



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 06:15 am BST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

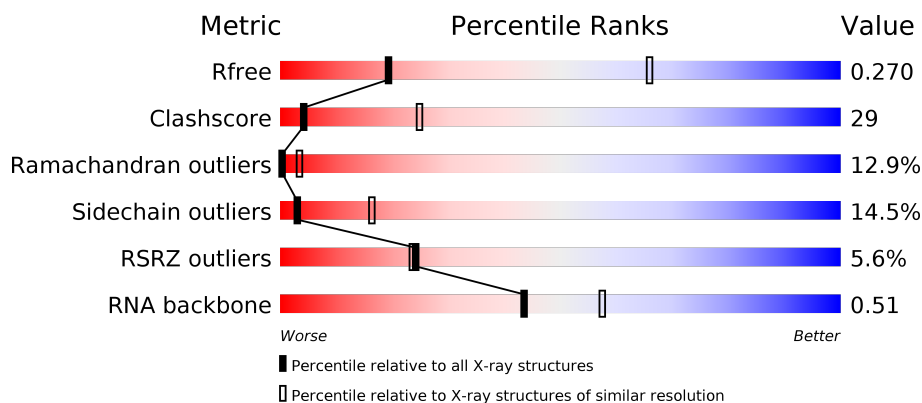
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>3%</div> <div>52%</div> <div>36%</div> <div>9%</div> <div>..</div> </div>
1	XA	1522	<div> <div>2%</div> <div>51%</div> <div>36%</div> <div>10%</div> <div>..</div> </div>
2	QB	256	<div> <div>11%</div> <div>17%</div> <div>59%</div> <div>16%</div> <div>7%</div> </div>
2	XB	256	<div> <div>7%</div> <div>17%</div> <div>59%</div> <div>16%</div> <div>7%</div> </div>

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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	

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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	

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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	

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

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Mol	Chain	Length	Quality of chain
53	R7	49	
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	QF	201	-	-	-	X
57	MG	RA	3091	-	-	-	X
57	MG	RA	3139	-	-	-	X
57	MG	RA	3199	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3223	-	-	-	X
57	MG	RA	3228	-	-	-	X
57	MG	XA	1657	-	-	-	X
57	MG	XA	1658	-	-	-	X
57	MG	XA	1673	-	-	-	X
57	MG	YA	3085	-	-	-	X
57	MG	YA	3122	-	-	-	X
57	MG	YA	3166	-	-	-	X
57	MG	YA	3177	-	-	-	X
57	MG	YA	3206	-	-	-	X

## 2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	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 SufA6.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RS	111	Total	C	N	O	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 L19.

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	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 L27.

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

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

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



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

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

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

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

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

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).

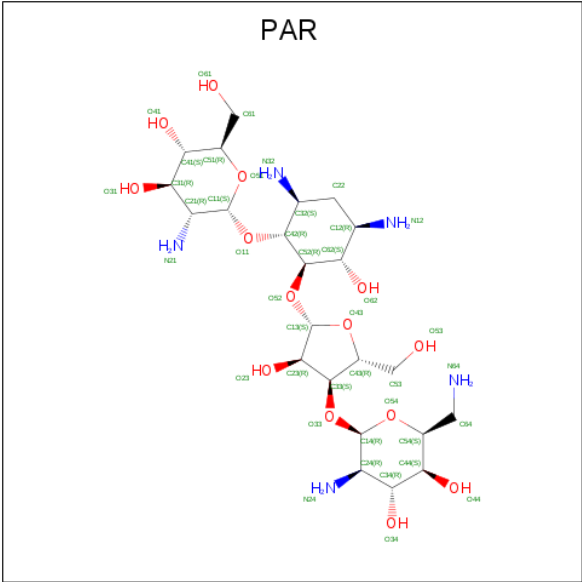
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RE	2	Total	Mg	0	0
			2	2		
57	RR	2	Total	Mg	0	0
			2	2		
57	XA	74	Total	Mg	0	0
			74	74		
57	QA	65	Total	Mg	0	0
			65	65		
57	Y0	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R0	1	Total 1	Mg 1	0	0
57	QX	1	Total 1	Mg 1	0	0
57	YA	268	Total 268	Mg 268	0	0
57	YB	4	Total 4	Mg 4	0	0
57	QF	1	Total 1	Mg 1	0	0
57	QM	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RA	241	Total 241	Mg 241	0	0
57	QH	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	YP	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	QV	1	Total 1	Mg 1	0	0
57	YE	1	Total 1	Mg 1	0	0

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

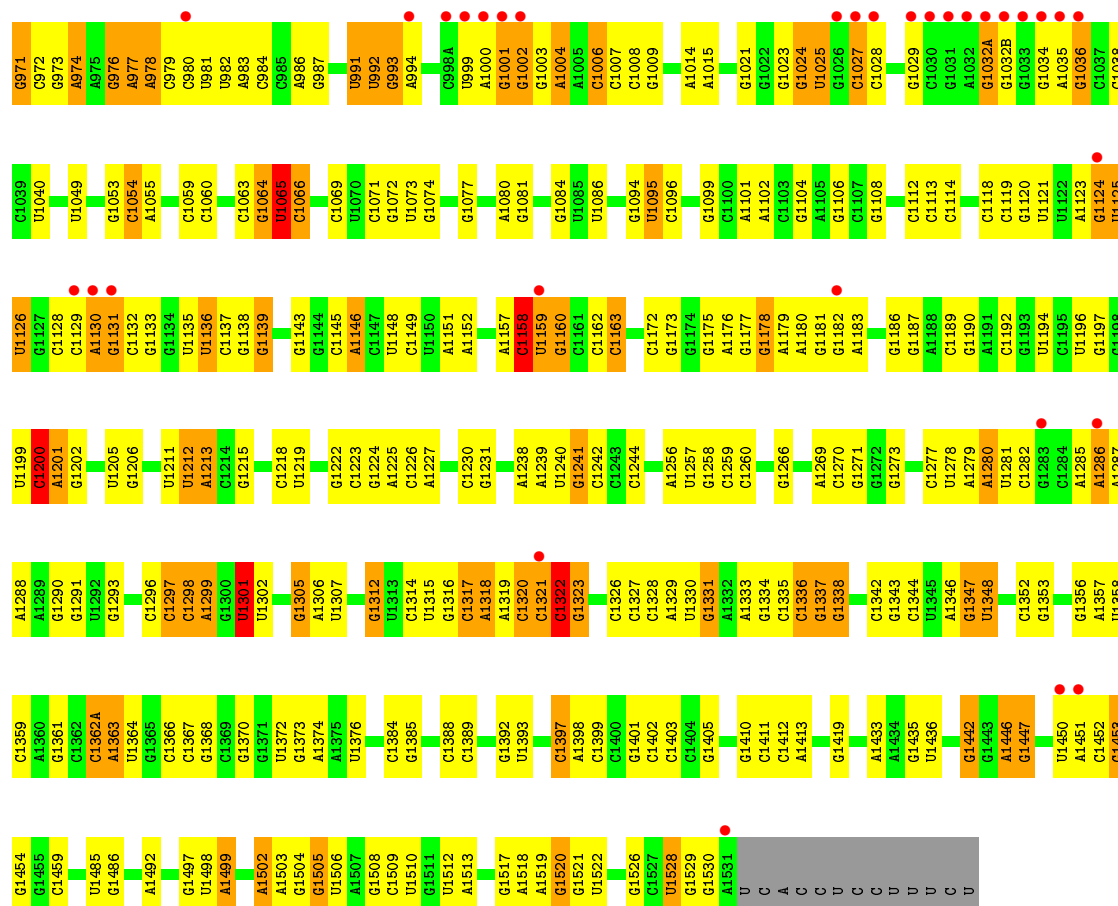


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total	C	N	O	0	0
			42	23	5	14		
58	XA	1	Total	C	N	O	0	0
			42	23	5	14		

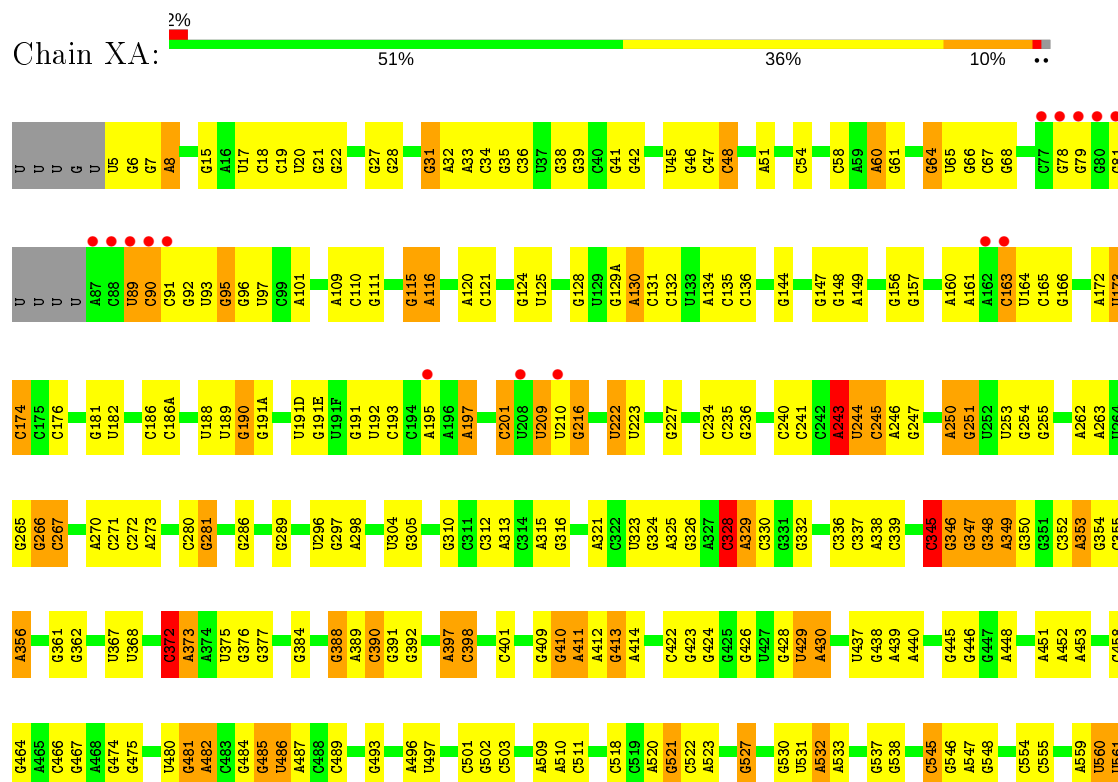
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

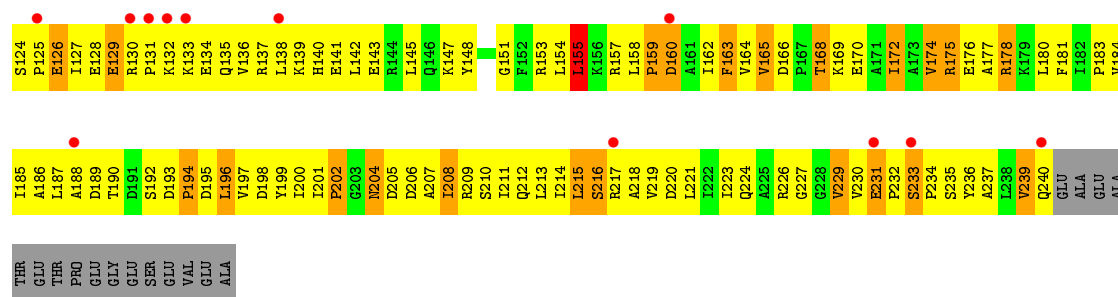




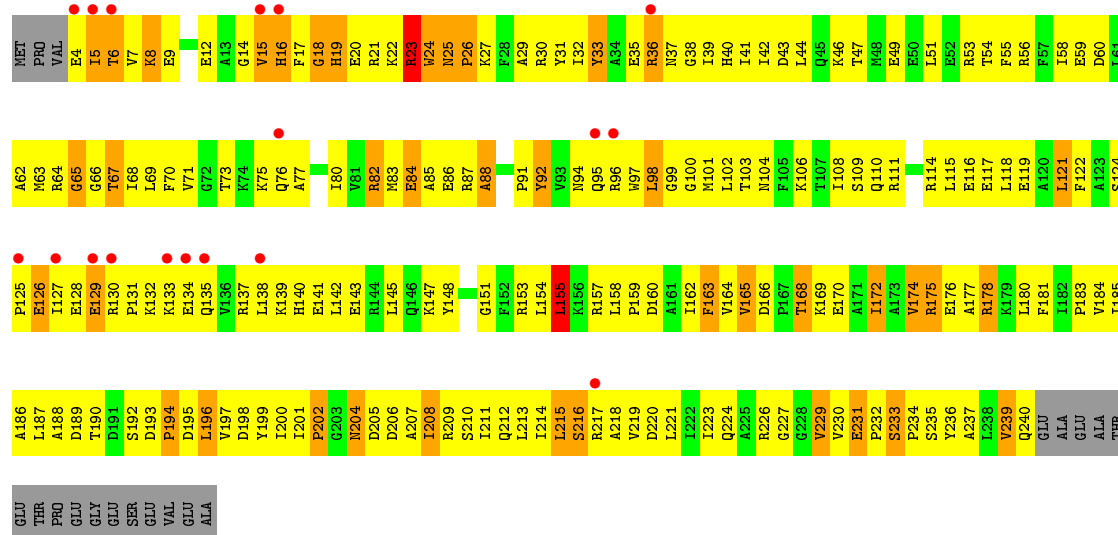
• Molecule 1: 16S rRNA



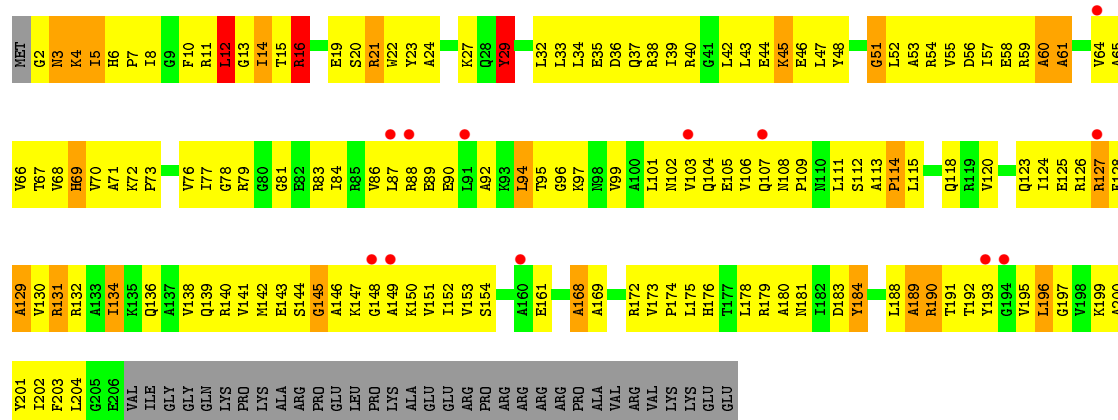




• Molecule 2: 30S ribosomal protein S2



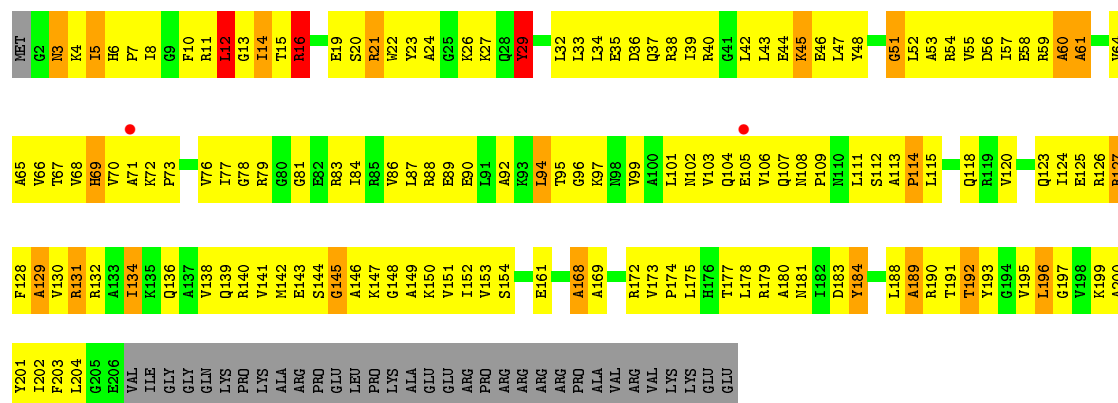
• Molecule 3: 30S ribosomal protein S3



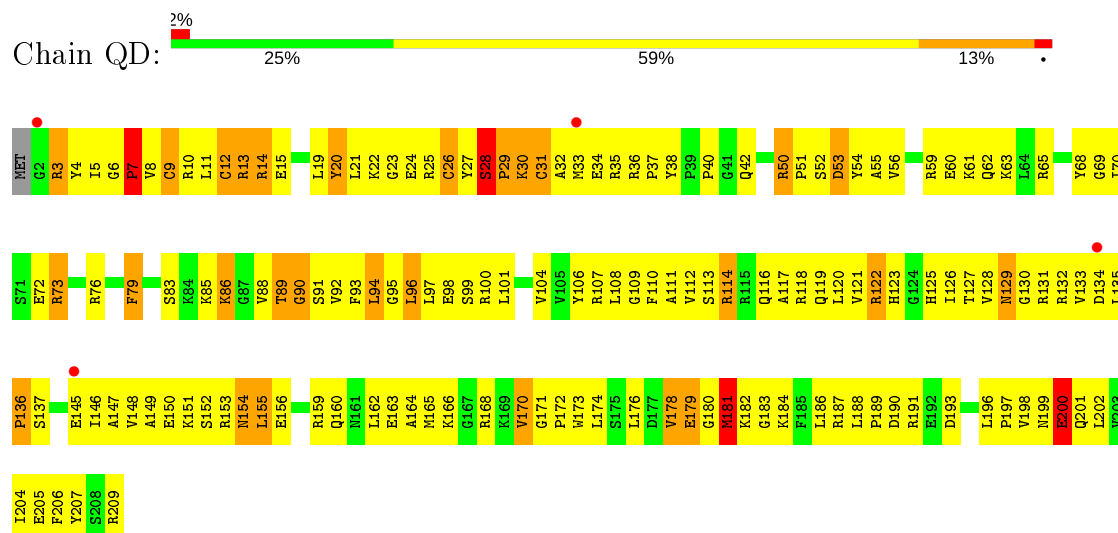
• Molecule 3: 30S ribosomal protein S3



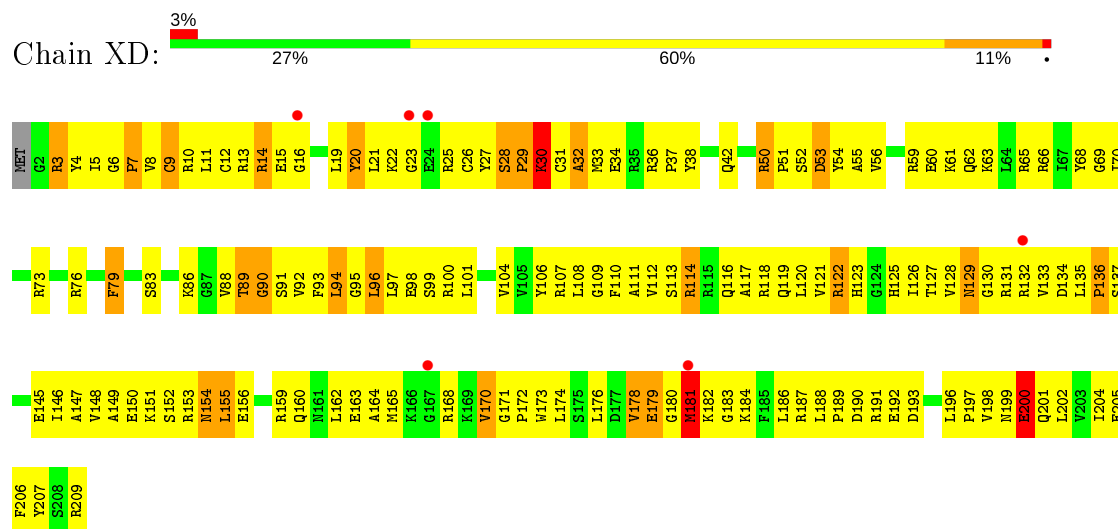




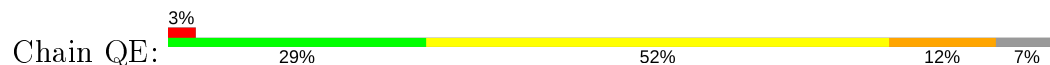
### • Molecule 4: 30S ribosomal protein S4

