



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:01 PM GMT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



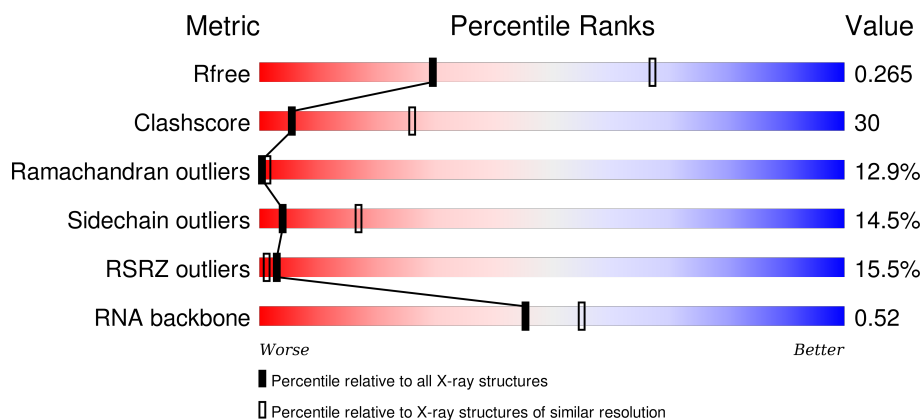
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)
RNA backbone	2183	1016 (3.58-2.70)

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. 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>19%</div> <div> <div></div> <div>50%</div> <div>37%</div> <div>10%</div> <div>..</div> </div> </div>
1	XA	1522	<div> <div>20%</div> <div> <div></div> <div>50%</div> <div>37%</div> <div>11%</div> <div>..</div> </div> </div>
2	QB	256	<div> <div>18%</div> <div> <div></div> <div>17%</div> <div>58%</div> <div>16%</div> <div>7%</div> </div> </div>
2	XB	256	<div> <div>9%</div> <div> <div></div> <div>17%</div> <div>59%</div> <div>16%</div> <div>7%</div> </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	QA	1615	-	-	-	X
57	MG	QA	1631	-	-	-	X
57	MG	QA	1657	-	-	-	X
57	MG	RA	3005	-	-	-	X
57	MG	RA	3029	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3035	-	-	-	X
57	MG	RA	3039	-	-	-	X
57	MG	RA	3053	-	-	-	X
57	MG	RA	3056	-	-	-	X
57	MG	RA	3060	-	-	-	X
57	MG	RA	3063	-	-	-	X
57	MG	RA	3088	-	-	-	X
57	MG	RA	3099	-	-	-	X
57	MG	RA	3125	-	-	-	X
57	MG	RA	3126	-	-	-	X
57	MG	RA	3131	-	-	-	X
57	MG	RA	3192	-	-	-	X
57	MG	RA	3200	-	-	-	X
57	MG	RA	3204	-	-	-	X
57	MG	RA	3220	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3230	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3238	-	-	-	X
57	MG	Y7	101	-	-	-	X
57	MG	YA	3015	-	-	-	X
57	MG	YA	3020	-	-	-	X
57	MG	YA	3023	-	-	-	X
57	MG	YA	3027	-	-	-	X
57	MG	YA	3034	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3099	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3144	-	-	-	X
57	MG	YA	3171	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3219	-	-	-	X
57	MG	YA	3240	-	-	-	X
57	MG	YA	3255	-	-	-	X
57	MG	YA	3258	-	-	-	X
57	MG	YA	3259	-	-	-	X
58	PAR	QA	1670	-	-	-	X
58	PAR	XA	1675	-	-	-	X



## 2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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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 Pro.

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

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

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

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

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

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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 L11.

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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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 L22.

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	69	Total	Mg	0	0
			69	69		
57	RP	1	Total	Mg	0	0
			1	1		
57	YA	265	Total	Mg	0	0
			265	265		
57	QM	1	Total	Mg	0	0
			1	1		
57	XX	1	Total	Mg	0	0
			1	1		

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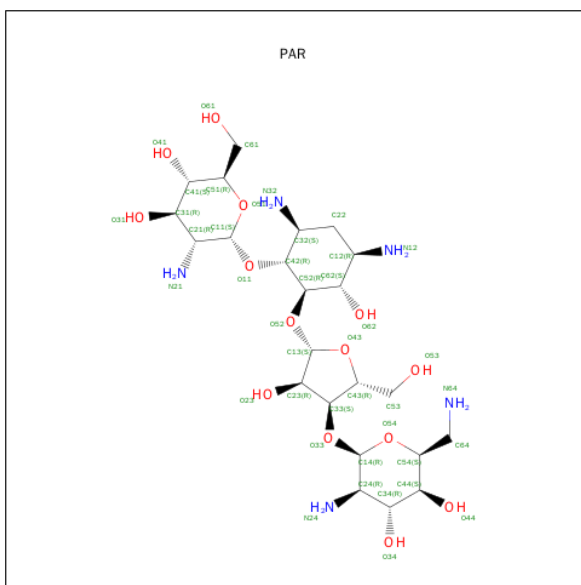


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QV	1	Total 1	Mg 1	0	0
57	XA	74	Total 74	Mg 74	0	0
57	R0	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	RA	240	Total 240	Mg 240	0	0
57	YP	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	YB	3	Total 3	Mg 3	0	0
57	XV	2	Total 2	Mg 2	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	YE	2	Total 2	Mg 2	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 42	C 23	N 5	O 14	0	0
58	XA	1	Total 42	C 23	N 5	O 14	0	0

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

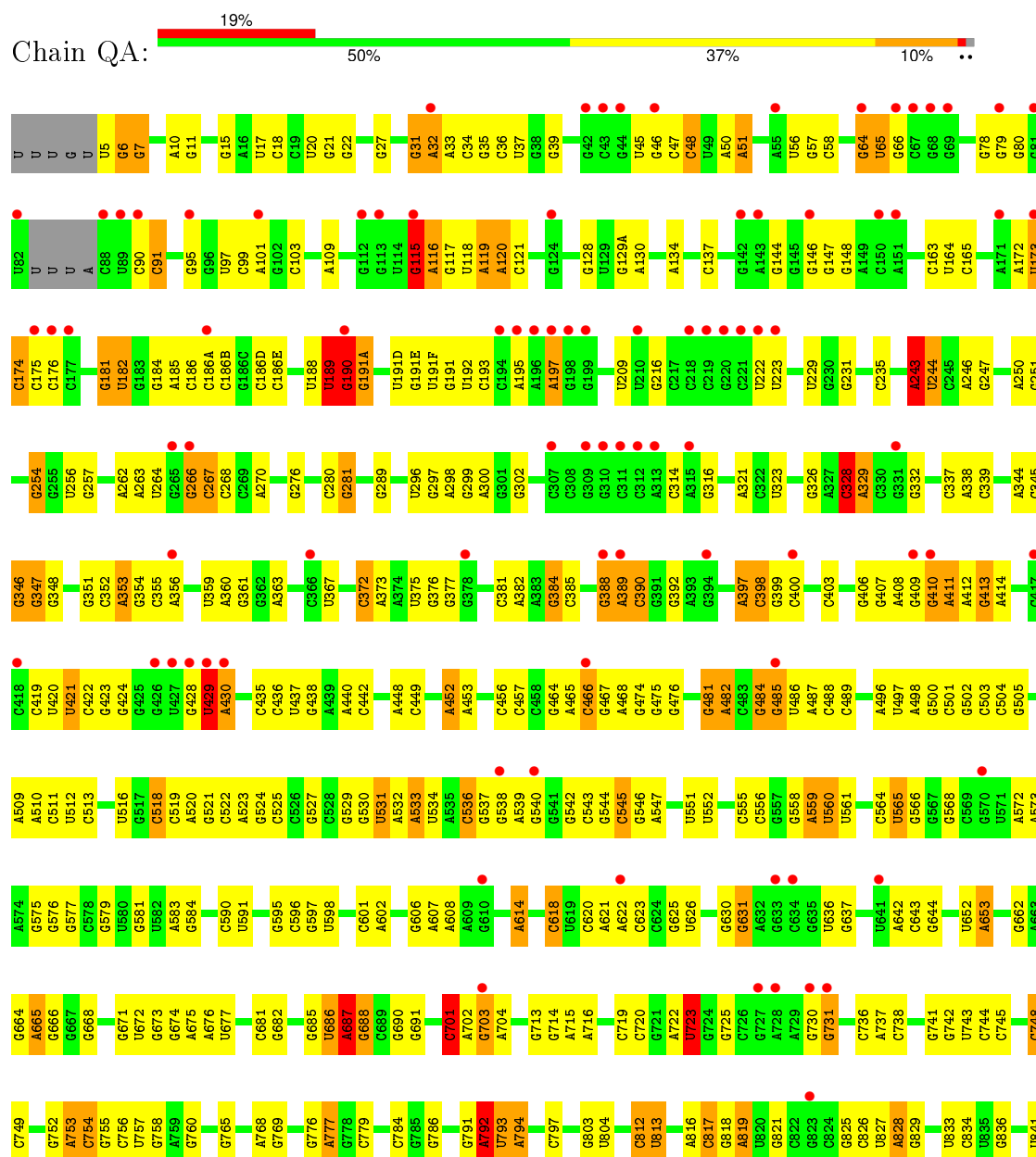
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	XD	1	Total Zn 1 1	0	0
59	QD	1	Total Zn 1 1	0	0
59	QN	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0



