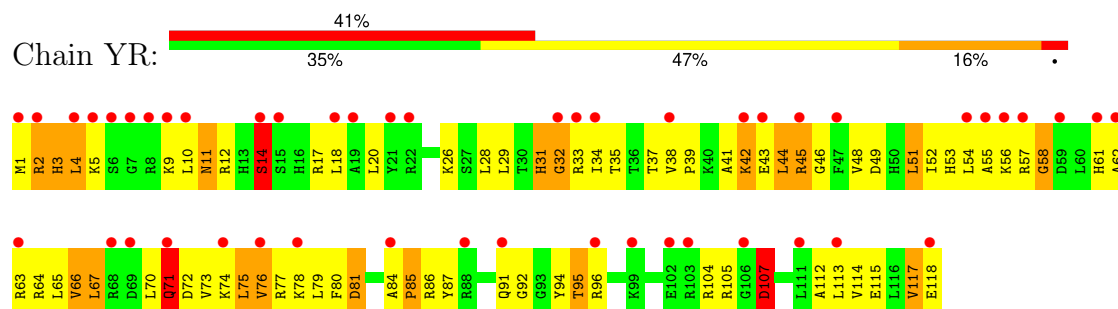
• Molecule 36: 50S ribosomal protein L15



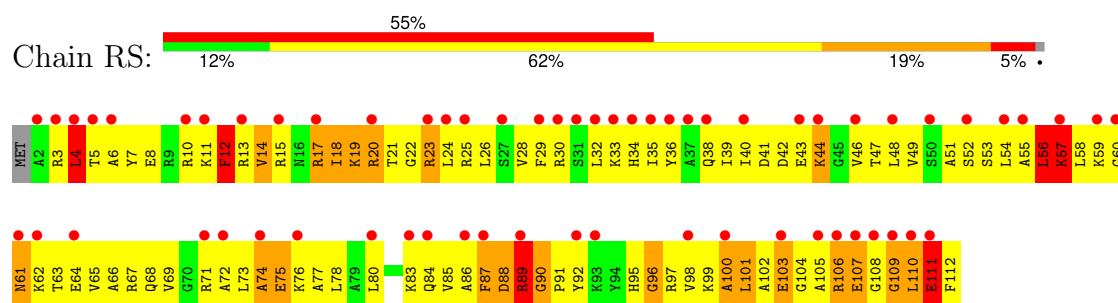
• Molecule 37: 50S ribosomal protein L16



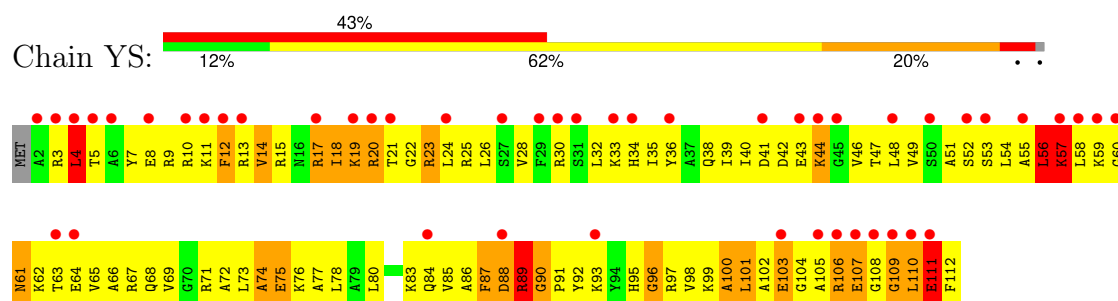
- Molecule 37: 50S ribosomal protein L16



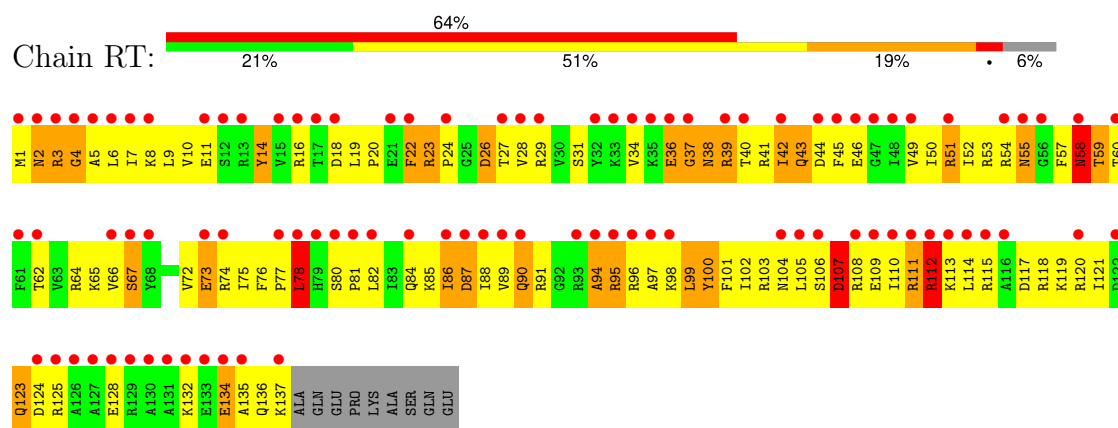
- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

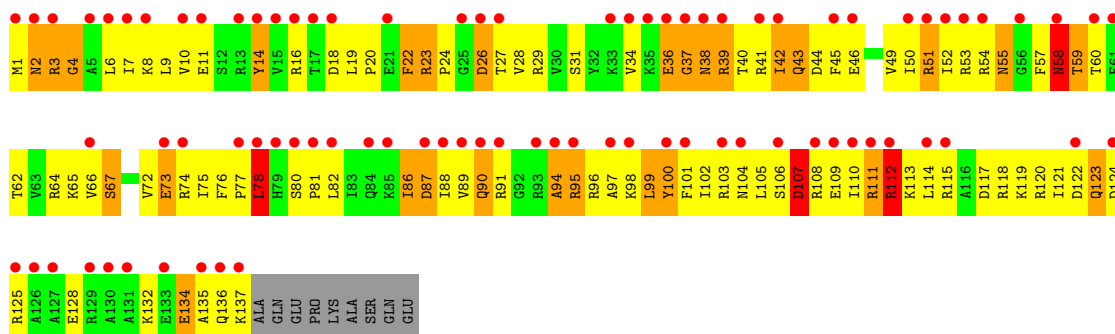


- Molecule 39: 50S ribosomal protein L18

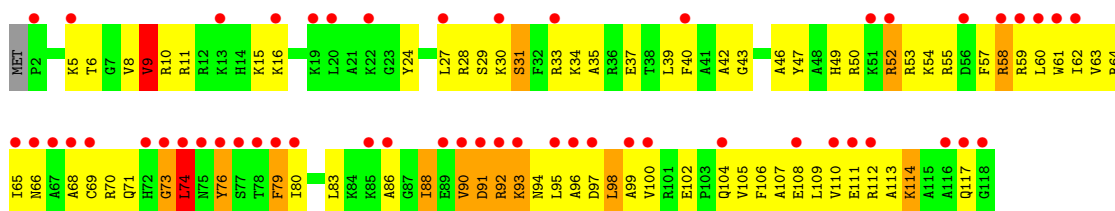


- Molecule 39: 50S ribosomal protein L18

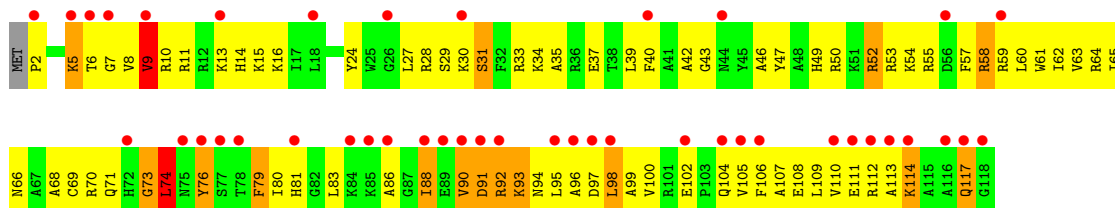




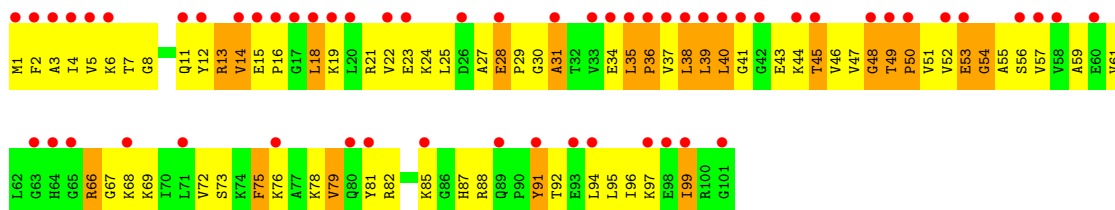
• Molecule 40: 50S ribosomal protein L19



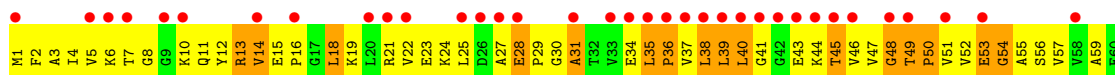
• Molecule 40: 50S ribosomal protein L19

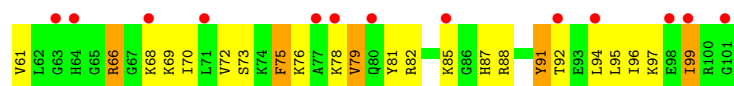


• Molecule 41: 50S ribosomal protein L20

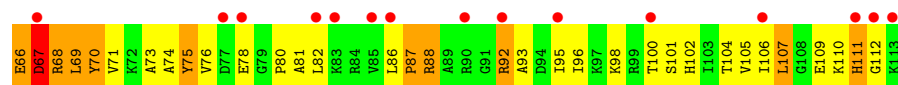


• Molecule 41: 50S ribosomal protein L20

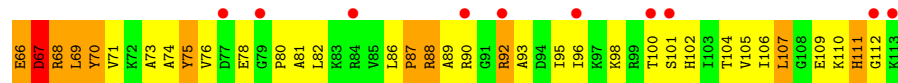
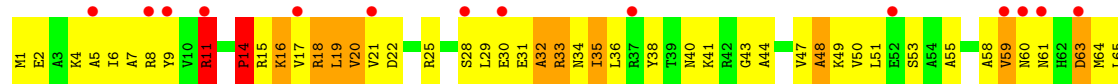




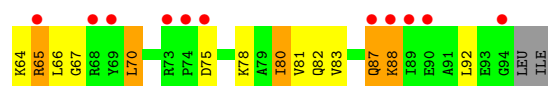
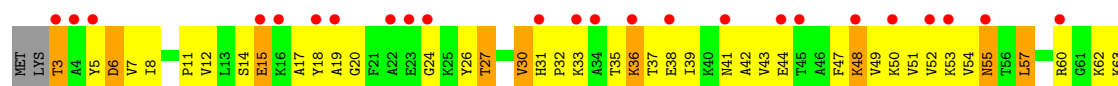
• Molecule 42: 50S ribosomal protein L21



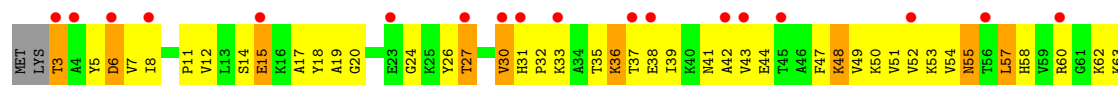
• Molecule 42: 50S ribosomal protein L21



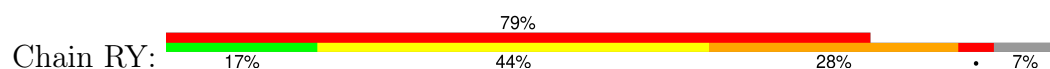
• Molecule 43: 50S ribosomal protein L22



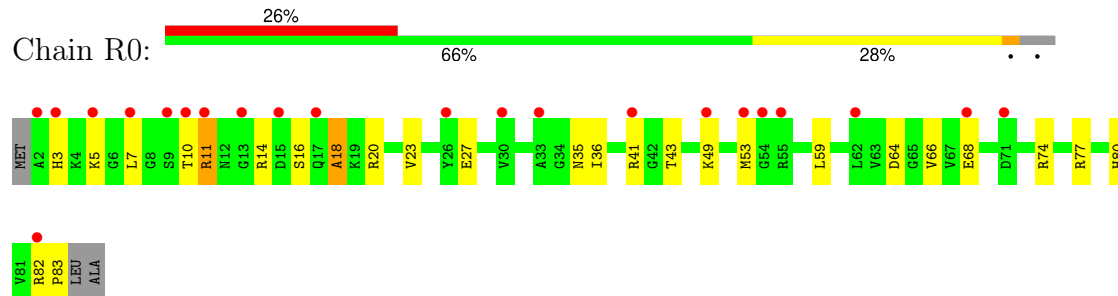
• Molecule 43: 50S ribosomal protein L22



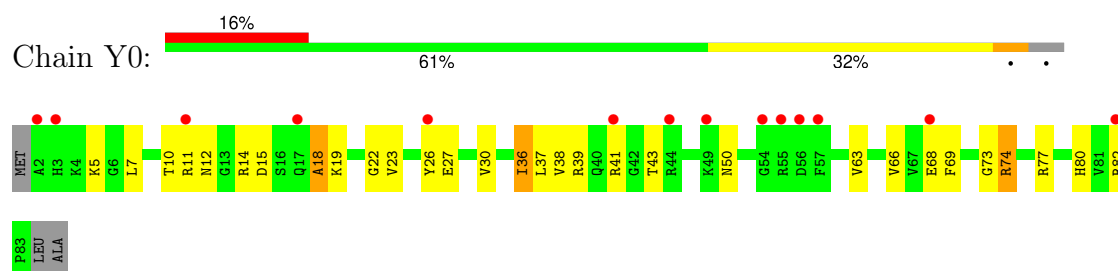
• Molecule 44: 50S ribosomal protein L23



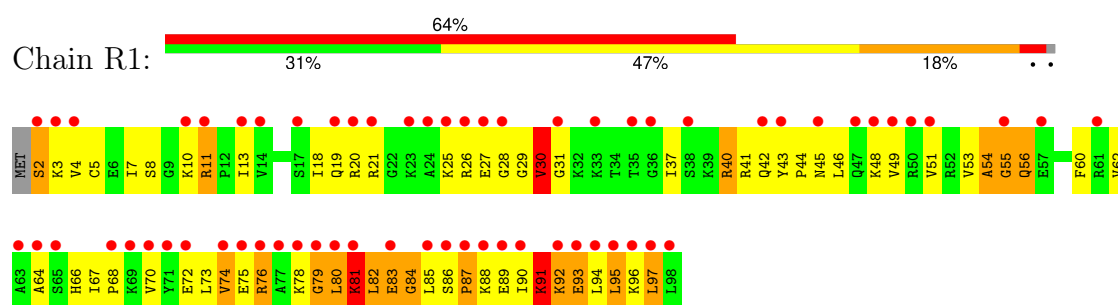
- Molecule 46: 50S ribosomal protein L25