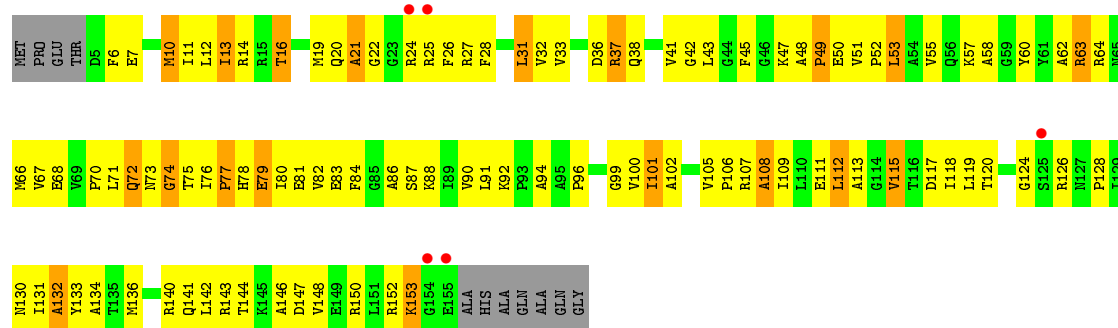


### • Molecule 4: 30S ribosomal protein S4

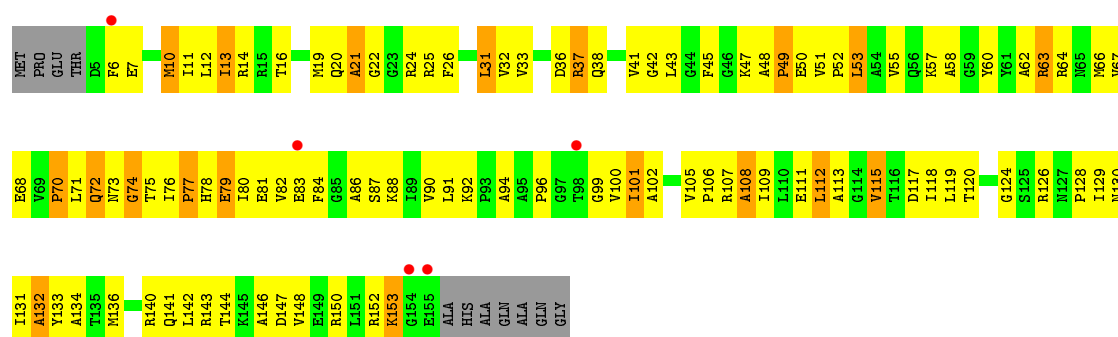


### • Molecule 5: 30S ribosomal protein S5

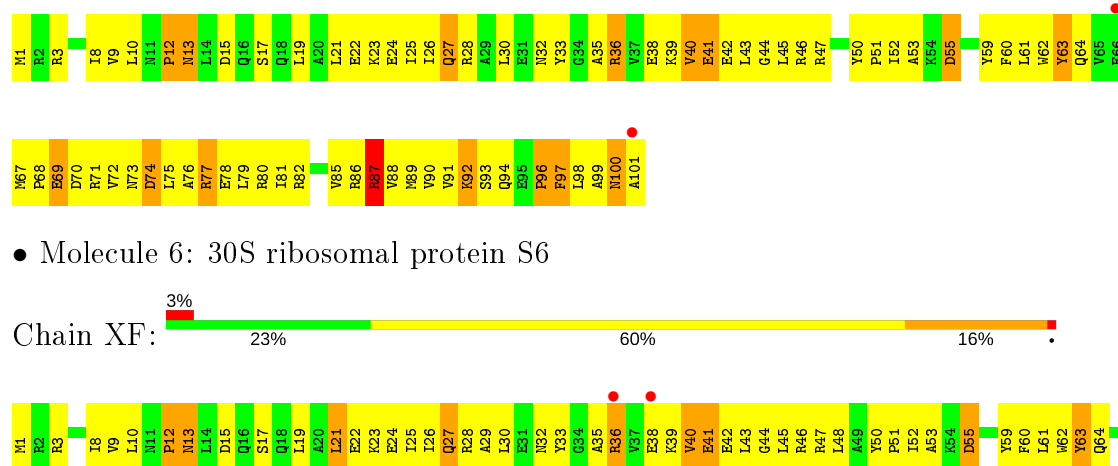




• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

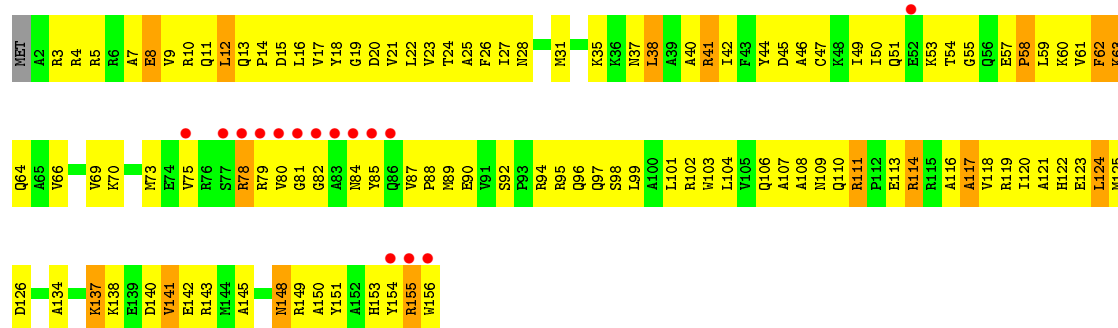


• Molecule 6: 30S ribosomal protein S6

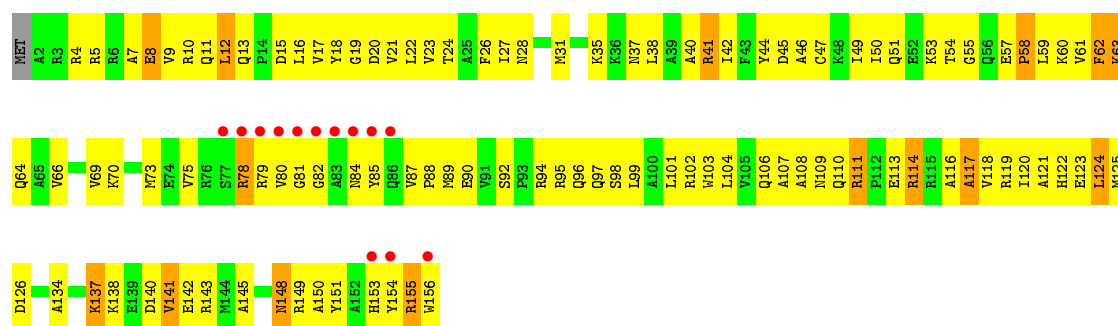


• Molecule 7: 30S ribosomal protein S7

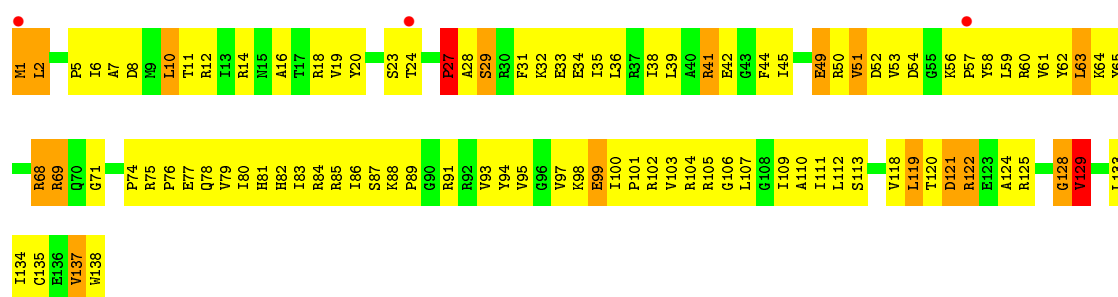




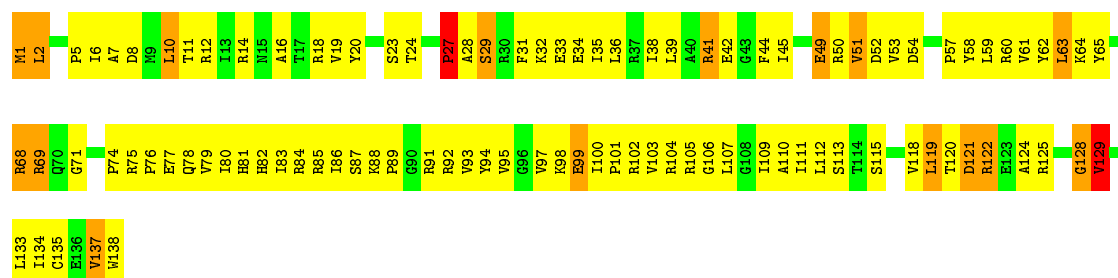
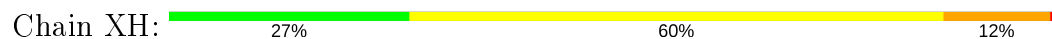
• Molecule 7: 30S ribosomal protein S7



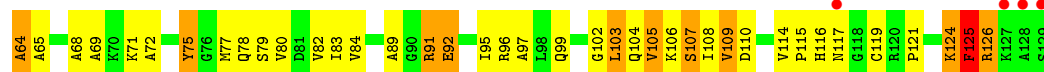
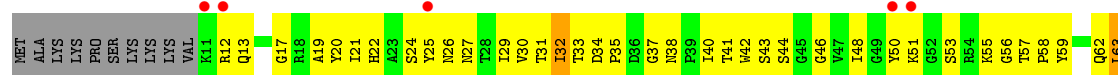
• Molecule 8: 30S ribosomal protein S8



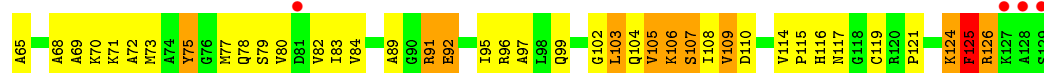
• Molecule 8: 30S ribosomal protein S8



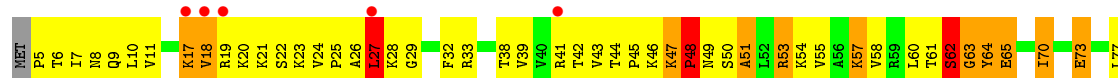




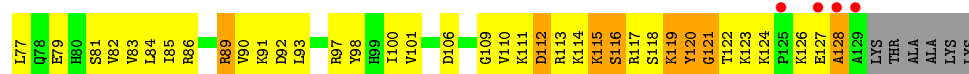
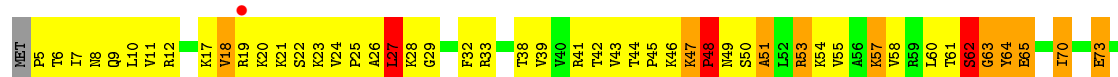
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

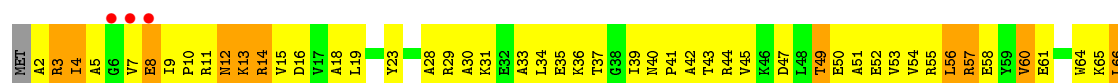


- Molecule 13: 30S ribosomal protein S13

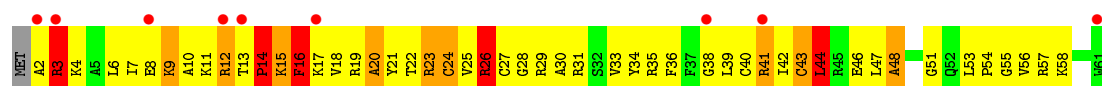
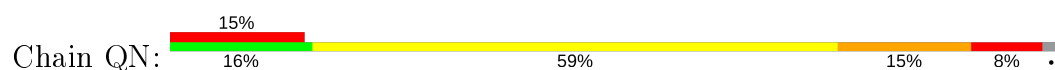




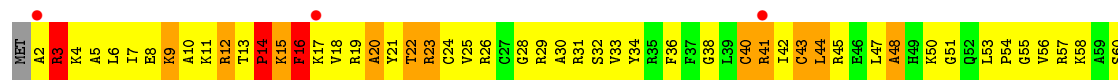
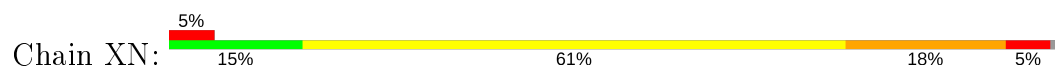
- Molecule 13: 30S ribosomal protein S13



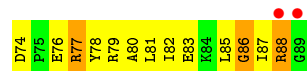
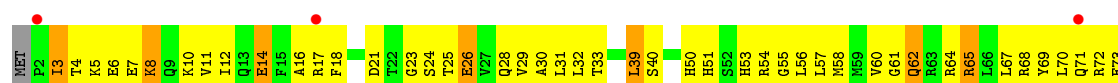
- Molecule 14: 30S ribosomal protein S14



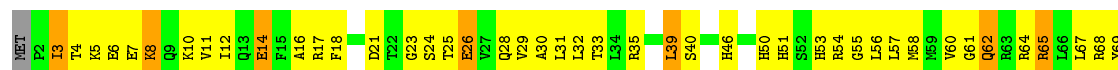
- Molecule 14: 30S ribosomal protein S14

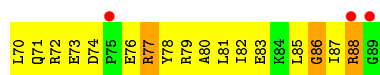


- Molecule 15: 30S ribosomal protein S15

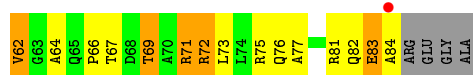
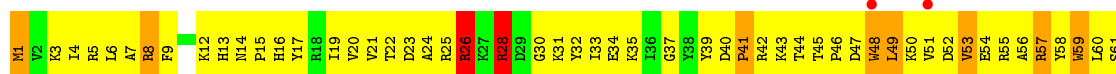


- Molecule 15: 30S ribosomal protein S15

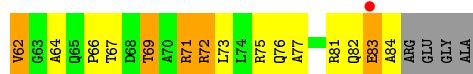




- Molecule 16: 30S ribosomal protein S16



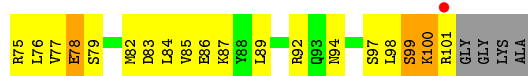
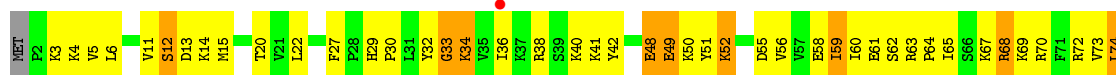
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



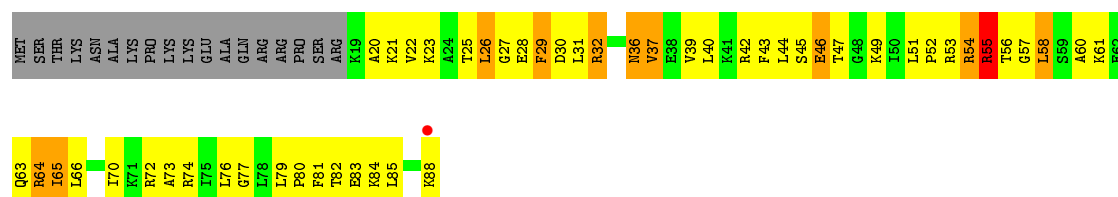
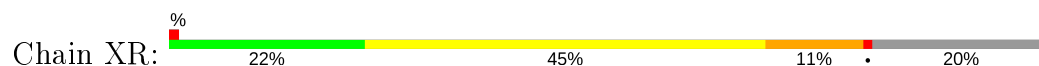
- Molecule 17: 30S ribosomal protein S17



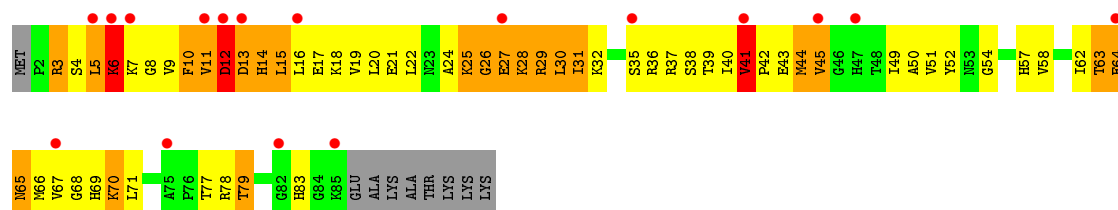
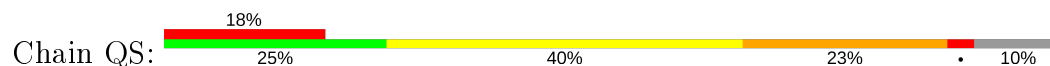
- Molecule 18: 30S ribosomal protein S18



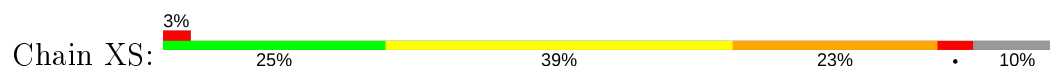
- Molecule 18: 30S ribosomal protein S18



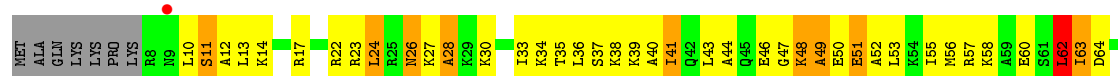
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

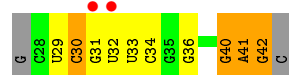


- Molecule 20: 30S ribosomal protein S20

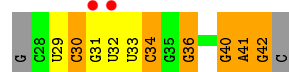
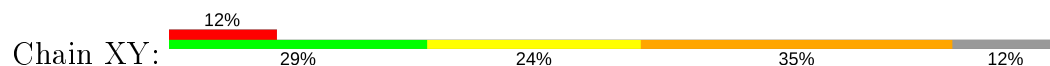




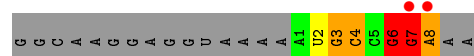




- Molecule 23: messenger RNA



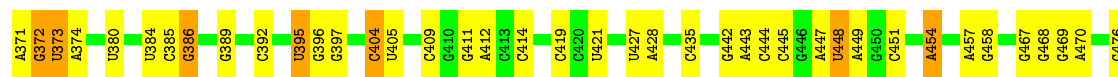
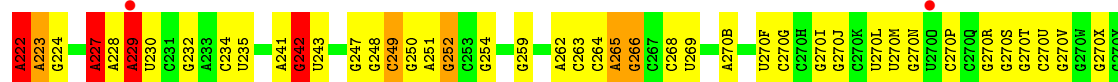
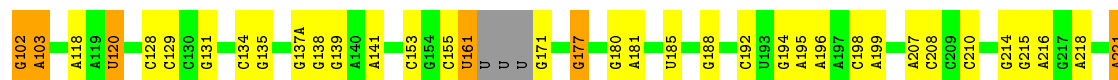
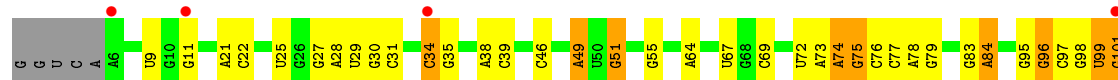
- Molecule 24: A-site ASL SufA6