### 3 Residue-property plots

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

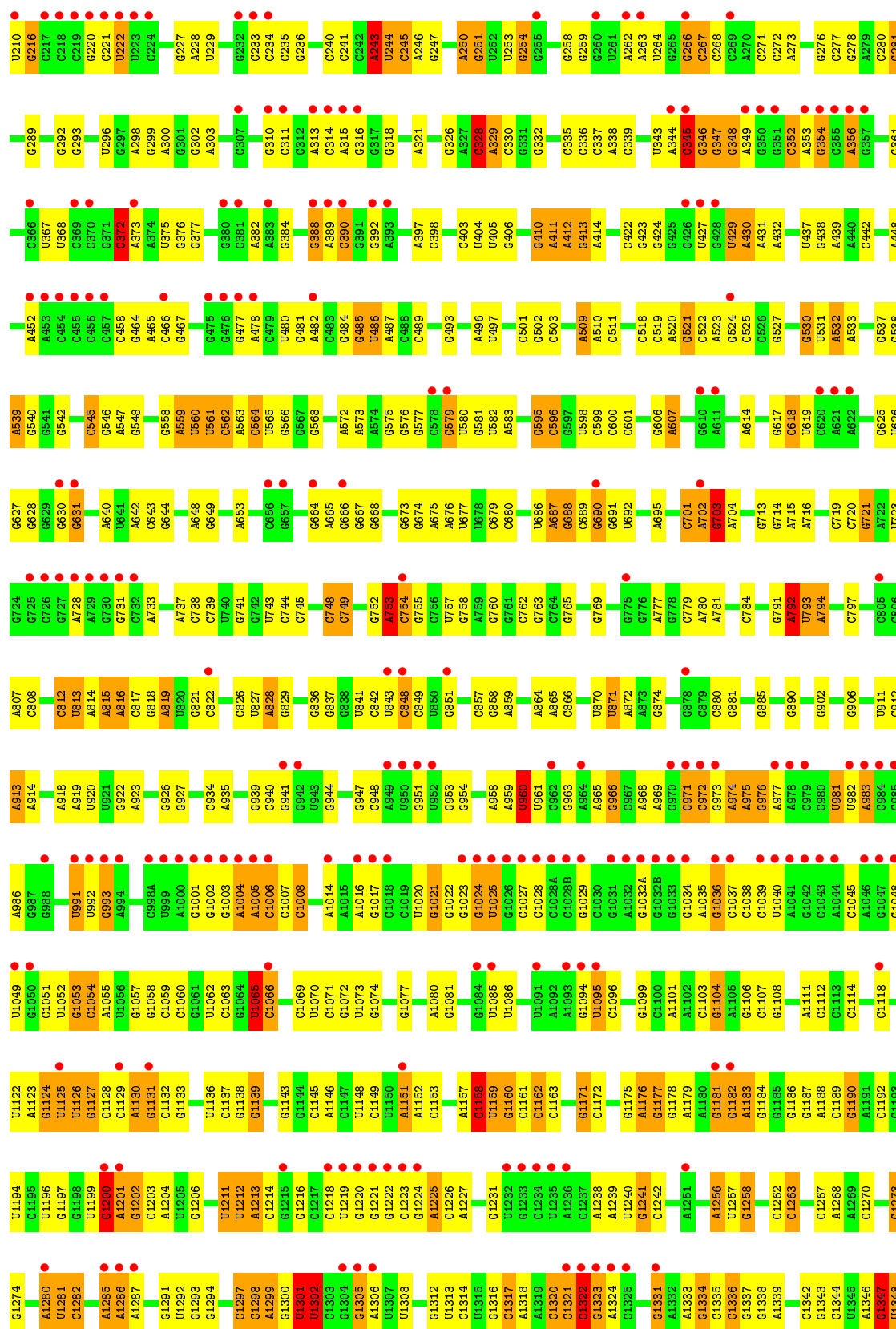
#### • Molecule 1: 16S rRNA



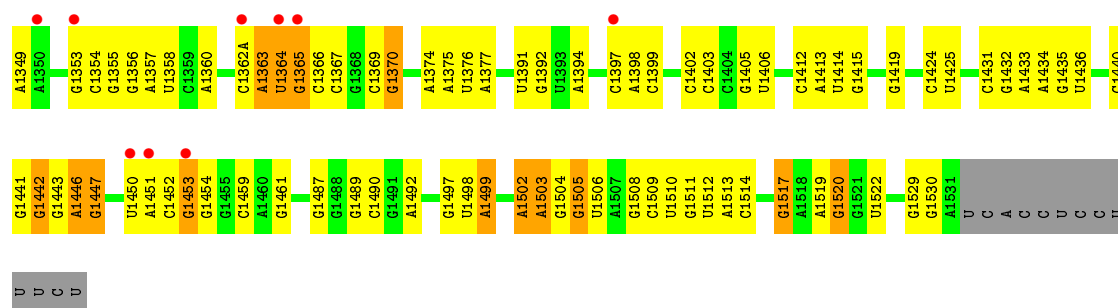




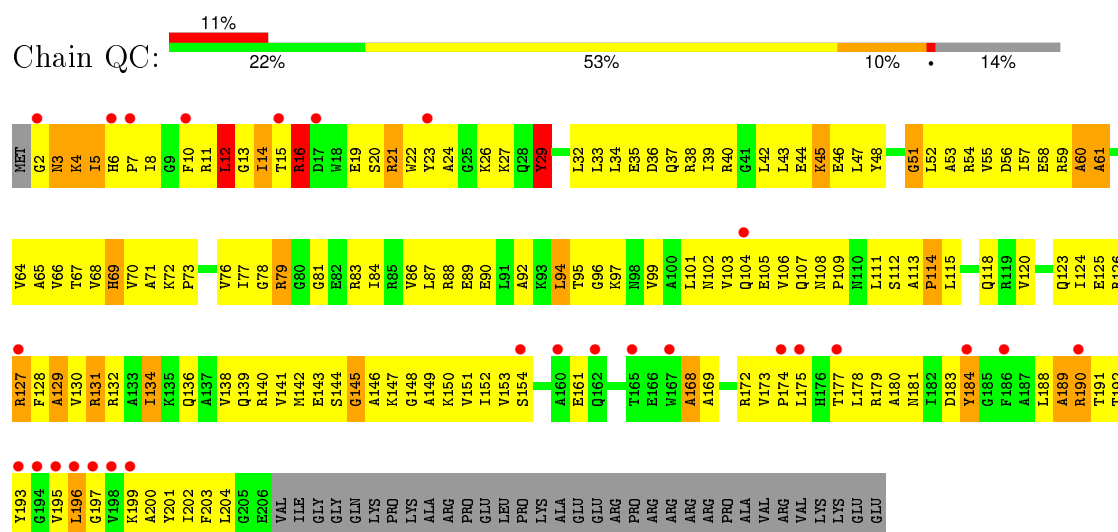




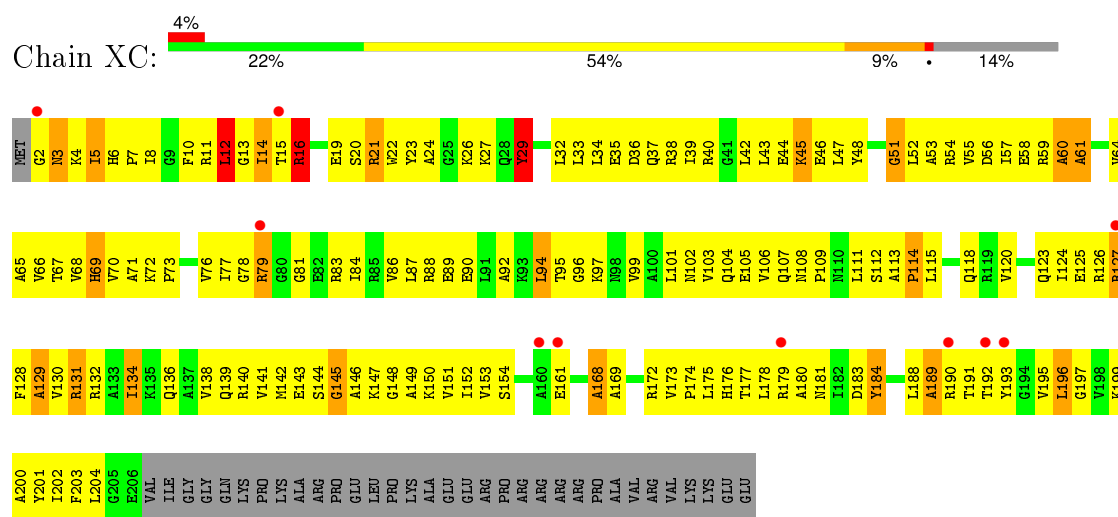




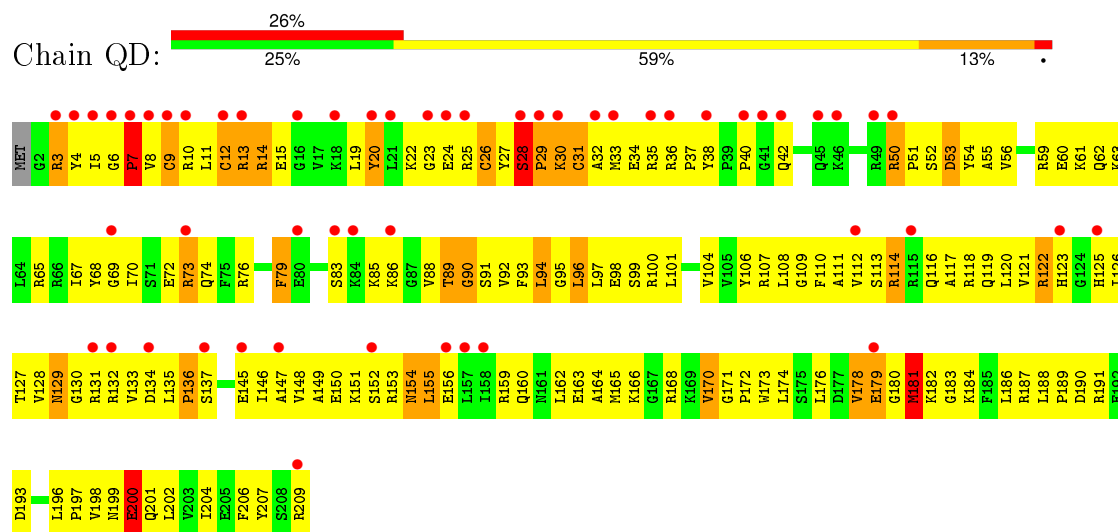




- Molecule 3: 30S ribosomal protein S3

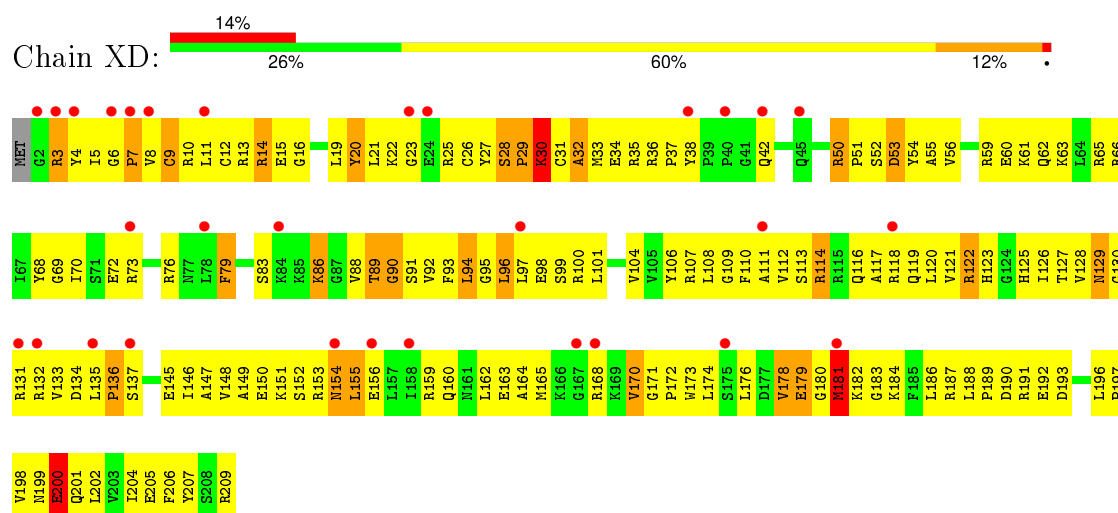


- Molecule 4: 30S ribosomal protein S4

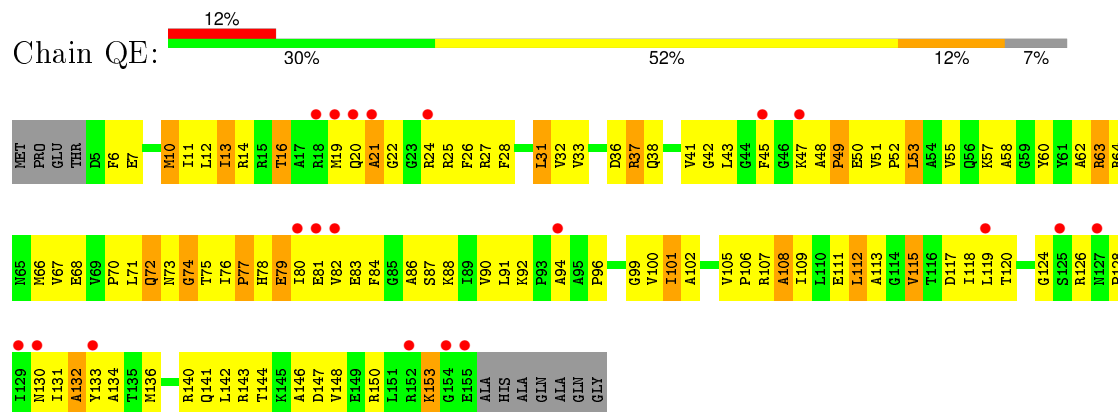


- Molecule 4: 30S ribosomal protein S4

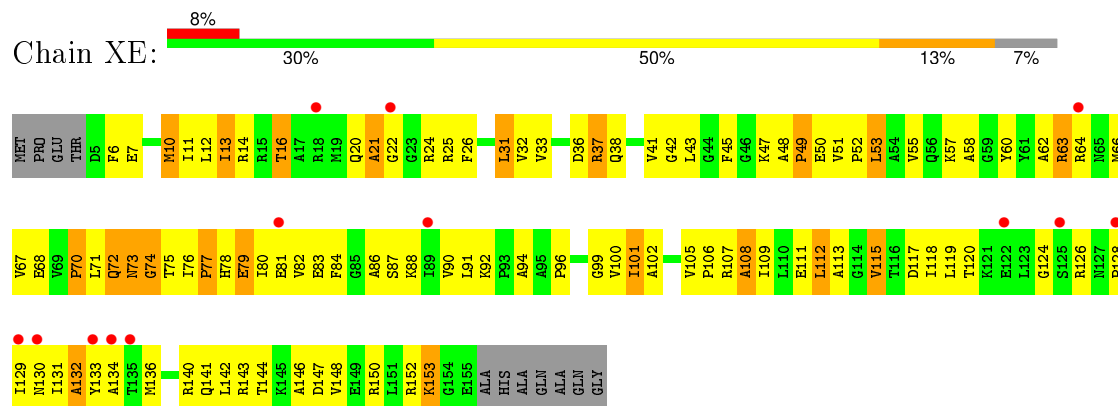




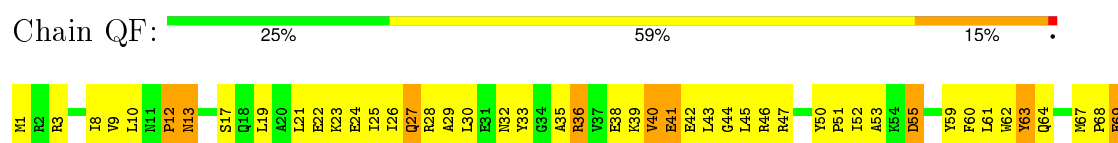
• Molecule 5: 30S ribosomal protein S5



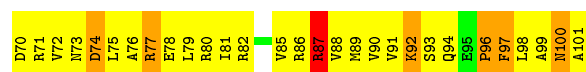
• Molecule 5: 30S ribosomal protein S5



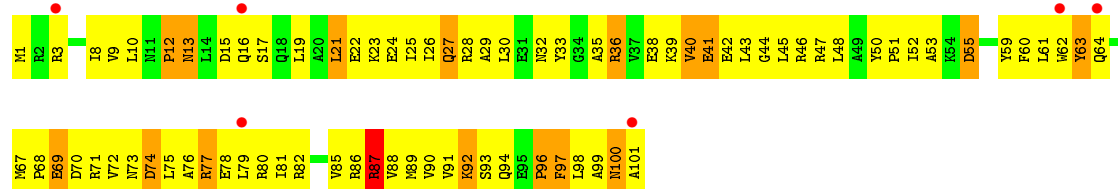
• Molecule 6: 30S ribosomal protein S6



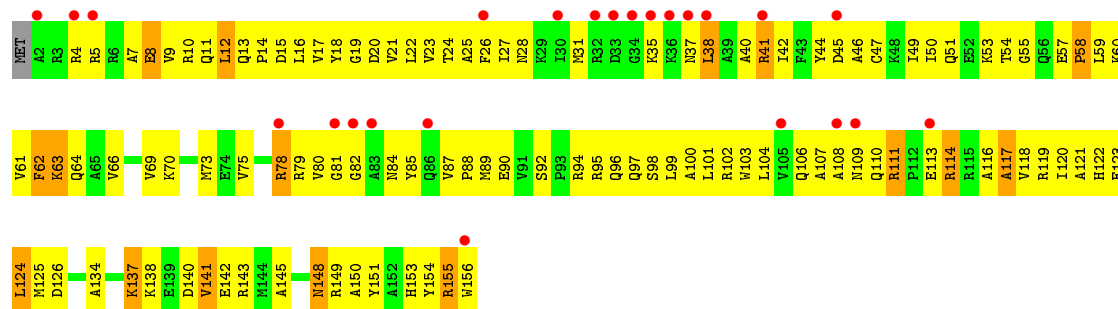




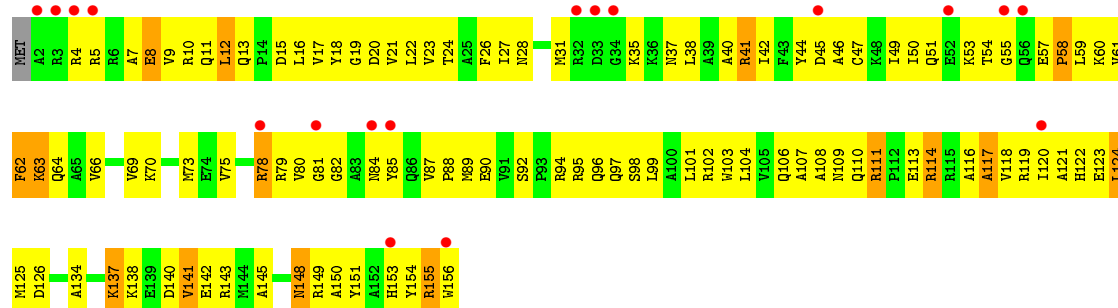
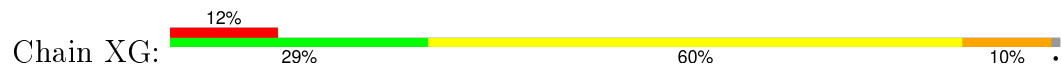
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7