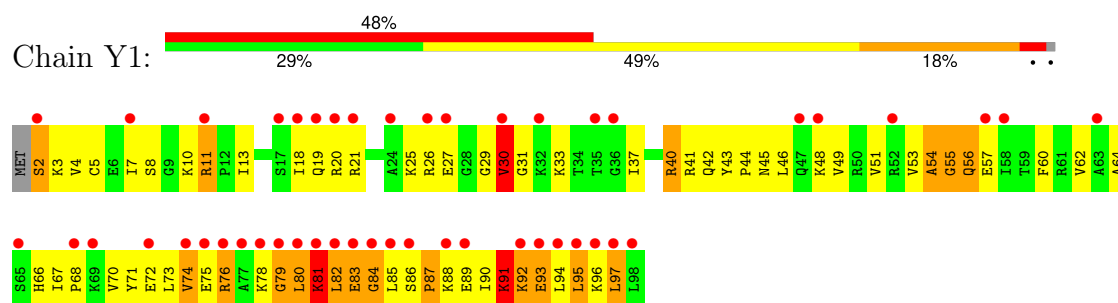
- Molecule 46: 50S ribosomal protein L25



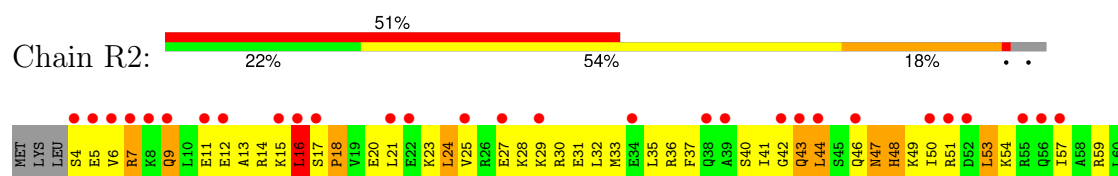
- Molecule 47: 50S ribosomal protein L27

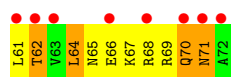


- Molecule 47: 50S ribosomal protein L27

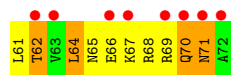
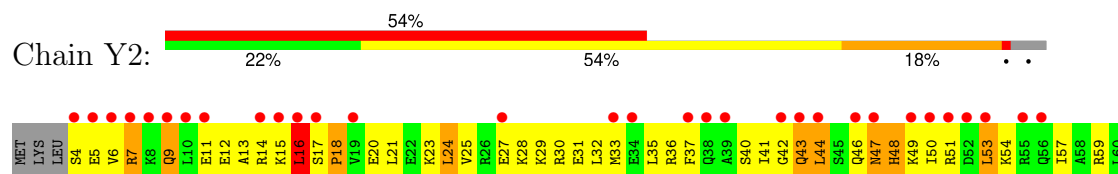


- Molecule 48: 50S ribosomal protein L28

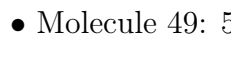
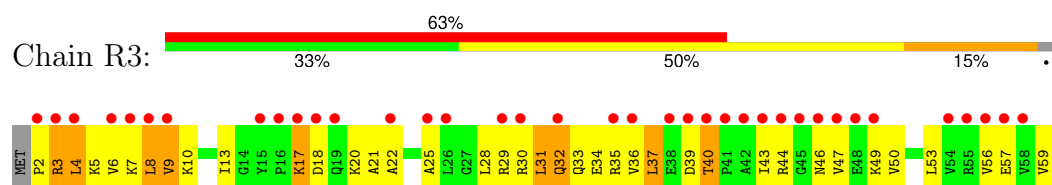




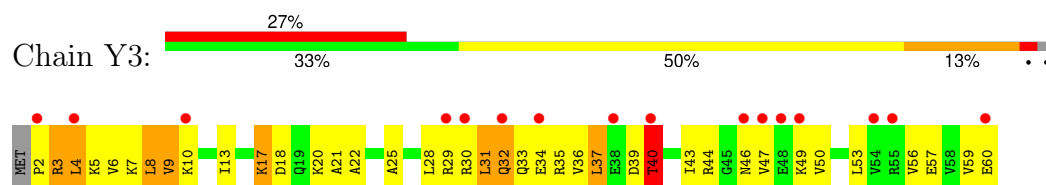
- Molecule 48: 50S ribosomal protein L28



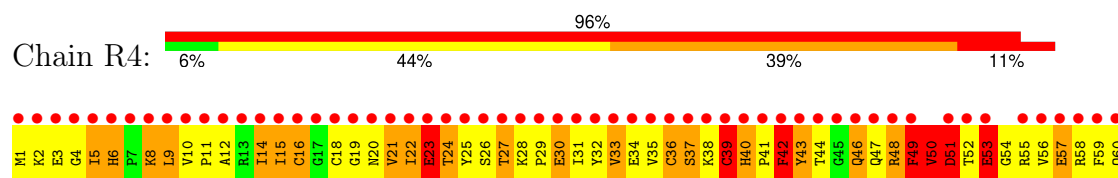
- Molecule 49: 50S ribosomal protein L29



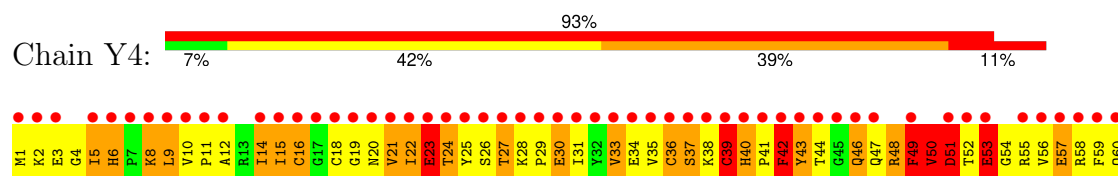
- Molecule 49: 50S ribosomal protein L29



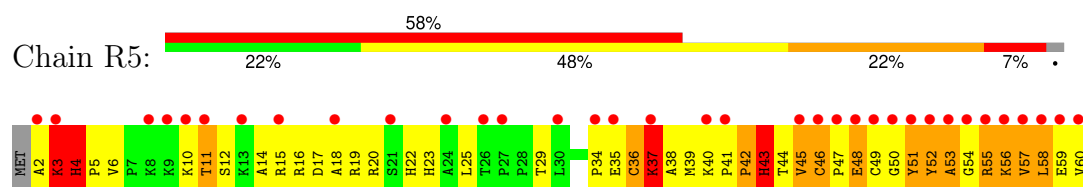
- Molecule 50: 50S ribosomal protein L30



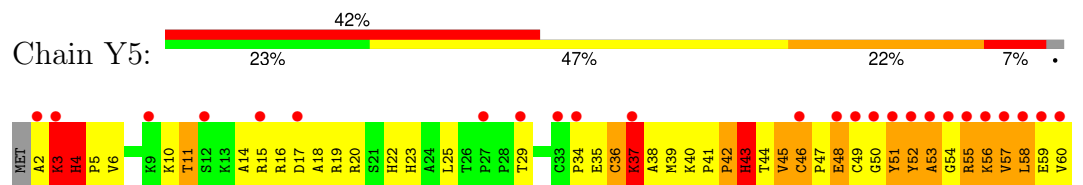
- Molecule 50: 50S ribosomal protein L30



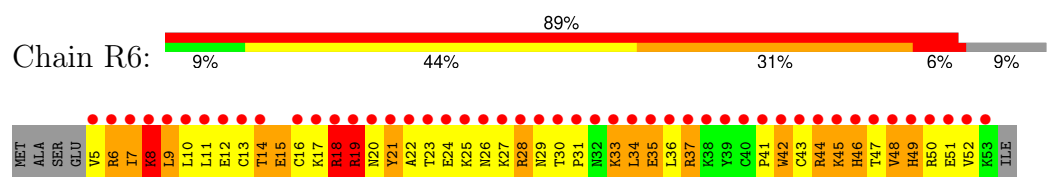
- Molecule 51: 50S ribosomal protein L32



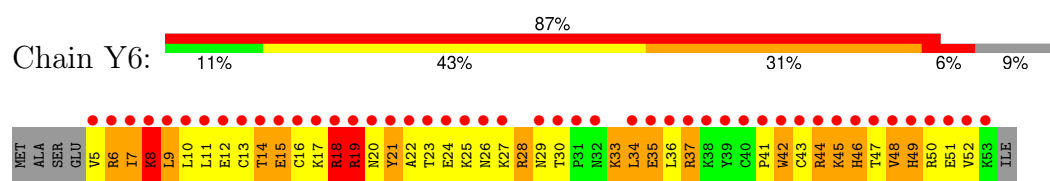
- Molecule 51: 50S ribosomal protein L32



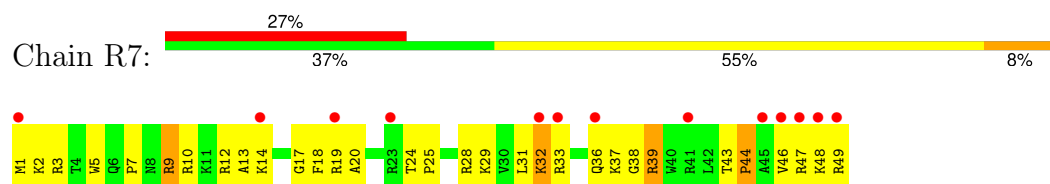
- Molecule 52: 50S ribosomal protein L33



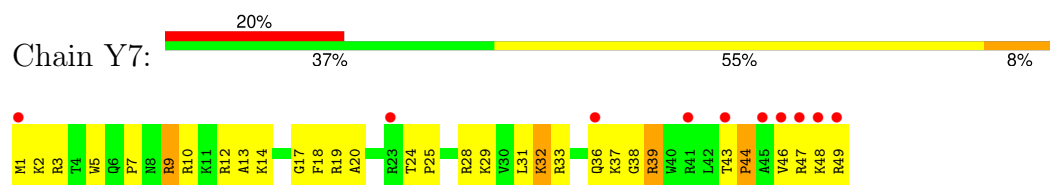
- Molecule 52: 50S ribosomal protein L33



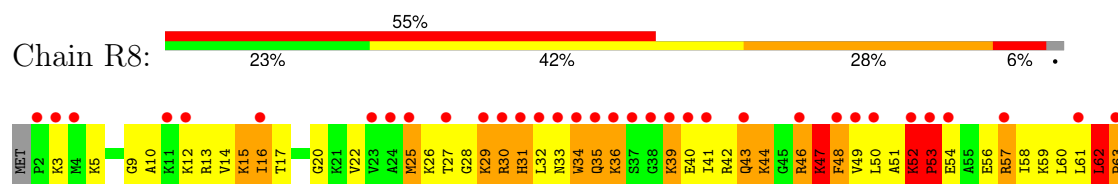
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34

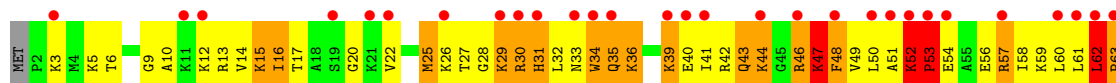
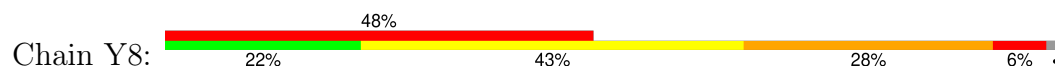


- Molecule 54: 50S ribosomal protein L35





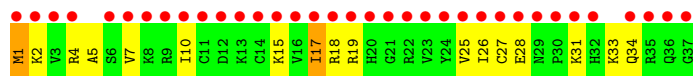
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.21Å 448.45Å 619.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.60 – 3.14 189.60 – 3.14	Depositor EDS
% Data completeness (in resolution range)	99.6 (189.60-3.14) 99.7 (189.60-3.14)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.230 , 0.262 0.232 , 0.263	Depositor DCC
R_{free} test set	46777 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	291998	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/36098	0.89	48/56341 (0.1%)
1	XA	0.37	0/36101	0.89	50/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.61	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.37	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.39	1/1836 (0.1%)	0.81	3/2859 (0.1%)
22	XV	0.42	1/1836 (0.1%)	0.84	4/2859 (0.1%)
23	QY	0.24	0/333	0.81	0/517
23	XY	0.24	0/333	0.74	0/517
24	QX	0.65	0/189	1.41	5/292 (1.7%)
24	XX	0.39	0/189	1.08	2/292 (0.7%)
25	RA	0.39	0/69521	0.88	70/108529 (0.1%)
25	YA	0.43	1/69543 (0.0%)	0.92	116/108563 (0.1%)
26	RB	0.32	0/2878	0.84	0/4490
26	YB	0.36	0/2878	0.88	1/4490 (0.0%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.28	0/1151	0.56	0/1558
32	YI	0.27	0/1151	0.58	0/1558
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.50	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.45	0/892	0.83	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.46	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.77	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.27	0/1493	0.52	0/2026
45	YZ	0.28	0/1493	0.54	0/2026
46	R0	0.30	0/657	0.54	0/874
46	Y0	0.34	0/657	0.53	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.83	1/771 (0.1%)
48	Y2	0.50	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.72	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.59	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.79	0/40	1.81	1/60 (1.7%)
56	Z8	0.77	0/40	1.81	1/60 (1.7%)
All	All	0.41	5/316375 (0.0%)	0.86	364/472993 (0.1%)

All (5) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	1	C	OP3-P	-10.56	1.48	1.61
22	XV	1	C	OP3-P	-10.53	1.48	1.61
27	RD	236	GLY	C-N	8.57	1.53	1.34
25	YA	774	A	N9-C4	-5.56	1.34	1.37
27	RD	241	PRO	N-CD	5.19	1.55	1.47