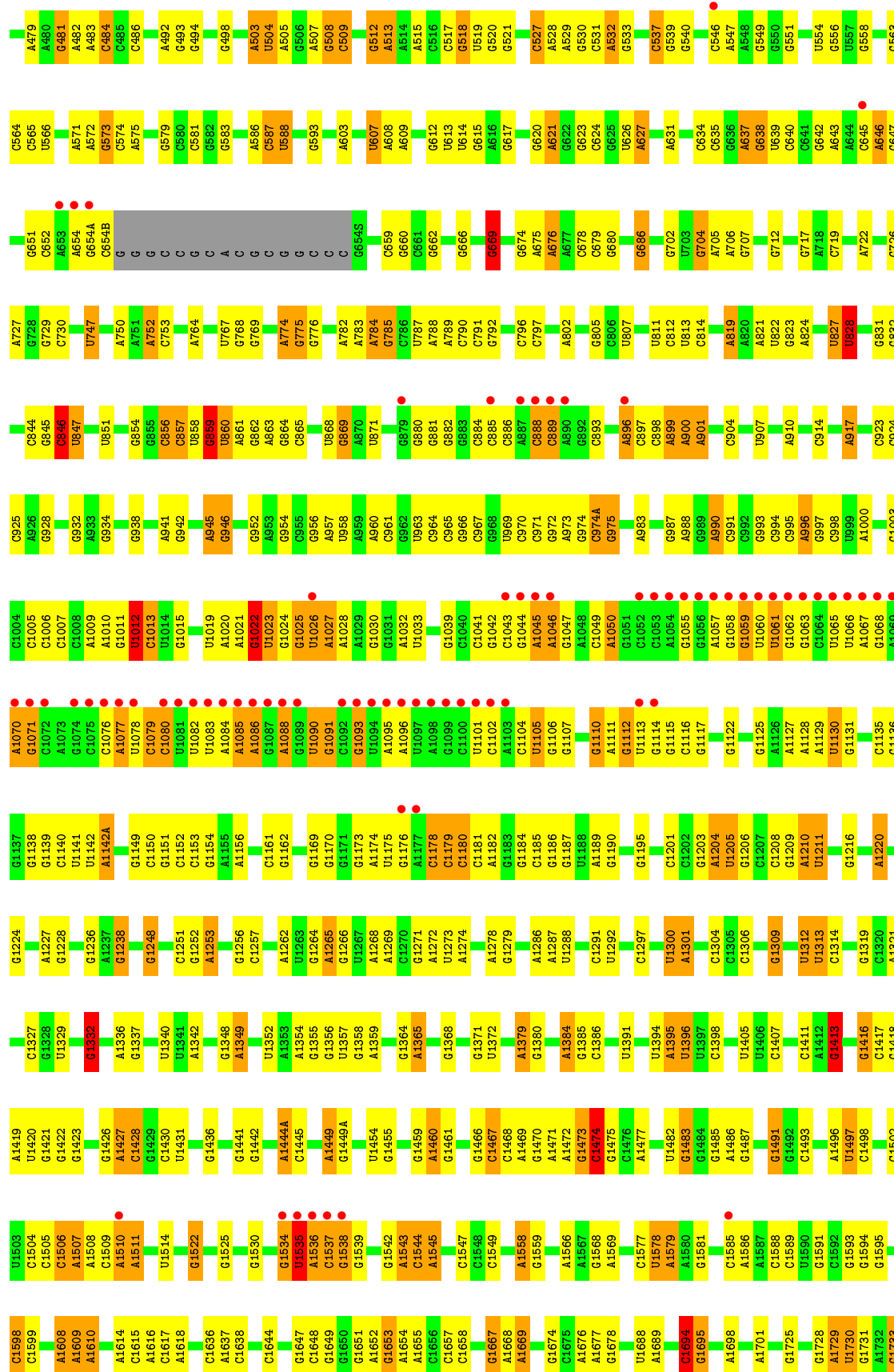


- Molecule 24: A-site ASL SufA6



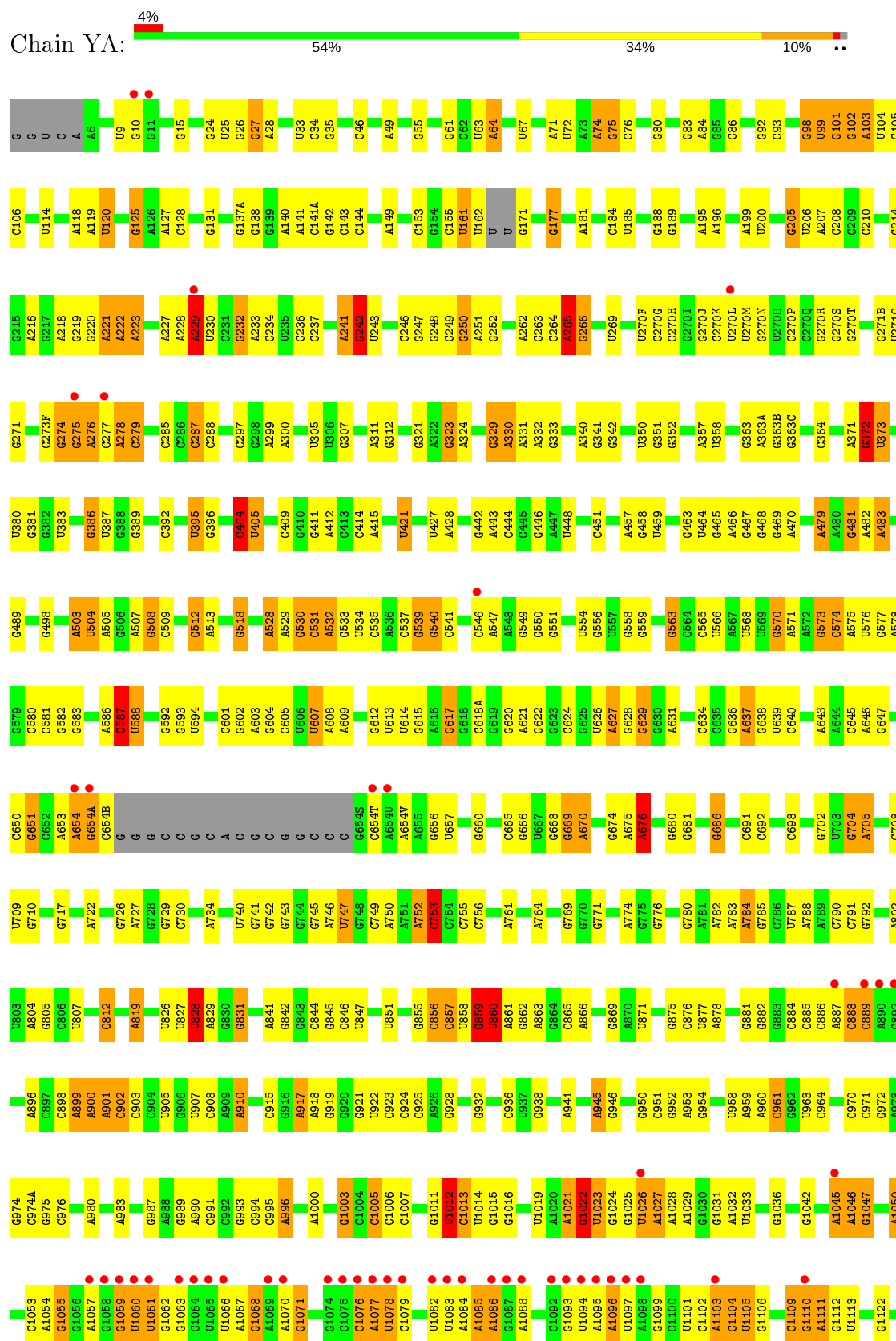
- Molecule 25: 23S rRNA



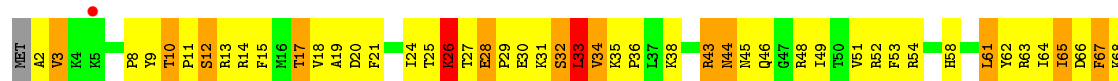


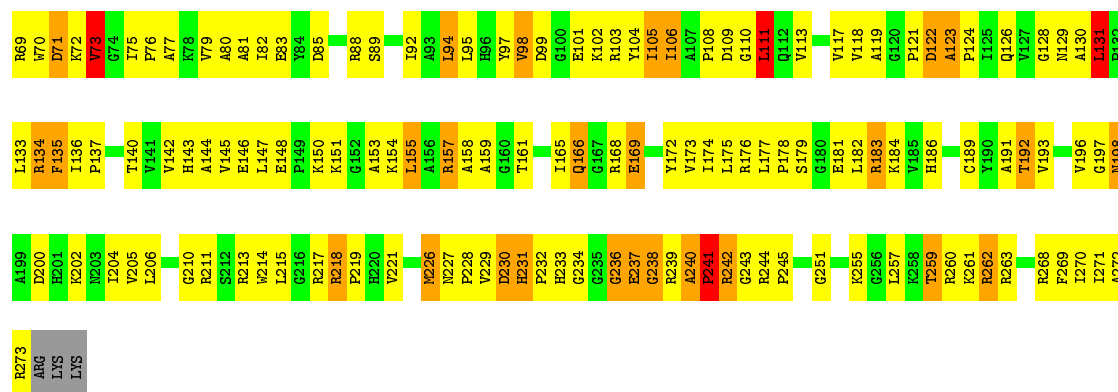


● Molecule 25: 23S rRNA

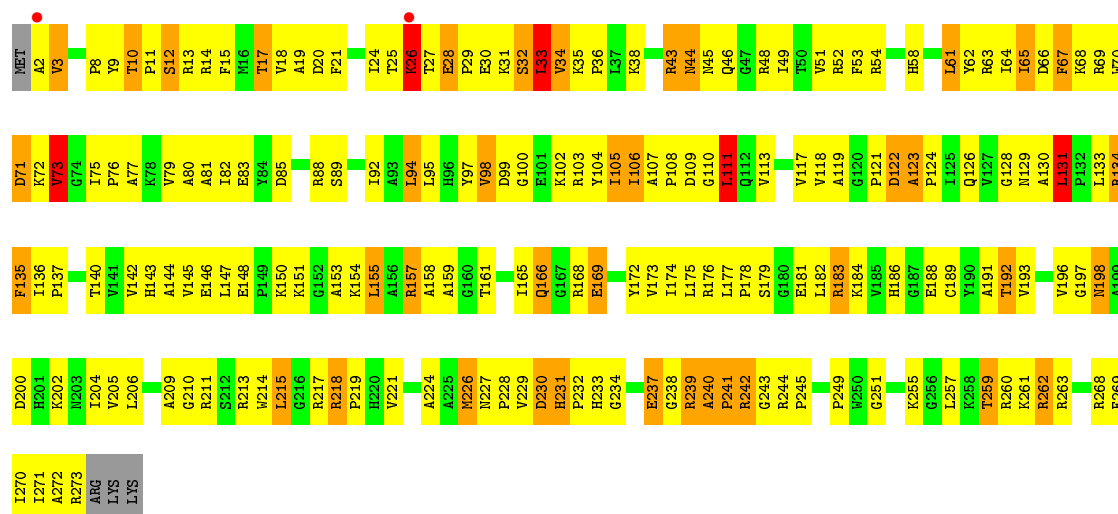


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G2383	G2299	G2193	G2124	A2033	G1948	A1830	A1729	A1610	U1514	G1429	U1341	G1238	A1128
G2385	C2306	A2198	G2125	U2034	G1949	C1830	G1730	C1617	U1516	C1430	U1342	G1239	A1129
G2389	G2307	G2208	G2126	G2035	G1950	U1834	G1731	A1618	G1517	C1431	A1349	U1240	U1130
U2390	A2309	C2208	G2127	C2039	U1951	U1835	G1732	G1636	U1518	C1432	U1352	A1241	C1135
G2391	A2310	G2210	G2128	A2042	A1952	G1835	G1733	A1637	G1519	A1434	U1353	G1250	G1136
A2392	G2311	G2211	U2130	C2043	U1955	C1836	C1742	A1637	U1520	G1441	A1354	C1251	G1137
A2393	C2312	A2212	G2131	G2046	U1956	U1847	G1743	C1648	G1522	G1442	G1357	G1252	G1138
C2394	G2313	G2213	U2132	U2047	C1957	A1848	G1750	A1648	G1525	A1444	U1358	A1253	G1139
G2395	G2314	G2215	G2133	G2048	C1958	U1849	G1751	G1651	A1528	A1445	A1359	U1141	U1141
G2396	G2315	G2216	A2134	U2047	G1959	A1848	G1752	A1652	A1529	G1445	G1359	G1256	U1142
U2401	C2316	G2217	C2136	A2051	C1959	A1883	G1754	G1653	A1530	A1445	A1359	C1257	A1142
A2402	G2317	G2218	C2137	G2052	U1963	A1883	A1755	G1654	A1531	A1445	A1359	G1257	A1142A
G2403	G2318	G2219	G2138	G2053	G1964	G1888	U1756	A1654	G1530	A1449	G1364	A1262	G1151
C2404	G2319	G2224	G2140	A2054	C1965	A1889	U1757	A1654	G1531	A1449A	A1365	U1263	C1152
G2405	A2320	A2225	G2141	G2055	A1966	G1889	A1762	C1657	C1533	U1454	G1368	U1264	C1153
U2406	G2321	G2226	G2142	G2056	C1967	G1889	G1763	G1658	U1534	G1455	G1369	A1265	G1154
U2407	A2322	A2227	C2145	A2059	G1968	G1889	G1764	G1667	U1535	C1458	U1372	U1267	A1155
G2410	G2323	U2233	C2146	A2060	A1969	U1864	A1773	A1669	A1536	A1460	A1379	A1268	C1161
G2414	G2324	G2234	G2147	G2061	A1970	G1869	U1779	U1672	G1538	G1461	A1384	G1270	G1162
G2415	G2325	G2234	G2148	G2062	A1971	G1870	U1780	U1673	G1539	G1461	A1384	G1271	G1169
U2419	A2326	G2238	U2150	A2063	A1972	A1871	U1781	G1674	U1540	C1464	G1385	A1272	G1170
C2420	G2327	U2244	G2151	G2068	G1973	G1878	U1782	C1675	A1542	C1467	C1386	U1273	G1171
U2423	G2328	U2243	G2152	G2069	A1978	C1882	A1783	G1676	A1543	A1471	U1390	G1278	G1173
C2424	G2329	U2244	G2153	G2070	G1979	G1883	U1784	G1677	A1544	G1478	U1391	G1279	A1174
A2425	G2330	G2246	G2154	A2071	G1980	G1883	U1785	G1678	A1545	G1479	U1392	U1287	U1175
G2426	G2331	G2246	G2155	G2072	A1981	A1884	A1787	G1681	C1549	A1472	A1393	A1287	A1177
G2427	G2332	G2247	G2156	G2073	C1982	G1888	U1790	G1682	A1558	C1474	U1394	C1281	C1178
G2428	A2333	U2249	G2157	C2073	G1989	A1889	A1791	G1683	A1559	G1478	U1395	U1292	C1179
G2429	G2334	G2250	G2158	U2074	U1991	G1896	U1792	C1684	G1566	G1479	U1406	C1293	C1180
A2430	U2344	C2263	G2160	C2078	G1992	G1899	U1794	U1688	A1566	G1480	G1407	U1300	G1187
U2435	G2345	G2264	G2161	U2079	U1993	G1899	U1795	A1689	A1567	U1482	C1403	U1301	U1188
G2436	G2346	C2264	G2162	C2079	C1994	C1902	U1796	A1690	A1568	G1483	C1404	A1302	U1189
C2437	C2347	A2267	G2163	U2086	G1998	G1903	U1797	A1691	C1577	G1484	U1405	G1309	G1190
U2438	G2350	A2268	G2164	G2087	G1998	G1906	U1798	U1692	C1578	G1485	G1406	G1309	A1194
A2439	G2353	A2269	U2167	U2096	G2002	G1906	G1799	U1693	U1578	A1490	C1407	U1312	G1195
C2441	G2361	G2275	A2169	G2100	C2007	A1913	G1801	G1695	A1579	G1491	C1408	U1313	C1196
C2442	G2362	G2276	A2170	G2105	C2008	A1916	G1802	G1696	A1580	G1492	C1411	U1314	G1203
G2443	C2363	G2277	U2172	G2106	G2009	U1917	G1803	G1697	G1581	G1493	A1412	A1317	A1204
G2444	G2364	G2277	G2173	G2107	U2011	A1918	G1813	A1698	C1582	A1496	G1413	G1318	U1205
G2445	G2365	G2277	G2174	G2108	G2012	A1919	G1814	G1699	A1586	U1497	G1415	G1319	G1206
G2446	A2369	C2283	C2175	C2111	A2013	C1920	A1815	A1700	A1586	G1500	G1416	G1319	G1206
G2447	G2370	C2284	A2176	U2113	A2014	G1929	G1816	G1703	G1593	G1500	G1417	C1320	A1210
A2448	G2371	C2285	C2177	A2114	A2015	G1930	G1816	G1704	G1594	C1505	G1418	A1321	U1211
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A2450	G2373	A2287	U2180	G2116	A2020	U1931	G1820	U1706	G1598	A1507	U1420	G1330	C1218
A2451	C2374	A2288	G2181	A2117	G2021	A1932	A1821	U1716	C1598	A1508	G1421	A1331	G1219
C2452	G2375	U2291	U2118	U2022	G2023	G1933	G1822	G1717	G1605	C1509	G1424	G1332	G1219
G2455	A2376	C2292	G2182	A2119	G2023	G1933	G1822	G1717	G1606	A1510	G1425	G1336	A1221
C2456	G2377	C2292	C2183	A2119	G2023	G1933	G1822	G1717	G1606	A1510	G1426	A1336	G1337
C2463	G2378	C2295	G2190	G2121	A2030	A1936	A1825	G1725	A1608	G1512	A1427	G1337	G1337
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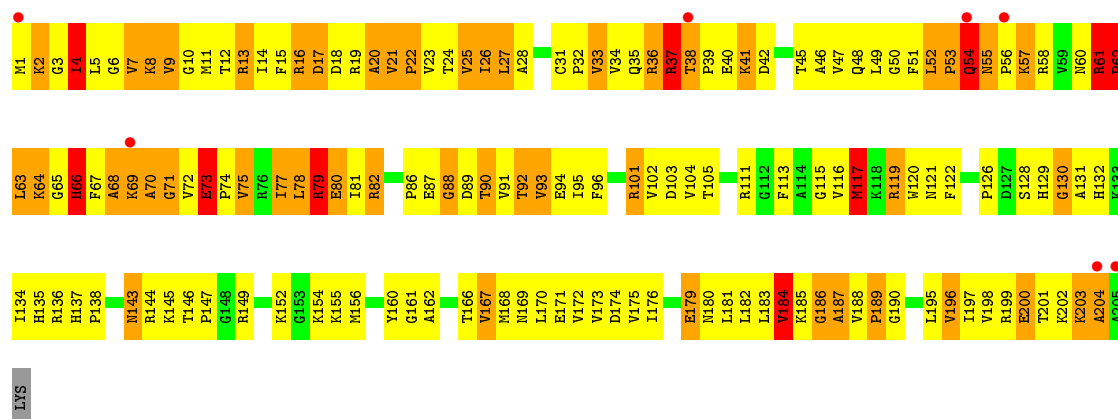




• Molecule 27: 50S ribosomal protein L2

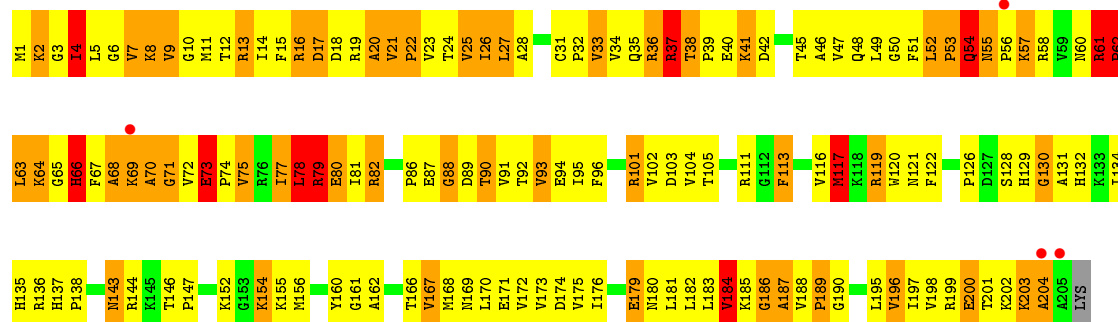
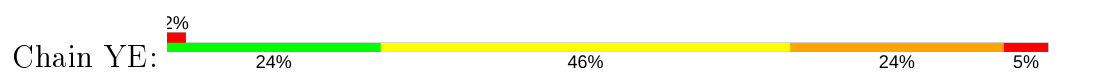