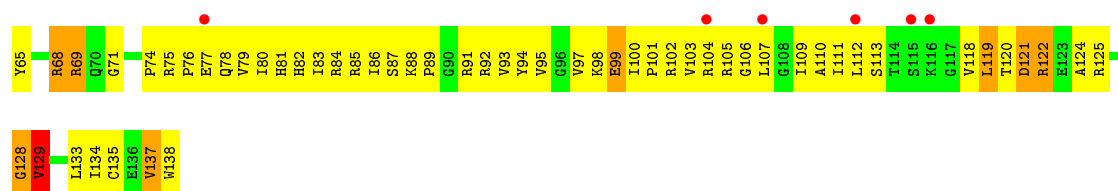
• Molecule 7: 30S ribosomal protein S7



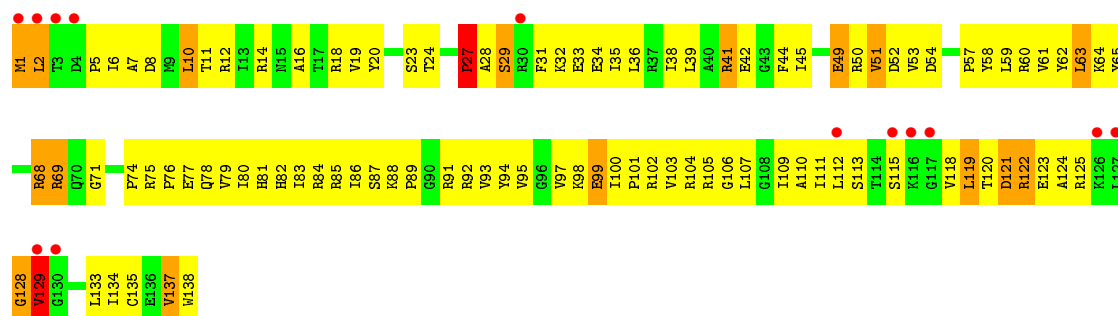
• Molecule 8: 30S ribosomal protein S8



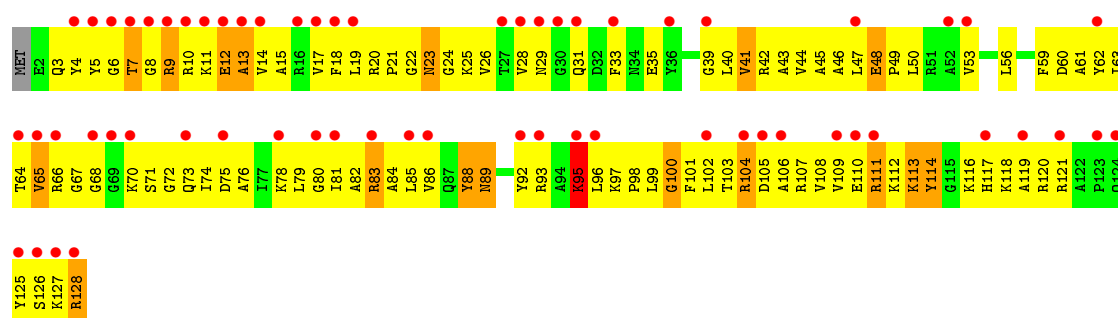




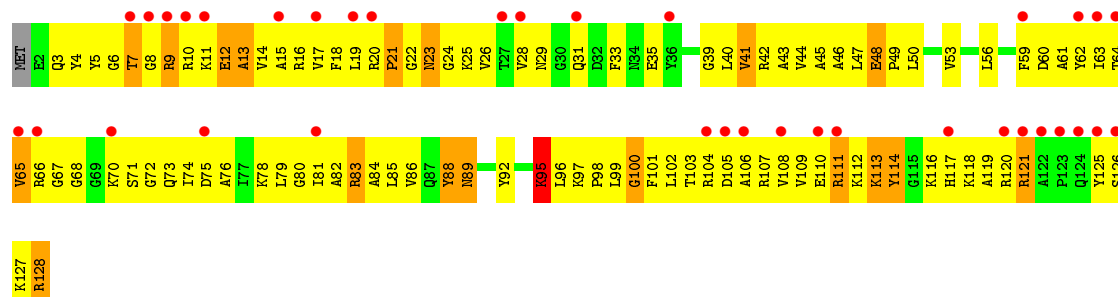
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9



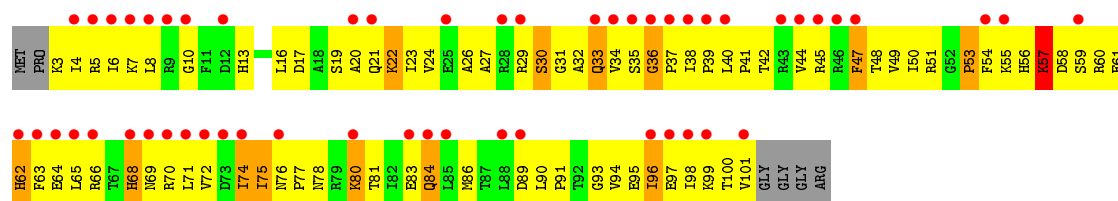
• Molecule 9: 30S ribosomal protein S9



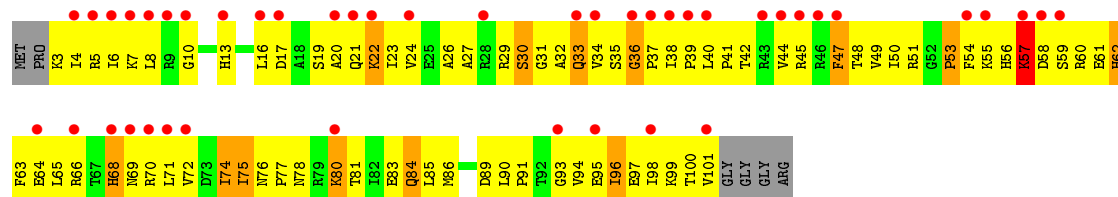
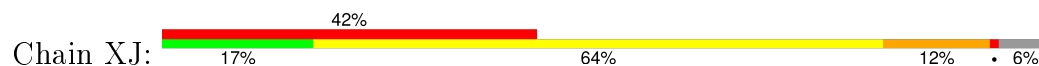
• Molecule 10: 30S ribosomal protein S10



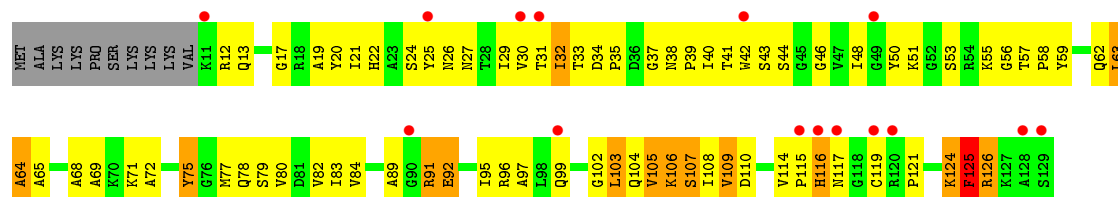




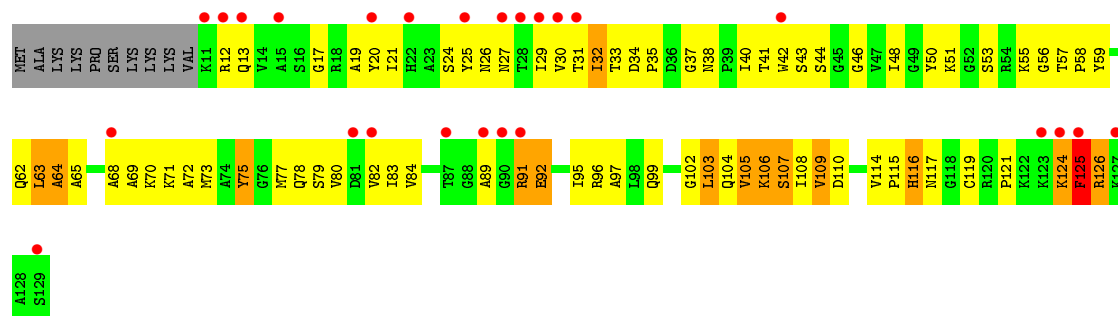
• Molecule 10: 30S ribosomal protein S10



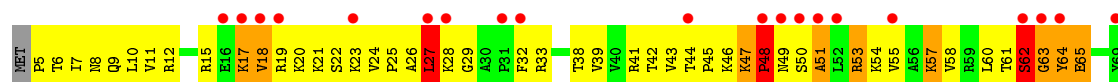
• Molecule 11: 30S ribosomal protein S11



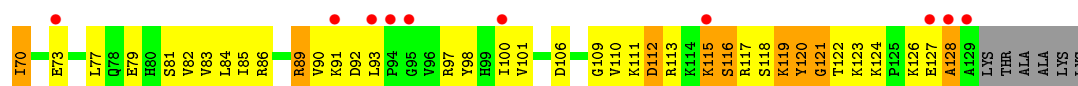
• Molecule 11: 30S ribosomal protein S11



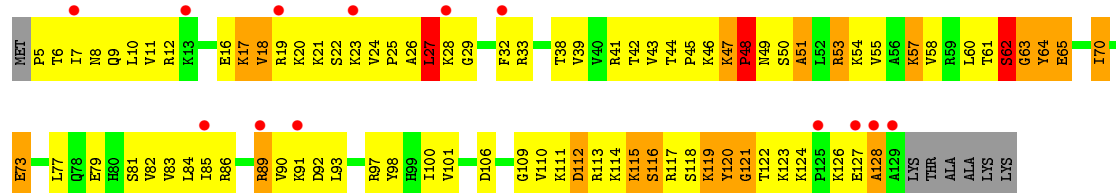
• Molecule 12: 30S ribosomal protein S12



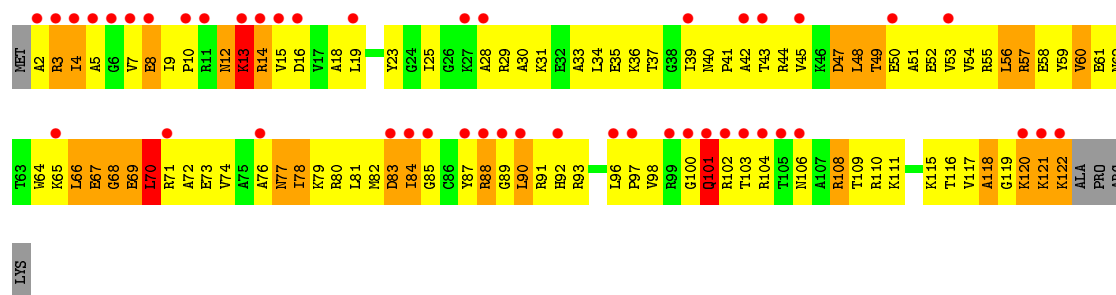




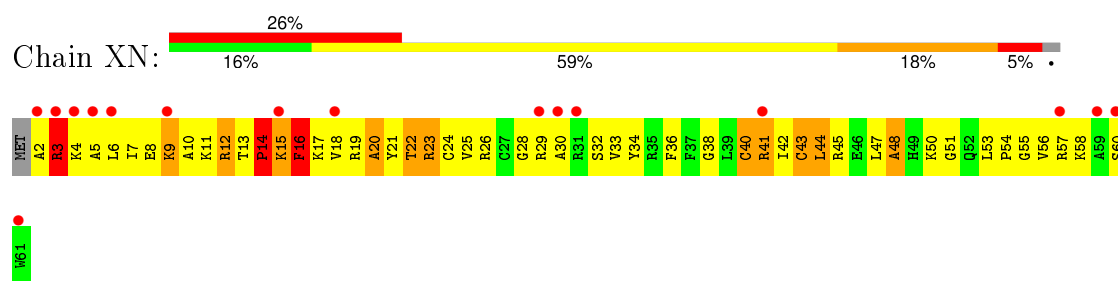
- Molecule 12: 30S ribosomal protein S12



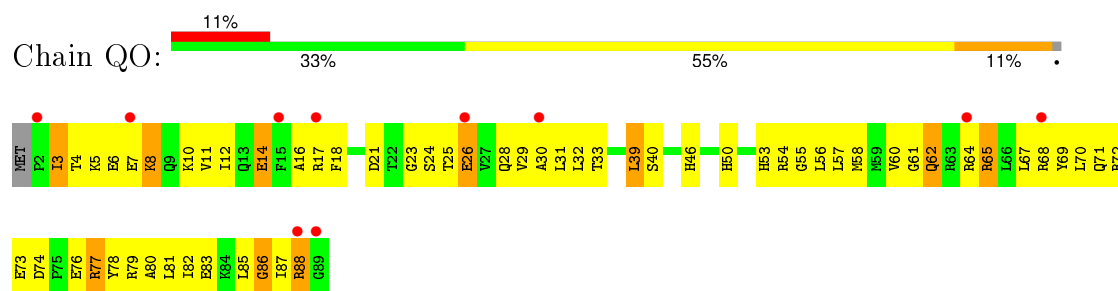
- Molecule 13: 30S ribosomal protein S13