The worst 5 of 364 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	XL	47	LYS	C-N-CD	-20.45	75.61	120.60
12	QL	47	LYS	C-N-CD	-20.44	75.62	120.60
25	YA	2506	U	N3-C2-O2	-10.56	114.81	122.20
28	YE	21	VAL	C-N-CD	-10.11	98.35	120.60
28	RE	21	VAL	C-N-CD	-10.09	98.41	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	576	0
1	XA	32249	0	16279	575	1
2	QB	1924	0	1975	287	0
2	XB	1924	0	1975	293	0
3	QC	1605	0	1668	212	0
3	XC	1605	0	1668	215	2
4	QD	1703	0	1765	261	0
4	XD	1703	0	1764	217	0
5	QE	1155	0	1213	140	0
5	XE	1155	0	1213	141	0
6	QF	843	0	857	97	0
6	XF	843	0	857	101	0
7	QG	1257	0	1296	148	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	143	0
8	QH	1116	0	1175	148	0
8	XH	1116	0	1177	154	0
9	QI	1010	0	1037	145	0
9	XI	1010	0	1037	153	0
10	QJ	801	0	849	152	0
10	XJ	801	0	849	141	0
11	QK	885	0	904	103	2
11	XK	885	0	904	109	0
12	QL	975	0	1062	107	0
12	XL	975	0	1062	110	0
13	QM	964	0	1034	163	0
13	XM	964	0	1034	150	0
14	QN	492	0	529	100	0
14	XN	492	0	529	94	0
15	QO	734	0	771	73	0
15	XO	734	0	771	72	0
16	QP	705	0	725	115	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	85	0
17	XQ	834	0	904	78	0
18	QR	574	0	644	66	0
18	XR	574	0	644	69	0
19	QS	674	0	699	103	0
19	XS	674	0	699	136	0
20	QT	763	0	860	108	0
20	XT	763	0	861	103	0
21	QU	217	0	234	27	0
21	XU	217	0	234	28	0
22	QV	1644	0	836	22	0
22	XV	1644	0	836	15	0
23	QY	323	0	165	2	0
23	XY	323	0	165	6	0
24	QX	170	0	88	2	0
24	XX	170	0	88	1	0
25	RA	62071	0	31288	992	0
25	YA	62091	0	31296	935	0
26	RB	2573	0	1306	62	0
26	YB	2573	0	1306	26	0
27	RD	2115	0	2195	319	0
27	YD	2115	0	2195	332	0
28	RE	1568	0	1634	270	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	265	0
29	RF	1585	0	1632	181	0
29	YF	1585	0	1632	180	0
30	RG	1474	0	1535	211	0
30	YG	1474	0	1535	193	0
31	RH	1307	0	1382	225	0
31	YH	1307	0	1382	221	0
32	RI	1136	0	1223	42	1
32	YI	1136	0	1223	40	0
33	RN	1104	0	1180	191	0
33	YN	1104	0	1180	183	0
34	RO	933	0	996	123	0
34	YO	933	0	996	123	0
35	RP	1145	0	1228	250	0
35	YP	1145	0	1228	245	0
36	RQ	1122	0	1179	159	0
36	YQ	1122	0	1179	158	0
37	RR	968	0	1033	113	0
37	YR	968	0	1033	113	0
38	RS	882	0	943	165	0
38	YS	882	0	943	159	0
39	RT	1141	0	1202	154	0
39	YT	1141	0	1202	153	0
40	RU	964	0	1022	131	0
40	YU	964	0	1022	137	0
41	RV	779	0	852	129	0
41	YV	779	0	852	136	3
42	RW	900	0	964	99	0
42	YW	900	0	964	100	0
43	RX	725	0	778	69	0
43	YX	725	0	778	74	0
44	RY	785	0	878	163	0
44	YY	785	0	878	151	0
45	RZ	1461	0	1493	46	0
45	YZ	1461	0	1493	57	0
46	R0	648	0	672	20	0
46	Y0	648	0	672	28	0
47	R1	763	0	848	146	0
47	Y1	763	0	848	142	0
48	R2	581	0	629	81	0
48	Y2	581	0	629	77	0
49	R3	469	0	518	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	41	0
50	R4	581	0	574	153	0
50	Y4	581	0	574	164	0
51	R5	459	0	480	77	0
51	Y5	459	0	480	75	3
52	R6	424	0	450	92	0
52	Y6	424	0	450	89	0
53	R7	430	0	480	43	0
53	Y7	430	0	480	44	0
54	R8	517	0	582	106	0
54	Y8	517	0	582	103	0
55	R9	307	0	338	18	0
55	Y9	307	0	338	18	0
56	Z6	74	0	51	6	0
56	Z8	74	0	51	7	0
57	QA	69	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	240	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	74	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	265	0	0	0	0
57	YB	3	0	0	0	0
57	YE	2	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	1	0	0	0	0
58	QA	42	0	45	3	0
58	XA	42	0	45	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291998	0	198367	14453	6

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 30.

The worst 5 of 14453 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.55
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	1.49	0.71
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.70	0.50
11:QK:99:GLN:OE1	3:XC:79:ARG:NE[4_555]	2.04	0.16
41:YV:50:PRO:CG	51:Y5:60:VAL:O[4_445]	2.14	0.06
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	1
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	1
3	QC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	2
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	2
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	2
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	2
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	2
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	2
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	0	3
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	0	3
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	2
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	0	2
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	2
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	2
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	1
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	1
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	2
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	2
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	4
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	4
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	1
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	1
13	QM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	0
13	XM	119/126 (94%)	71 (60%)	26 (22%)	22 (18%)	0	0
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	0
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	0
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	5
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	5
16	QP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	0	1
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	1
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	3
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	1
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	1
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	0
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	0
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	0
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	0
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	0
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	0
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	5
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	5
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	2
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	2
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	1
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	1
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
32	RI	144/148 (97%)	102 (71%)	27 (19%)	15 (10%)	0	2
32	YI	144/148 (97%)	103 (72%)	25 (17%)	16 (11%)	0	1
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	0
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	0
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	4
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	4
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	2
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	2
37	RR	116/118 (98%)	83 (72%)	19 (16%)	14 (12%)	0	1
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	1
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	0
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	0
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	4
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	4
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	2
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	2
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	1
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	1
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1	7
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1	7
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
45	RZ	181/206 (88%)	126 (70%)	35 (19%)	20 (11%)	0	2
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	0	2
46	R0	80/85 (94%)	71 (89%)	7 (9%)	2 (2%)	4	19
46	Y0	80/85 (94%)	72 (90%)	6 (8%)	2 (2%)	4	19
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	1
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	1
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	1
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	1
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1	8
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1	8
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	6
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	0
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	0
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7666 (67%)	2321 (20%)	1483 (13%)	0	1

5 of 1483 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	4	16
2	XB	205/220 (93%)	181 (88%)	24 (12%)	4	16
3	QC	159/188 (85%)	143 (90%)	16 (10%)	6	21
3	XC	159/188 (85%)	143 (90%)	16 (10%)	6	21
4	QD	180/181 (99%)	160 (89%)	20 (11%)	5	18
4	XD	180/181 (99%)	165 (92%)	15 (8%)	9	29
5	QE	116/123 (94%)	108 (93%)	8 (7%)	13	36
5	XE	116/123 (94%)	107 (92%)	9 (8%)	10	32
6	QF	90/90 (100%)	76 (84%)	14 (16%)	2	8
6	XF	90/90 (100%)	76 (84%)	14 (16%)	2	8
7	QG	126/127 (99%)	114 (90%)	12 (10%)	7	24
7	XG	126/127 (99%)	115 (91%)	11 (9%)	8	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	106 (89%)	13 (11%)	5	19
8	XH	119/119 (100%)	106 (89%)	13 (11%)	5	19
9	QI	98/99 (99%)	87 (89%)	11 (11%)	5	18
9	XI	98/99 (99%)	87 (89%)	11 (11%)	5	18
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	8	26
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	8	26
11	QK	90/99 (91%)	81 (90%)	9 (10%)	6	21
11	XK	90/99 (91%)	81 (90%)	9 (10%)	6	21
12	QL	104/109 (95%)	90 (86%)	14 (14%)	3	12
12	XL	104/109 (95%)	90 (86%)	14 (14%)	3	12
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	7
13	XM	97/101 (96%)	81 (84%)	16 (16%)	2	7
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	5
14	XN	49/50 (98%)	44 (90%)	5 (10%)	6	20
15	QO	79/80 (99%)	73 (92%)	6 (8%)	11	32
15	XO	79/80 (99%)	73 (92%)	6 (8%)	11	32
16	QP	72/74 (97%)	63 (88%)	9 (12%)	3	14
16	XP	72/74 (97%)	63 (88%)	9 (12%)	3	14
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	15	39
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	15	39
18	QR	61/77 (79%)	54 (88%)	7 (12%)	4	17
18	XR	61/77 (79%)	54 (88%)	7 (12%)	4	17
19	QS	73/80 (91%)	62 (85%)	11 (15%)	2	9
19	XS	73/80 (91%)	62 (85%)	11 (15%)	2	9
20	QT	76/82 (93%)	68 (90%)	8 (10%)	5	20
20	XT	76/82 (93%)	68 (90%)	8 (10%)	5	20
21	QU	20/22 (91%)	19 (95%)	1 (5%)	20	46
21	XU	20/22 (91%)	19 (95%)	1 (5%)	20	46
27	RD	214/218 (98%)	177 (83%)	37 (17%)	1	6
27	YD	214/218 (98%)	177 (83%)	37 (17%)	1	6
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	0	2
29	RF	161/166 (97%)	140 (87%)	21 (13%)	3	13
29	YF	161/166 (97%)	140 (87%)	21 (13%)	3	13
30	RG	155/156 (99%)	130 (84%)	25 (16%)	2	8
30	YG	155/156 (99%)	130 (84%)	25 (16%)	2	8
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	4
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	4
32	RI	122/124 (98%)	100 (82%)	22 (18%)	1	6
32	YI	122/124 (98%)	98 (80%)	24 (20%)	1	4
33	RN	117/119 (98%)	98 (84%)	19 (16%)	2	8
33	YN	117/119 (98%)	98 (84%)	19 (16%)	2	8
34	RO	100/100 (100%)	90 (90%)	10 (10%)	6	21
34	YO	100/100 (100%)	90 (90%)	10 (10%)	6	21
35	RP	116/116 (100%)	89 (77%)	27 (23%)	0	2
35	YP	116/116 (100%)	89 (77%)	27 (23%)	0	2
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	8
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	2	8
37	RR	101/101 (100%)	84 (83%)	17 (17%)	1	7
37	YR	101/101 (100%)	84 (83%)	17 (17%)	1	7
38	RS	87/88 (99%)	74 (85%)	13 (15%)	2	10
38	YS	87/88 (99%)	74 (85%)	13 (15%)	2	10
39	RT	120/127 (94%)	97 (81%)	23 (19%)	1	5
39	YT	120/127 (94%)	97 (81%)	23 (19%)	1	5
40	RU	93/94 (99%)	80 (86%)	13 (14%)	3	11
40	YU	93/94 (99%)	80 (86%)	13 (14%)	3	11
41	RV	82/82 (100%)	71 (87%)	11 (13%)	3	12
41	YV	82/82 (100%)	71 (87%)	11 (13%)	3	12
42	RW	92/92 (100%)	77 (84%)	15 (16%)	2	7
42	YW	92/92 (100%)	77 (84%)	15 (16%)	2	7
43	RX	74/78 (95%)	63 (85%)	11 (15%)	2	10
43	YX	74/78 (95%)	63 (85%)	11 (15%)	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	70 (82%)	15 (18%)	1	6
44	YY	85/91 (93%)	70 (82%)	15 (18%)	1	6
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	2	10
45	YZ	162/179 (90%)	142 (88%)	20 (12%)	4	15
46	R0	65/67 (97%)	58 (89%)	7 (11%)	5	19
46	Y0	65/67 (97%)	63 (97%)	2 (3%)	35	60
47	R1	82/83 (99%)	67 (82%)	15 (18%)	1	5
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	5
48	R2	64/67 (96%)	57 (89%)	7 (11%)	5	19
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	5	19
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	3
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	3
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	0
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	0
51	R5	51/52 (98%)	39 (76%)	12 (24%)	0	2
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	0	2
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	4
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	4
53	R7	42/42 (100%)	39 (93%)	3 (7%)	12	35
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	12	35
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	1
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	1
55	R9	34/34 (100%)	32 (94%)	2 (6%)	16	41
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	16	41
All	All	9702/10066 (96%)	8299 (86%)	1403 (14%)	2	10

5 of 1403 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	YD	43	ARG
35	YP	99	LEU
27	YD	237	GLU
27	YD	33	LEU
30	YG	159	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
3	XC	181	ASN
13	XM	101	GLN
47	Y1	56	GLN
5	XE	78	HIS
7	XG	148	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	293 (19%)	45 (3%)
1	XA	1498/1522 (98%)	299 (19%)	47 (3%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	21 (27%)	1 (1%)
23	QY	14/17 (82%)	4 (28%)	1 (7%)
23	XY	14/17 (82%)	4 (28%)	1 (7%)
24	QX	7/25 (28%)	4 (57%)	0
24	XX	7/25 (28%)	3 (42%)	2 (28%)
25	RA	2879/2916 (98%)	618 (21%)	67 (2%)
25	YA	2880/2916 (98%)	612 (21%)	64 (2%)
26	RB	119/122 (97%)	24 (20%)	2 (1%)
26	YB	119/122 (97%)	29 (24%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9364 (98%)	1932 (21%)	232 (2%)

5 of 1932 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	RB	66	A
25	YA	2566	A
1	XA	703	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	YA	2481	G
25	YA	1085	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	PPU	Z8	76	25,56	33,40,41	2.67	8 (24%)	33,57,60	2.64	8 (24%)
56	PPU	Z6	76	25,56	33,40,41	2.68	7 (21%)	33,57,60	2.65	8 (24%)
23	1MG	QY	37	23	19,26,27	2.53	3 (15%)	18,39,42	2.24	5 (27%)
23	1MG	XY	37	23	19,26,27	2.49	3 (15%)	18,39,42	2.13	5 (27%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.62	1.41	1.23
56	Z8	76	PPU	O-C	9.54	1.41	1.23
23	QY	37	1MG	C2-N2	7.81	1.47	1.34
23	XY	37	1MG	C2-N2	7.75	1.47	1.34
56	Z6	76	PPU	C9-N6	-6.22	1.32	1.45

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.56	110.18	123.20
56	Z8	76	PPU	C3'-N3'-C	-8.55	110.19	123.20
23	QY	37	1MG	N2-C2-N1	6.82	124.27	118.79
23	XY	37	1MG	N2-C2-N1	5.69	123.36	118.79
56	Z8	76	PPU	N3-C2-N1	-5.36	121.40	128.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	7	0
56	Z6	76	PPU	5	0
23	XY	37	1MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 682 ligands modelled in this entry, 680 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	XA	1675	-	44,45,45	1.33	6 (13%)	63,67,67	1.30	4 (6%)
58	PAR	QA	1670	-	44,45,45	1.27	6 (13%)	63,67,67	1.33	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	PAR	XA	1675	-	-	6/18/94/94	0/4/4/4
58	PAR	QA	1670	-	-	8/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1670	PAR	C52-C42	3.14	1.58	1.52
58	XA	1675	PAR	C52-C42	3.04	1.58	1.52
58	QA	1670	PAR	O54-C14	2.90	1.49	1.41
58	XA	1675	PAR	O54-C14	2.85	1.49	1.41
58	XA	1675	PAR	C11-C21	2.83	1.57	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1675	PAR	O33-C14-C24	5.00	116.26	108.08
58	XA	1675	PAR	C14-O54-C54	4.32	122.16	113.72
58	QA	1670	PAR	O33-C14-C24	4.04	114.69	108.08
58	QA	1670	PAR	C14-O54-C54	3.81	121.16	113.72
58	QA	1670	PAR	O11-C42-C52	3.16	115.45	107.42