• Molecule 28: 50S ribosomal protein L3

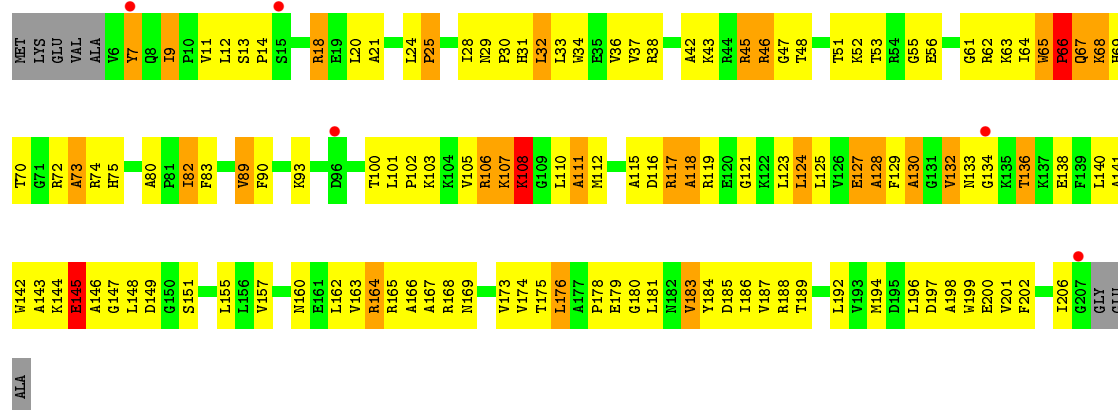


• Molecule 28: 50S ribosomal protein L3

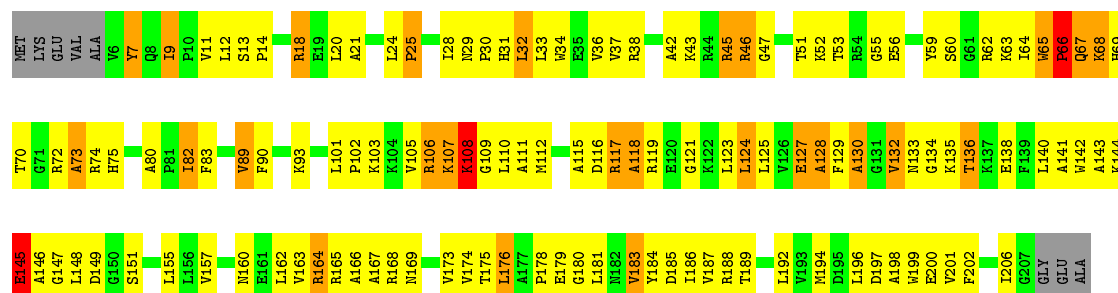




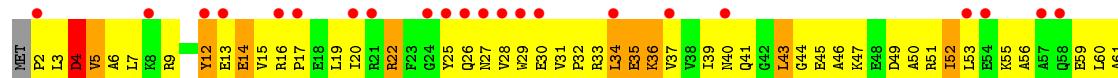
• Molecule 29: 50S ribosomal protein L4

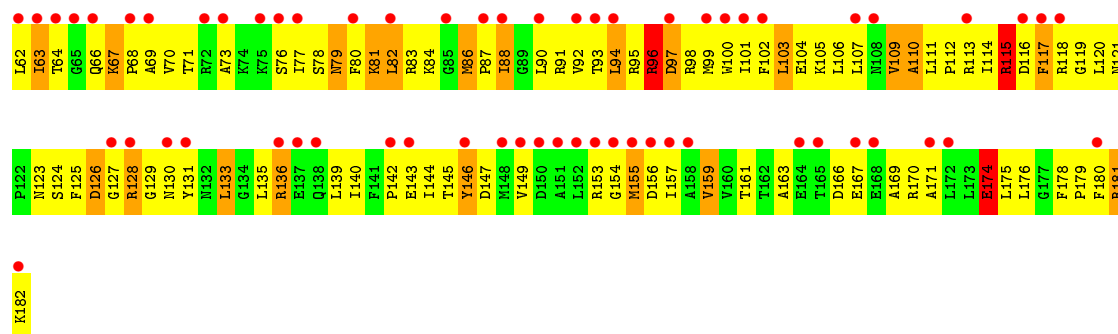


• Molecule 29: 50S ribosomal protein L4

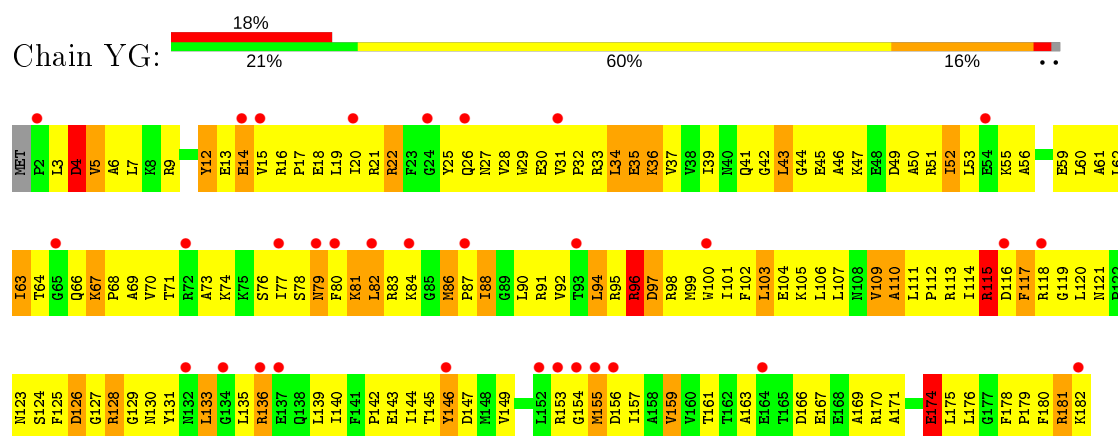


• Molecule 30: 50S ribosomal protein L5

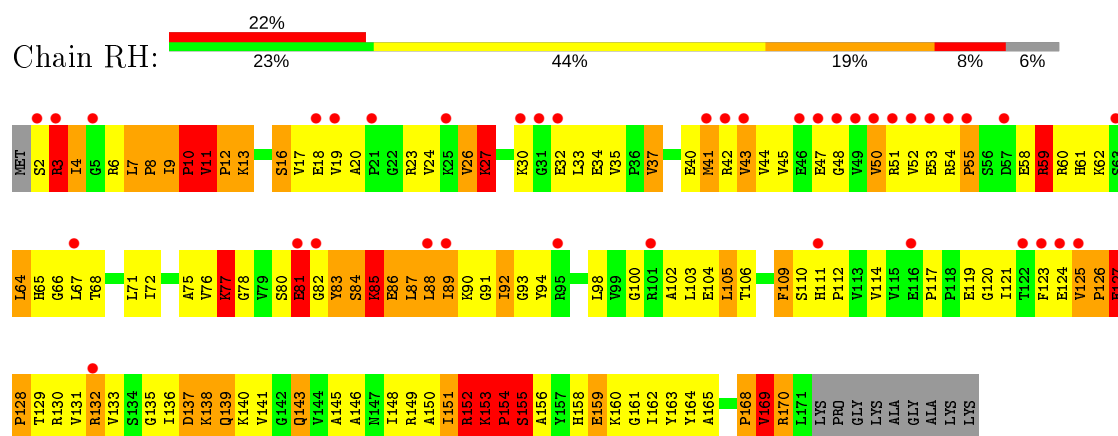




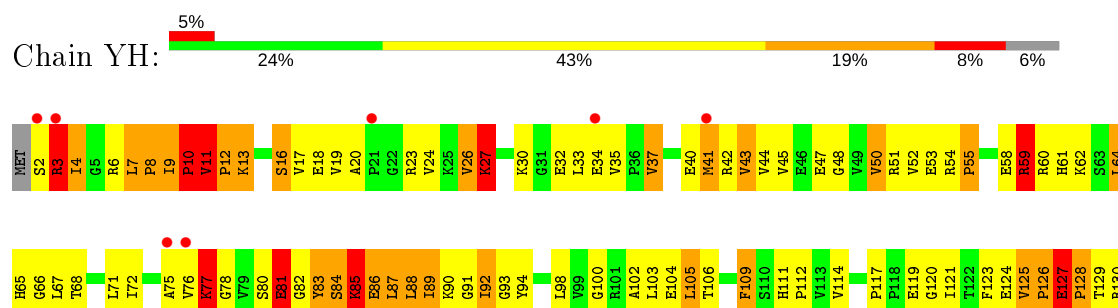
• Molecule 30: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L6

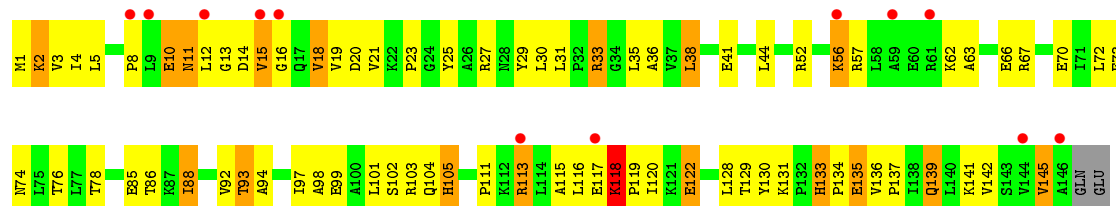


• Molecule 31: 50S ribosomal protein L6

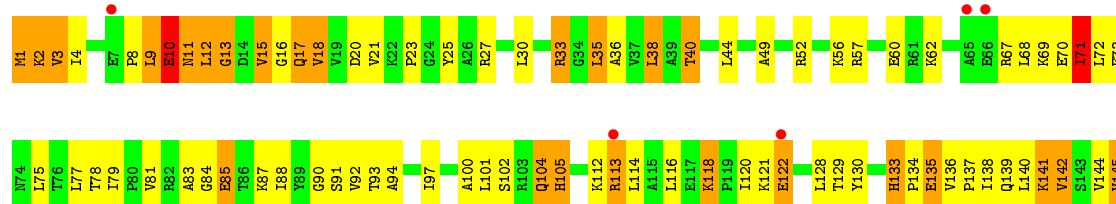
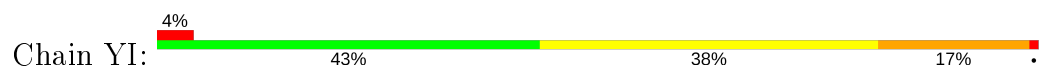




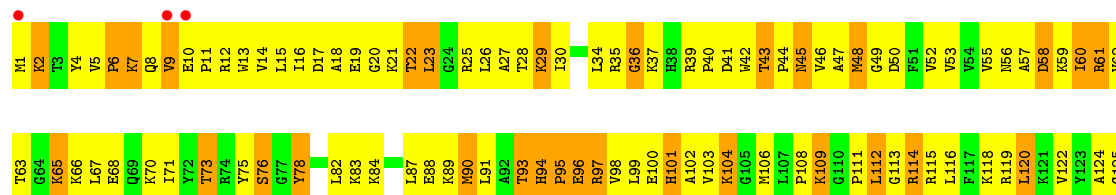
- Molecule 32: 50S ribosomal protein L9



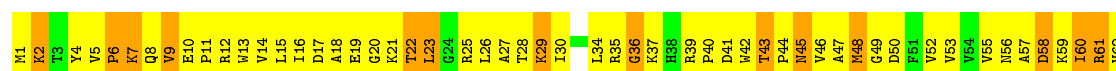
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13

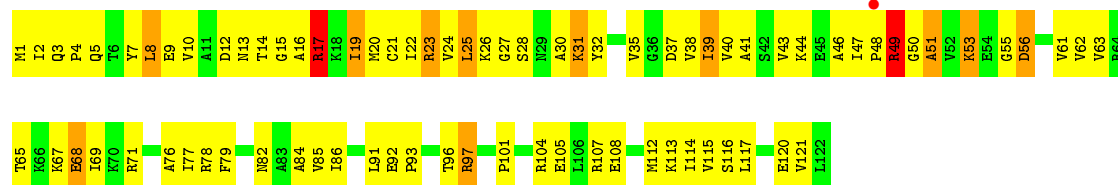


- Molecule 33: 50S ribosomal protein L13

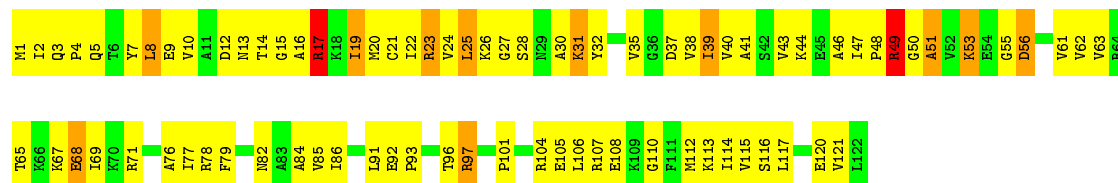




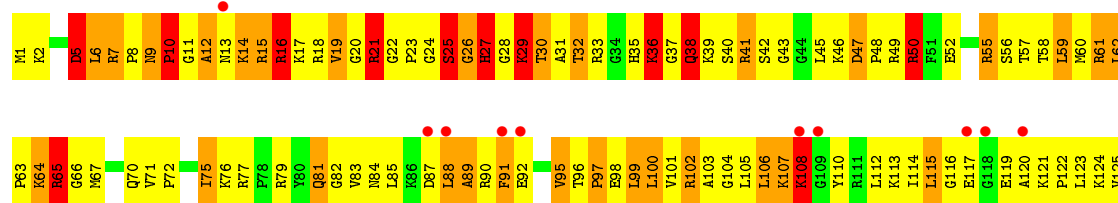
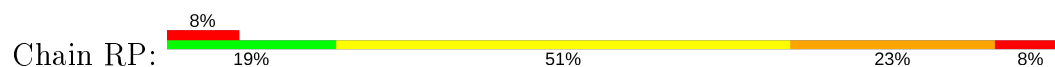
• Molecule 34: 50S ribosomal protein L14



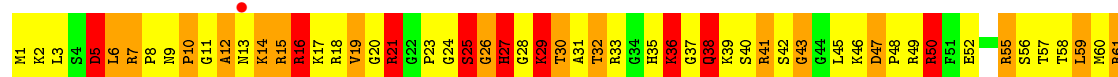
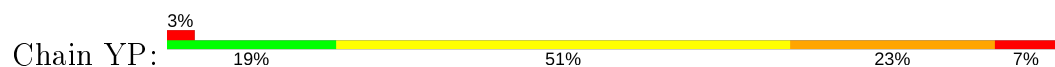
• Molecule 34: 50S ribosomal protein L14

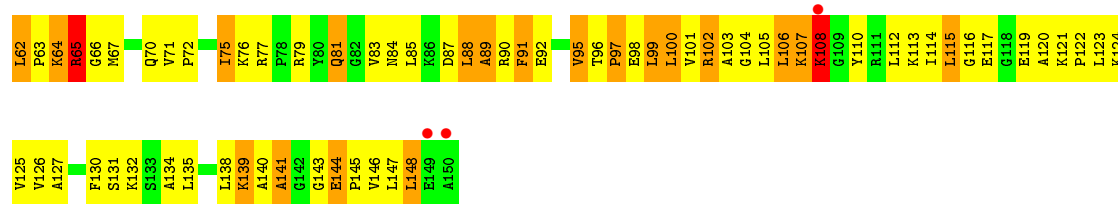


• Molecule 35: 50S ribosomal protein L15

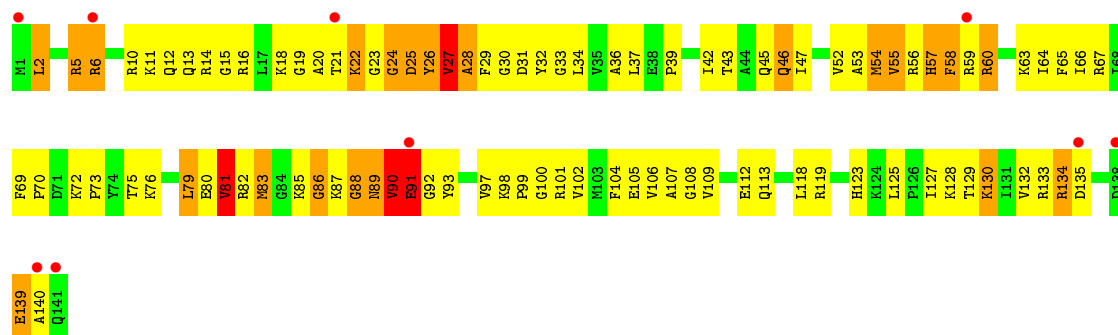


• Molecule 35: 50S ribosomal protein L15

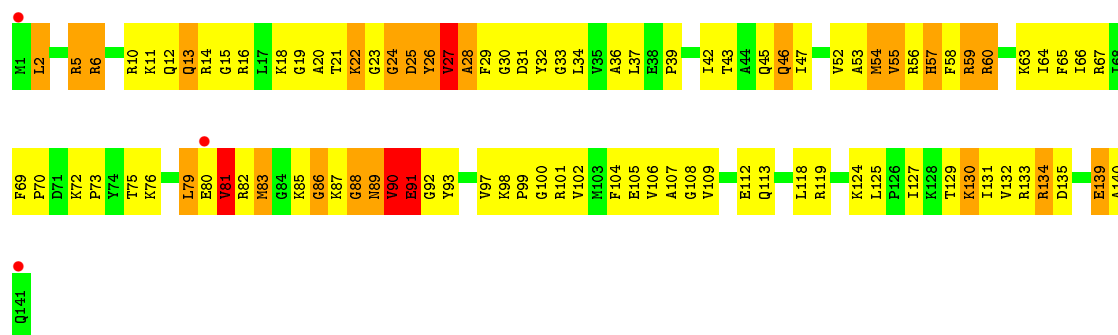




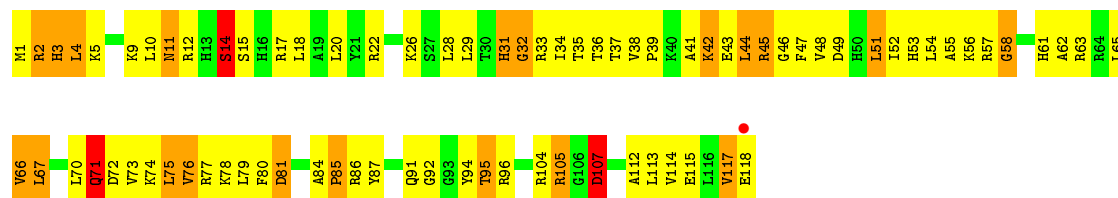
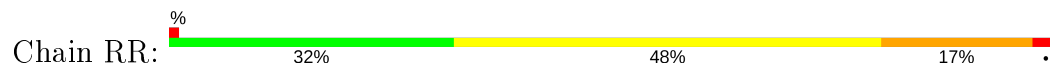
• Molecule 36: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L16

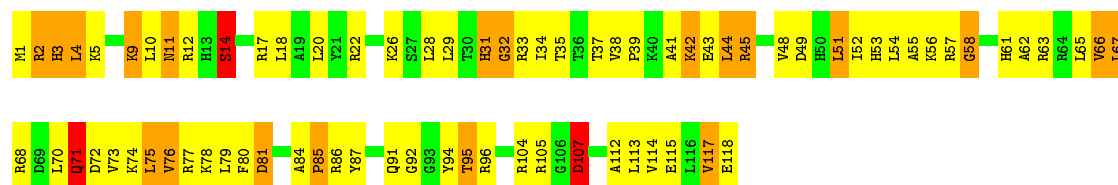


• Molecule 37: 50S ribosomal protein L17

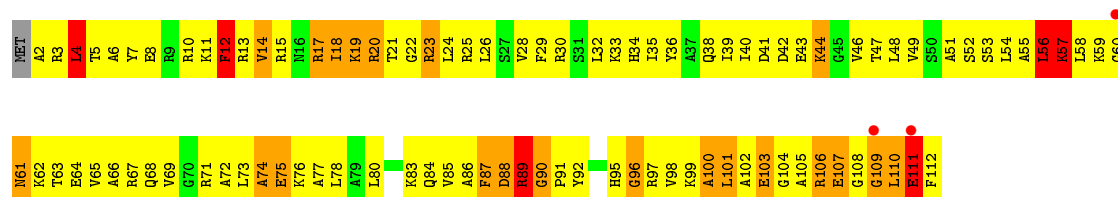
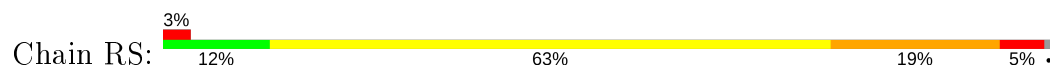