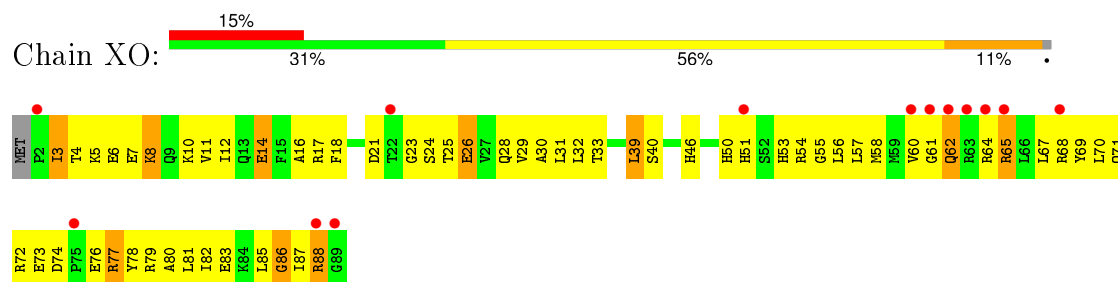




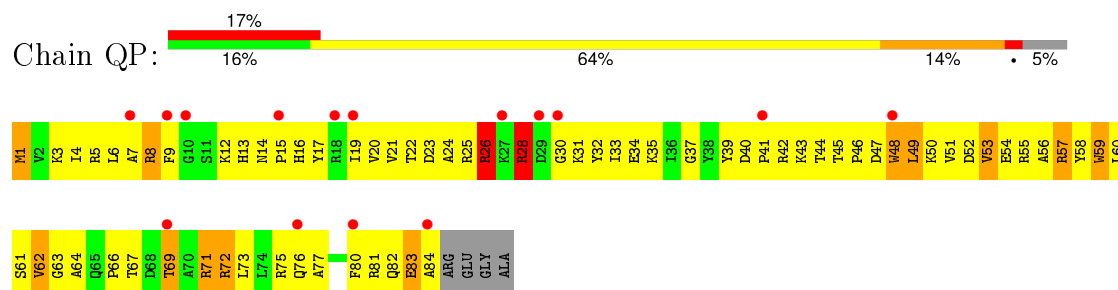
- Molecule 15: 30S ribosomal protein S15



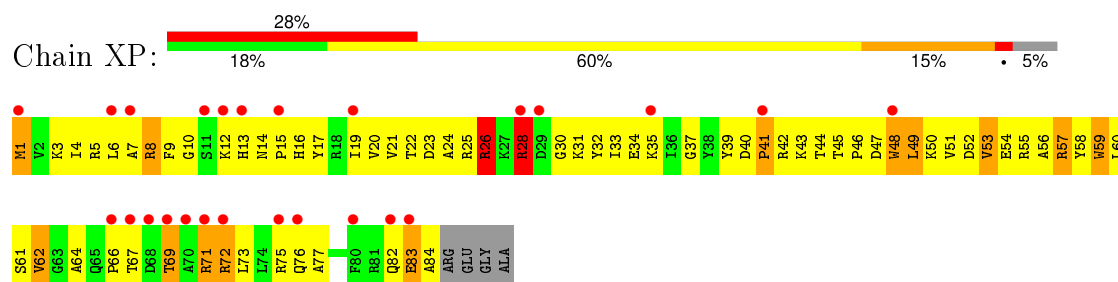
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

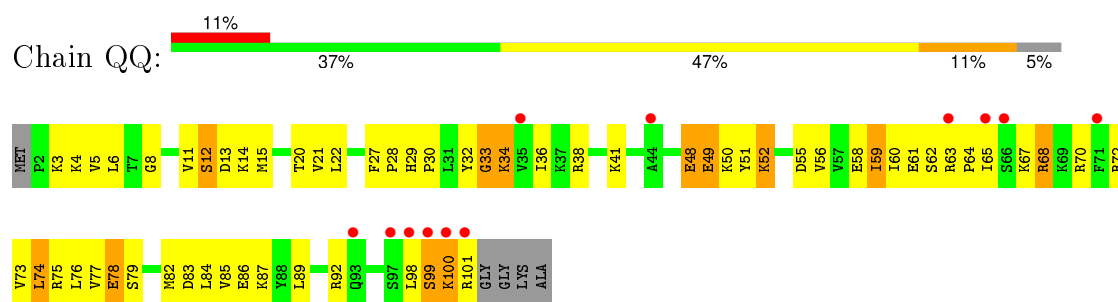


- Molecule 16: 30S ribosomal protein S16

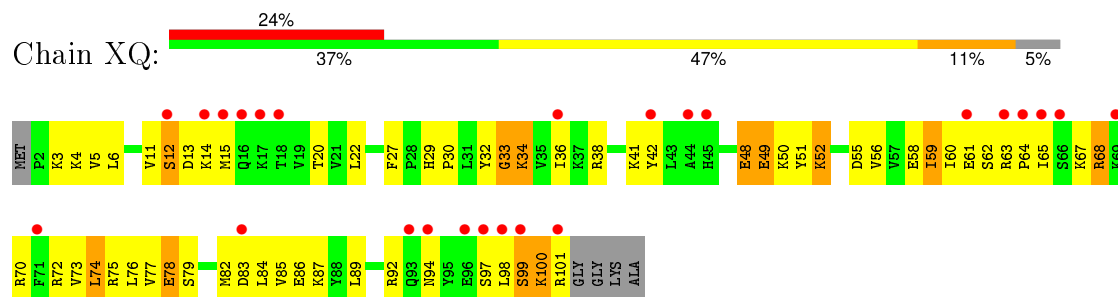


- Molecule 17: 30S ribosomal protein S17

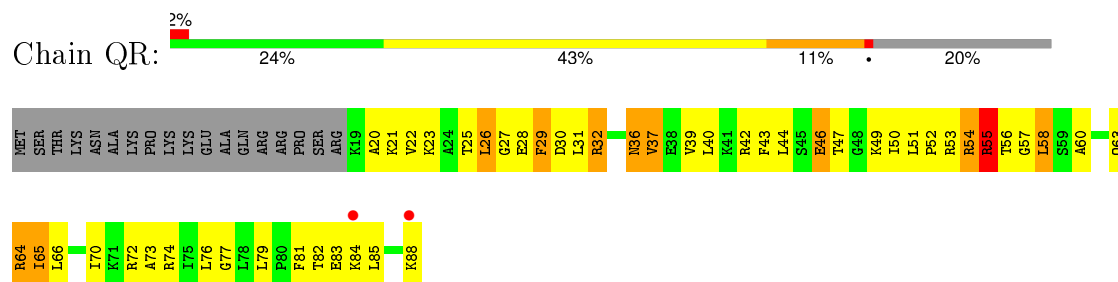




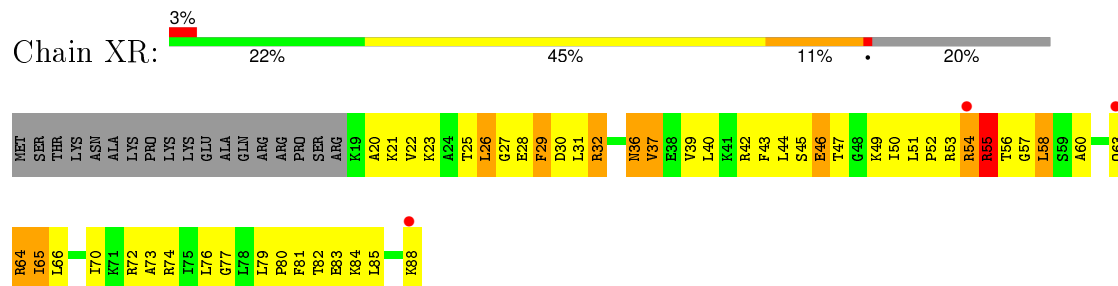
• Molecule 17: 30S ribosomal protein S17



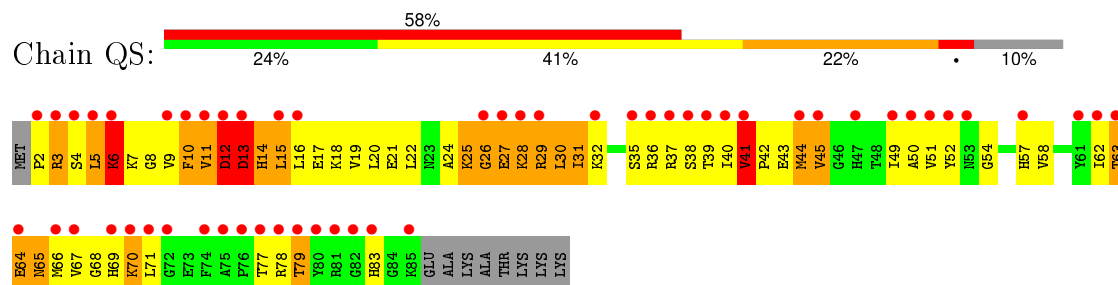
• Molecule 18: 30S ribosomal protein S18



• Molecule 18: 30S ribosomal protein S18

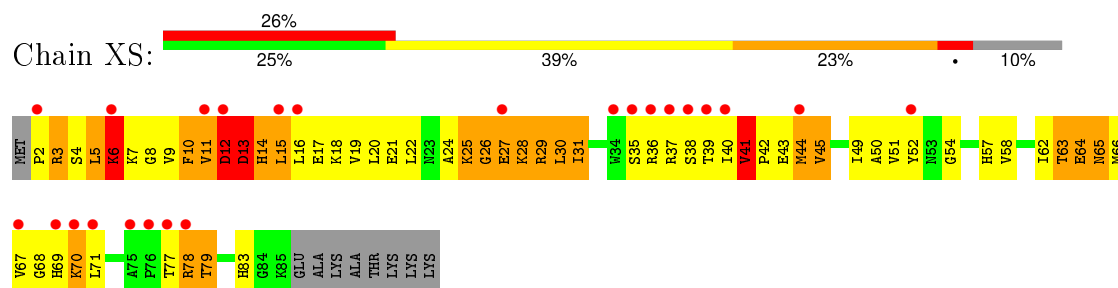


• Molecule 19: 30S ribosomal protein S19

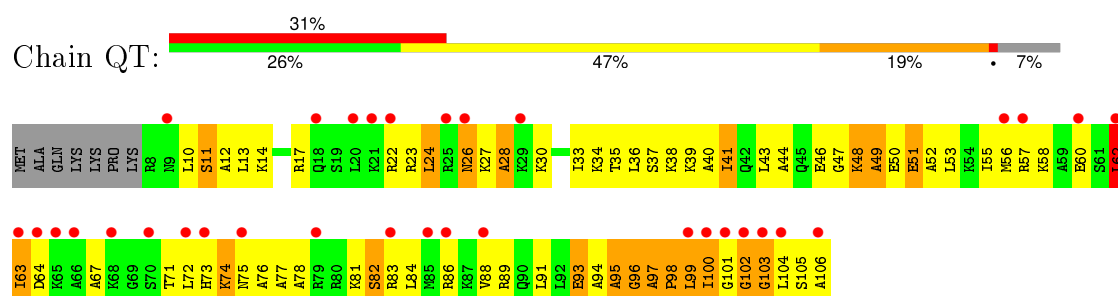




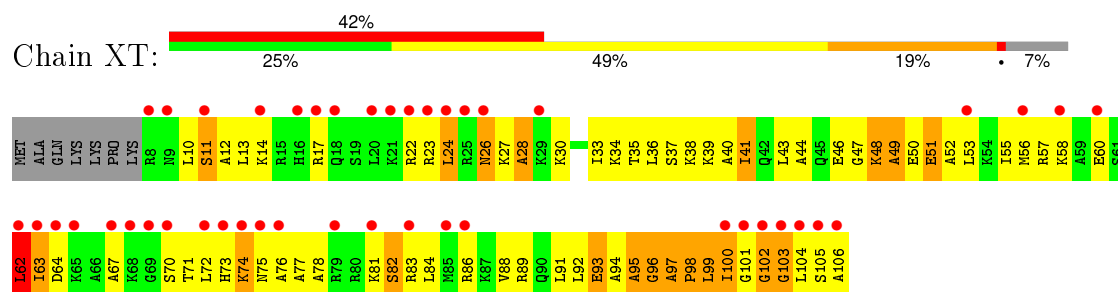
- Molecule 19: 30S ribosomal protein S19



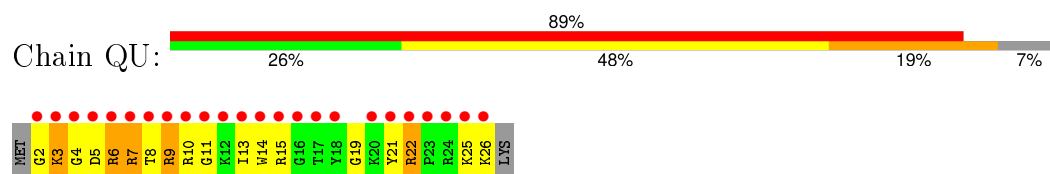
- Molecule 20: 30S ribosomal protein S20



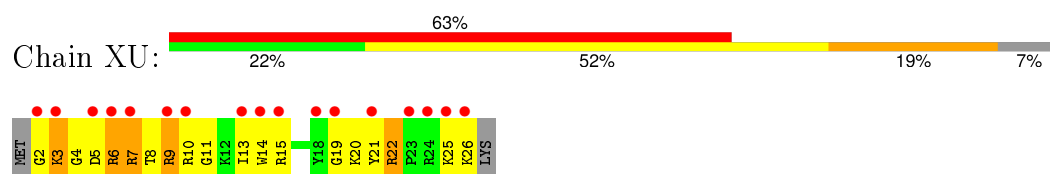
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



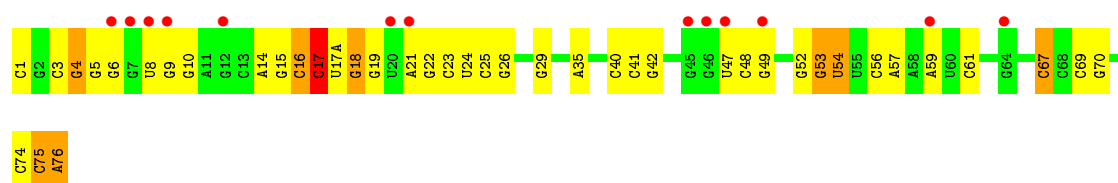
- Molecule 21: 30S ribosomal protein S21