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

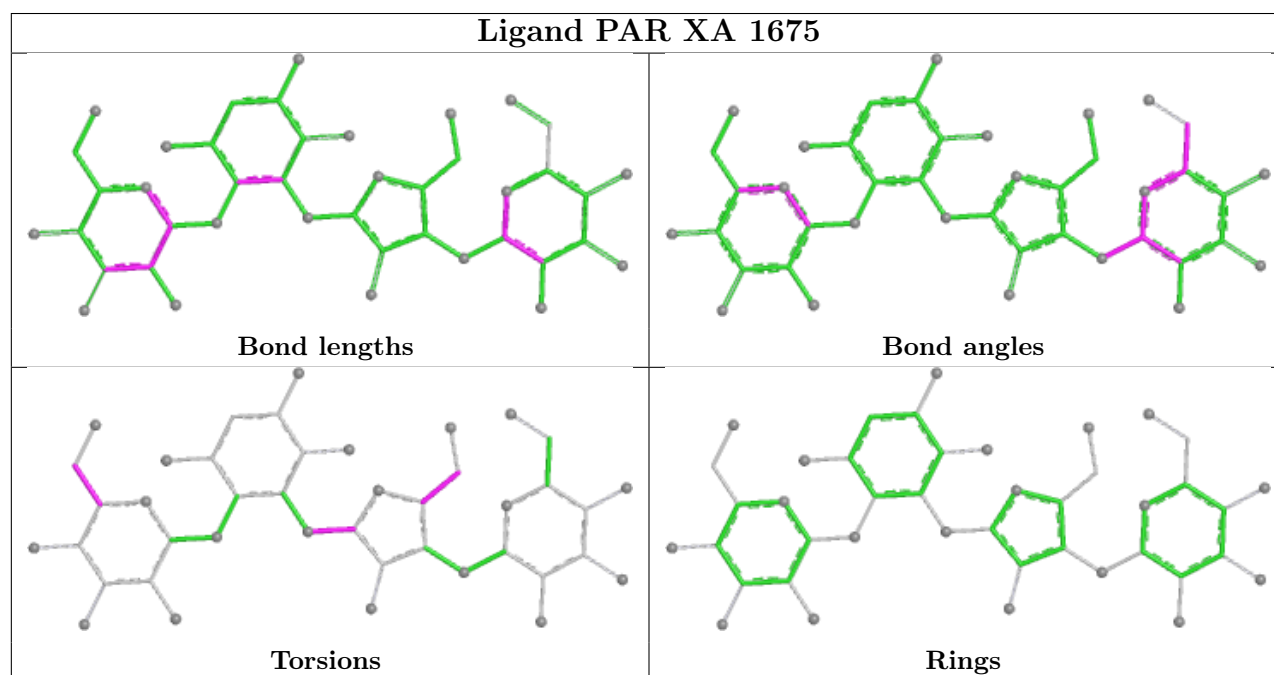
Mol	Chain	Res	Type	Atoms
58	QA	1670	PAR	C44-C54-C64-N64
58	QA	1670	PAR	O54-C54-C64-N64
58	XA	1675	PAR	O51-C51-C61-O61
58	QA	1670	PAR	O51-C51-C61-O61
58	XA	1675	PAR	C41-C51-C61-O61

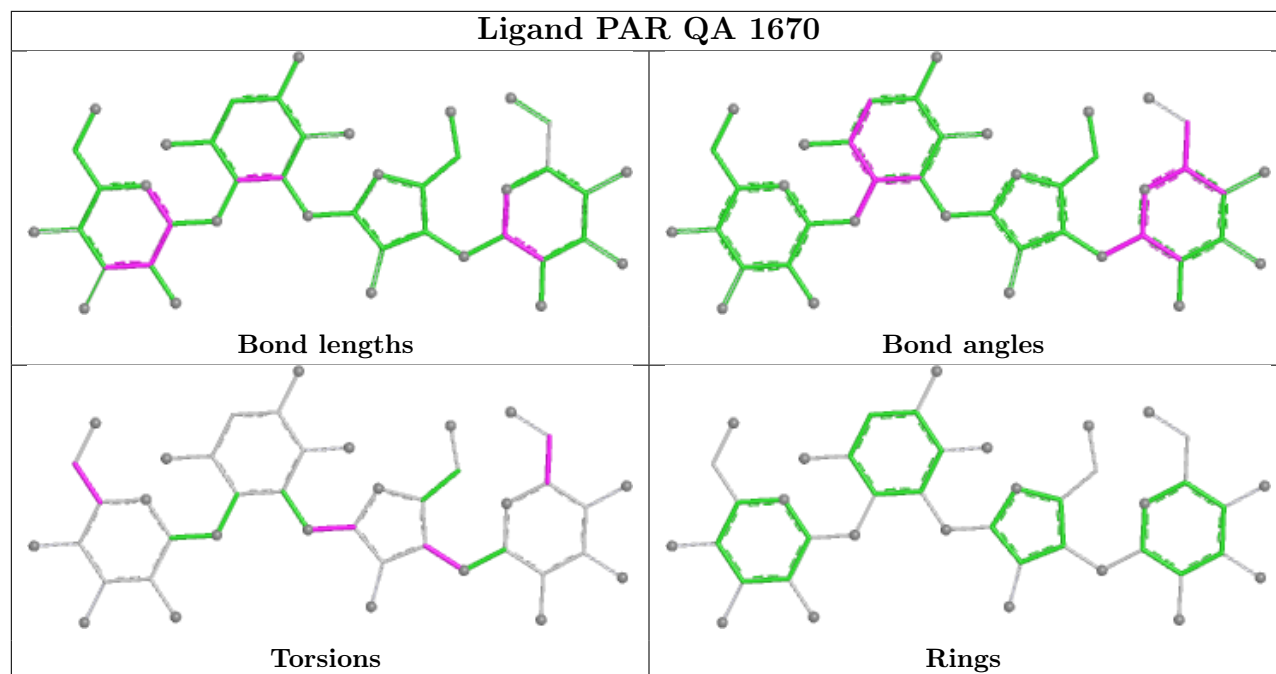
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1675	PAR	1	0
58	QA	1670	PAR	3	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	QA	1500/1522 (98%)	1.64	440 (29%)	1	1	27, 67, 148, 352	0
1	XA	1500/1522 (98%)	1.47	382 (25%)	2	1	18, 55, 149, 326	0
2	QB	237/256 (92%)	3.34	179 (75%)	0	0	54, 126, 215, 288	0
2	XB	237/256 (92%)	3.15	182 (76%)	0	0	43, 102, 177, 293	0
3	QC	205/239 (85%)	3.00	159 (77%)	0	0	56, 108, 175, 255	0
3	XC	205/239 (85%)	2.54	122 (59%)	0	0	30, 78, 132, 181	0
4	QD	208/209 (99%)	2.88	134 (64%)	0	0	41, 79, 136, 185	0
4	XD	208/209 (99%)	2.94	136 (65%)	0	0	30, 74, 134, 231	0
5	QE	151/162 (93%)	2.75	101 (66%)	0	0	42, 85, 148, 260	0
5	XE	151/162 (93%)	2.14	83 (54%)	0	0	23, 61, 121, 196	0
6	QF	101/101 (100%)	2.34	55 (54%)	0	0	30, 74, 112, 155	0
6	XF	101/101 (100%)	2.21	52 (51%)	0	0	26, 69, 110, 146	0
7	QG	155/156 (99%)	3.05	98 (63%)	0	0	46, 97, 158, 302	0
7	XG	155/156 (99%)	2.62	85 (54%)	0	0	35, 82, 149, 230	0
8	QH	138/138 (100%)	2.74	94 (68%)	0	0	39, 83, 130, 174	0
8	XH	138/138 (100%)	2.43	84 (60%)	0	0	34, 68, 117, 169	0
9	QI	127/128 (99%)	3.51	97 (76%)	0	0	48, 117, 170, 243	0
9	XI	127/128 (99%)	3.06	98 (77%)	0	0	33, 91, 152, 203	0
10	QJ	99/105 (94%)	4.52	94 (94%)	0	0	53, 140, 243, 282	0
10	XJ	99/105 (94%)	3.40	79 (79%)	0	0	21, 100, 169, 213	0
11	QK	119/129 (92%)	3.16	85 (71%)	0	0	42, 77, 149, 228	0
11	XK	119/129 (92%)	2.51	67 (56%)	0	0	28, 70, 134, 196	0
12	QL	125/132 (94%)	2.77	67 (53%)	0	0	35, 69, 140, 262	0
12	XL	125/132 (94%)	2.15	54 (43%)	1	0	22, 51, 113, 282	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%)	3.22	86 (71%)	0	0	43, 108, 185, 410	0
13	XM	121/126 (96%)	2.87	81 (66%)	0	0	36, 86, 141, 273	0
14	QN	60/61 (98%)	3.16	45 (75%)	0	0	59, 101, 150, 166	0
14	XN	60/61 (98%)	2.86	41 (68%)	0	0	36, 67, 127, 143	0
15	QO	88/89 (98%)	2.41	49 (55%)	0	0	32, 78, 150, 180	0
15	XO	88/89 (98%)	1.92	41 (46%)	0	0	27, 62, 111, 129	0
16	QP	84/88 (95%)	2.72	59 (70%)	0	0	38, 71, 115, 186	0
16	XP	84/88 (95%)	2.64	57 (67%)	0	0	39, 73, 119, 211	0
17	QQ	100/105 (95%)	2.85	63 (63%)	0	0	44, 79, 131, 161	0
17	XQ	100/105 (95%)	2.55	54 (54%)	0	0	35, 75, 127, 166	0
18	QR	70/88 (79%)	2.29	35 (50%)	0	0	28, 73, 141, 149	0
18	XR	70/88 (79%)	1.96	27 (38%)	1	0	27, 66, 118, 171	0
19	QS	84/93 (90%)	3.54	76 (90%)	0	0	80, 119, 195, 275	0
19	XS	84/93 (90%)	2.90	60 (71%)	0	0	47, 88, 168, 219	0
20	QT	99/106 (93%)	2.91	67 (67%)	0	0	37, 82, 140, 220	0
20	XT	99/106 (93%)	3.09	77 (77%)	0	0	28, 86, 149, 177	0
21	QU	25/27 (92%)	3.68	19 (76%)	0	0	45, 98, 150, 185	0
21	XU	25/27 (92%)	3.36	21 (84%)	0	0	43, 69, 139, 153	0
22	QV	77/77 (100%)	1.82	29 (37%)	1	0	27, 73, 146, 212	0
22	XV	77/77 (100%)	1.42	20 (25%)	2	1	17, 59, 103, 207	0
23	QY	14/17 (82%)	2.54	7 (50%)	0	0	69, 116, 169, 189	0
23	XY	14/17 (82%)	2.28	4 (28%)	1	1	41, 102, 143, 157	0
24	QX	8/25 (32%)	2.72	3 (37%)	1	0	49, 58, 151, 164	0
24	XX	8/25 (32%)	1.40	2 (25%)	2	1	32, 38, 89, 104	0
25	RA	2882/2916 (98%)	1.20	520 (18%)	4	2	13, 44, 212, 472	0
25	YA	2883/2916 (98%)	0.95	416 (14%)	7	4	7, 35, 201, 461	0
26	RB	120/122 (98%)	1.80	43 (35%)	1	0	43, 69, 105, 120	0
26	YB	120/122 (98%)	0.93	10 (8%)	19	11	29, 51, 71, 110	0
27	RD	272/276 (98%)	1.97	117 (43%)	1	0	9, 42, 81, 176	0
27	YD	272/276 (98%)	1.68	89 (32%)	1	0	5, 35, 71, 188	0
28	RE	205/206 (99%)	2.40	97 (47%)	0	0	11, 56, 123, 335	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	2.25	104 (50%)	0	0	2, 52, 123, 250	0
29	RF	202/210 (96%)	2.35	110 (54%)	0	0	15, 62, 132, 185	0
29	YF	202/210 (96%)	1.83	73 (36%)	1	0	8, 45, 121, 194	0
30	RG	181/182 (99%)	6.55	180 (99%)	0	0	79, 156, 284, 386	0
30	YG	181/182 (99%)	4.04	167 (92%)	0	0	30, 89, 155, 309	0
31	RH	170/180 (94%)	3.74	150 (88%)	0	0	79, 145, 235, 306	0
31	YH	170/180 (94%)	3.28	124 (72%)	0	0	31, 79, 122, 167	0
32	RI	146/148 (98%)	2.65	87 (59%)	0	0	25, 87, 178, 297	0
32	YI	146/148 (98%)	2.39	77 (52%)	0	0	22, 83, 152, 183	0
33	RN	138/140 (98%)	2.37	76 (55%)	0	0	26, 64, 124, 179	0
33	YN	138/140 (98%)	2.07	58 (42%)	1	0	16, 54, 108, 166	0
34	RO	122/122 (100%)	2.44	70 (57%)	0	0	22, 55, 103, 142	0
34	YO	122/122 (100%)	1.97	52 (42%)	1	0	16, 48, 78, 126	0
35	RP	150/150 (100%)	2.96	99 (66%)	0	0	18, 68, 154, 247	0
35	YP	150/150 (100%)	2.39	79 (52%)	0	0	9, 53, 126, 253	0
36	RQ	141/141 (100%)	2.99	83 (58%)	0	0	28, 67, 128, 178	0
36	YQ	141/141 (100%)	2.49	69 (48%)	0	0	14, 47, 124, 154	0
37	RR	118/118 (100%)	1.78	45 (38%)	1	0	18, 48, 81, 170	0
37	YR	118/118 (100%)	1.83	48 (40%)	1	0	20, 46, 85, 137	0
38	RS	111/112 (99%)	2.41	62 (55%)	0	0	38, 76, 131, 184	0
38	YS	111/112 (99%)	1.95	48 (43%)	1	0	28, 58, 106, 195	0
39	RT	137/146 (93%)	2.95	94 (68%)	0	0	29, 67, 161, 259	0
39	YT	137/146 (93%)	2.77	84 (61%)	0	0	27, 61, 152, 303	0
40	RU	117/118 (99%)	2.20	53 (45%)	1	0	20, 54, 114, 221	0
40	YU	117/118 (99%)	1.98	43 (36%)	1	0	19, 39, 97, 221	0
41	RV	101/101 (100%)	2.49	58 (57%)	0	0	21, 77, 140, 320	0
41	YV	101/101 (100%)	2.24	48 (47%)	0	0	13, 63, 124, 304	0
42	RW	113/113 (100%)	1.60	31 (27%)	2	1	19, 41, 99, 220	0
42	YW	113/113 (100%)	1.32	24 (21%)	3	2	15, 41, 95, 193	0
43	RX	92/96 (95%)	1.82	35 (38%)	1	0	26, 53, 87, 135	0
43	YX	92/96 (95%)	1.42	26 (28%)	1	1	12, 39, 76, 116	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	4.85	87 (85%)	0	0	40, 99, 177, 285	0
44	YY	102/110 (92%)	3.15	70 (68%)	0	0	31, 73, 155, 210	0
45	RZ	183/206 (88%)	2.92	120 (65%)	0	0	41, 93, 178, 292	0
45	YZ	183/206 (88%)	2.55	98 (53%)	0	0	32, 71, 179, 271	0
46	R0	82/85 (96%)	1.56	22 (26%)	2	1	18, 49, 71, 179	0
46	Y0	82/85 (96%)	0.98	14 (17%)	5	3	11, 34, 60, 87	0
47	R1	97/98 (98%)	2.92	63 (64%)	0	0	21, 51, 160, 335	0
47	Y1	97/98 (98%)	2.29	47 (48%)	0	0	16, 49, 139, 210	0
48	R2	69/72 (95%)	2.37	37 (53%)	0	0	28, 69, 143, 169	0
48	Y2	69/72 (95%)	2.69	39 (56%)	0	0	19, 59, 119, 177	0
49	R3	59/60 (98%)	2.57	38 (64%)	0	0	31, 71, 112, 169	0
49	Y3	59/60 (98%)	1.62	16 (27%)	2	1	22, 49, 91, 198	0
50	R4	71/71 (100%)	5.17	68 (95%)	0	0	107, 211, 311, 396	0
50	Y4	71/71 (100%)	5.11	66 (92%)	0	0	66, 156, 274, 384	0
51	R5	59/60 (98%)	2.98	35 (59%)	0	0	8, 49, 223, 238	0
51	Y5	59/60 (98%)	2.24	25 (42%)	1	0	11, 49, 223, 335	0
52	R6	49/54 (90%)	5.35	48 (97%)	0	0	86, 175, 268, 291	0
52	Y6	49/54 (90%)	4.92	47 (95%)	0	0	76, 163, 229, 312	0
53	R7	49/49 (100%)	1.52	13 (26%)	2	1	16, 29, 87, 168	0
53	Y7	49/49 (100%)	1.18	10 (20%)	3	2	8, 23, 87, 176	0
54	R8	64/65 (98%)	2.72	36 (56%)	0	0	20, 53, 102, 208	0
54	Y8	64/65 (98%)	2.36	31 (48%)	0	0	16, 44, 97, 214	0
55	R9	37/37 (100%)	4.78	36 (97%)	0	0	82, 138, 203, 344	0
55	Y9	37/37 (100%)	4.48	35 (94%)	0	0	57, 119, 223, 246	0
56	Z6	2/3 (66%)	2.74	2 (100%)	0	0	33, 33, 33, 47	0
56	Z8	2/3 (66%)	2.50	2 (100%)	0	0	24, 24, 24, 36	0
All	All	20873/21492 (97%)	2.08	8804 (42%)	1	0	2, 61, 174, 472	0