• Molecule 37: 50S ribosomal protein L17

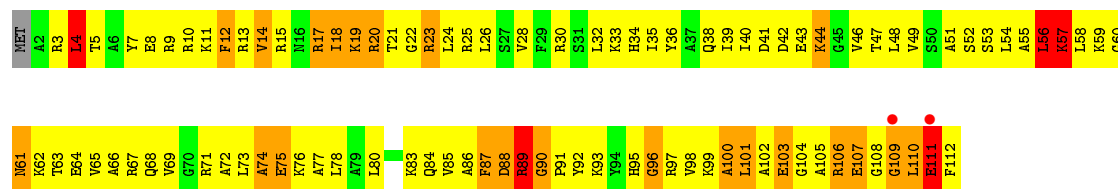
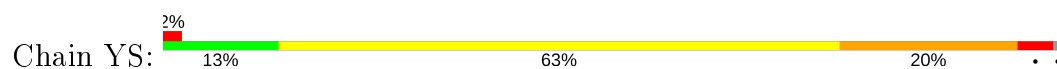




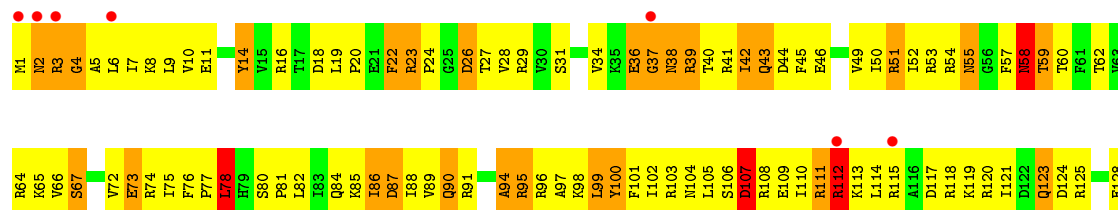
• Molecule 38: 50S ribosomal protein L18



• Molecule 38: 50S ribosomal protein L18

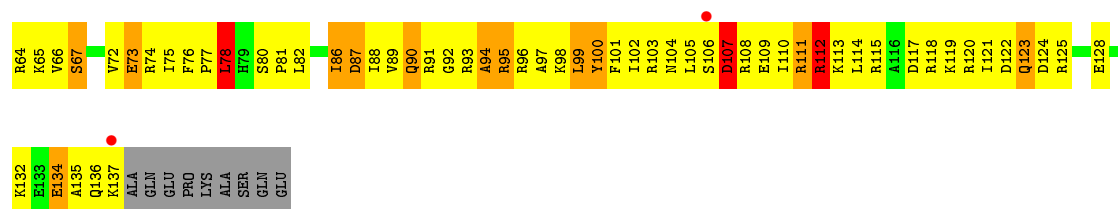


• Molecule 39: 50S ribosomal protein L19

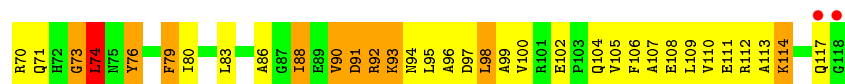


• Molecule 39: 50S ribosomal protein L19





• Molecule 40: 50S ribosomal protein L20



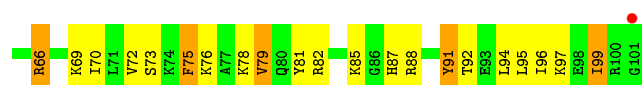
• Molecule 40: 50S ribosomal protein L20



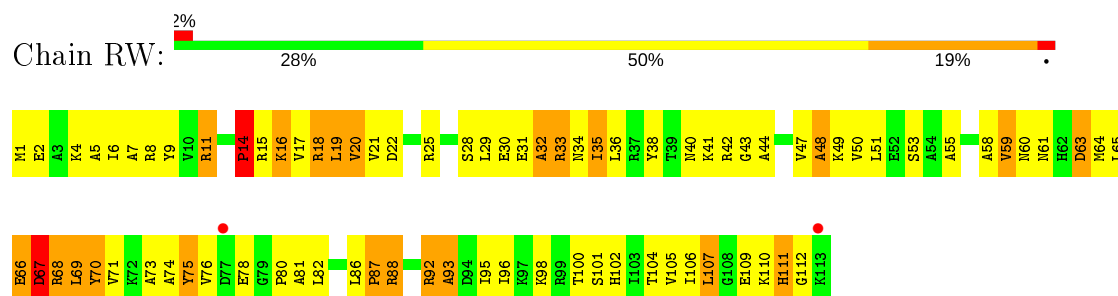
• Molecule 41: 50S ribosomal protein L21



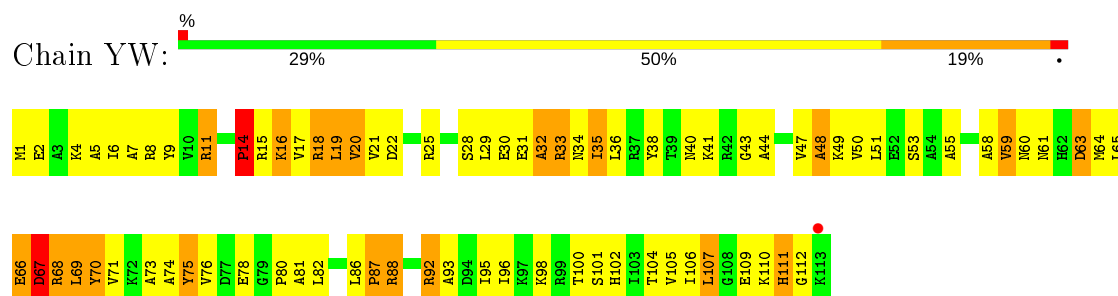
• Molecule 41: 50S ribosomal protein L21



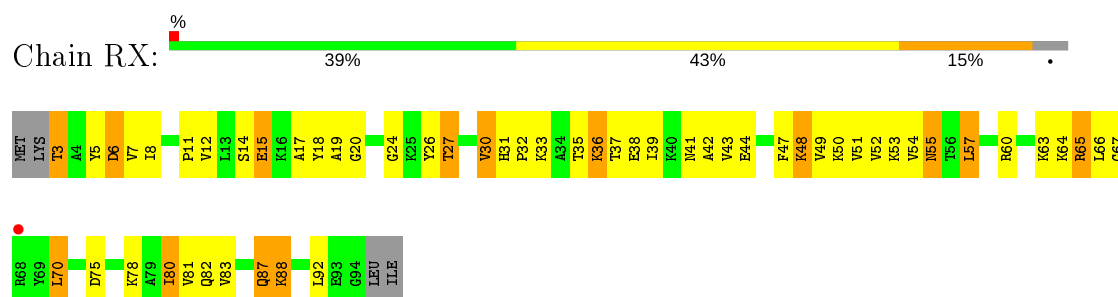
- Molecule 42: 50S ribosomal protein L22



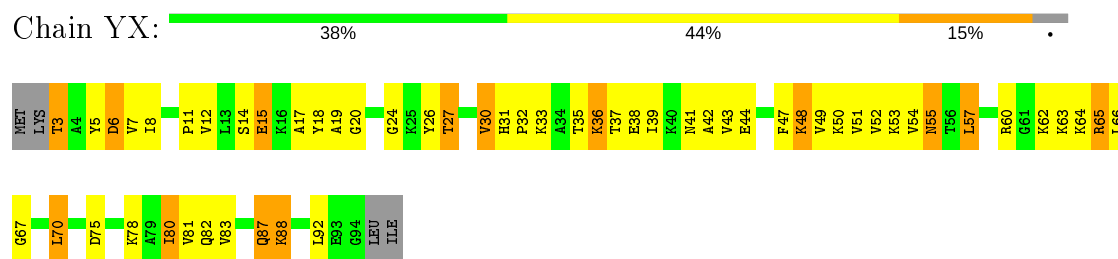
- Molecule 42: 50S ribosomal protein L22



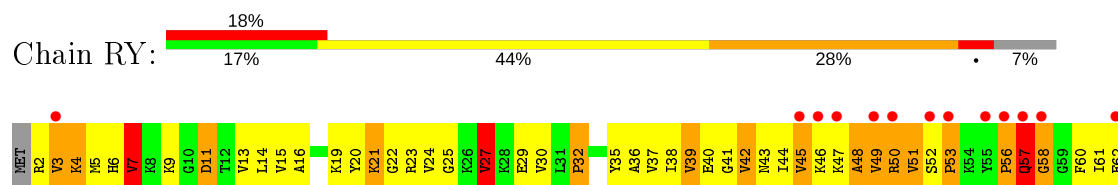
- Molecule 43: 50S ribosomal protein L23



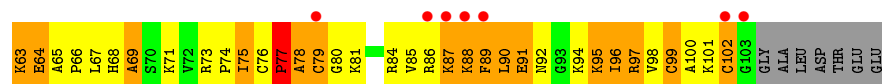
- Molecule 43: 50S ribosomal protein L23



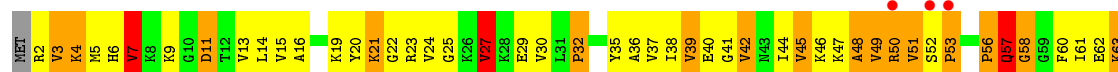
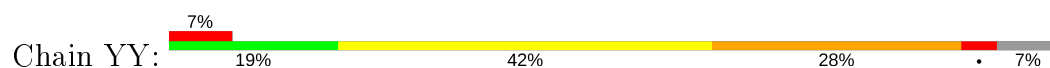
- Molecule 44: 50S ribosomal protein L24



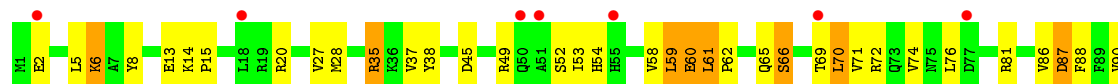




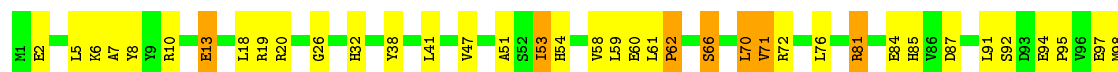
- Molecule 44: 50S ribosomal protein L24



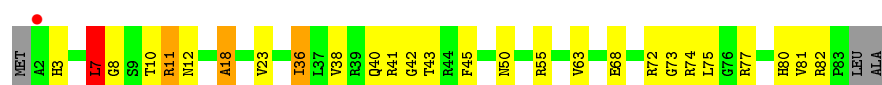
- Molecule 45: 50S ribosomal protein L25




- Molecule 45: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27

Chain Y0: 



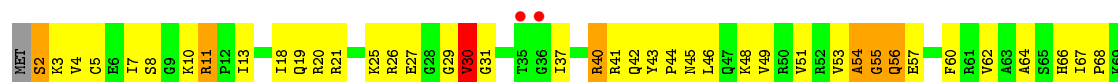
- Molecule 47: 50S ribosomal protein L28

Chain R1: 



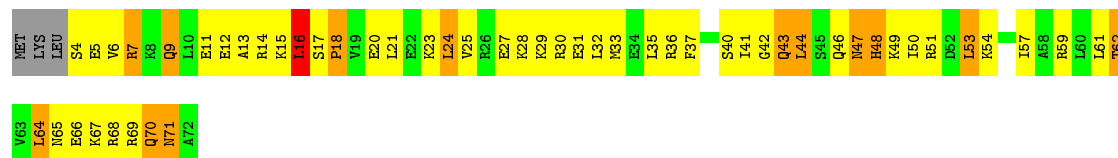
- Molecule 47: 50S ribosomal protein L28

Chain Y1: 

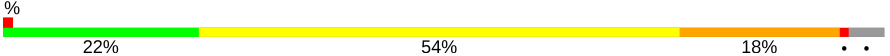


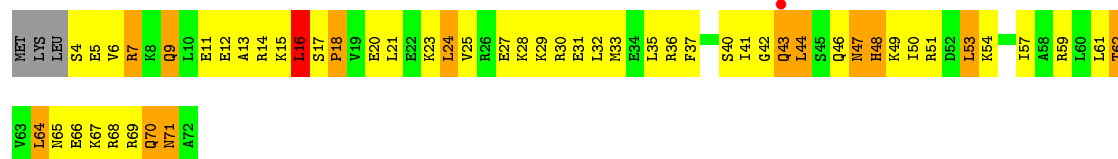
- Molecule 48: 50S ribosomal protein L29

Chain R2: 



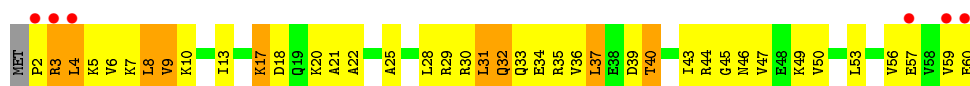
- Molecule 48: 50S ribosomal protein L29

Chain Y2: 

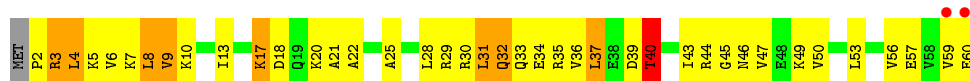


- Molecule 49: 50S ribosomal protein L30

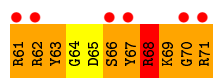
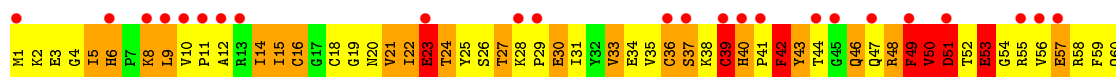
Chain R3: 



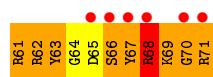
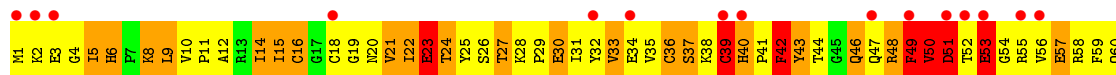
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31



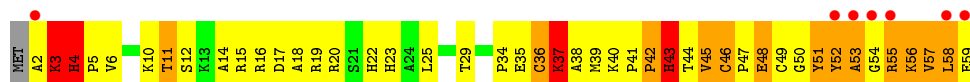
- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32

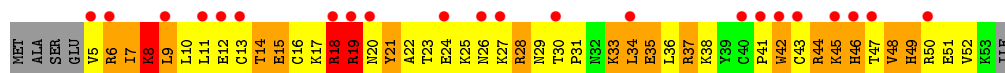


- Molecule 51: 50S ribosomal protein L32

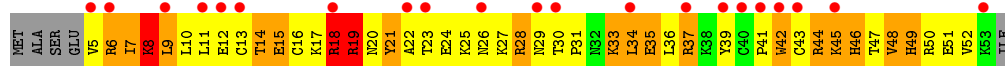


- Molecule 52: 50S ribosomal protein L33





- Molecule 52: 50S ribosomal protein L33



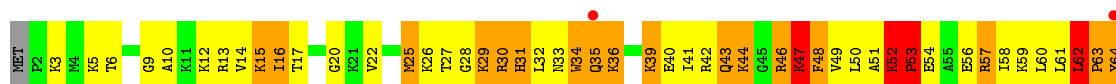
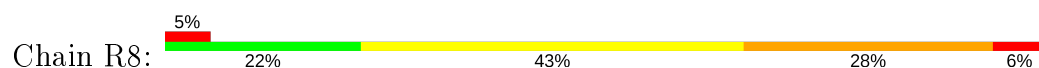
- Molecule 53: 50S ribosomal protein L34



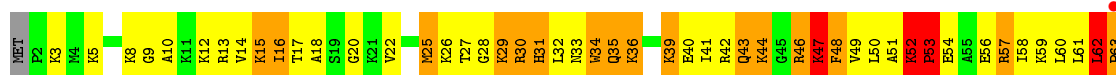
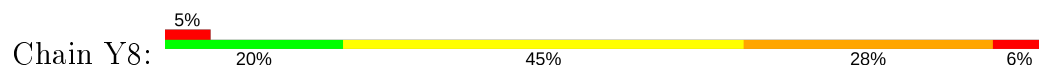
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35

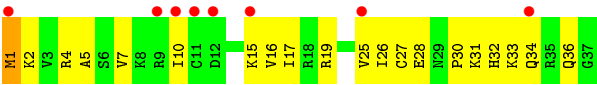


- Molecule 54: 50S ribosomal protein L35

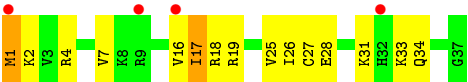


- Molecule 55: 50S ribosomal protein L36





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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, MG, PAR, 1MG, PPU

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

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

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



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

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

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

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

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

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 14284 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:YN:32:SER:CB	14:YN:41:ARG:HB3	1.23	1.55
14:YN:32:SER:HB3	14:YN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

The worst 5 of 17 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YV:50:PRO:C	51:Y5:60:VAL:O[4_445]	1.47	0.73
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.50	0.70
41:YV:51:VAL:N	51:Y5:60:VAL:C[4_445]	1.60	0.60
41:YV:50:PRO:CG	51:Y5:60:VAL:CA[4_445]	1.78	0.42
41:YV:50:PRO:CA	51:Y5:60:VAL:O[4_445]	1.83	0.37

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	QB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	<b>0</b> <b>3</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	3
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	7
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	7
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	6
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	5
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	6
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	5
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	7
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	7
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	6
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	7
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	3
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	3
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	7
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	6
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	11
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	9
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	4
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	4
13	QM	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	2
13	XM	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	2
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	1
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	1
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	10
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	10
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	8
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	4
18	XR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	4
19	QS	82/93 (88%)	47 (57%)	17 (21%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	1
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	1
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	1
21	XU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	1
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	10
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	10
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	6
29	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	6
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	4
30	YG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	4
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	102 (71%)	29 (20%)	13 (9%)	1	7
32	YI	144/148 (97%)	101 (70%)	26 (18%)	17 (12%)	0	4
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	9
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	9
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	6
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	6
37	RR	116/118 (98%)	83 (72%)	19 (16%)	14 (12%)	0	4
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	1
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
40	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	9
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	9
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	6
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	6
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	15
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	15
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
45	RZ	181/206 (88%)	126 (70%)	40 (22%)	15 (8%)	1	8
45	YZ	181/206 (88%)	125 (69%)	38 (21%)	18 (10%)	0	6
46	R0	80/85 (94%)	68 (85%)	9 (11%)	3 (4%)	3	24
46	Y0	80/85 (94%)	71 (89%)	9 (11%)	0	100	100
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	4
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	4
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	3
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	16
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	16
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	13
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7650 (67%)	2346 (20%)	1474 (13%)	0	3

5 of 1474 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

Mol	Chain	Res	Type
49	R3	8	LEU
7	XG	84	ASN
45	YZ	144	LEU
50	R4	49	PHE
2	XB	63	MET

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

Mol	Chain	Res	Type
48	R2	9	GLN
6	XF	64	GLN
44	YY	57	GLN
49	R3	19	GLN
2	XB	204	ASN

### 5.3.3 RNA ⓘ

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

5 of 1931 RNA backbone outliers are listed below:

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

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2481	G
1	XA	266	G
25	YA	1929	G

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Mol	Chain	Res	Type
25	RA	2610	C
1	XA	5	U

## 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	$\# Z  > 2$
23	1MG	QY	37	23	18,26,27	2.74	3 (16%)	19,39,42	1.74	3 (15%)
56	PPU	Z6	76	25,56	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z8	76	57,56	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
23	1MG	XY	37	23	18,26,27	2.75	3 (16%)	19,39,42	1.73	3 (15%)