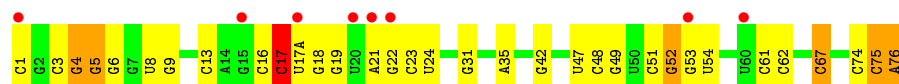
- Molecule 22: P-site tRNA fMet







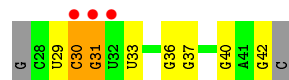
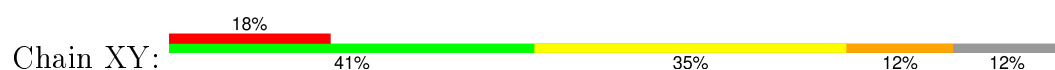
- Molecule 22: P-site tRNA fMet



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



- Molecule 24: A-site ASL Pro



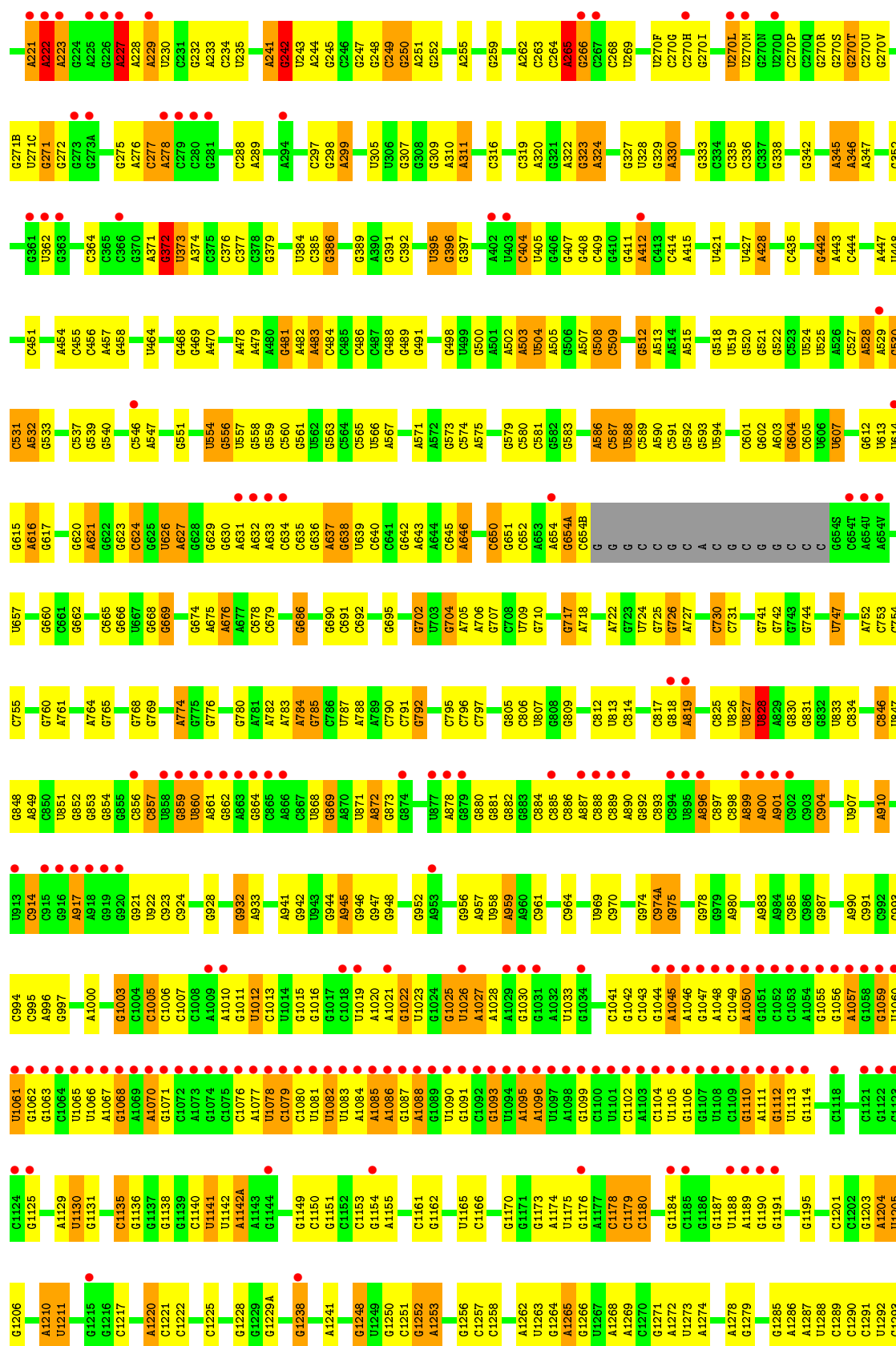
- Molecule 24: A-site ASL Pro



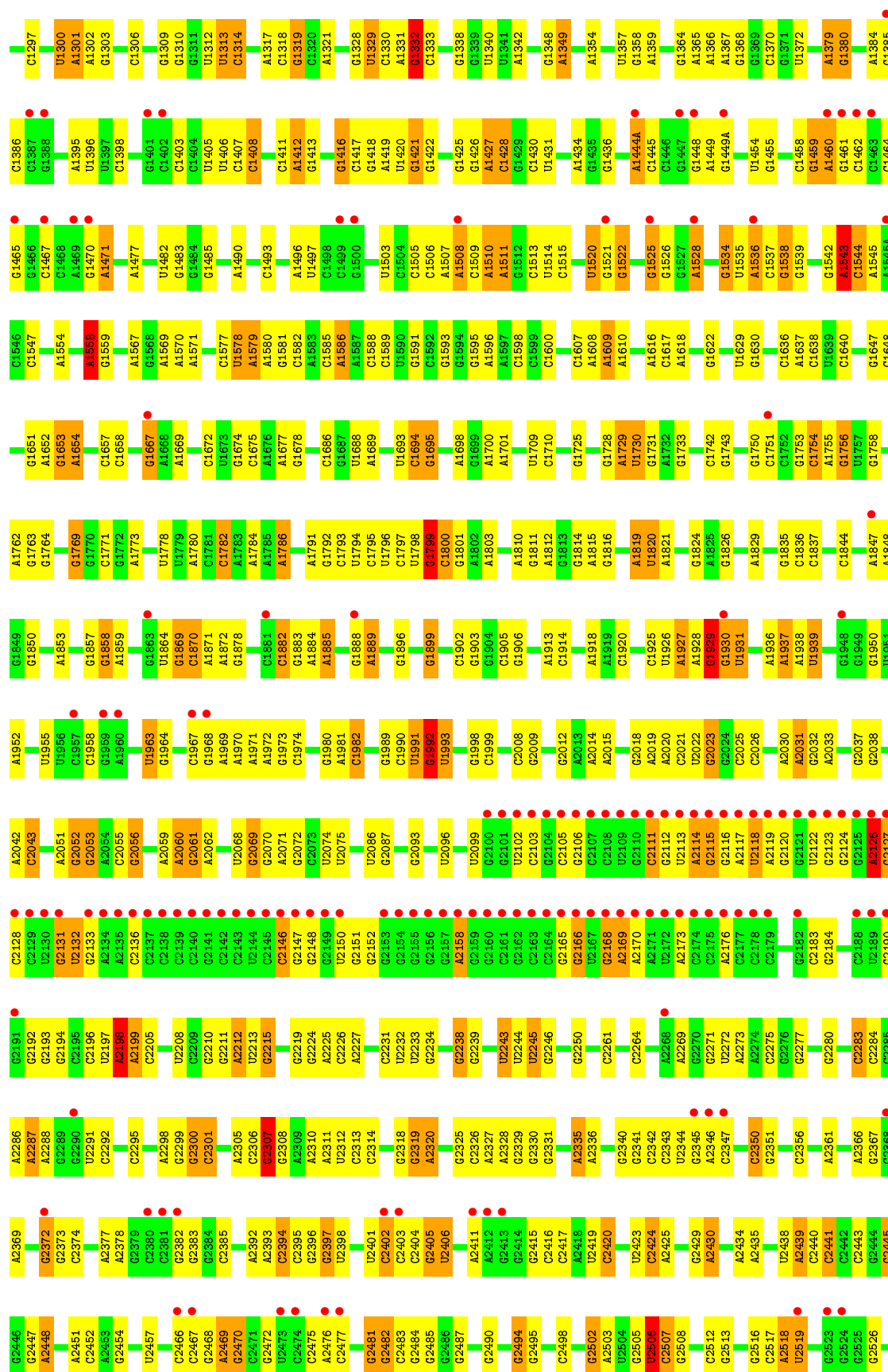
- Molecule 25: 23S rRNA



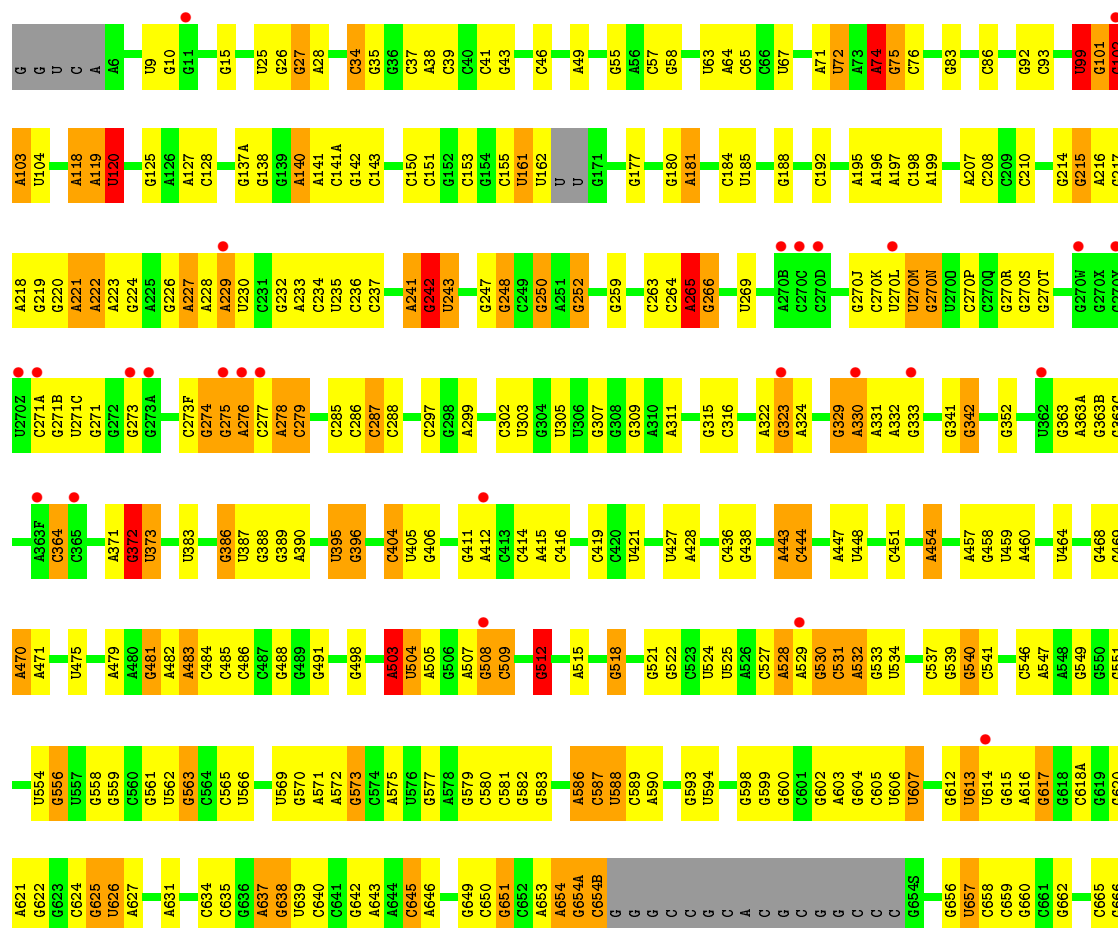








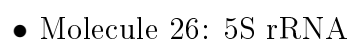




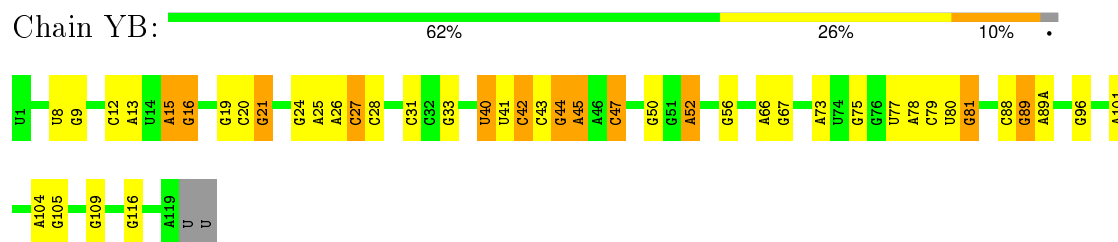


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U1796	C1589	G1705	C1589	U1336	G1240	U1141	A1087	A990	C885	A788	G669
C1797	C1592	U1706	C1592	G1337	A1241	A1142	A1069	C991	C886	A789	G674
U1798	C1592	G1707	C1592	U1338	A1242	A1142A	A1070	C992	C887	C790	A675
G1799	A1597	G1708	A1597	G1339	G1244	C1153	G1071	C993	C888	C791	A675
C1800	C1598	U1709	C1598	U1340	G1244	C1154	C1072	C994	C889	C792	A676
G1801	C1599	C1710	C1599	U1341	G1250	G1155	A1073	C995	C890	C795	G686
A1802	C1600	G1717	C1600	G1342	C1251	A1155	G1074	C996	C891	C796	G702
A1803	A1603	G1718	A1603	A1349	C1252	C1161	G1075	C997	A896	C797	U703
A1809	G1607	G1725	G1607	U1352	A1253	G1162	G1076	G1002	C897	A802	G704
A1812	A1608	G1728	A1608	A1353	G1256	G1163	A1077	G1003	C898	A802	G704
G1813	A1609	U1729	A1609	G1354	C1257	U1164	U1078	G1003	A899	G805	G717
G1814	A1610	U1730	A1610	A1355	G1267	U1165	C1079	C1004	A900	G806	G717
A1815	G1617	A1731	G1617	G1359	U1267	C1166	C1080	C1005	A901	U807	A722
G1816	C1617	A1732	C1617	A1359	A1268	U1175	U1082	C1006	C902	U807	A722
A1819	A1618	G1733	A1618	C1363	G1269	U1176	A1088	G1015	G916	G812	G723
U1820	A1637	G1734	A1637	G1364	G1270	A1177	A1089	G1016	A918	U827	U724
A1821	C1640	G1743	C1640	A1444A	G1271	C1178	U1090	U1019	G919	U828	U725
G1824	G1647	A1749	G1647	G1365	G1272	C1179	G1093	A1020	G920	G831	G726
A1825	C1648	G1750	C1648	A1448	U1273	C1180	U1094	A1021	G921	G842	G742
G1826	G1653	C1751	G1653	G1449	U1273	G1186	A1095	G1022	G928	A841	A746
C1827	A1654	G1752	A1654	A1365	G1279	U1187	U1096	U1023	G932	U846	U747
G1828	G1657	C1753	G1657	A1366	U1281	U1188	A1097	G1024	G932	U847	G748
A1829	U1659	G1754	U1659	G1386	A1287	G1189	C1099	U1025	A941	G848	A751
G1835	A1667	A1755	A1667	C1387	C1291	G1190	U1101	A1026	G942	G849	A752
A1836	C1667	G1756	C1667	G1388	U1292	C1196	C1102	A1028	G943	A859	C753
C1837	A1668	A1756	A1668	G1389	U1292	C1196	A1103	A1029	G944	C850	C754
G1842	A1669	G1762	A1669	U1390	C1293	C1200	C1104	G1030	G946	U851	C755
C1843	G1674	G1763	G1674	U1391	U1300	C1201	U1105	U1033	G952	C856	C756
G1845	C1675	C1771	C1675	U1394	A1301	G1202	G1106	A1045	G952	C857	A761
G1846	A1676	G1772	A1676	A1395	A1302	G1203	U1108	A1046	A953	U858	A761
U1854	G1677	A1773	G1677	U1396	A1308	A1204	C1109	G1047	A957	C859	A764
G1858	G1681	U1778	G1681	U1397	A1309	U1205	G1111	A1048	U958	U860	G769
A1859	U1688	U1779	U1688	C1398	G1309	G1206	G1112	C1049	A959	A861	G770
U1864	A1689	A1780	A1689	G1399	U1313	U1211	U1113	A1050	G961	G862	G770
G1869	U1693	G1781	G1693	G1400	C1314	U1212	G1114	A1054	C961	G864	G771
C1870	C1694	C1782	C1694	G1401	G1314	G1212	U1130	U1060	U979	C865	A774
A1871	G1695	A1783	G1695	C1402	G1319	C1217	G1122	G1055	G974	A866	G775
G1872	G1696	G1784	G1696	C1403	C1320	C1218	G1125	G1056	C974A	U870	G776
A1873	G1697	A1785	G1697	U1405	A1321	G1219	A1126	A1057	G975	A871	G776
C1882	A1698	U1786	A1698	U1406	A1322	U1221	G1130	G1058	G978	A872	G780
A1883	G1699	G1787	G1699	C1407	A1322	C1221	G1131	U1061	A980	A878	A781
G1884	A1700	C1788	A1700	C1408	U1329	C1330	U1130	U1060	U979	A878	A782
U1889	A1701	A1789	A1701	C1411	C1330	C1332	G1131	U1061	A980	G881	A783
G1890	C1585	C1790	C1585	U1415	G1332	G1225	C1135	G1063	A983	A882	A784
A1899	A1586	G1702	A1586	G1500	C1333	G1228	C1136	C1064	A984	G882	G785