The worst 5 of 8804 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	22.8
30	RG	154	GLY	17.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	QG	81	GLY	17.4
7	QG	82	GLY	16.4
30	RG	72	ARG	16.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PPU	Z8	76	37/38	0.85	0.24	37,37,37,37	0
56	PPU	Z6	76	37/38	0.86	0.26	41,41,41,41	0
23	1MG	QY	37	24/25	0.92	0.12	63,63,63,63	0
23	1MG	XY	37	24/25	0.92	0.13	45,45,45,45	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	YA	3105	1/1	0.26	0.24	21,21,21,21	0
57	MG	RA	3222	1/1	0.29	0.58	93,93,93,93	0
57	MG	YA	3120	1/1	0.33	0.55	63,63,63,63	0
57	MG	RA	3192	1/1	0.37	0.25	79,79,79,79	0
57	MG	RA	3120	1/1	0.37	0.36	60,60,60,60	0
57	MG	YA	3139	1/1	0.37	0.27	70,70,70,70	0
57	MG	YA	3165	1/1	0.39	0.37	54,54,54,54	0
57	MG	QA	1657	1/1	0.49	0.26	58,58,58,58	0
57	MG	QA	1629	1/1	0.59	0.24	43,43,43,43	0
57	MG	QA	1626	1/1	0.59	0.20	59,59,59,59	0
57	MG	RA	3195	1/1	0.59	0.26	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3091	1/1	0.59	0.39	73,73,73,73	0
57	MG	QA	1637	1/1	0.62	0.25	57,57,57,57	0
57	MG	QA	1609	1/1	0.63	0.18	34,34,34,34	0
57	MG	XA	1672	1/1	0.63	0.17	40,40,40,40	0
57	MG	XA	1655	1/1	0.64	0.30	81,81,81,81	0
57	MG	RA	3207	1/1	0.64	0.37	47,47,47,47	0
57	MG	RA	3139	1/1	0.69	0.24	49,49,49,49	0
57	MG	QA	1645	1/1	0.70	0.23	53,53,53,53	0
57	MG	RA	3194	1/1	0.71	0.18	44,44,44,44	0
57	MG	RA	3101	1/1	0.71	0.15	7,7,7,7	0
57	MG	RA	3135	1/1	0.72	0.16	16,16,16,16	0
57	MG	RA	3204	1/1	0.72	0.27	82,82,82,82	0
57	MG	RA	3226	1/1	0.72	0.18	48,48,48,48	0
57	MG	XA	1621	1/1	0.73	0.22	29,29,29,29	0
57	MG	YA	3084	1/1	0.73	0.22	10,10,10,10	0
57	MG	YA	3127	1/1	0.75	0.17	26,26,26,26	0
57	MG	XA	1631	1/1	0.75	0.20	35,35,35,35	0
57	MG	YA	3164	1/1	0.75	0.15	36,36,36,36	0
57	MG	RA	3232	1/1	0.75	0.14	30,30,30,30	0
57	MG	YA	3222	1/1	0.75	0.14	34,34,34,34	0
57	MG	YA	3172	1/1	0.76	0.14	43,43,43,43	0
57	MG	RA	3212	1/1	0.76	0.20	42,42,42,42	0
57	MG	RA	3221	1/1	0.77	0.18	62,62,62,62	0
57	MG	RA	3058	1/1	0.77	0.23	37,37,37,37	0
57	MG	QA	1658	1/1	0.77	0.20	63,63,63,63	0
57	MG	RA	3215	1/1	0.77	0.20	48,48,48,48	0
57	MG	YA	3130	1/1	0.77	0.15	17,17,17,17	0
57	MG	XA	1663	1/1	0.79	0.12	44,44,44,44	0
58	PAR	QA	1670	42/42	0.79	0.30	56,56,56,56	0
57	MG	RA	3061	1/1	0.80	0.07	9,9,9,9	0
57	MG	XA	1630	1/1	0.80	0.17	16,16,16,16	0
57	MG	YA	3135	1/1	0.80	0.22	21,21,21,21	0
57	MG	YA	3196	1/1	0.80	0.21	28,28,28,28	0
57	MG	RA	3200	1/1	0.80	0.11	38,38,38,38	0
57	MG	YA	3241	1/1	0.80	0.16	46,46,46,46	0
57	MG	YA	3244	1/1	0.80	0.12	25,25,25,25	0
57	MG	YA	3158	1/1	0.80	0.13	24,24,24,24	0
57	MG	XA	1624	1/1	0.81	0.17	55,55,55,55	0
57	MG	YA	3204	1/1	0.81	0.09	19,19,19,19	0
57	MG	QA	1663	1/1	0.81	0.13	82,82,82,82	0
57	MG	XA	1671	1/1	0.81	0.14	71,71,71,71	0
57	MG	RA	3119	1/1	0.81	0.16	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XA	1633	1/1	0.81	0.22	37,37,37,37	0
57	MG	YA	3259	1/1	0.82	0.37	43,43,43,43	0
57	MG	YA	3237	1/1	0.82	0.14	44,44,44,44	0
57	MG	YA	3207	1/1	0.83	0.48	80,80,80,80	0
57	MG	YA	3220	1/1	0.83	0.17	52,52,52,52	0
57	MG	YA	3221	1/1	0.83	0.15	19,19,19,19	0
57	MG	XA	1654	1/1	0.83	0.20	53,53,53,53	0
57	MG	YA	3071	1/1	0.83	0.16	10,10,10,10	0
57	MG	QH	201	1/1	0.83	0.09	58,58,58,58	0
57	MG	XA	1622	1/1	0.83	0.17	26,26,26,26	0
57	MG	YA	3198	1/1	0.83	0.28	59,59,59,59	0
57	MG	RA	3115	1/1	0.83	0.14	7,7,7,7	0
57	MG	QA	1664	1/1	0.84	0.13	40,40,40,40	0
57	MG	YA	3202	1/1	0.84	0.18	59,59,59,59	0
57	MG	RA	3155	1/1	0.84	0.18	24,24,24,24	0
57	MG	YA	3016	1/1	0.84	0.14	8,8,8,8	0
57	MG	YA	3155	1/1	0.84	0.21	53,53,53,53	0
57	MG	RA	3177	1/1	0.84	0.21	38,38,38,38	0
57	MG	YA	3161	1/1	0.84	0.16	25,25,25,25	0
57	MG	RA	3227	1/1	0.84	0.20	73,73,73,73	0
57	MG	RA	3130	1/1	0.84	0.11	46,46,46,46	0
57	MG	RA	3193	1/1	0.84	0.39	51,51,51,51	0
57	MG	YA	3173	1/1	0.84	0.12	43,43,43,43	0
57	MG	QA	1654	1/1	0.84	0.18	79,79,79,79	0
58	PAR	XA	1675	42/42	0.84	0.25	49,49,49,49	0
57	MG	RB	201	1/1	0.85	0.11	59,59,59,59	0
57	MG	RD	301	1/1	0.85	0.20	41,41,41,41	0
57	MG	XA	1661	1/1	0.85	0.12	48,48,48,48	0
57	MG	XA	1609	1/1	0.85	0.12	22,22,22,22	0
57	MG	XA	1667	1/1	0.85	0.11	32,32,32,32	0
57	MG	YA	3174	1/1	0.85	0.10	19,19,19,19	0
57	MG	XA	1610	1/1	0.85	0.11	42,42,42,42	0
57	MG	RA	3218	1/1	0.85	0.25	29,29,29,29	0
57	MG	XA	1647	1/1	0.85	0.17	49,49,49,49	0
57	MG	XA	1649	1/1	0.85	0.18	30,30,30,30	0
57	MG	RB	202	1/1	0.86	0.10	54,54,54,54	0
57	MG	RA	3123	1/1	0.86	0.18	28,28,28,28	0
57	MG	RA	3156	1/1	0.86	0.25	44,44,44,44	0
57	MG	RA	3164	1/1	0.86	0.29	36,36,36,36	0
57	MG	YA	3208	1/1	0.86	0.18	55,55,55,55	0
57	MG	YA	3214	1/1	0.86	0.10	35,35,35,35	0
57	MG	YA	3064	1/1	0.86	0.10	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3176	1/1	0.86	0.09	24,24,24,24	0
57	MG	YA	3072	1/1	0.86	0.19	17,17,17,17	0
57	MG	RA	3072	1/1	0.86	0.12	13,13,13,13	0
57	MG	YA	3239	1/1	0.86	0.21	46,46,46,46	0
57	MG	YA	3170	1/1	0.86	0.12	38,38,38,38	0
57	MG	QA	1618	1/1	0.86	0.25	42,42,42,42	0
57	MG	RA	3034	1/1	0.86	0.37	30,30,30,30	0
57	MG	YB	201	1/1	0.86	0.26	35,35,35,35	0
57	MG	XA	1665	1/1	0.86	0.10	44,44,44,44	0
57	MG	YA	3129	1/1	0.86	0.20	27,27,27,27	0
57	MG	YA	3194	1/1	0.87	0.08	41,41,41,41	0
57	MG	RA	3124	1/1	0.87	0.20	23,23,23,23	0
57	MG	YA	3128	1/1	0.87	0.20	26,26,26,26	0
57	MG	RA	3187	1/1	0.87	0.27	63,63,63,63	0
57	MG	QA	1656	1/1	0.87	0.16	52,52,52,52	0
57	MG	RA	3050	1/1	0.87	0.23	31,31,31,31	0
57	MG	RA	3223	1/1	0.87	0.09	23,23,23,23	0
57	MG	YA	3144	1/1	0.87	0.24	35,35,35,35	0
57	MG	YA	3151	1/1	0.87	0.18	25,25,25,25	0
57	MG	RA	3112	1/1	0.87	0.22	25,25,25,25	0
57	MG	QA	1668	1/1	0.87	0.08	42,42,42,42	0
57	MG	YA	3227	1/1	0.87	0.17	13,13,13,13	0
57	MG	QA	1620	1/1	0.87	0.21	28,28,28,28	0
57	MG	RA	3001	1/1	0.87	0.12	11,11,11,11	0
57	MG	RA	3173	1/1	0.87	0.08	15,15,15,15	0
57	MG	YA	3242	1/1	0.87	0.34	72,72,72,72	0
57	MG	RA	3084	1/1	0.87	0.10	9,9,9,9	0
57	MG	YA	3171	1/1	0.87	0.35	32,32,32,32	0
57	MG	YA	3265	1/1	0.87	0.25	27,27,27,27	0
57	MG	RE	302	1/1	0.87	0.20	23,23,23,23	0
57	MG	Y0	101	1/1	0.87	0.12	7,7,7,7	0
57	MG	YA	3107	1/1	0.87	0.15	11,11,11,11	0
57	MG	XA	1656	1/1	0.87	0.12	31,31,31,31	0
57	MG	QA	1638	1/1	0.88	0.16	27,27,27,27	0
57	MG	RA	3234	1/1	0.88	0.22	48,48,48,48	0
57	MG	XA	1635	1/1	0.88	0.26	41,41,41,41	0
57	MG	RA	3013	1/1	0.88	0.24	20,20,20,20	0
57	MG	RA	3142	1/1	0.88	0.11	39,39,39,39	0
57	MG	YA	3075	1/1	0.88	0.21	28,28,28,28	0
57	MG	RA	3151	1/1	0.88	0.12	18,18,18,18	0
57	MG	YA	3229	1/1	0.88	0.08	24,24,24,24	0
57	MG	RA	3219	1/1	0.88	0.17	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3220	1/1	0.88	0.18	56,56,56,56	0
57	MG	YA	3111	1/1	0.88	0.22	34,34,34,34	0
57	MG	XA	1658	1/1	0.88	0.35	46,46,46,46	0
57	MG	XA	1660	1/1	0.88	0.08	30,30,30,30	0
57	MG	YA	3247	1/1	0.88	0.09	30,30,30,30	0
57	MG	RA	3023	1/1	0.88	0.32	14,14,14,14	0
57	MG	YA	3195	1/1	0.88	0.15	35,35,35,35	0
57	MG	RA	3062	1/1	0.88	0.11	56,56,56,56	0
57	MG	RA	3160	1/1	0.88	0.21	51,51,51,51	0
57	MG	RA	3127	1/1	0.88	0.15	23,23,23,23	0
57	MG	QA	1649	1/1	0.88	0.17	39,39,39,39	0
57	MG	RA	3078	1/1	0.89	0.16	22,22,22,22	0
57	MG	YA	3160	1/1	0.89	0.09	12,12,12,12	0
57	MG	RA	3010	1/1	0.89	0.26	78,78,78,78	0
57	MG	YA	3162	1/1	0.89	0.10	20,20,20,20	0
57	MG	QA	1662	1/1	0.89	0.14	53,53,53,53	0
57	MG	RA	3153	1/1	0.89	0.22	51,51,51,51	0
57	MG	QA	1655	1/1	0.89	0.17	51,51,51,51	0
57	MG	RA	3108	1/1	0.89	0.19	24,24,24,24	0
57	MG	YA	3024	1/1	0.89	0.33	16,16,16,16	0
57	MG	YA	3052	1/1	0.89	0.11	21,21,21,21	0
57	MG	QA	1602	1/1	0.89	0.16	18,18,18,18	0
57	MG	YA	3189	1/1	0.89	0.16	23,23,23,23	0
57	MG	YA	3243	1/1	0.89	0.14	42,42,42,42	0
57	MG	YA	3192	1/1	0.89	0.14	30,30,30,30	0
57	MG	RA	3047	1/1	0.89	0.19	9,9,9,9	0
57	MG	RA	3167	1/1	0.89	0.09	29,29,29,29	0
57	MG	YA	3145	1/1	0.89	0.09	11,11,11,11	0
57	MG	YA	3197	1/1	0.89	0.10	44,44,44,44	0
57	MG	YB	203	1/1	0.89	0.17	37,37,37,37	0
57	MG	YP	201	1/1	0.89	0.12	23,23,23,23	0
57	MG	YA	3146	1/1	0.89	0.36	57,57,57,57	0
57	MG	RA	3205	1/1	0.89	0.14	46,46,46,46	0
57	MG	RA	3137	1/1	0.89	0.15	10,10,10,10	0
57	MG	RA	3056	1/1	0.90	0.27	17,17,17,17	0
57	MG	R0	101	1/1	0.90	0.10	11,11,11,11	0
57	MG	YA	3137	1/1	0.90	0.10	6,6,6,6	0
57	MG	YA	3068	1/1	0.90	0.24	17,17,17,17	0
57	MG	YA	3228	1/1	0.90	0.13	22,22,22,22	0
57	MG	YA	3179	1/1	0.90	0.15	35,35,35,35	0
57	MG	YA	3233	1/1	0.90	0.08	34,34,34,34	0
57	MG	YA	3236	1/1	0.90	0.25	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3182	1/1	0.90	0.14	24,24,24,24	0
57	MG	RA	3092	1/1	0.90	0.11	9,9,9,9	0
57	MG	QA	1613	1/1	0.90	0.22	21,21,21,21	0
57	MG	RA	3128	1/1	0.90	0.25	31,31,31,31	0
57	MG	QA	1650	1/1	0.90	0.21	49,49,49,49	0
57	MG	RA	3132	1/1	0.90	0.16	22,22,22,22	0
57	MG	YA	3246	1/1	0.90	0.22	21,21,21,21	0
57	MG	QA	1639	1/1	0.90	0.17	36,36,36,36	0
57	MG	QA	1660	1/1	0.90	0.18	35,35,35,35	0
57	MG	YA	3263	1/1	0.90	0.19	33,33,33,33	0
57	MG	RA	3175	1/1	0.90	0.10	21,21,21,21	0
57	MG	YA	3203	1/1	0.90	0.10	27,27,27,27	0
57	MG	YA	3126	1/1	0.90	0.20	22,22,22,22	0
57	MG	QA	1619	1/1	0.90	0.18	33,33,33,33	0
57	MG	RA	3002	1/1	0.90	0.28	36,36,36,36	0
57	MG	RA	3180	1/1	0.90	0.14	34,34,34,34	0
57	MG	YA	3219	1/1	0.90	0.51	52,52,52,52	0
57	MG	RA	3025	1/1	0.91	0.12	15,15,15,15	0
57	MG	RA	3178	1/1	0.91	0.12	22,22,22,22	0
57	MG	XA	1645	1/1	0.91	0.19	29,29,29,29	0
57	MG	XA	1646	1/1	0.91	0.23	45,45,45,45	0
57	MG	YA	3200	1/1	0.91	0.18	26,26,26,26	0
57	MG	RA	3179	1/1	0.91	0.09	15,15,15,15	0
57	MG	RA	3026	1/1	0.91	0.12	8,8,8,8	0
57	MG	RA	3183	1/1	0.91	0.07	19,19,19,19	0