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
23	1MG	QY	37	23	-	0/3/25/26	0/3/3/3
56	PPU	Z6	76	25,56	-	2/21/43/44	0/4/4/4
56	PPU	Z8	76	57,56	-	2/21/43/44	0/4/4/4
23	1MG	XY	37	23	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.30	1.41	1.23
56	Z6	76	PPU	O-C	9.27	1.41	1.23
23	XY	37	1MG	C4-N3	8.66	1.49	1.35
23	QY	37	1MG	C4-N3	8.57	1.49	1.35
23	QY	37	1MG	C2-N2	6.72	1.47	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z8	76	PPU	C3'-N3'-C	-8.60	110.23	123.21
56	Z6	76	PPU	C3'-N3'-C	-8.58	110.27	123.21
23	XY	37	1MG	C2-N3-C4	4.74	120.77	115.36
56	Z8	76	PPU	N3-C2-N1	-4.71	121.31	128.68
23	QY	37	1MG	C2-N3-C4	4.71	120.73	115.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 12 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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



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

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

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

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

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

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

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

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

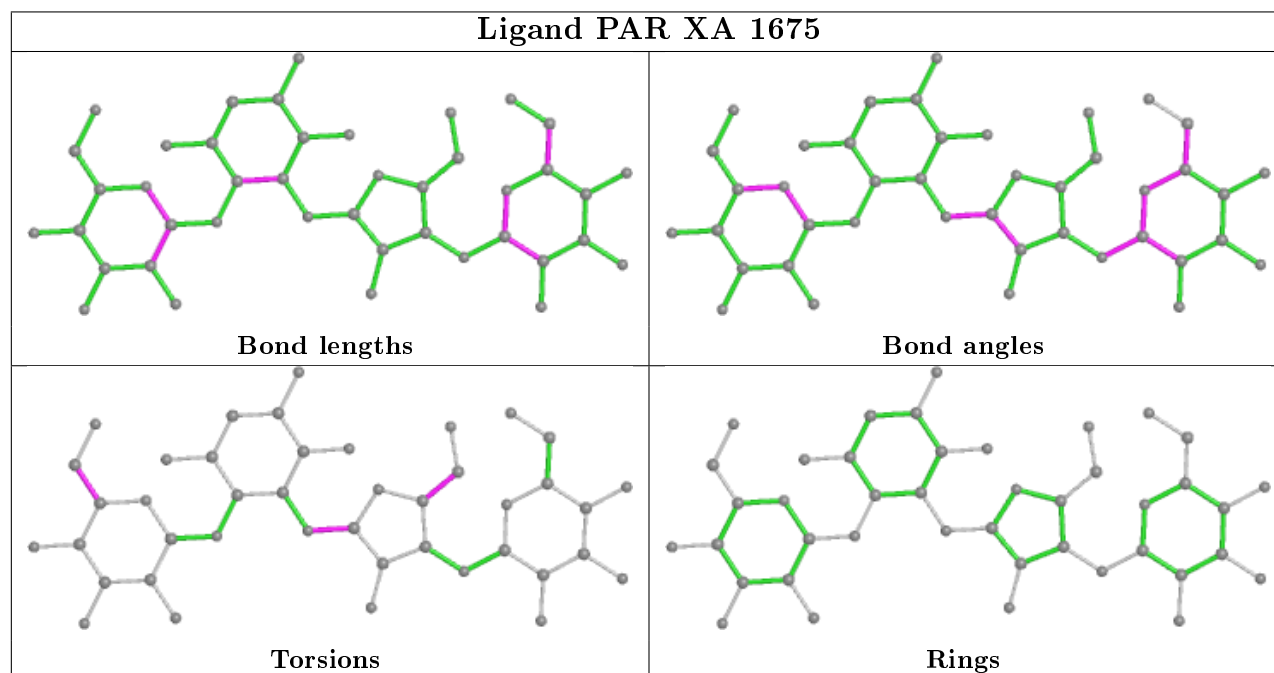
Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	XA	1675	PAR	O51-C51-C61-O61
58	QA	1666	PAR	O51-C51-C61-O61
58	XA	1675	PAR	C41-C51-C61-O61

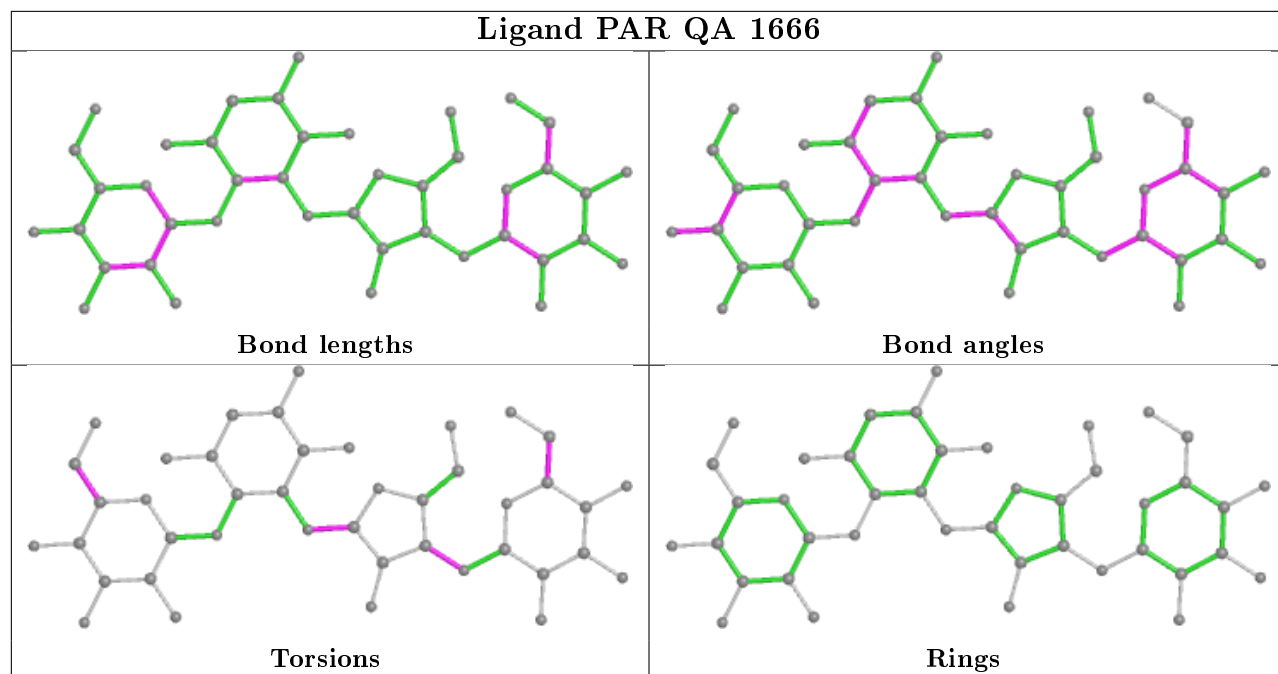
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

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

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

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

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

The worst 5 of 1170 RSRZ outliers are listed below:

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

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

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	PPU	Z6	76	37/38	0.83	0.36	73,73,73,73	0
56	PPU	Z8	76	37/38	0.86	0.35	70,70,70,70	0
23	1MG	QY	37	24/25	0.91	0.22	86,86,86,86	0
23	1MG	XY	37	24/25	0.94	0.17	62,62,62,62	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
57	MG	RA	3130	1/1	0.07	0.30	94,94,94,94	0
57	MG	QH	201	1/1	0.28	0.21	74,74,74,74	0
57	MG	RA	3115	1/1	0.41	0.30	47,47,47,47	0
57	MG	QA	1625	1/1	0.43	0.32	94,94,94,94	0
57	MG	QA	1657	1/1	0.43	0.28	108,108,108,108	0
57	MG	RA	3139	1/1	0.44	0.53	51,51,51,51	0
57	MG	YA	3085	1/1	0.45	0.58	65,65,65,65	0
57	MG	YA	3167	1/1	0.47	0.37	42,42,42,42	0
57	MG	QA	1608	1/1	0.50	0.31	68,68,68,68	0
57	MG	RA	3163	1/1	0.50	0.35	79,79,79,79	0
57	MG	XA	1654	1/1	0.52	0.34	58,58,58,58	0