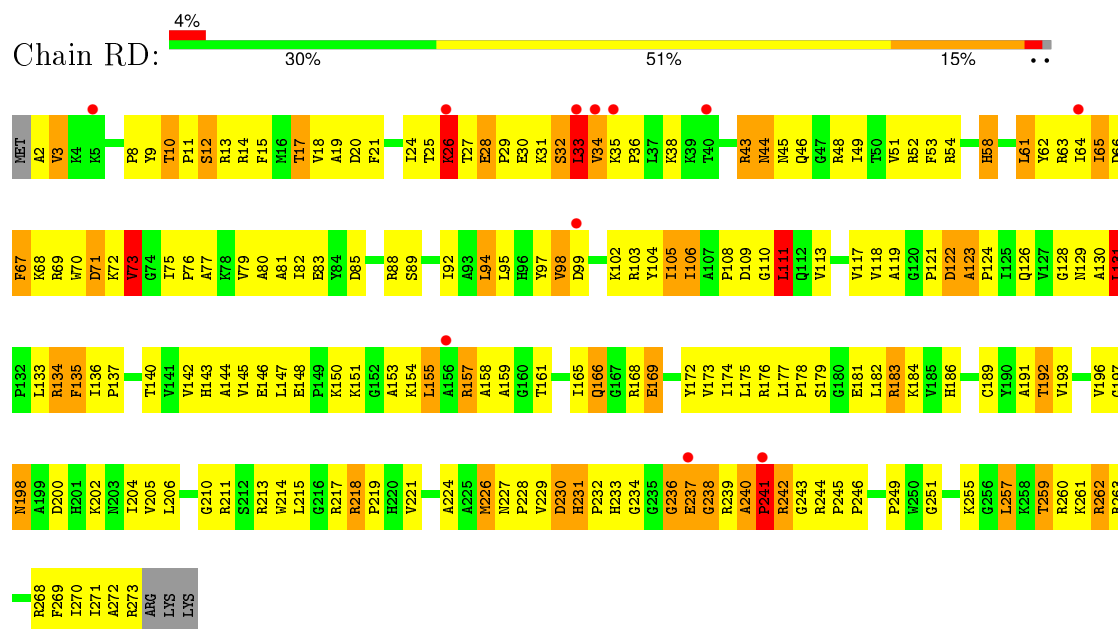




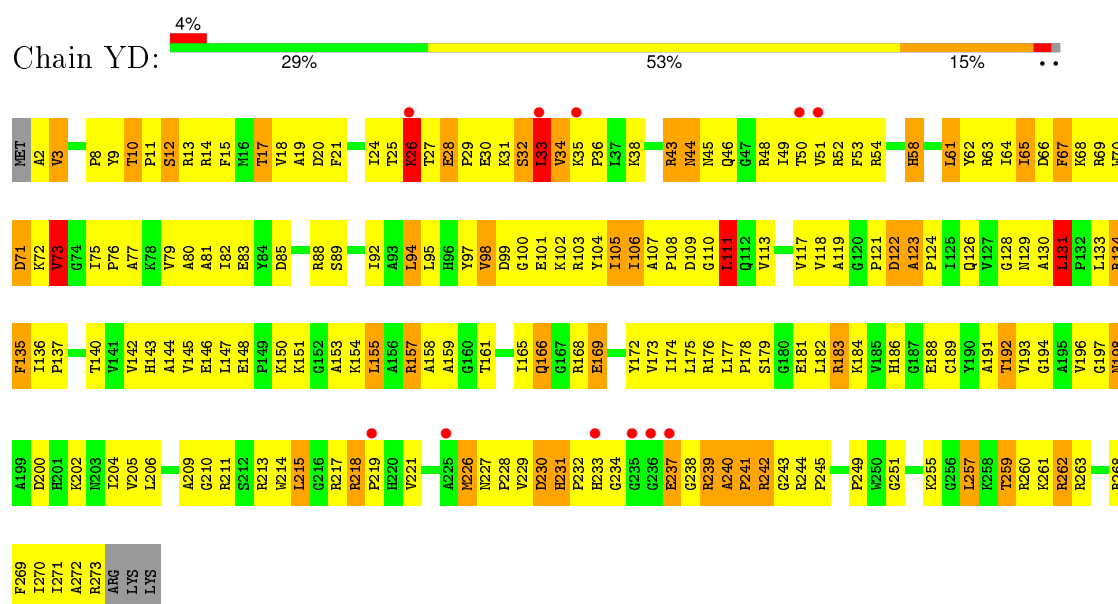




- Molecule 27: 50S ribosomal protein L2



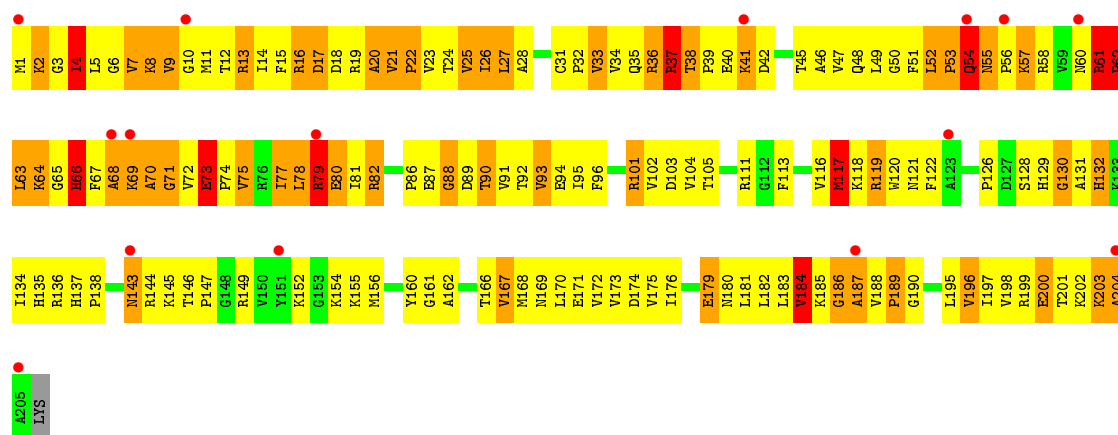
- Molecule 27: 50S ribosomal protein L2



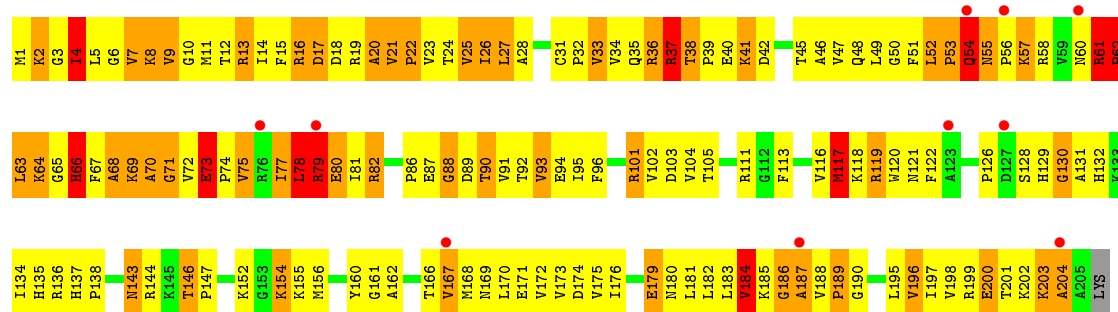
- Molecule 28: 50S ribosomal protein L3



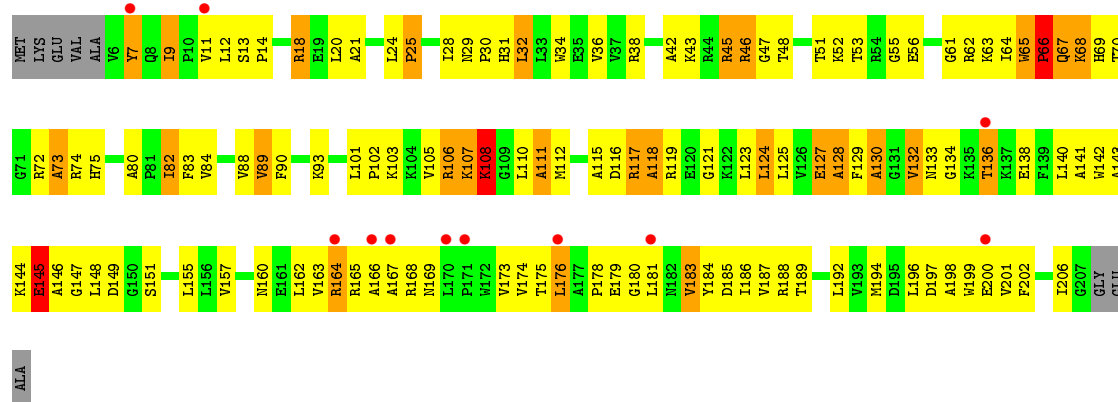




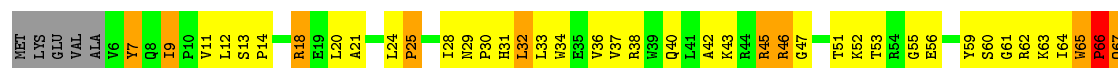
• Molecule 28: 50S ribosomal protein L3



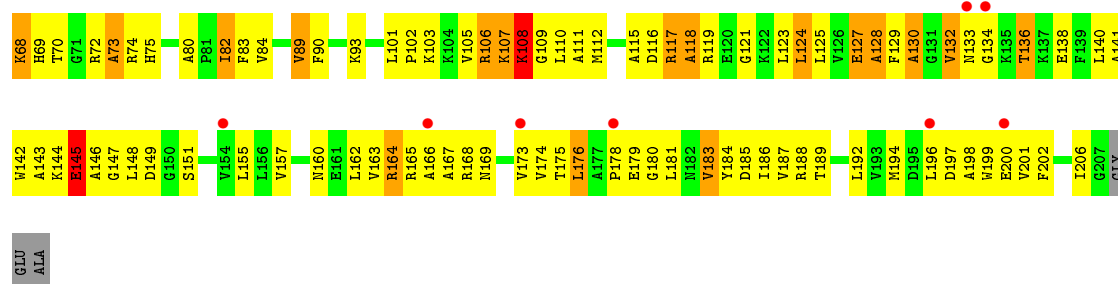
• Molecule 29: 50S ribosomal protein L4



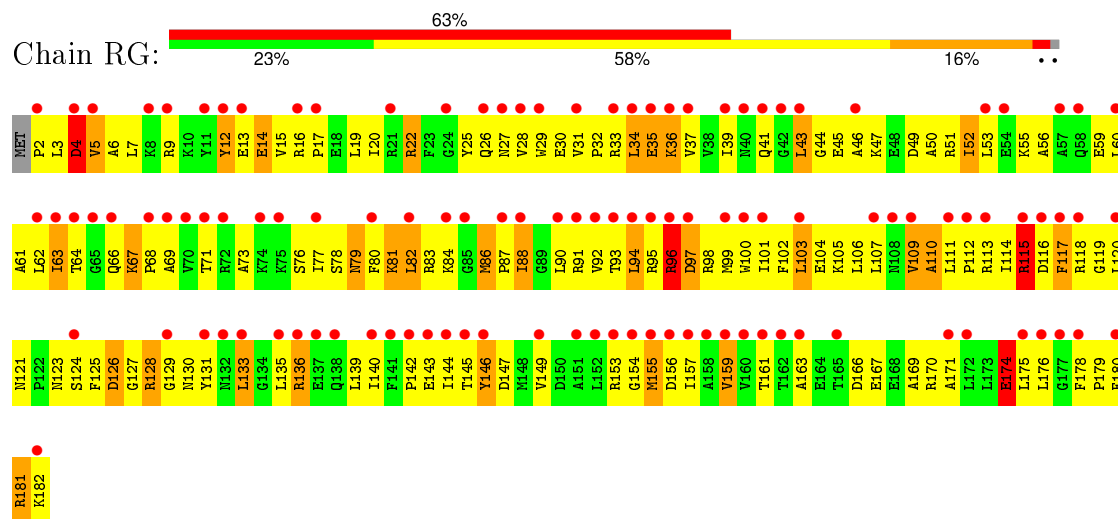
• Molecule 29: 50S ribosomal protein L4



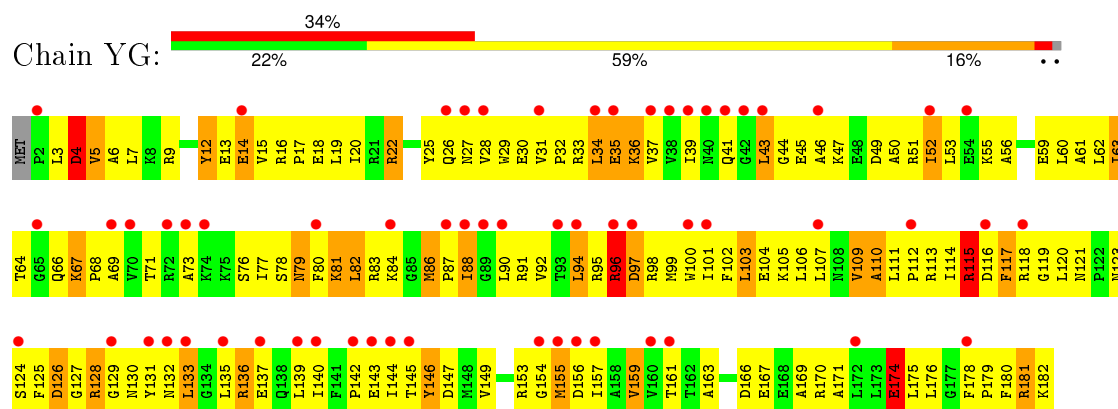




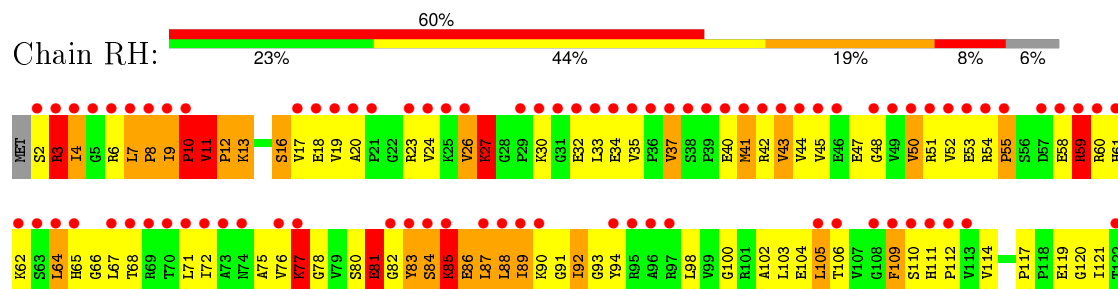
• Molecule 30: 50S ribosomal protein L5