57	MG	RA	3059	1/1	0.91	0.11	2,2,2,2	0
57	MG	RA	3154	1/1	0.91	0.15	22,22,22,22	0
57	MG	YA	3209	1/1	0.91	0.16	27,27,27,27	0
57	MG	QA	1659	1/1	0.91	0.22	39,39,39,39	0
57	MG	YA	3215	1/1	0.91	0.12	25,25,25,25	0
57	MG	YA	3216	1/1	0.91	0.23	59,59,59,59	0
57	MG	RA	3045	1/1	0.91	0.16	16,16,16,16	0
57	MG	RA	3110	1/1	0.91	0.13	9,9,9,9	0
57	MG	RA	3197	1/1	0.91	0.16	55,55,55,55	0
57	MG	RA	3163	1/1	0.91	0.18	38,38,38,38	0
57	MG	RA	3201	1/1	0.91	0.10	24,24,24,24	0
57	MG	YA	3147	1/1	0.91	0.10	8,8,8,8	0
57	MG	RP	201	1/1	0.91	0.30	30,30,30,30	0
57	MG	RR	202	1/1	0.91	0.09	19,19,19,19	0
57	MG	YA	3235	1/1	0.91	0.08	29,29,29,29	0
57	MG	XA	1674	1/1	0.91	0.12	25,25,25,25	0
57	MG	YA	3159	1/1	0.91	0.10	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3012	1/1	0.91	0.29	9,9,9,9	0
57	MG	QA	1633	1/1	0.91	0.22	44,44,44,44	0
57	MG	RA	3076	1/1	0.91	0.20	15,15,15,15	0
57	MG	YA	3029	1/1	0.91	0.18	12,12,12,12	0
57	MG	YA	3037	1/1	0.91	0.12	1,1,1,1	0
57	MG	YA	3166	1/1	0.91	0.35	58,58,58,58	0
57	MG	YA	3046	1/1	0.91	0.15	8,8,8,8	0
57	MG	YA	3254	1/1	0.91	0.13	7,7,7,7	0
57	MG	RA	3171	1/1	0.91	0.12	33,33,33,33	0
57	MG	YA	3260	1/1	0.91	0.11	14,14,14,14	0
57	MG	RA	3209	1/1	0.91	0.17	50,50,50,50	0
57	MG	YA	3065	1/1	0.91	0.17	8,8,8,8	0
57	MG	RA	3118	1/1	0.91	0.10	33,33,33,33	0
57	MG	RA	3213	1/1	0.91	0.12	29,29,29,29	0
57	MG	YE	302	1/1	0.91	0.15	10,10,10,10	0
57	MG	XA	1626	1/1	0.91	0.13	19,19,19,19	0
57	MG	RA	3138	1/1	0.91	0.13	12,12,12,12	0
57	MG	QA	1669	1/1	0.91	0.10	45,45,45,45	0
57	MG	YA	3102	1/1	0.91	0.21	12,12,12,12	0
57	MG	QA	1631	1/1	0.92	0.10	46,46,46,46	0
57	MG	RA	3090	1/1	0.92	0.16	23,23,23,23	0
57	MG	RA	3199	1/1	0.92	0.08	29,29,29,29	0
57	MG	QA	1647	1/1	0.92	0.09	23,23,23,23	0
57	MG	RA	3044	1/1	0.92	0.15	24,24,24,24	0
57	MG	RA	3143	1/1	0.92	0.18	40,40,40,40	0
57	MG	RA	3144	1/1	0.92	0.23	17,17,17,17	0
57	MG	XA	1657	1/1	0.92	0.16	31,31,31,31	0
57	MG	YA	3106	1/1	0.92	0.07	9,9,9,9	0
57	MG	YA	3234	1/1	0.92	0.09	21,21,21,21	0
57	MG	RF	301	1/1	0.92	0.09	40,40,40,40	0
57	MG	RA	3149	1/1	0.92	0.18	32,32,32,32	0
57	MG	YA	3178	1/1	0.92	0.19	35,35,35,35	0
57	MG	RA	3099	1/1	0.92	0.23	24,24,24,24	0
57	MG	QA	1630	1/1	0.92	0.19	48,48,48,48	0
57	MG	YA	3183	1/1	0.92	0.13	30,30,30,30	0
57	MG	XA	1603	1/1	0.92	0.22	38,38,38,38	0
57	MG	XA	1666	1/1	0.92	0.11	43,43,43,43	0
57	MG	RA	3069	1/1	0.92	0.09	21,21,21,21	0
57	MG	RA	3181	1/1	0.92	0.19	48,48,48,48	0
57	MG	XA	1617	1/1	0.92	0.20	14,14,14,14	0
57	MG	RA	3217	1/1	0.92	0.08	28,28,28,28	0
57	MG	QA	1634	1/1	0.92	0.16	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3140	1/1	0.92	0.16	20,20,20,20	0
57	MG	QA	1651	1/1	0.92	0.20	35,35,35,35	0
57	MG	RA	3188	1/1	0.92	0.14	39,39,39,39	0
57	MG	YB	202	1/1	0.92	0.11	20,20,20,20	0
57	MG	RA	3190	1/1	0.92	0.08	38,38,38,38	0
57	MG	RA	3158	1/1	0.92	0.23	51,51,51,51	0
57	MG	YA	3045	1/1	0.92	0.21	2,2,2,2	0
57	MG	RA	3134	1/1	0.92	0.20	44,44,44,44	0
57	MG	QA	1644	1/1	0.92	0.10	40,40,40,40	0
57	MG	XA	1638	1/1	0.92	0.18	16,16,16,16	0
59	ZN	XD	301	1/1	0.92	0.27	45,45,45,45	0
57	MG	XA	1653	1/1	0.93	0.15	60,60,60,60	0
57	MG	YA	3085	1/1	0.93	0.12	71,71,71,71	0
57	MG	RA	3174	1/1	0.93	0.07	38,38,38,38	0
57	MG	YA	3103	1/1	0.93	0.18	31,31,31,31	0
57	MG	RA	3202	1/1	0.93	0.09	21,21,21,21	0
57	MG	RA	3068	1/1	0.93	0.08	21,21,21,21	0
57	MG	QA	1632	1/1	0.93	0.12	35,35,35,35	0
57	MG	RA	3145	1/1	0.93	0.17	27,27,27,27	0
57	MG	YA	3201	1/1	0.93	0.06	14,14,14,14	0
57	MG	YA	3116	1/1	0.93	0.18	36,36,36,36	0
57	MG	YA	3117	1/1	0.93	0.13	18,18,18,18	0
57	MG	RA	3208	1/1	0.93	0.08	19,19,19,19	0
57	MG	RA	3070	1/1	0.93	0.25	26,26,26,26	0
57	MG	RA	3100	1/1	0.93	0.16	9,9,9,9	0
57	MG	RA	3057	1/1	0.93	0.17	11,11,11,11	0
57	MG	YA	3210	1/1	0.93	0.14	37,37,37,37	0
57	MG	XA	1606	1/1	0.93	0.18	17,17,17,17	0
57	MG	RA	3214	1/1	0.93	0.15	18,18,18,18	0
57	MG	QA	1615	1/1	0.93	0.10	23,23,23,23	0
57	MG	YA	3217	1/1	0.93	0.06	29,29,29,29	0
57	MG	RA	3131	1/1	0.93	0.27	41,41,41,41	0
57	MG	QA	1607	1/1	0.93	0.10	40,40,40,40	0
57	MG	RA	3157	1/1	0.93	0.21	49,49,49,49	0
57	MG	RA	3133	1/1	0.93	0.08	28,28,28,28	0
57	MG	YA	3018	1/1	0.93	0.25	13,13,13,13	0
57	MG	YA	3023	1/1	0.93	0.20	16,16,16,16	0
57	MG	RA	3111	1/1	0.93	0.16	22,22,22,22	0
57	MG	YA	3149	1/1	0.93	0.06	16,16,16,16	0
57	MG	YA	3150	1/1	0.93	0.20	61,61,61,61	0
57	MG	RA	3081	1/1	0.93	0.16	30,30,30,30	0
57	MG	YA	3152	1/1	0.93	0.17	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3113	1/1	0.93	0.26	32,32,32,32	0
57	MG	YA	3156	1/1	0.93	0.17	33,33,33,33	0
57	MG	YA	3039	1/1	0.93	0.15	19,19,19,19	0
57	MG	YA	3042	1/1	0.93	0.13	19,19,19,19	0
57	MG	YA	3044	1/1	0.93	0.35	7,7,7,7	0
57	MG	XA	1632	1/1	0.93	0.14	17,17,17,17	0
57	MG	QA	1640	1/1	0.93	0.16	51,51,51,51	0
57	MG	YA	3048	1/1	0.93	0.21	10,10,10,10	0
57	MG	YA	3249	1/1	0.93	0.12	26,26,26,26	0
57	MG	YA	3253	1/1	0.93	0.25	18,18,18,18	0
57	MG	YA	3049	1/1	0.93	0.30	14,14,14,14	0
57	MG	RA	3169	1/1	0.93	0.20	35,35,35,35	0
57	MG	YA	3063	1/1	0.93	0.10	13,13,13,13	0
57	MG	RA	3228	1/1	0.93	0.28	58,58,58,58	0
57	MG	XA	1641	1/1	0.93	0.08	40,40,40,40	0
57	MG	RA	3230	1/1	0.93	0.20	18,18,18,18	0
57	MG	YA	3069	1/1	0.93	0.19	15,15,15,15	0
57	MG	RA	3088	1/1	0.93	0.15	19,19,19,19	0
57	MG	QA	1666	1/1	0.93	0.16	36,36,36,36	0
57	MG	YA	3180	1/1	0.93	0.28	49,49,49,49	0
57	MG	RA	3240	1/1	0.93	0.14	25,25,25,25	0
57	MG	YA	3078	1/1	0.93	0.16	19,19,19,19	0
57	MG	YA	3186	1/1	0.93	0.21	39,39,39,39	0
57	MG	YA	3188	1/1	0.93	0.09	32,32,32,32	0
57	MG	QA	1606	1/1	0.94	0.14	22,22,22,22	0
57	MG	RA	3203	1/1	0.94	0.18	35,35,35,35	0
57	MG	QA	1622	1/1	0.94	0.09	32,32,32,32	0
57	MG	YA	3087	1/1	0.94	0.22	15,15,15,15	0
57	MG	YA	3096	1/1	0.94	0.17	10,10,10,10	0
57	MG	YA	3191	1/1	0.94	0.17	24,24,24,24	0
57	MG	XA	1659	1/1	0.94	0.09	34,34,34,34	0
57	MG	YA	3193	1/1	0.94	0.15	27,27,27,27	0
57	MG	QF	201	1/1	0.94	0.06	39,39,39,39	0
57	MG	RA	3042	1/1	0.94	0.12	3,3,3,3	0
57	MG	XA	1662	1/1	0.94	0.08	11,11,11,11	0
57	MG	QA	1617	1/1	0.94	0.12	19,19,19,19	0
57	MG	QA	1661	1/1	0.94	0.06	38,38,38,38	0
57	MG	YA	3115	1/1	0.94	0.13	17,17,17,17	0
57	MG	RA	3210	1/1	0.94	0.15	30,30,30,30	0
57	MG	XA	1604	1/1	0.94	0.10	15,15,15,15	0
57	MG	RA	3211	1/1	0.94	0.23	43,43,43,43	0
57	MG	YA	3123	1/1	0.94	0.11	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3125	1/1	0.94	0.11	11,11,11,11	0
57	MG	RA	3073	1/1	0.94	0.18	24,24,24,24	0
57	MG	RA	3075	1/1	0.94	0.06	15,15,15,15	0
57	MG	YA	3001	1/1	0.94	0.16	9,9,9,9	0
57	MG	YA	3003	1/1	0.94	0.20	10,10,10,10	0
57	MG	YA	3009	1/1	0.94	0.20	12,12,12,12	0
57	MG	QA	1643	1/1	0.94	0.12	22,22,22,22	0
57	MG	YA	3136	1/1	0.94	0.10	18,18,18,18	0
57	MG	RA	3049	1/1	0.94	0.09	8,8,8,8	0
57	MG	YA	3138	1/1	0.94	0.06	10,10,10,10	0
57	MG	QA	1612	1/1	0.94	0.14	13,13,13,13	0
57	MG	RA	3152	1/1	0.94	0.12	14,14,14,14	0
57	MG	YA	3141	1/1	0.94	0.06	16,16,16,16	0
57	MG	YA	3142	1/1	0.94	0.09	28,28,28,28	0
57	MG	RA	3122	1/1	0.94	0.18	29,29,29,29	0
57	MG	YA	3027	1/1	0.94	0.21	0,0,0,0	0
57	MG	YA	3028	1/1	0.94	0.18	9,9,9,9	0
57	MG	RA	3053	1/1	0.94	0.21	16,16,16,16	0
57	MG	YA	3148	1/1	0.94	0.08	14,14,14,14	0
57	MG	YA	3030	1/1	0.94	0.19	20,20,20,20	0
57	MG	YA	3032	1/1	0.94	0.21	4,4,4,4	0
57	MG	YA	3240	1/1	0.94	0.12	43,43,43,43	0
57	MG	YA	3034	1/1	0.94	0.20	9,9,9,9	0
57	MG	YA	3036	1/1	0.94	0.12	5,5,5,5	0
57	MG	YA	3153	1/1	0.94	0.11	21,21,21,21	0
57	MG	RA	3189	1/1	0.94	0.09	34,34,34,34	0
57	MG	RA	3085	1/1	0.94	0.12	16,16,16,16	0
57	MG	YA	3041	1/1	0.94	0.14	5,5,5,5	0
57	MG	RA	3191	1/1	0.94	0.12	21,21,21,21	0
57	MG	YA	3251	1/1	0.94	0.20	20,20,20,20	0
57	MG	RA	3224	1/1	0.94	0.19	52,52,52,52	0
57	MG	XA	1636	1/1	0.94	0.08	5,5,5,5	0
57	MG	YA	3258	1/1	0.94	0.17	11,11,11,11	0
57	MG	RA	3126	1/1	0.94	0.34	33,33,33,33	0
57	MG	XA	1639	1/1	0.94	0.13	35,35,35,35	0
57	MG	RA	3087	1/1	0.94	0.14	34,34,34,34	0
57	MG	XA	1644	1/1	0.94	0.09	27,27,27,27	0
57	MG	YA	3169	1/1	0.94	0.07	20,20,20,20	0
57	MG	RA	3012	1/1	0.94	0.13	8,8,8,8	0
57	MG	QA	1635	1/1	0.94	0.06	33,33,33,33	0
57	MG	RA	3161	1/1	0.94	0.07	27,27,27,27	0
57	MG	XA	1648	1/1	0.94	0.15	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3022	1/1	0.94	0.16	16,16,16,16	0
57	MG	RA	3239	1/1	0.94	0.11	19,19,19,19	0
57	MG	QA	1603	1/1	0.94	0.10	7,7,7,7	0
57	MG	RA	3060	1/1	0.94	0.24	8,8,8,8	0
57	MG	RA	3148	1/1	0.95	0.24	36,36,36,36	0
57	MG	RA	3055	1/1	0.95	0.09	7,7,7,7	0
57	MG	YA	3177	1/1	0.95	0.05	20,20,20,20	0
57	MG	YA	3073	1/1	0.95	0.12	7,7,7,7	0
57	MG	YA	3074	1/1	0.95	0.04	6,6,6,6	0
57	MG	RA	3030	1/1	0.95	0.18	12,12,12,12	0
57	MG	YA	3181	1/1	0.95	0.26	34,34,34,34	0
57	MG	YA	3077	1/1	0.95	0.20	16,16,16,16	0
57	MG	RA	3114	1/1	0.95	0.17	20,20,20,20	0
57	MG	RA	3079	1/1	0.95	0.12	17,17,17,17	0
57	MG	QA	1614	1/1	0.95	0.18	26,26,26,26	0
57	MG	RA	3082	1/1	0.95	0.13	42,42,42,42	0
57	MG	YA	3091	1/1	0.95	0.08	21,21,21,21	0
57	MG	RA	3198	1/1	0.95	0.08	20,20,20,20	0
57	MG	YA	3099	1/1	0.95	0.13	7,7,7,7	0
57	MG	YA	3100	1/1	0.95	0.19	13,13,13,13	0
57	MG	RA	3083	1/1	0.95	0.14	11,11,11,11	0
57	MG	RA	3035	1/1	0.95	0.21	11,11,11,11	0
57	MG	RA	3040	1/1	0.95	0.21	21,21,21,21	0
57	MG	XA	1664	1/1	0.95	0.32	51,51,51,51	0
57	MG	YA	3199	1/1	0.95	0.38	18,18,18,18	0
57	MG	RA	3159	1/1	0.95	0.10	30,30,30,30	0
57	MG	R5	101	1/1	0.95	0.10	19,19,19,19	0
57	MG	RA	3086	1/1	0.95	0.19	14,14,14,14	0
57	MG	XA	1669	1/1	0.95	0.23	41,41,41,41	0
57	MG	XA	1670	1/1	0.95	0.14	29,29,29,29	0
57	MG	YA	3206	1/1	0.95	0.06	15,15,15,15	0