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3118	1/1	0.78	0.28	49,49,49,49	0
57	MG	YA	3151	1/1	0.78	0.21	38,38,38,38	0
57	MG	XA	1673	1/1	0.78	0.49	56,56,56,56	0
59	ZN	XN	101	1/1	0.78	0.22	103,103,103,103	0
57	MG	QA	1654	1/1	0.78	0.21	69,69,69,69	0
57	MG	QA	1637	1/1	0.78	0.30	66,66,66,66	0
57	MG	RA	3091	1/1	0.78	0.42	65,65,65,65	0
57	MG	RA	3177	1/1	0.79	0.25	47,47,47,47	0
57	MG	YA	3191	1/1	0.79	0.21	22,22,22,22	0
57	MG	RA	3209	1/1	0.79	0.14	23,23,23,23	0
57	MG	RA	3138	1/1	0.79	0.27	17,17,17,17	0
57	MG	YA	3153	1/1	0.80	0.38	33,33,33,33	0
57	MG	YA	3016	1/1	0.80	0.21	20,20,20,20	0
57	MG	RA	3199	1/1	0.80	0.43	72,72,72,72	0
57	MG	RA	3188	1/1	0.80	0.20	53,53,53,53	0
57	MG	QA	1661	1/1	0.80	0.12	41,41,41,41	0
57	MG	YA	3072	1/1	0.81	0.32	15,15,15,15	0
57	MG	RA	3157	1/1	0.81	0.24	48,48,48,48	0
57	MG	RA	3210	1/1	0.81	0.14	51,51,51,51	0
57	MG	YA	3118	1/1	0.81	0.33	33,33,33,33	0
57	MG	YA	3218	1/1	0.81	0.20	47,47,47,47	0
57	MG	YA	3185	1/1	0.81	0.25	34,34,34,34	0
57	MG	RA	3233	1/1	0.81	0.34	42,42,42,42	0
57	MG	RA	3241	1/1	0.81	0.23	36,36,36,36	0
57	MG	YA	3175	1/1	0.81	0.13	42,42,42,42	0
57	MG	QA	1617	1/1	0.81	0.62	50,50,50,50	0
59	ZN	R9	101	1/1	0.82	0.09	112,112,112,112	0
57	MG	YA	3250	1/1	0.82	0.27	37,37,37,37	0
57	MG	QA	1618	1/1	0.82	0.30	42,42,42,42	0
57	MG	YA	3262	1/1	0.82	0.37	24,24,24,24	0
57	MG	RA	3179	1/1	0.83	0.28	29,29,29,29	0
57	MG	RA	3122	1/1	0.83	0.28	29,29,29,29	0
57	MG	YA	3230	1/1	0.83	0.14	35,35,35,35	0
57	MG	XA	1638	1/1	0.83	0.37	91,91,91,91	0
57	MG	RA	3135	1/1	0.83	0.28	55,55,55,55	0
57	MG	XA	1620	1/1	0.83	0.21	30,30,30,30	0
57	MG	XA	1649	1/1	0.83	0.35	48,48,48,48	0
57	MG	XA	1668	1/1	0.83	0.19	30,30,30,30	0
57	MG	RA	3180	1/1	0.83	0.29	33,33,33,33	0
57	MG	RA	3171	1/1	0.83	0.18	46,46,46,46	0
57	MG	XA	1662	1/1	0.84	0.10	47,47,47,47	0
57	MG	QA	1624	1/1	0.84	0.27	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1664	1/1	0.84	0.26	35,35,35,35	0
57	MG	RA	3133	1/1	0.84	0.13	51,51,51,51	0
57	MG	RA	3103	1/1	0.84	0.17	26,26,26,26	0
57	MG	QM	201	1/1	0.84	0.13	66,66,66,66	0
57	MG	RA	3226	1/1	0.85	0.29	38,38,38,38	0
57	MG	YA	3168	1/1	0.85	0.30	52,52,52,52	0
57	MG	RA	3075	1/1	0.85	0.14	39,39,39,39	0
57	MG	XA	1661	1/1	0.85	0.21	28,28,28,28	0
57	MG	YA	3238	1/1	0.85	0.97	154,154,154,154	0
57	MG	XA	1651	1/1	0.85	0.40	59,59,59,59	0
57	MG	RA	3172	1/1	0.85	0.28	31,31,31,31	0
57	MG	RA	3222	1/1	0.85	0.27	50,50,50,50	0
57	MG	RA	3170	1/1	0.85	0.18	41,41,41,41	0
57	MG	RA	3220	1/1	0.85	0.37	58,58,58,58	0
57	MG	YA	3164	1/1	0.86	0.27	22,22,22,22	0
57	MG	RA	3161	1/1	0.86	0.25	33,33,33,33	0
57	MG	YA	3232	1/1	0.86	0.27	28,28,28,28	0
57	MG	XA	1614	1/1	0.86	0.24	57,57,57,57	0
57	MG	YA	3127	1/1	0.86	0.17	13,13,13,13	0
57	MG	QA	1638	1/1	0.86	0.21	54,54,54,54	0
57	MG	YA	3251	1/1	0.86	0.35	60,60,60,60	0
57	MG	XA	1666	1/1	0.86	0.09	61,61,61,61	0
57	MG	YA	3124	1/1	0.86	0.16	16,16,16,16	0
57	MG	RA	3134	1/1	0.86	0.16	42,42,42,42	0
57	MG	YA	3172	1/1	0.86	0.18	48,48,48,48	0
57	MG	XA	1656	1/1	0.86	0.21	45,45,45,45	0
57	MG	YP	201	1/1	0.86	0.19	153,153,153,153	0
57	MG	RA	3189	1/1	0.86	0.28	33,33,33,33	0
57	MG	RA	3126	1/1	0.86	0.58	39,39,39,39	0
57	MG	RA	3159	1/1	0.87	0.25	40,40,40,40	0
57	MG	YA	3174	1/1	0.87	0.13	27,27,27,27	0
58	PAR	QA	1666	42/42	0.87	0.30	84,84,84,84	0
57	MG	XA	1611	1/1	0.87	0.20	8,8,8,8	0
57	MG	RA	3127	1/1	0.87	0.23	36,36,36,36	0
57	MG	YA	3265	1/1	0.87	0.23	36,36,36,36	0
58	PAR	XA	1675	42/42	0.87	0.33	74,74,74,74	0
57	MG	YB	201	1/1	0.87	0.21	51,51,51,51	0
57	MG	RA	3185	1/1	0.87	0.34	45,45,45,45	0
57	MG	RA	3206	1/1	0.87	0.32	26,26,26,26	0
57	MG	YA	3146	1/1	0.87	0.25	40,40,40,40	0
57	MG	R0	101	1/1	0.87	0.18	32,32,32,32	0
57	MG	YA	3235	1/1	0.87	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1641	1/1	0.87	0.20	17,17,17,17	0
57	MG	YA	3193	1/1	0.87	0.32	35,35,35,35	0
57	MG	YP	202	1/1	0.87	0.19	31,31,31,31	0
57	MG	QA	1650	1/1	0.88	0.12	27,27,27,27	0
57	MG	RA	3229	1/1	0.88	0.28	41,41,41,41	0
57	MG	QA	1601	1/1	0.88	0.32	58,58,58,58	0
57	MG	YA	3243	1/1	0.88	0.27	32,32,32,32	0
57	MG	RA	3235	1/1	0.88	0.35	29,29,29,29	0
57	MG	RA	3142	1/1	0.88	0.17	59,59,59,59	0
57	MG	RA	3191	1/1	0.88	0.25	38,38,38,38	0
57	MG	RD	301	1/1	0.88	0.30	38,38,38,38	0
57	MG	RA	3008	1/1	0.88	0.24	47,47,47,47	0
57	MG	RA	3195	1/1	0.88	0.36	85,85,85,85	0
57	MG	RA	3162	1/1	0.88	0.17	39,39,39,39	0
57	MG	RA	3207	1/1	0.88	0.36	105,105,105,105	0
57	MG	RR	202	1/1	0.88	0.18	20,20,20,20	0
57	MG	YA	3213	1/1	0.88	0.09	31,31,31,31	0
57	MG	YA	3220	1/1	0.88	0.20	53,53,53,53	0
57	MG	YA	3012	1/1	0.88	0.36	5,5,5,5	0
57	MG	YA	3150	1/1	0.88	0.14	31,31,31,31	0
57	MG	RA	3026	1/1	0.88	0.11	3,3,3,3	0
57	MG	YA	3157	1/1	0.88	0.23	49,49,49,49	0
57	MG	YA	3195	1/1	0.88	0.24	44,44,44,44	0
57	MG	YA	3154	1/1	0.88	0.24	38,38,38,38	0
57	MG	YA	3223	1/1	0.88	0.34	42,42,42,42	0
57	MG	YA	3152	1/1	0.89	0.14	43,43,43,43	0
57	MG	QA	1632	1/1	0.89	0.23	40,40,40,40	0
57	MG	XA	1665	1/1	0.89	0.32	46,46,46,46	0
57	MG	XA	1628	1/1	0.89	0.10	19,19,19,19	0
57	MG	RA	3002	1/1	0.89	0.31	41,41,41,41	0
57	MG	RA	3131	1/1	0.89	0.27	31,31,31,31	0
57	MG	YA	3234	1/1	0.89	0.17	28,28,28,28	0
57	MG	RF	301	1/1	0.89	0.21	65,65,65,65	0
57	MG	RA	3044	1/1	0.89	0.30	37,37,37,37	0
57	MG	YA	3248	1/1	0.89	0.13	32,32,32,32	0
57	MG	YA	3219	1/1	0.89	0.19	33,33,33,33	0
57	MG	QA	1636	1/1	0.89	0.10	34,34,34,34	0
57	MG	RA	3009	1/1	0.89	0.16	26,26,26,26	0
57	MG	XA	1670	1/1	0.89	0.22	79,79,79,79	0
57	MG	XA	1652	1/1	0.89	0.25	64,64,64,64	0
57	MG	YA	3054	1/1	0.89	0.17	3,3,3,3	0
57	MG	RA	3184	1/1	0.89	0.28	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3217	1/1	0.89	0.12	49,49,49,49	0
57	MG	RA	3205	1/1	0.89	0.22	54,54,54,54	0
57	MG	RA	3183	1/1	0.89	0.38	44,44,44,44	0
57	MG	YA	3226	1/1	0.89	0.17	20,20,20,20	0
57	MG	YA	3143	1/1	0.89	0.29	66,66,66,66	0
57	MG	YA	3253	1/1	0.89	0.34	25,25,25,25	0
57	MG	RA	3049	1/1	0.90	0.11	14,14,14,14	0
57	MG	XA	1663	1/1	0.90	0.27	35,35,35,35	0
57	MG	QA	1656	1/1	0.90	0.20	100,100,100,100	0
57	MG	YA	3209	1/1	0.90	0.15	29,29,29,29	0
57	MG	RA	3057	1/1	0.90	0.41	34,34,34,34	0
57	MG	RA	3151	1/1	0.90	0.13	22,22,22,22	0
57	MG	QA	1612	1/1	0.90	0.28	18,18,18,18	0
59	ZN	XD	301	1/1	0.90	0.27	45,45,45,45	0
57	MG	RA	3059	1/1	0.90	0.21	15,15,15,15	0
57	MG	YA	3082	1/1	0.90	1.03	80,80,80,80	0
57	MG	YA	3139	1/1	0.90	0.21	33,33,33,33	0
57	MG	QA	1629	1/1	0.90	0.13	47,47,47,47	0
57	MG	RA	3039	1/1	0.90	0.10	14,14,14,14	0
57	MG	YA	3221	1/1	0.90	1.00	42,42,42,42	0
57	MG	YA	3176	1/1	0.90	0.11	32,32,32,32	0
57	MG	RA	3014	1/1	0.90	0.23	3,3,3,3	0
57	MG	RA	3211	1/1	0.90	0.26	38,38,38,38	0
57	MG	YA	3108	1/1	0.90	0.41	20,20,20,20	0
57	MG	YA	3069	1/1	0.90	0.28	13,13,13,13	0
57	MG	QA	1626	1/1	0.90	0.17	29,29,29,29	0
57	MG	YA	3246	1/1	0.90	0.36	29,29,29,29	0
57	MG	XA	1634	1/1	0.90	0.20	43,43,43,43	0
57	MG	YA	3186	1/1	0.90	0.33	44,44,44,44	0
57	MG	RA	3160	1/1	0.90	0.18	42,42,42,42	0
57	MG	RA	3182	1/1	0.91	0.31	55,55,55,55	0
57	MG	YA	3110	1/1	0.91	0.25	11,11,11,11	0
57	MG	RA	3143	1/1	0.91	0.18	30,30,30,30	0
57	MG	YA	3241	1/1	0.91	0.20	39,39,39,39	0
57	MG	XA	1672	1/1	0.91	0.10	23,23,23,23	0
57	MG	RA	3068	1/1	0.91	0.20	37,37,37,37	0
57	MG	QA	1619	1/1	0.91	0.16	43,43,43,43	0
57	MG	XA	1659	1/1	0.91	0.21	41,41,41,41	0
57	MG	YA	3149	1/1	0.91	0.20	25,25,25,25	0
57	MG	XA	1618	1/1	0.91	0.28	33,33,33,33	0
57	MG	QA	1603	1/1	0.91	0.40	22,22,22,22	0
57	MG	YA	3254	1/1	0.91	0.31	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3165	1/1	0.91	0.44	43,43,43,43	0
57	MG	YA	3266	1/1	0.91	0.22	11,11,11,11	0
57	MG	YA	3163	1/1	0.91	0.21	29,29,29,29	0
57	MG	RA	3238	1/1	0.91	0.19	31,31,31,31	0
57	MG	RA	3224	1/1	0.91	0.16	40,40,40,40	0
57	MG	QA	1647	1/1	0.91	0.28	58,58,58,58	0
57	MG	YA	3229	1/1	0.91	0.18	20,20,20,20	0
57	MG	XA	1619	1/1	0.91	0.25	33,33,33,33	0
57	MG	RA	3236	1/1	0.91	0.25	34,34,34,34	0
57	MG	XA	1621	1/1	0.91	0.35	32,32,32,32	0
57	MG	YA	3224	1/1	0.91	0.10	35,35,35,35	0
57	MG	YA	3038	1/1	0.91	0.25	4,4,4,4	0
57	MG	RA	3145	1/1	0.92	0.27	14,14,14,14	0
57	MG	RA	3167	1/1	0.92	0.15	56,56,56,56	0
57	MG	RA	3216	1/1	0.92	0.10	31,31,31,31	0
57	MG	RA	3239	1/1	0.92	0.38	24,24,24,24	0
57	MG	XA	1606	1/1	0.92	0.28	29,29,29,29	0
57	MG	RA	3116	1/1	0.92	0.21	2,2,2,2	0
57	MG	YA	3236	1/1	0.92	0.21	40,40,40,40	0
57	MG	YA	3201	1/1	0.92	0.58	23,23,23,23	0
57	MG	QA	1662	1/1	0.92	0.11	63,63,63,63	0
57	MG	QA	1644	1/1	0.92	0.14	36,36,36,36	0
57	MG	RA	3104	1/1	0.92	0.11	6,6,6,6	0
57	MG	XA	1642	1/1	0.92	0.18	37,37,37,37	0
57	MG	RA	3010	1/1	0.92	0.15	48,48,48,48	0
57	MG	RB	202	1/1	0.92	0.10	46,46,46,46	0
57	MG	YA	3179	1/1	0.92	0.10	40,40,40,40	0
57	MG	RA	3121	1/1	0.92	0.27	45,45,45,45	0
57	MG	YA	3133	1/1	0.92	0.17	12,12,12,12	0
57	MG	YA	3158	1/1	0.92	0.18	16,16,16,16	0
57	MG	YA	3202	1/1	0.92	0.15	33,33,33,33	0
57	MG	RA	3148	1/1	0.92	0.23	39,39,39,39	0
57	MG	RA	3141	1/1	0.92	0.32	34,34,34,34	0
57	MG	XA	1627	1/1	0.92	0.10	24,24,24,24	0
57	MG	RA	3212	1/1	0.92	0.18	37,37,37,37	0
57	MG	RA	3174	1/1	0.92	0.15	26,26,26,26	0
57	MG	RA	3055	1/1	0.92	0.22	21,21,21,21	0
57	MG	YA	3184	1/1	0.92	0.20	35,35,35,35	0
57	MG	YA	3252	1/1	0.92	0.36	41,41,41,41	0
57	MG	QA	1658	1/1	0.92	0.13	52,52,52,52	0
57	MG	RA	3178	1/1	0.92	0.16	30,30,30,30	0
57	MG	RE	302	1/1	0.92	0.10	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3249	1/1	0.92	0.21	34,34,34,34	0
57	MG	RA	3227	1/1	0.92	0.12	64,64,64,64	0
57	MG	YA	3217	1/1	0.92	0.24	38,38,38,38	0
57	MG	RA	3213	1/1	0.92	0.13	44,44,44,44	0
57	MG	YA	3212	1/1	0.92	0.20	67,67,67,67	0
57	MG	RA	3037	1/1	0.92	0.27	26,26,26,26	0
57	MG	RA	3166	1/1	0.92	0.16	53,53,53,53	0
57	MG	YA	3187	1/1	0.92	0.13	19,19,19,19	0
59	ZN	QD	301	1/1	0.92	0.26	53,53,53,53	0
57	MG	YA	3075	1/1	0.92	0.13	23,23,23,23	0
57	MG	QA	1602	1/1	0.93	0.23	24,24,24,24	0
57	MG	YA	3227	1/1	0.93	0.20	26,26,26,26	0
57	MG	QA	1641	1/1	0.93	0.12	22,22,22,22	0
57	MG	YA	3130	1/1	0.93	0.47	52,52,52,52	0
57	MG	RA	3137	1/1	0.93	0.24	36,36,36,36	0
57	MG	YA	3042	1/1	0.93	0.28	11,11,11,11	0
57	MG	RA	3100	1/1	0.93	0.24	43,43,43,43	0
57	MG	RA	3001	1/1	0.93	0.14	2,2,2,2	0
57	MG	QA	1627	1/1	0.93	0.15	92,92,92,92	0
57	MG	RA	3119	1/1	0.93	0.23	28,28,28,28	0
57	MG	XA	1613	1/1	0.93	0.08	14,14,14,14	0
57	MG	YA	3170	1/1	0.93	0.10	26,26,26,26	0
57	MG	RA	3146	1/1	0.93	0.16	37,37,37,37	0
57	MG	XA	1607	1/1	0.93	0.21	25,25,25,25	0
57	MG	RA	3225	1/1	0.93	0.18	51,51,51,51	0
57	MG	QA	1622	1/1	0.93	0.17	33,33,33,33	0
57	MG	YA	3100	1/1	0.93	0.28	7,7,7,7	0
57	MG	QA	1615	1/1	0.93	0.09	66,66,66,66	0
57	MG	YA	3134	1/1	0.93	0.09	37,37,37,37	0
57	MG	YA	3197	1/1	0.93	0.26	16,16,16,16	0
57	MG	YA	3147	1/1	0.93	0.26	28,28,28,28	0
57	MG	RA	3041	1/1	0.93	0.22	20,20,20,20	0
57	MG	RA	3097	1/1	0.93	0.18	7,7,7,7	0
57	MG	YA	3225	1/1	0.93	0.14	21,21,21,21	0
57	MG	YA	3128	1/1	0.93	0.33	34,34,34,34	0
57	MG	RA	3111	1/1	0.93	0.18	20,20,20,20	0
57	MG	XA	1653	1/1	0.93	0.24	62,62,62,62	0
57	MG	YA	3200	1/1	0.93	0.38	39,39,39,39	0
57	MG	XA	1671	1/1	0.93	0.10	43,43,43,43	0
57	MG	YA	3169	1/1	0.93	0.14	30,30,30,30	0
57	MG	RA	3079	1/1	0.93	0.23	32,32,32,32	0
57	MG	XA	1646	1/1	0.93	0.15	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3197	1/1	0.93	0.10	42,42,42,42	0
57	MG	YA	3073	1/1	0.93	0.18	7,7,7,7	0
57	MG	QA	1663	1/1	0.93	0.12	85,85,85,85	0
57	MG	RA	3203	1/1	0.93	0.34	61,61,61,61	0
57	MG	RA	3128	1/1	0.93	0.13	55,55,55,55	0
57	MG	YA	3083	1/1	0.93	0.09	0,0,0,0	0
57	MG	YA	3215	1/1	0.93	0.15	24,24,24,24	0
57	MG	RA	3011	1/1	0.93	0.34	48,48,48,48	0
57	MG	YA	3145	1/1	0.93	0.14	23,23,23,23	0
57	MG	RA	3078	1/1	0.93	0.30	34,34,34,34	0
57	MG	RA	3098	1/1	0.93	0.24	11,11,11,11	0
57	MG	YA	3097	1/1	0.93	0.28	30,30,30,30	0
57	MG	YA	3060	1/1	0.93	0.23	24,24,24,24	0
57	MG	QA	1646	1/1	0.93	0.28	46,46,46,46	0
57	MG	QA	1605	1/1	0.93	0.40	15,15,15,15	0
57	MG	XA	1650	1/1	0.93	0.20	31,31,31,31	0
57	MG	YA	3180	1/1	0.93	0.14	31,31,31,31	0
57	MG	RA	3072	1/1	0.94	0.20	16,16,16,16	0
57	MG	RA	3214	1/1	0.94	0.14	44,44,44,44	0
57	MG	QA	1659	1/1	0.94	0.11	24,24,24,24	0
57	MG	RA	3152	1/1	0.94	0.15	33,33,33,33	0
57	MG	RA	3186	1/1	0.94	0.16	52,52,52,52	0
57	MG	YA	3233	1/1	0.94	0.31	32,32,32,32	0
57	MG	RA	3187	1/1	0.94	0.08	25,25,25,25	0
57	MG	YA	3192	1/1	0.94	0.07	19,19,19,19	0
57	MG	YA	3135	1/1	0.94	0.47	40,40,40,40	0
57	MG	RA	3196	1/1	0.94	0.33	46,46,46,46	0
57	MG	YA	3239	1/1	0.94	0.11	27,27,27,27	0
57	MG	YA	3101	1/1	0.94	0.45	24,24,24,24	0
57	MG	RA	3012	1/1	0.94	0.13	14,14,14,14	0
57	MG	QA	1640	1/1	0.94	0.26	37,37,37,37	0
57	MG	YA	3092	1/1	0.94	0.20	25,25,25,25	0
57	MG	YA	3173	1/1	0.94	0.53	32,32,32,32	0
57	MG	XA	1636	1/1	0.94	0.38	23,23,23,23	0
57	MG	RA	3058	1/1	0.94	0.22	27,27,27,27	0
57	MG	YA	3115	1/1	0.94	0.14	32,32,32,32	0
57	MG	RA	3028	1/1	0.94	0.22	37,37,37,37	0
57	MG	YA	3181	1/1	0.94	0.17	36,36,36,36	0
57	MG	YA	3071	1/1	0.94	0.12	18,18,18,18	0
57	MG	RA	3234	1/1	0.94	0.27	44,44,44,44	0
57	MG	YA	3025	1/1	0.94	0.12	4,4,4,4	0
57	MG	RA	3198	1/1	0.94	0.21	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3033	1/1	0.94	0.33	11,11,11,11	0
57	MG	YA	3076	1/1	0.94	0.12	25,25,25,25	0
57	MG	RA	3158	1/1	0.94	0.17	52,52,52,52	0
57	MG	RA	3150	1/1	0.94	0.17	32,32,32,32	0
57	MG	RA	3070	1/1	0.94	0.16	11,11,11,11	0
57	MG	YE	301	1/1	0.94	0.14	8,8,8,8	0
57	MG	YA	3046	1/1	0.94	0.34	11,11,11,11	0
57	MG	YA	3222	1/1	0.94	0.39	40,40,40,40	0
57	MG	YA	3105	1/1	0.94	0.22	7,7,7,7	0
57	MG	QA	1633	1/1	0.94	0.26	20,20,20,20	0
57	MG	RA	3201	1/1	0.94	0.11	22,22,22,22	0
57	MG	RA	3090	1/1	0.94	0.23	7,7,7,7	0
57	MG	XA	1639	1/1	0.94	0.16	59,59,59,59	0
57	MG	YA	3140	1/1	0.94	0.18	3,3,3,3	0
57	MG	RA	3082	1/1	0.94	0.36	26,26,26,26	0
57	MG	RA	3147	1/1	0.94	0.12	14,14,14,14	0
57	MG	YA	3247	1/1	0.94	0.22	26,26,26,26	0
57	MG	YA	3142	1/1	0.94	0.26	14,14,14,14	0
57	MG	YA	3003	1/1	0.94	0.17	9,9,9,9	0
57	MG	QA	1610	1/1	0.94	0.28	22,22,22,22	0
57	MG	YA	3267	1/1	0.94	0.20	40,40,40,40	0
57	MG	QA	1631	1/1	0.94	0.11	41,41,41,41	0
57	MG	YA	3035	1/1	0.94	0.34	12,12,12,12	0
57	MG	RA	3019	1/1	0.94	0.30	21,21,21,21	0
57	MG	QA	1665	1/1	0.94	0.23	29,29,29,29	0
57	MG	YA	3079	1/1	0.94	0.28	18,18,18,18	0
57	MG	YA	3160	1/1	0.94	0.14	14,14,14,14	0
57	MG	QA	1613	1/1	0.94	0.14	22,22,22,22	0
57	MG	XA	1632	1/1	0.94	0.31	27,27,27,27	0
57	MG	YA	3001	1/1	0.94	0.37	7,7,7,7	0
57	MG	XA	1623	1/1	0.94	0.07	27,27,27,27	0
57	MG	YA	3204	1/1	0.94	0.09	32,32,32,32	0
57	MG	YA	3047	1/1	0.95	0.24	13,13,13,13	0
57	MG	RA	3023	1/1	0.95	0.33	8,8,8,8	0
57	MG	YA	3039	1/1	0.95	0.12	14,14,14,14	0
57	MG	RA	3032	1/1	0.95	0.23	44,44,44,44	0
57	MG	YA	3045	1/1	0.95	0.30	2,2,2,2	0
57	MG	YA	3009	1/1	0.95	0.44	16,16,16,16	0
57	MG	QA	1616	1/1	0.95	0.14	18,18,18,18	0
57	MG	YA	3198	1/1	0.95	0.15	21,21,21,21	0
57	MG	RA	3155	1/1	0.95	0.21	41,41,41,41	0
57	MG	RA	3192	1/1	0.95	0.12	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3034	1/1	0.95	0.30	23,23,23,23	0
57	MG	RA	3136	1/1	0.95	0.21	26,26,26,26	0
57	MG	YA	3148	1/1	0.95	0.36	39,39,39,39	0
57	MG	YA	3125	1/1	0.95	0.16	65,65,65,65	0
57	MG	RA	3016	1/1	0.95	0.28	4,4,4,4	0
57	MG	YA	3196	1/1	0.95	0.07	11,11,11,11	0
57	MG	RA	3109	1/1	0.95	0.16	21,21,21,21	0
57	MG	YA	3049	1/1	0.95	0.17	12,12,12,12	0
57	MG	RA	3240	1/1	0.95	0.27	23,23,23,23	0
57	MG	YA	3034	1/1	0.95	0.29	7,7,7,7	0
57	MG	RA	3092	1/1	0.95	0.19	35,35,35,35	0
57	MG	RA	3096	1/1	0.95	0.35	22,22,22,22	0
57	MG	RA	3054	1/1	0.95	0.09	14,14,14,14	0
57	MG	YA	3052	1/1	0.95	0.18	1,1,1,1	0
57	MG	RA	3035	1/1	0.95	0.34	27,27,27,27	0
57	MG	YA	3093	1/1	0.95	0.19	18,18,18,18	0
59	ZN	QN	101	1/1	0.95	0.10	87,87,87,87	0
57	MG	RA	3064	1/1	0.95	0.34	3,3,3,3	0
57	MG	YA	3161	1/1	0.95	0.19	29,29,29,29	0
57	MG	YA	3056	1/1	0.95	0.17	7,7,7,7	0
57	MG	YA	3109	1/1	0.95	0.29	11,11,11,11	0
57	MG	XA	1626	1/1	0.95	0.17	27,27,27,27	0
57	MG	YA	3183	1/1	0.95	0.10	21,21,21,21	0
57	MG	RA	3013	1/1	0.95	0.38	26,26,26,26	0
57	MG	YA	3194	1/1	0.95	0.11	34,34,34,34	0
57	MG	RA	3231	1/1	0.95	0.33	14,14,14,14	0
57	MG	RA	3169	1/1	0.95	0.18	44,44,44,44	0
57	MG	XA	1609	1/1	0.95	0.16	28,28,28,28	0
57	MG	YA	3006	1/1	0.95	0.19	1,1,1,1	0
57	MG	RA	3024	1/1	0.95	0.17	17,17,17,17	0
57	MG	R5	101	1/1	0.95	0.26	51,51,51,51	0
57	MG	XA	1667	1/1	0.95	0.10	55,55,55,55	0
57	MG	YA	3064	1/1	0.95	0.16	19,19,19,19	0
57	MG	RA	3132	1/1	0.95	0.30	14,14,14,14	0
57	MG	YA	3188	1/1	0.95	0.12	18,18,18,18	0
57	MG	YA	3165	1/1	0.95	0.13	21,21,21,21	0
57	MG	YA	3237	1/1	0.95	0.18	9,9,9,9	0
57	MG	YA	3055	1/1	0.95	0.18	37,37,37,37	0
57	MG	YA	3144	1/1	0.95	0.15	13,13,13,13	0
57	MG	QA	1635	1/1	0.95	0.15	49,49,49,49	0
57	MG	RA	3173	1/1	0.95	0.11	90,90,90,90	0
57	MG	QA	1660	1/1	0.95	0.45	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1660	1/1	0.95	0.25	54,54,54,54	0
57	MG	YB	204	1/1	0.95	0.15	45,45,45,45	0
57	MG	RA	3153	1/1	0.95	0.12	21,21,21,21	0
57	MG	YA	3068	1/1	0.95	0.17	26,26,26,26	0
57	MG	RA	3112	1/1	0.95	0.26	14,14,14,14	0
57	MG	XA	1669	1/1	0.95	0.22	17,17,17,17	0
57	MG	YA	3062	1/1	0.95	0.11	18,18,18,18	0
57	MG	YA	3070	1/1	0.95	0.21	5,5,5,5	0
57	MG	YA	3208	1/1	0.95	0.12	30,30,30,30	0
57	MG	YA	3178	1/1	0.95	0.14	10,10,10,10	0
59	ZN	Y9	101	1/1	0.95	0.10	87,87,87,87	0
57	MG	YA	3171	1/1	0.95	0.20	22,22,22,22	0
57	MG	RA	3087	1/1	0.95	0.12	27,27,27,27	0
57	MG	QA	1639	1/1	0.95	0.18	45,45,45,45	0
57	MG	YA	3136	1/1	0.96	0.09	29,29,29,29	0
57	MG	YA	3018	1/1	0.96	0.21	6,6,6,6	0
57	MG	RA	3022	1/1	0.96	0.43	23,23,23,23	0
57	MG	QA	1651	1/1	0.96	0.30	31,31,31,31	0
57	MG	XA	1603	1/1	0.96	0.20	24,24,24,24	0
57	MG	QA	1642	1/1	0.96	0.13	25,25,25,25	0
57	MG	QA	1606	1/1	0.96	0.15	44,44,44,44	0
57	MG	RA	3176	1/1	0.96	0.16	27,27,27,27	0
57	MG	YA	3089	1/1	0.96	0.18	5,5,5,5	0
57	MG	QA	1607	1/1	0.96	0.10	21,21,21,21	0
57	MG	YA	3244	1/1	0.96	0.27	34,34,34,34	0
57	MG	QA	1645	1/1	0.96	0.08	37,37,37,37	0
57	MG	YA	3057	1/1	0.96	0.12	1,1,1,1	0
57	MG	RA	3050	1/1	0.96	0.28	13,13,13,13	0
57	MG	RA	3208	1/1	0.96	0.18	69,69,69,69	0
57	MG	RA	3125	1/1	0.96	0.19	29,29,29,29	0
57	MG	RA	3045	1/1	0.96	0.27	23,23,23,23	0
57	MG	YA	3041	1/1	0.96	0.28	2,2,2,2	0
57	MG	QA	1653	1/1	0.96	0.12	82,82,82,82	0
57	MG	RA	3110	1/1	0.96	0.09	12,12,12,12	0
57	MG	YA	3104	1/1	0.96	0.08	22,22,22,22	0
57	MG	XA	1655	1/1	0.96	0.30	47,47,47,47	0
57	MG	QA	1611	1/1	0.96	0.13	20,20,20,20	0
57	MG	QA	1614	1/1	0.96	0.28	31,31,31,31	0
57	MG	YA	3131	1/1	0.96	0.17	15,15,15,15	0
57	MG	XA	1612	1/1	0.96	0.20	18,18,18,18	0
57	MG	YA	3065	1/1	0.96	0.25	25,25,25,25	0
57	MG	YA	3211	1/1	0.96	0.17	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3005	1/1	0.96	0.31	11,11,11,11	0
57	MG	RA	3046	1/1	0.96	0.14	19,19,19,19	0
57	MG	XA	1624	1/1	0.96	0.45	39,39,39,39	0
57	MG	XA	1605	1/1	0.96	0.17	7,7,7,7	0
57	MG	RA	3113	1/1	0.96	0.14	22,22,22,22	0
57	MG	RA	3219	1/1	0.96	0.18	36,36,36,36	0
57	MG	RA	3237	1/1	0.96	0.15	13,13,13,13	0
57	MG	RA	3081	1/1	0.96	0.24	27,27,27,27	0
57	MG	YA	3112	1/1	0.96	0.25	23,23,23,23	0
57	MG	YA	3214	1/1	0.96	0.15	28,28,28,28	0
57	MG	YA	3080	1/1	0.96	0.14	11,11,11,11	0
57	MG	Y5	101	1/1	0.96	0.22	18,18,18,18	0
57	MG	YA	3031	1/1	0.96	0.39	26,26,26,26	0
57	MG	YA	3023	1/1	0.96	0.27	14,14,14,14	0
57	MG	YA	3123	1/1	0.96	0.14	28,28,28,28	0
57	MG	YA	3203	1/1	0.96	0.14	18,18,18,18	0
57	MG	YA	3189	1/1	0.96	0.08	33,33,33,33	0
57	MG	YA	3059	1/1	0.96	0.24	15,15,15,15	0
57	MG	RA	3164	1/1	0.96	0.09	27,27,27,27	0
57	MG	YA	3182	1/1	0.96	0.50	55,55,55,55	0
57	MG	RA	3077	1/1	0.96	0.27	24,24,24,24	0
57	MG	RA	3190	1/1	0.96	0.15	33,33,33,33	0
57	MG	XA	1625	1/1	0.96	0.17	14,14,14,14	0
57	MG	QA	1623	1/1	0.96	0.24	29,29,29,29	0
57	MG	QA	1634	1/1	0.96	0.12	39,39,39,39	0
57	MG	RA	3129	1/1	0.96	0.16	38,38,38,38	0
57	MG	XA	1631	1/1	0.96	0.14	39,39,39,39	0
57	MG	YA	3159	1/1	0.96	0.14	19,19,19,19	0
57	MG	RA	3063	1/1	0.96	0.45	12,12,12,12	0
57	MG	YB	203	1/1	0.96	0.21	43,43,43,43	0
57	MG	XA	1617	1/1	0.96	0.15	10,10,10,10	0
57	MG	RA	3053	1/1	0.97	0.17	13,13,13,13	0
57	MG	YA	3137	1/1	0.97	0.08	21,21,21,21	0
57	MG	RA	3030	1/1	0.97	0.17	5,5,5,5	0
57	MG	YA	3061	1/1	0.97	0.19	16,16,16,16	0
57	MG	YA	3126	1/1	0.97	0.13	17,17,17,17	0
57	MG	RA	3086	1/1	0.97	0.20	2,2,2,2	0
57	MG	YA	3029	1/1	0.97	0.14	5,5,5,5	0
57	MG	YA	3240	1/1	0.97	0.13	31,31,31,31	0
57	MG	YA	3087	1/1	0.97	0.32	6,6,6,6	0
57	MG	QA	1630	1/1	0.97	0.14	26,26,26,26	0
57	MG	RA	3232	1/1	0.97	0.34	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3040	1/1	0.97	0.16	9,9,9,9	0
57	MG	YA	3090	1/1	0.97	0.28	12,12,12,12	0
57	MG	YA	3028	1/1	0.97	0.10	3,3,3,3	0
57	MG	YA	3261	1/1	0.97	0.29	18,18,18,18	0
57	MG	YA	3048	1/1	0.97	0.33	6,6,6,6	0
57	MG	RA	3088	1/1	0.97	0.26	25,25,25,25	0
57	MG	YA	3120	1/1	0.97	0.17	18,18,18,18	0
57	MG	YA	3102	1/1	0.97	0.44	11,11,11,11	0
57	MG	RA	3060	1/1	0.97	0.19	3,3,3,3	0
57	MG	YA	3205	1/1	0.97	0.12	37,37,37,37	0
57	MG	YA	3078	1/1	0.97	0.17	8,8,8,8	0
57	MG	RA	3144	1/1	0.97	0.20	11,11,11,11	0
57	MG	YA	3066	1/1	0.97	0.08	20,20,20,20	0
57	MG	QA	1648	1/1	0.97	0.12	47,47,47,47	0
57	MG	XA	1604	1/1	0.97	0.44	20,20,20,20	0
57	MG	RA	3006	1/1	0.97	0.19	7,7,7,7	0
57	MG	YA	3024	1/1	0.97	0.23	1,1,1,1	0
57	MG	RA	3069	1/1	0.97	0.06	28,28,28,28	0
57	MG	YA	3033	1/1	0.97	0.23	10,10,10,10	0
57	MG	RA	3066	1/1	0.97	0.24	11,11,11,11	0
57	MG	YA	3098	1/1	0.97	0.15	19,19,19,19	0
57	MG	RA	3108	1/1	0.97	0.28	32,32,32,32	0
57	MG	YA	3014	1/1	0.97	0.24	3,3,3,3	0
57	MG	RA	3117	1/1	0.97	0.11	10,10,10,10	0
57	MG	RA	3175	1/1	0.97	0.10	40,40,40,40	0
57	MG	QA	1609	1/1	0.97	0.12	14,14,14,14	0
57	MG	RA	3027	1/1	0.97	0.26	3,3,3,3	0
57	MG	YA	3216	1/1	0.97	0.10	18,18,18,18	0
57	MG	RA	3202	1/1	0.97	0.10	31,31,31,31	0
57	MG	XA	1637	1/1	0.97	0.26	39,39,39,39	0
57	MG	RA	3154	1/1	0.97	0.10	28,28,28,28	0
57	MG	XA	1630	1/1	0.97	0.14	18,18,18,18	0
57	MG	RA	3025	1/1	0.97	0.25	22,22,22,22	0
57	MG	YA	3095	1/1	0.97	0.33	5,5,5,5	0
57	MG	YA	3094	1/1	0.97	0.11	5,5,5,5	0
57	MG	YA	3099	1/1	0.97	0.17	2,2,2,2	0
57	MG	RA	3051	1/1	0.97	0.14	18,18,18,18	0
57	MG	RA	3036	1/1	0.97	0.27	4,4,4,4	0
57	MG	RR	201	1/1	0.97	0.16	7,7,7,7	0
57	MG	RA	3029	1/1	0.97	0.22	6,6,6,6	0
57	MG	YA	3268	1/1	0.97	0.30	21,21,21,21	0
57	MG	YA	3077	1/1	0.97	0.28	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3048	1/1	0.97	0.38	18,18,18,18	0
57	MG	YA	3113	1/1	0.97	0.07	19,19,19,19	0
57	MG	RA	3107	1/1	0.97	0.12	27,27,27,27	0
57	MG	YA	3256	1/1	0.97	0.13	11,11,11,11	0
57	MG	YA	3199	1/1	0.97	0.14	30,30,30,30	0
57	MG	Y0	101	1/1	0.97	0.22	20,20,20,20	0
57	MG	YA	3096	1/1	0.97	0.37	7,7,7,7	0
57	MG	XA	1635	1/1	0.97	0.27	26,26,26,26	0
57	MG	RA	3074	1/1	0.97	0.12	7,7,7,7	0
57	MG	YA	3114	1/1	0.97	0.27	9,9,9,9	0
57	MG	QA	1604	1/1	0.97	0.23	10,10,10,10	0
57	MG	RA	3124	1/1	0.97	0.10	28,28,28,28	0
57	MG	XA	1643	1/1	0.97	0.18	25,25,25,25	0
57	MG	RA	3114	1/1	0.97	0.14	35,35,35,35	0
57	MG	YA	3088	1/1	0.97	0.29	17,17,17,17	0
57	MG	RA	3093	1/1	0.97	0.25	10,10,10,10	0
57	MG	YA	3026	1/1	0.97	0.29	0,0,0,0	0
57	MG	XA	1647	1/1	0.97	0.10	25,25,25,25	0
57	MG	RA	3073	1/1	0.97	0.21	23,23,23,23	0
57	MG	RB	201	1/1	0.97	0.10	54,54,54,54	0
57	MG	QA	1652	1/1	0.97	0.12	31,31,31,31	0
57	MG	YA	3044	1/1	0.97	0.31	4,4,4,4	0
57	MG	RA	3215	1/1	0.97	0.19	20,20,20,20	0
57	MG	YA	3103	1/1	0.97	0.31	26,26,26,26	0
57	MG	QV	101	1/1	0.97	0.14	24,24,24,24	0
57	MG	RA	3061	1/1	0.97	0.23	32,32,32,32	0
57	MG	YA	3022	1/1	0.97	0.22	11,11,11,11	0
57	MG	XA	1633	1/1	0.97	0.23	30,30,30,30	0
57	MG	RE	301	1/1	0.97	0.21	30,30,30,30	0
57	MG	RA	3043	1/1	0.97	0.11	14,14,14,14	0
57	MG	YA	3156	1/1	0.97	0.13	20,20,20,20	0
57	MG	RA	3102	1/1	0.97	0.20	5,5,5,5	0
57	MG	RA	3047	1/1	0.97	0.33	13,13,13,13	0
57	MG	YA	3259	1/1	0.97	0.30	14,14,14,14	0
57	MG	YA	3258	1/1	0.98	0.38	9,9,9,9	0
57	MG	QA	1621	1/1	0.98	0.15	35,35,35,35	0
57	MG	XA	1601	1/1	0.98	0.26	7,7,7,7	0
57	MG	YA	3111	1/1	0.98	0.06	5,5,5,5	0
57	MG	RA	3042	1/1	0.98	0.31	18,18,18,18	0
57	MG	YA	3138	1/1	0.98	0.12	15,15,15,15	0
57	MG	RA	3038	1/1	0.98	0.18	8,8,8,8	0
57	MG	XA	1645	1/1	0.98	0.28	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1616	1/1	0.98	0.31	14,14,14,14	0
57	MG	XA	1622	1/1	0.98	0.08	33,33,33,33	0
57	MG	RA	3149	1/1	0.98	0.22	28,28,28,28	0
57	MG	RA	3004	1/1	0.98	0.26	2,2,2,2	0
57	MG	YA	3207	1/1	0.98	0.30	52,52,52,52	0
57	MG	YA	3019	1/1	0.98	0.25	0,0,0,0	0
57	MG	RA	3020	1/1	0.98	0.17	7,7,7,7	0
57	MG	XA	1674	1/1	0.98	0.13	35,35,35,35	0
57	MG	YA	3013	1/1	0.98	0.35	2,2,2,2	0
57	MG	RA	3003	1/1	0.98	0.39	15,15,15,15	0
57	MG	YA	3067	1/1	0.98	0.31	27,27,27,27	0
57	MG	RA	3065	1/1	0.98	0.19	23,23,23,23	0
57	MG	YA	3255	1/1	0.98	0.37	0,0,0,0	0
57	MG	YA	3036	1/1	0.98	0.24	9,9,9,9	0
57	MG	RA	3021	1/1	0.98	0.37	8,8,8,8	0
57	MG	RA	3007	1/1	0.98	0.26	11,11,11,11	0
57	MG	YA	3017	1/1	0.98	0.21	13,13,13,13	0
57	MG	RA	3018	1/1	0.98	0.15	9,9,9,9	0
57	MG	RA	3089	1/1	0.98	0.26	6,6,6,6	0
57	MG	YA	3264	1/1	0.98	0.20	3,3,3,3	0
57	MG	RA	3230	1/1	0.98	0.17	15,15,15,15	0
57	MG	YA	3119	1/1	0.98	0.11	22,22,22,22	0
57	MG	YA	3004	1/1	0.98	0.13	5,5,5,5	0
57	MG	RA	3095	1/1	0.98	0.23	6,6,6,6	0
57	MG	RA	3067	1/1	0.98	0.20	12,12,12,12	0
57	MG	YA	3116	1/1	0.98	0.27	12,12,12,12	0
57	MG	YA	3011	1/1	0.98	0.28	25,25,25,25	0
57	MG	RA	3099	1/1	0.98	0.31	19,19,19,19	0
57	MG	YA	3005	1/1	0.98	0.09	7,7,7,7	0
57	MG	RA	3071	1/1	0.98	0.28	18,18,18,18	0
57	MG	RA	3094	1/1	0.98	0.35	23,23,23,23	0
57	MG	RA	3052	1/1	0.98	0.12	9,9,9,9	0
57	MG	QA	1620	1/1	0.98	0.10	29,29,29,29	0
57	MG	YA	3032	1/1	0.98	0.27	3,3,3,3	0
57	MG	YA	3086	1/1	0.98	0.27	58,58,58,58	0
57	MG	RA	3080	1/1	0.98	0.29	15,15,15,15	0
57	MG	YA	3228	1/1	0.98	0.20	4,4,4,4	0
57	MG	YA	3010	1/1	0.98	0.20	0,0,0,0	0
57	MG	RA	3106	1/1	0.98	0.24	28,28,28,28	0
57	MG	YA	3007	1/1	0.98	0.14	2,2,2,2	0
57	MG	RA	3040	1/1	0.98	0.17	3,3,3,3	0
57	MG	YA	3257	1/1	0.98	0.12	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3056	1/1	0.98	0.37	12,12,12,12	0
57	MG	YA	3190	1/1	0.98	0.12	13,13,13,13	0
57	MG	YA	3043	1/1	0.98	0.30	12,12,12,12	0
57	MG	YA	3121	1/1	0.98	0.16	31,31,31,31	0
57	MG	YA	3015	1/1	0.98	0.43	3,3,3,3	0
57	MG	RA	3105	1/1	0.98	0.13	6,6,6,6	0
57	MG	XA	1602	1/1	0.98	0.16	16,16,16,16	0
57	MG	YA	3231	1/1	0.98	0.17	23,23,23,23	0
57	MG	RA	3123	1/1	0.98	0.20	19,19,19,19	0
57	MG	YA	3263	1/1	0.98	0.10	15,15,15,15	0
57	MG	RA	3140	1/1	0.98	0.16	27,27,27,27	0
57	MG	RA	3017	1/1	0.98	0.19	7,7,7,7	0
57	MG	XA	1644	1/1	0.98	0.12	21,21,21,21	0
57	MG	YA	3063	1/1	0.98	0.21	17,17,17,17	0
57	MG	YA	3027	1/1	0.98	0.21	9,9,9,9	0
57	MG	XA	1640	1/1	0.98	0.10	187,187,187,187	0
57	MG	RA	3181	1/1	0.98	0.15	43,43,43,43	0
57	MG	YA	3260	1/1	0.98	0.29	11,11,11,11	0
57	MG	YA	3030	1/1	0.98	0.49	19,19,19,19	0
57	MG	YA	3008	1/1	0.98	0.23	22,22,22,22	0
57	MG	YA	3050	1/1	0.98	0.27	6,6,6,6	0
57	MG	RA	3085	1/1	0.98	0.16	11,11,11,11	0
57	MG	RA	3015	1/1	0.98	0.16	19,19,19,19	0
57	MG	YA	3020	1/1	0.99	0.46	13,13,13,13	0
57	MG	YA	3037	1/1	0.99	0.11	2,2,2,2	0
57	MG	YA	3002	1/1	0.99	0.29	9,9,9,9	0
57	MG	RA	3031	1/1	0.99	0.24	7,7,7,7	0
57	MG	YA	3053	1/1	0.99	0.17	11,11,11,11	0
57	MG	YA	3021	1/1	0.99	0.30	17,17,17,17	0
57	MG	RA	3083	1/1	0.99	0.26	13,13,13,13	0
57	MG	RA	3076	1/1	0.99	0.12	6,6,6,6	0
57	MG	YA	3084	1/1	0.99	0.38	6,6,6,6	0
57	MG	YA	3081	1/1	0.99	0.23	5,5,5,5	0
57	MG	YA	3058	1/1	0.99	0.34	11,11,11,11	0
57	MG	YA	3074	1/1	0.99	0.32	22,22,22,22	0
57	MG	XA	1610	1/1	0.99	0.20	19,19,19,19	0
57	MG	XA	1615	1/1	0.99	0.27	30,30,30,30	0
57	MG	YA	3091	1/1	0.99	0.32	7,7,7,7	0
57	MG	YA	3051	1/1	0.99	0.20	4,4,4,4	0