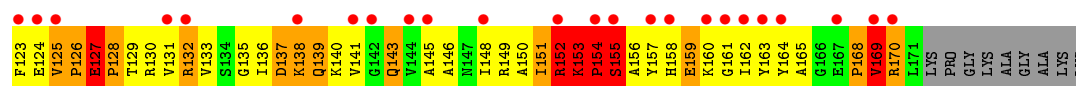
• Molecule 30: 50S ribosomal protein L5



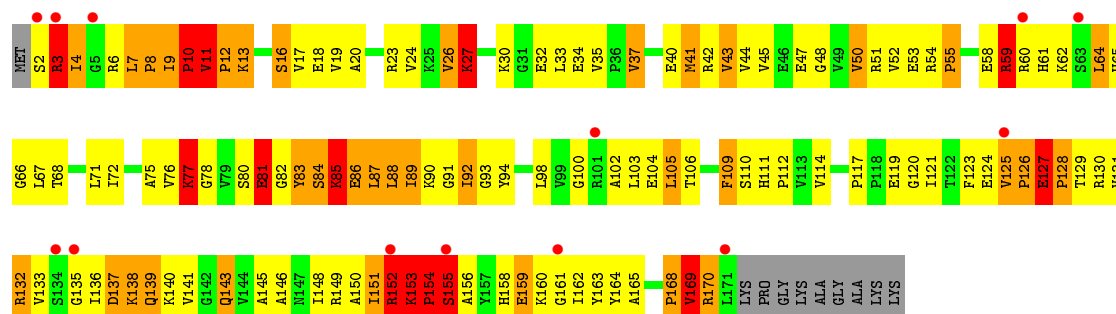
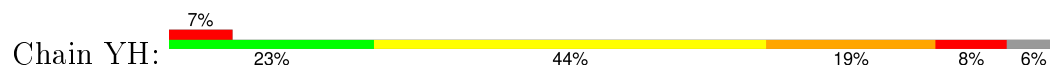
• Molecule 31: 50S ribosomal protein L6



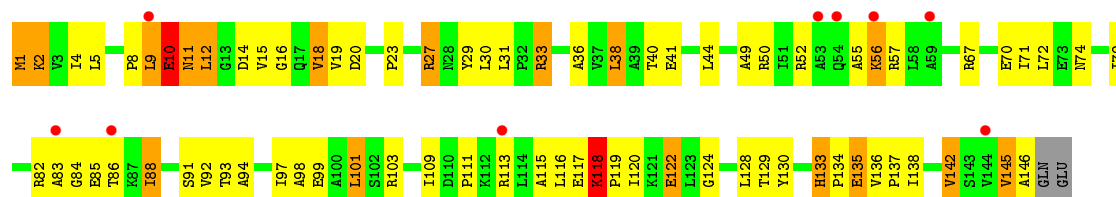




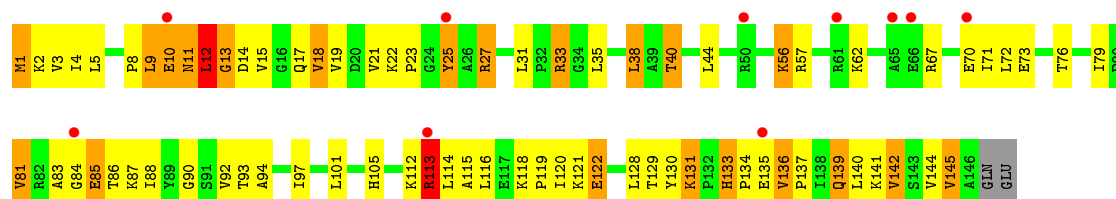
• Molecule 31: 50S ribosomal protein L6



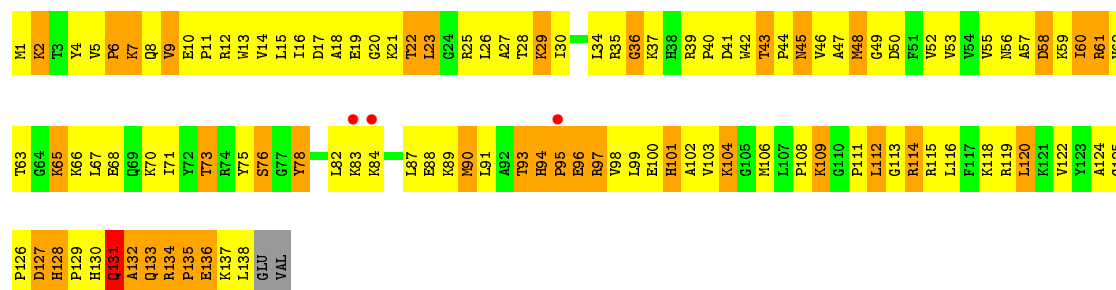
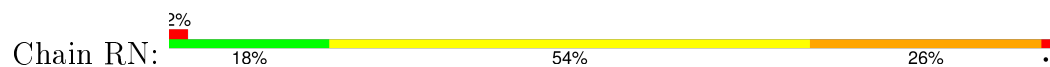
• Molecule 32: 50S ribosomal protein L9



• Molecule 32: 50S ribosomal protein L9

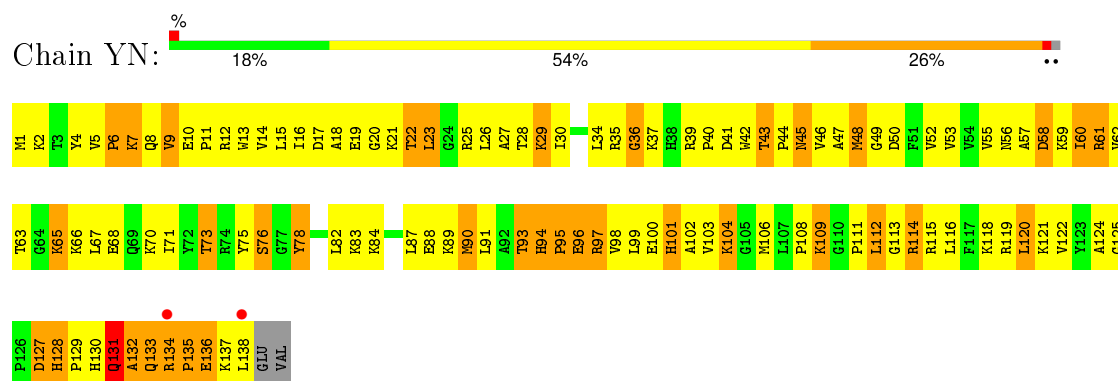


• Molecule 33: 50S ribosomal protein L11

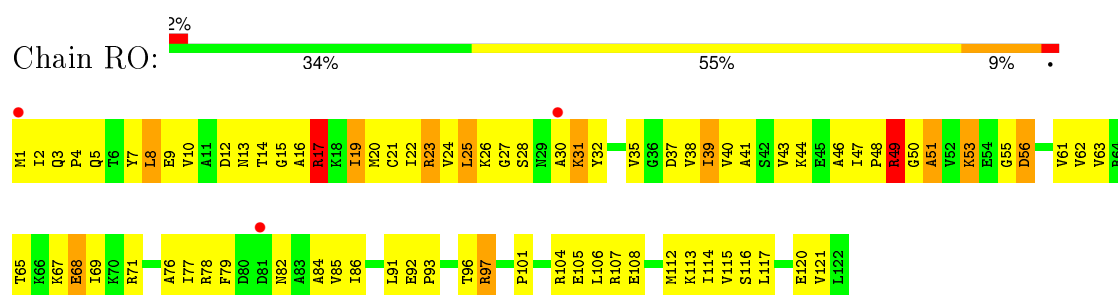




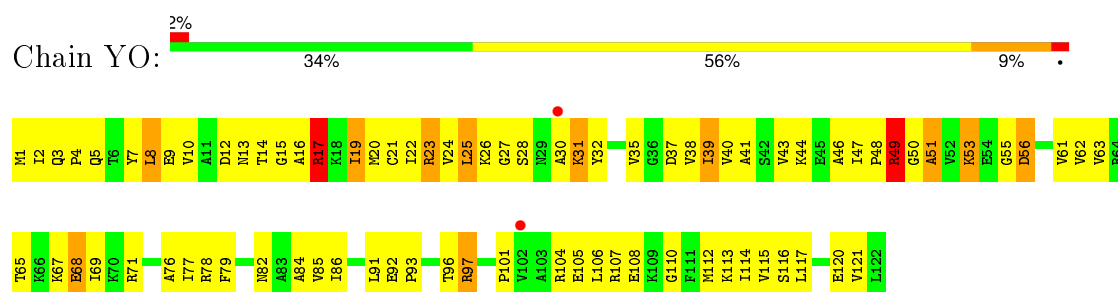
- Molecule 33: 50S ribosomal protein L11