57	MG	YA	3118	1/1	0.95	0.24	25,25,25,25	0
57	MG	RA	3125	1/1	0.95	0.20	28,28,28,28	0
57	MG	XA	1605	1/1	0.95	0.10	16,16,16,16	0
57	MG	RA	3041	1/1	0.95	0.15	2,2,2,2	0
57	MG	YA	3211	1/1	0.95	0.04	14,14,14,14	0
57	MG	YA	3213	1/1	0.95	0.08	29,29,29,29	0
57	MG	XA	1608	1/1	0.95	0.20	23,23,23,23	0
57	MG	RA	3011	1/1	0.95	0.32	32,32,32,32	0
57	MG	RA	3089	1/1	0.95	0.06	8,8,8,8	0
57	MG	XA	1612	1/1	0.95	0.14	13,13,13,13	0
57	MG	YA	3015	1/1	0.95	0.25	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3132	1/1	0.95	0.05	18,18,18,18	0
57	MG	YA	3134	1/1	0.95	0.11	21,21,21,21	0
57	MG	XA	1614	1/1	0.95	0.19	7,7,7,7	0
57	MG	YA	3224	1/1	0.95	0.05	24,24,24,24	0
57	MG	YA	3225	1/1	0.95	0.16	9,9,9,9	0
57	MG	QA	1648	1/1	0.95	0.10	12,12,12,12	0
57	MG	XA	1620	1/1	0.95	0.18	17,17,17,17	0
57	MG	RA	3170	1/1	0.95	0.05	25,25,25,25	0
57	MG	YA	3230	1/1	0.95	0.16	32,32,32,32	0
57	MG	YA	3232	1/1	0.95	0.07	23,23,23,23	0
57	MG	YA	3025	1/1	0.95	0.20	8,8,8,8	0
57	MG	RA	3064	1/1	0.95	0.15	5,5,5,5	0
57	MG	XA	1623	1/1	0.95	0.35	40,40,40,40	0
57	MG	RA	3172	1/1	0.95	0.07	23,23,23,23	0
57	MG	YA	3143	1/1	0.95	0.07	17,17,17,17	0
57	MG	YA	3238	1/1	0.95	0.11	24,24,24,24	0
57	MG	QA	1665	1/1	0.95	0.10	18,18,18,18	0
57	MG	XA	1628	1/1	0.95	0.16	27,27,27,27	0
57	MG	YA	3033	1/1	0.95	0.18	4,4,4,4	0
57	MG	XA	1629	1/1	0.95	0.19	29,29,29,29	0
57	MG	QA	1652	1/1	0.95	0.07	37,37,37,37	0
57	MG	RA	3048	1/1	0.95	0.06	1,1,1,1	0
57	MG	RA	3071	1/1	0.95	0.18	19,19,19,19	0
57	MG	YA	3040	1/1	0.95	0.18	8,8,8,8	0
57	MG	RA	3102	1/1	0.95	0.15	14,14,14,14	0
57	MG	RA	3103	1/1	0.95	0.08	8,8,8,8	0
57	MG	YA	3154	1/1	0.95	0.06	9,9,9,9	0
57	MG	RA	3105	1/1	0.95	0.18	18,18,18,18	0
57	MG	RA	3140	1/1	0.95	0.19	26,26,26,26	0
57	MG	RA	3141	1/1	0.95	0.15	33,33,33,33	0
57	MG	RA	3182	1/1	0.95	0.06	10,10,10,10	0
57	MG	YA	3262	1/1	0.95	0.12	38,38,38,38	0
57	MG	RA	3107	1/1	0.95	0.12	25,25,25,25	0
57	MG	YA	3050	1/1	0.95	0.28	9,9,9,9	0
57	MG	RA	3185	1/1	0.95	0.16	25,25,25,25	0
57	MG	YA	3163	1/1	0.95	0.11	28,28,28,28	0
57	MG	YA	3062	1/1	0.95	0.09	9,9,9,9	0
57	MG	QA	1627	1/1	0.95	0.15	26,26,26,26	0
57	MG	RA	3007	1/1	0.95	0.13	6,6,6,6	0
57	MG	YQ	201	1/1	0.95	0.06	25,25,25,25	0
57	MG	RA	3229	1/1	0.95	0.17	5,5,5,5	0
57	MG	RA	3008	1/1	0.95	0.08	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XA	1652	1/1	0.95	0.07	32,32,32,32	0
57	MG	YA	3070	1/1	0.95	0.16	8,8,8,8	0
59	ZN	XN	101	1/1	0.95	0.12	65,65,65,65	0
57	MG	RA	3077	1/1	0.96	0.19	6,6,6,6	0
57	MG	YA	3038	1/1	0.96	0.11	6,6,6,6	0
57	MG	RA	3027	1/1	0.96	0.18	3,3,3,3	0
57	MG	RA	3106	1/1	0.96	0.14	11,11,11,11	0
57	MG	RA	3029	1/1	0.96	0.09	2,2,2,2	0
57	MG	XA	1613	1/1	0.96	0.20	13,13,13,13	0
57	MG	RA	3136	1/1	0.96	0.08	9,9,9,9	0
57	MG	YA	3133	1/1	0.96	0.05	18,18,18,18	0
57	MG	YA	3205	1/1	0.96	0.46	38,38,38,38	0
57	MG	XA	1616	1/1	0.96	0.06	17,17,17,17	0
57	MG	RA	3165	1/1	0.96	0.08	19,19,19,19	0
57	MG	RA	3225	1/1	0.96	0.06	27,27,27,27	0
57	MG	RA	3166	1/1	0.96	0.12	43,43,43,43	0
57	MG	RA	3196	1/1	0.96	0.11	15,15,15,15	0
57	MG	RA	3003	1/1	0.96	0.16	14,14,14,14	0
57	MG	YA	3053	1/1	0.96	0.18	5,5,5,5	0
57	MG	YA	3054	1/1	0.96	0.10	49,49,49,49	0
57	MG	YA	3058	1/1	0.96	0.14	12,12,12,12	0
57	MG	YA	3060	1/1	0.96	0.14	4,4,4,4	0
57	MG	YA	3061	1/1	0.96	0.12	15,15,15,15	0
57	MG	QA	1653	1/1	0.96	0.07	36,36,36,36	0
57	MG	XA	1625	1/1	0.96	0.10	16,16,16,16	0
57	MG	XA	1668	1/1	0.96	0.10	19,19,19,19	0
57	MG	QA	1605	1/1	0.96	0.31	30,30,30,30	0
57	MG	RA	3039	1/1	0.96	0.12	2,2,2,2	0
57	MG	QA	1628	1/1	0.96	0.13	25,25,25,25	0
57	MG	YA	3226	1/1	0.96	0.10	3,3,3,3	0
57	MG	RA	3235	1/1	0.96	0.19	22,22,22,22	0
57	MG	XA	1673	1/1	0.96	0.07	26,26,26,26	0
57	MG	QA	1646	1/1	0.96	0.10	39,39,39,39	0
57	MG	XX	101	1/1	0.96	0.09	22,22,22,22	0
57	MG	QA	1616	1/1	0.96	0.05	40,40,40,40	0
57	MG	RA	3066	1/1	0.96	0.15	24,24,24,24	0
57	MG	YA	3004	1/1	0.96	0.13	5,5,5,5	0
57	MG	RA	3043	1/1	0.96	0.13	4,4,4,4	0
57	MG	YA	3079	1/1	0.96	0.12	12,12,12,12	0
57	MG	YA	3081	1/1	0.96	0.08	5,5,5,5	0
57	MG	YA	3083	1/1	0.96	0.20	7,7,7,7	0
57	MG	QA	1601	1/1	0.96	0.15	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3013	1/1	0.96	0.18	1,1,1,1	0
57	MG	RA	3018	1/1	0.96	0.10	9,9,9,9	0
57	MG	YA	3090	1/1	0.96	0.12	5,5,5,5	0
57	MG	RA	3021	1/1	0.96	0.17	2,2,2,2	0
57	MG	YA	3095	1/1	0.96	0.10	7,7,7,7	0
57	MG	RA	3093	1/1	0.96	0.15	9,9,9,9	0
57	MG	YA	3019	1/1	0.96	0.12	1,1,1,1	0
57	MG	YA	3248	1/1	0.96	0.22	26,26,26,26	0
57	MG	YA	3021	1/1	0.96	0.20	9,9,9,9	0
57	MG	YA	3250	1/1	0.96	0.12	40,40,40,40	0
57	MG	YA	3022	1/1	0.96	0.20	7,7,7,7	0
57	MG	YA	3175	1/1	0.96	0.22	37,37,37,37	0
57	MG	XA	1642	1/1	0.96	0.22	23,23,23,23	0
57	MG	YA	3255	1/1	0.96	0.21	13,13,13,13	0
57	MG	YA	3104	1/1	0.96	0.17	24,24,24,24	0
57	MG	XA	1643	1/1	0.96	0.14	29,29,29,29	0
57	MG	RA	3096	1/1	0.96	0.16	23,23,23,23	0
57	MG	YA	3261	1/1	0.96	0.18	8,8,8,8	0
57	MG	RA	3098	1/1	0.96	0.16	10,10,10,10	0
57	MG	QA	1623	1/1	0.96	0.14	37,37,37,37	0
57	MG	YA	3113	1/1	0.96	0.14	19,19,19,19	0
57	MG	YA	3185	1/1	0.96	0.06	10,10,10,10	0
57	MG	YA	3114	1/1	0.96	0.08	8,8,8,8	0
57	MG	YA	3187	1/1	0.96	0.04	29,29,29,29	0
57	MG	RA	3184	1/1	0.96	0.15	13,13,13,13	0
57	MG	QA	1624	1/1	0.96	0.09	27,27,27,27	0
57	MG	QA	1641	1/1	0.96	0.10	24,24,24,24	0
57	MG	XA	1650	1/1	0.96	0.10	26,26,26,26	0
57	MG	QA	1611	1/1	0.96	0.13	14,14,14,14	0
57	MG	YA	3121	1/1	0.96	0.06	18,18,18,18	0
59	ZN	QD	301	1/1	0.96	0.20	47,47,47,47	0
57	MG	XA	1607	1/1	0.96	0.27	31,31,31,31	0
57	MG	YA	3124	1/1	0.96	0.22	9,9,9,9	0
57	MG	RA	3063	1/1	0.97	0.26	6,6,6,6	0
57	MG	RA	3104	1/1	0.97	0.07	16,16,16,16	0
57	MG	XA	1601	1/1	0.97	0.13	4,4,4,4	0
57	MG	XA	1602	1/1	0.97	0.12	30,30,30,30	0
57	MG	YA	3088	1/1	0.97	0.08	1,1,1,1	0
57	MG	RA	3028	1/1	0.97	0.08	4,4,4,4	0
57	MG	RA	3129	1/1	0.97	0.07	21,21,21,21	0
57	MG	YA	3218	1/1	0.97	0.04	10,10,10,10	0
57	MG	YA	3093	1/1	0.97	0.06	13,13,13,13	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3216	1/1	0.97	0.18	43,43,43,43	0
57	MG	RA	3186	1/1	0.97	0.05	20,20,20,20	0
57	MG	YA	3097	1/1	0.97	0.16	19,19,19,19	0
57	MG	YA	3223	1/1	0.97	0.12	25,25,25,25	0
57	MG	QA	1608	1/1	0.97	0.05	13,13,13,13	0
57	MG	RA	3017	1/1	0.97	0.18	8,8,8,8	0
57	MG	YA	3101	1/1	0.97	0.22	8,8,8,8	0
57	MG	RA	3004	1/1	0.97	0.17	15,15,15,15	0
57	MG	RA	3109	1/1	0.97	0.07	8,8,8,8	0
57	MG	XA	1611	1/1	0.97	0.17	23,23,23,23	0
57	MG	RA	3051	1/1	0.97	0.12	3,3,3,3	0
57	MG	YA	3167	1/1	0.97	0.10	21,21,21,21	0
57	MG	RA	3162	1/1	0.97	0.04	18,18,18,18	0
57	MG	RA	3052	1/1	0.97	0.11	4,4,4,4	0
57	MG	YA	3110	1/1	0.97	0.05	15,15,15,15	0
57	MG	XA	1615	1/1	0.97	0.08	15,15,15,15	0
57	MG	RA	3019	1/1	0.97	0.15	19,19,19,19	0
57	MG	YA	3043	1/1	0.97	0.22	15,15,15,15	0
57	MG	RA	3006	1/1	0.97	0.22	18,18,18,18	0
57	MG	YA	3176	1/1	0.97	0.08	6,6,6,6	0
57	MG	XA	1618	1/1	0.97	0.17	7,7,7,7	0
57	MG	XA	1619	1/1	0.97	0.11	18,18,18,18	0
57	MG	YA	3047	1/1	0.97	0.23	6,6,6,6	0
57	MG	YA	3119	1/1	0.97	0.17	31,31,31,31	0
57	MG	YA	3245	1/1	0.97	0.12	38,38,38,38	0
57	MG	QA	1625	1/1	0.97	0.13	36,36,36,36	0
57	MG	QA	1604	1/1	0.97	0.15	12,12,12,12	0
57	MG	YA	3122	1/1	0.97	0.13	9,9,9,9	0
57	MG	YA	3184	1/1	0.97	0.20	20,20,20,20	0
57	MG	RA	3116	1/1	0.97	0.10	1,1,1,1	0
57	MG	RA	3117	1/1	0.97	0.10	3,3,3,3	0
57	MG	YA	3252	1/1	0.97	0.22	25,25,25,25	0
57	MG	RA	3024	1/1	0.97	0.08	5,5,5,5	0
57	MG	RA	3233	1/1	0.97	0.09	24,24,24,24	0
57	MG	RA	3097	1/1	0.97	0.15	14,14,14,14	0
57	MG	QM	201	1/1	0.97	0.08	55,55,55,55	0
57	MG	RA	3236	1/1	0.97	0.19	33,33,33,33	0
57	MG	XV	101	1/1	0.97	0.17	9,9,9,9	0
57	MG	RA	3237	1/1	0.97	0.10	26,26,26,26	0
57	MG	RA	3121	1/1	0.97	0.07	29,29,29,29	0
57	MG	YA	3002	1/1	0.97	0.23	9,9,9,9	0
57	MG	RA	3146	1/1	0.97	0.14	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3147	1/1	0.97	0.07	21,21,21,21	0
57	MG	YA	3007	1/1	0.97	0.13	9,9,9,9	0
57	MG	RA	3206	1/1	0.97	0.30	15,15,15,15	0
57	MG	YE	301	1/1	0.97	0.13	7,7,7,7	0
57	MG	YA	3011	1/1	0.97	0.27	20,20,20,20	0
57	MG	QA	1610	1/1	0.97	0.06	11,11,11,11	0
57	MG	XA	1637	1/1	0.97	0.30	24,24,24,24	0
57	MG	RE	301	1/1	0.97	0.10	1,1,1,1	0
57	MG	Y7	101	1/1	0.97	0.31	38,38,38,38	0
57	MG	YA	3076	1/1	0.97	0.22	7,7,7,7	0
57	MG	RA	3080	1/1	0.97	0.19	19,19,19,19	0
57	MG	RA	3150	1/1	0.97	0.07	25,25,25,25	0
59	ZN	QN	101	1/1	0.97	0.07	80,80,80,80	0
57	MG	QA	1636	1/1	0.97	0.04	16,16,16,16	0
57	MG	RA	3046	1/1	0.97	0.09	12,12,12,12	0
57	MG	RA	3031	1/1	0.98	0.07	16,16,16,16	0
57	MG	YA	3055	1/1	0.98	0.07	10,10,10,10	0
57	MG	YA	3056	1/1	0.98	0.13	8,8,8,8	0
57	MG	RA	3032	1/1	0.98	0.12	15,15,15,15	0
57	MG	RA	3033	1/1	0.98	0.15	3,3,3,3	0
57	MG	RA	3168	1/1	0.98	0.09	22,22,22,22	0
57	MG	RA	3238	1/1	0.98	0.27	32,32,32,32	0
57	MG	XA	1651	1/1	0.98	0.05	12,12,12,12	0
57	MG	QA	1667	1/1	0.98	0.08	32,32,32,32	0
57	MG	RA	3020	1/1	0.98	0.13	1,1,1,1	0
57	MG	YA	3066	1/1	0.98	0.13	16,16,16,16	0
57	MG	YA	3108	1/1	0.98	0.11	3,3,3,3	0
57	MG	YA	3109	1/1	0.98	0.20	10,10,10,10	0
57	MG	YA	3067	1/1	0.98	0.09	22,22,22,22	0
57	MG	XV	102	1/1	0.98	0.06	0,0,0,0	0
57	MG	YA	3112	1/1	0.98	0.07	15,15,15,15	0
57	MG	YA	3031	1/1	0.98	0.14	2,2,2,2	0
57	MG	YA	3157	1/1	0.98	0.12	30,30,30,30	0
57	MG	RA	3074	1/1	0.98	0.06	4,4,4,4	0
57	MG	RA	3036	1/1	0.98	0.12	4,4,4,4	0
57	MG	RA	3037	1/1	0.98	0.09	11,11,11,11	0
57	MG	RA	3014	1/1	0.98	0.19	9,9,9,9	0
57	MG	RA	3016	1/1	0.98	0.14	1,1,1,1	0
57	MG	YA	3006	1/1	0.98	0.24	9,9,9,9	0
57	MG	YA	3256	1/1	0.98	0.14	7,7,7,7	0
57	MG	YA	3257	1/1	0.98	0.12	3,3,3,3	0
57	MG	RA	3095	1/1	0.98	0.17	14,14,14,14	0