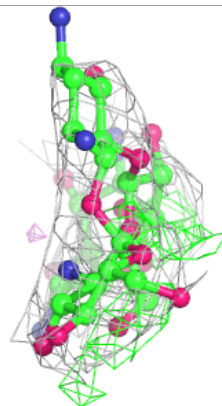
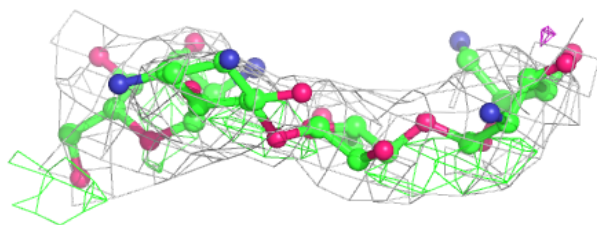
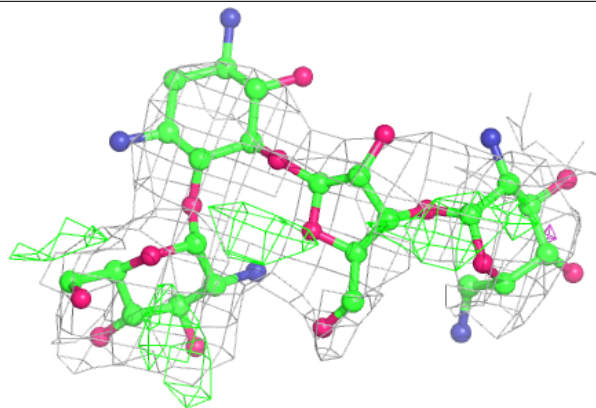
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different



orientation to approximate a three-dimensional view.

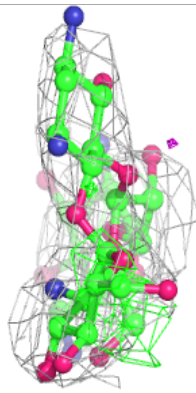
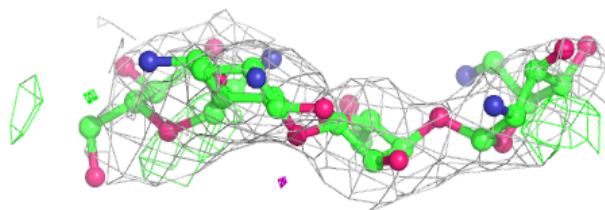
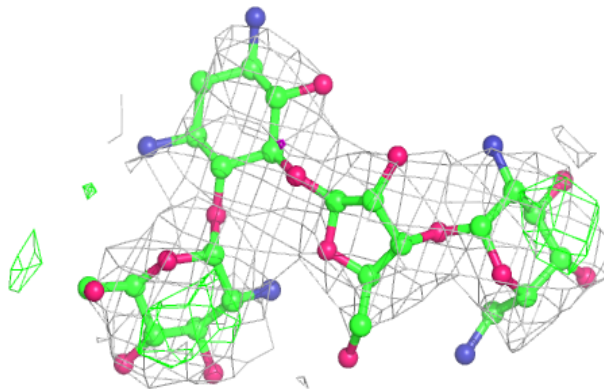
**Electron density around PAR QA 1666:**

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



**Electron density around PAR XA 1675:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.