Continued on next page...

Continued from previous page...

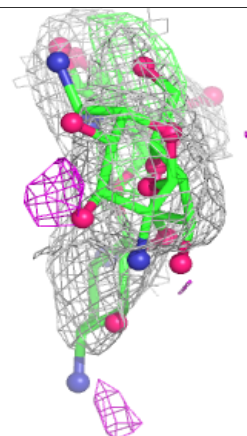
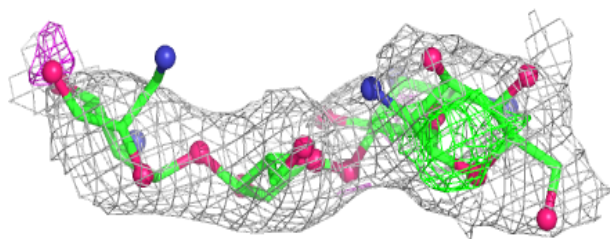
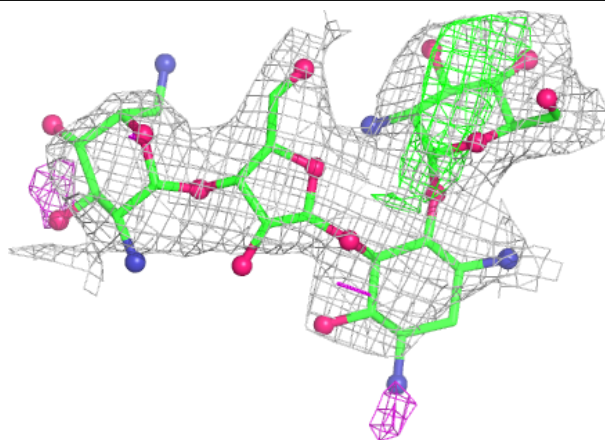
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3008	1/1	0.98	0.13	9,9,9,9	0
57	MG	YA	3212	1/1	0.98	0.07	9,9,9,9	0
57	MG	QV	101	1/1	0.98	0.09	26,26,26,26	0
57	MG	YA	3010	1/1	0.98	0.11	4,4,4,4	0
57	MG	RR	201	1/1	0.98	0.12	7,7,7,7	0
57	MG	YA	3264	1/1	0.98	0.04	24,24,24,24	0
57	MG	YA	3082	1/1	0.98	0.08	8,8,8,8	0
57	MG	XA	1640	1/1	0.98	0.05	31,31,31,31	0
57	MG	RA	3065	1/1	0.98	0.06	16,16,16,16	0
57	MG	YA	3014	1/1	0.98	0.11	3,3,3,3	0
57	MG	YA	3086	1/1	0.98	0.14	6,6,6,6	0
57	MG	RA	3005	1/1	0.98	0.24	13,13,13,13	0
57	MG	YA	3131	1/1	0.98	0.13	35,35,35,35	0
57	MG	RA	3231	1/1	0.98	0.21	9,9,9,9	0
57	MG	YA	3089	1/1	0.98	0.13	8,8,8,8	0
57	MG	YA	3017	1/1	0.98	0.12	2,2,2,2	0
57	MG	RA	3067	1/1	0.98	0.11	9,9,9,9	0
57	MG	YA	3092	1/1	0.98	0.12	30,30,30,30	0
57	MG	RA	3054	1/1	0.98	0.04	0,0,0,0	0
57	MG	YA	3094	1/1	0.98	0.09	2,2,2,2	0
57	MG	YA	3020	1/1	0.98	0.23	7,7,7,7	0
57	MG	YA	3231	1/1	0.98	0.04	19,19,19,19	0
57	MG	QA	1621	1/1	0.99	0.03	14,14,14,14	0
57	MG	RA	3015	1/1	0.99	0.10	2,2,2,2	0
57	MG	RA	3009	1/1	0.99	0.07	9,9,9,9	0
57	MG	YA	3051	1/1	0.99	0.09	2,2,2,2	0
57	MG	XA	1634	1/1	0.99	0.04	15,15,15,15	0
57	MG	YA	3168	1/1	0.99	0.04	13,13,13,13	0
57	MG	XA	1627	1/1	0.99	0.04	7,7,7,7	0
57	MG	YA	3080	1/1	0.99	0.19	10,10,10,10	0
57	MG	QA	1642	1/1	0.99	0.04	21,21,21,21	0
57	MG	RA	3038	1/1	0.99	0.14	9,9,9,9	0
57	MG	Y5	101	1/1	0.99	0.09	26,26,26,26	0
57	MG	YA	3035	1/1	0.99	0.10	5,5,5,5	0
57	MG	YA	3190	1/1	0.99	0.04	2,2,2,2	0
57	MG	YA	3098	1/1	0.99	0.08	16,16,16,16	0
57	MG	YA	3057	1/1	0.99	0.18	6,6,6,6	0
57	MG	YA	3026	1/1	0.99	0.21	8,8,8,8	0
57	MG	YA	3059	1/1	0.99	0.09	6,6,6,6	0
57	MG	RA	3094	1/1	0.99	0.04	9,9,9,9	0
57	MG	YA	3005	1/1	1.00	0.03	1,1,1,1	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

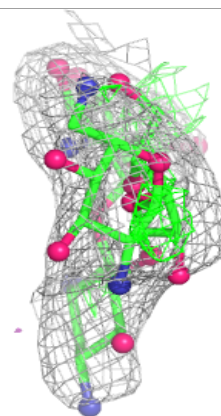
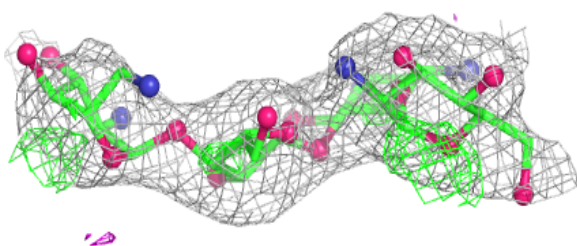
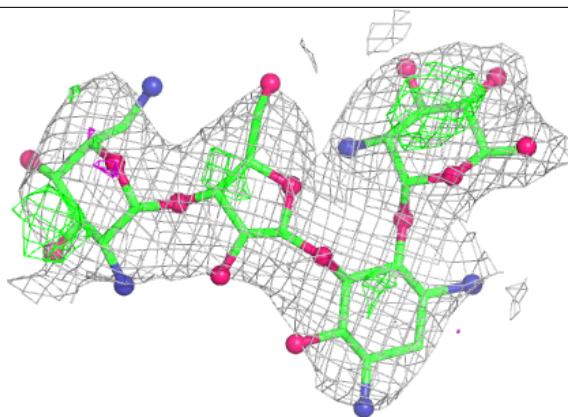
Electron density around PAR QA 1670:

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



Electron density around PAR XA 1675:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.