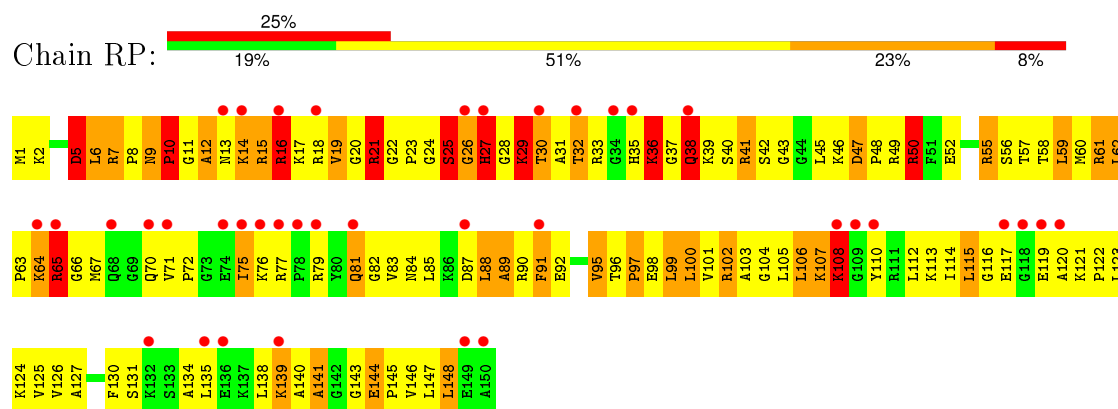
- Molecule 34: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L13

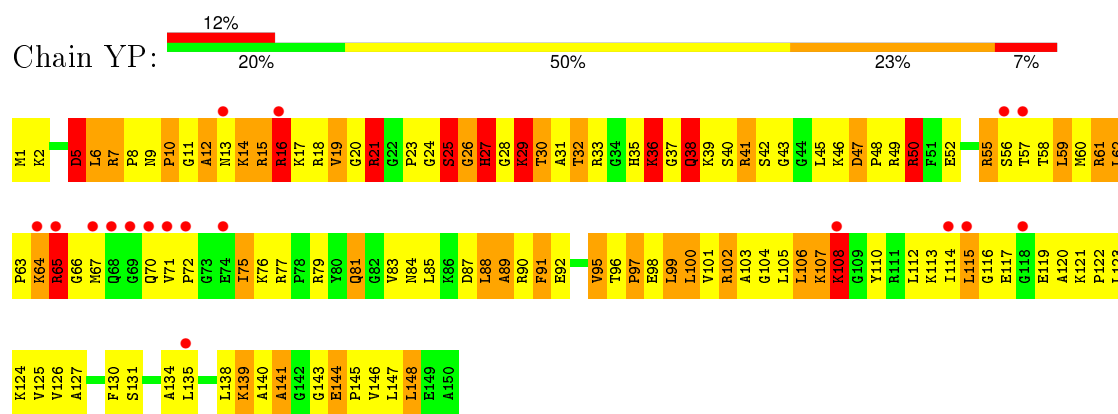


- Molecule 35: 50S ribosomal protein L14

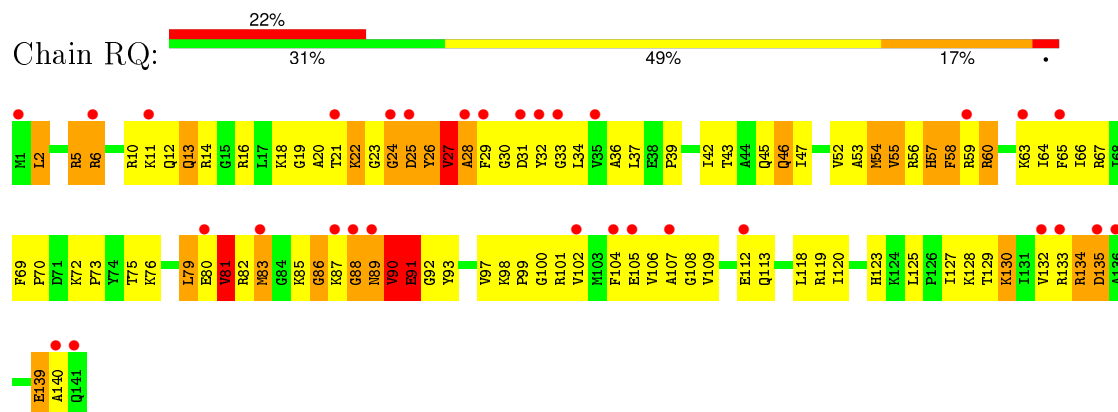


- Molecule 35: 50S ribosomal protein L14

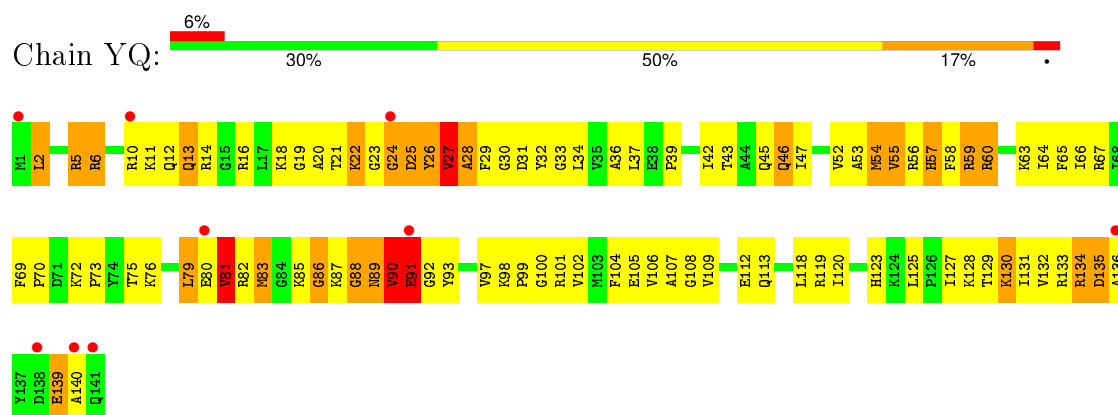




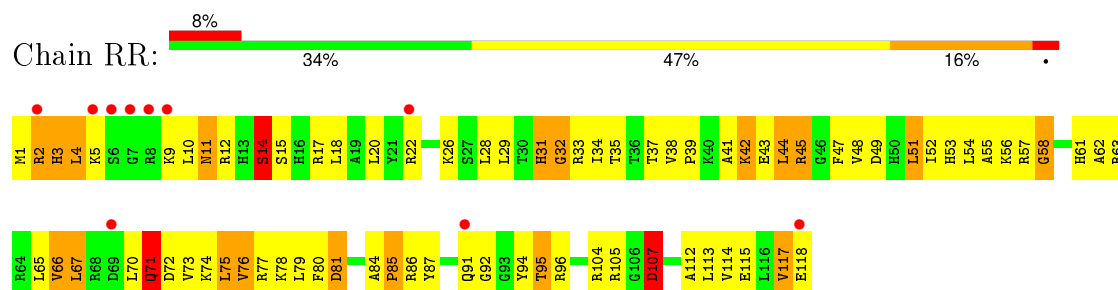
• Molecule 36: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L15

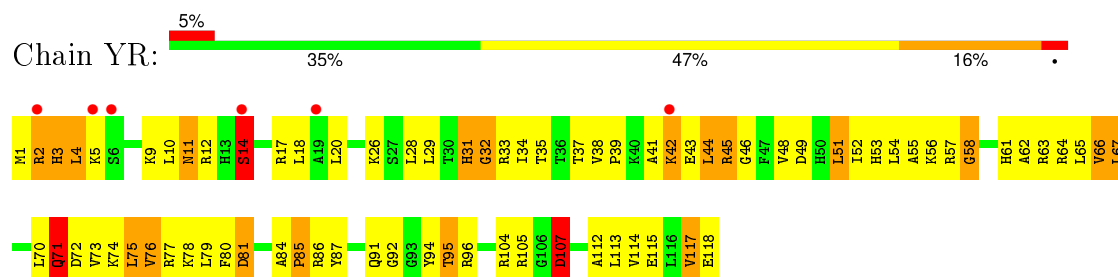


• Molecule 37: 50S ribosomal protein L16

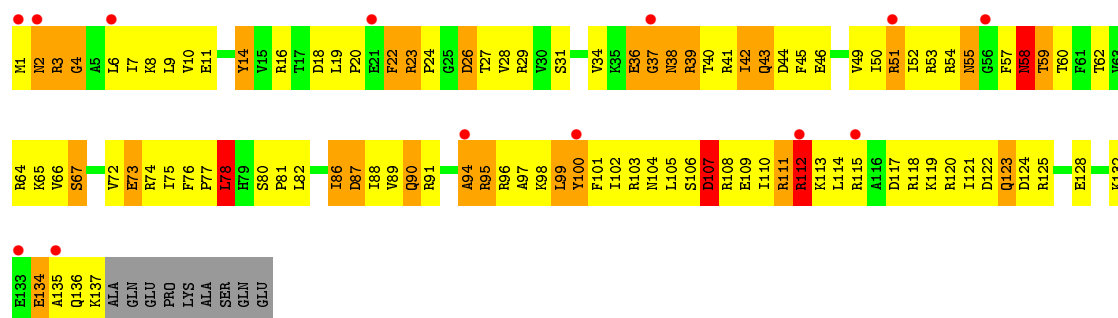




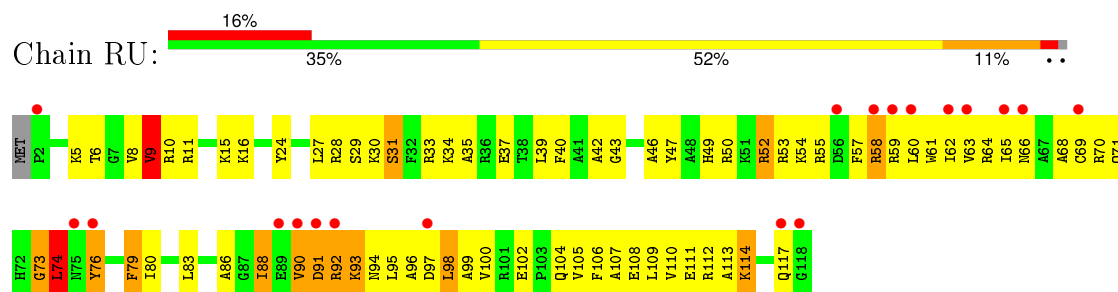
- Molecule 37: 50S ribosomal protein L16



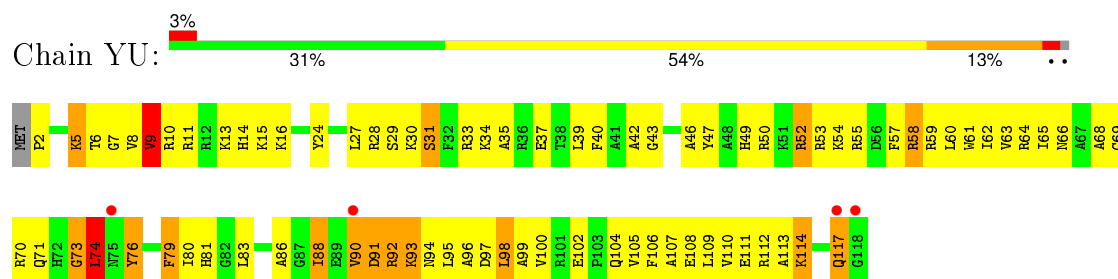




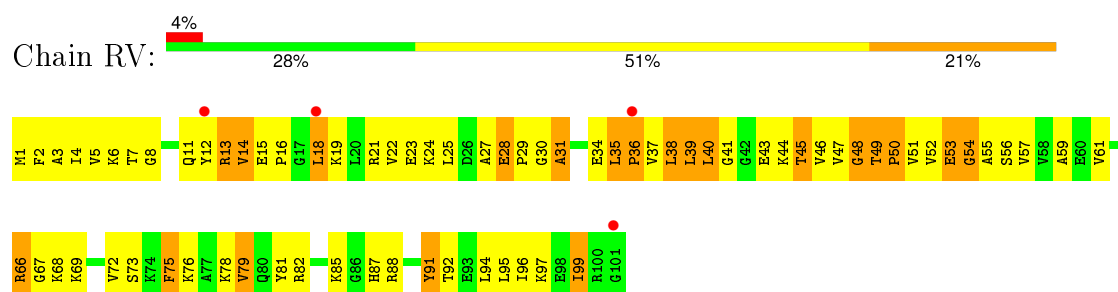
- Molecule 40: 50S ribosomal protein L19



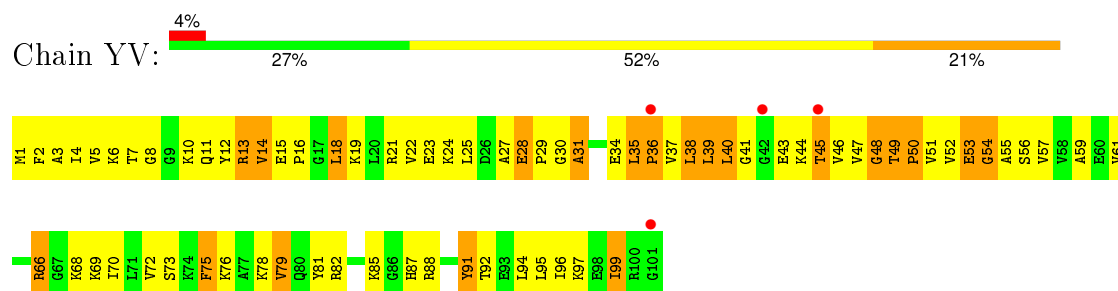
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L20

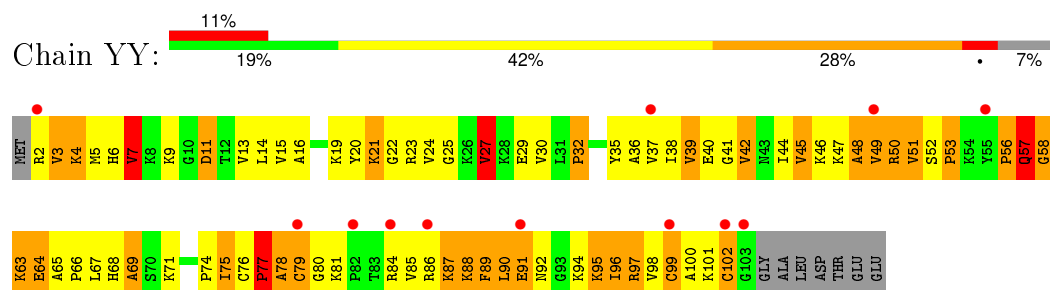




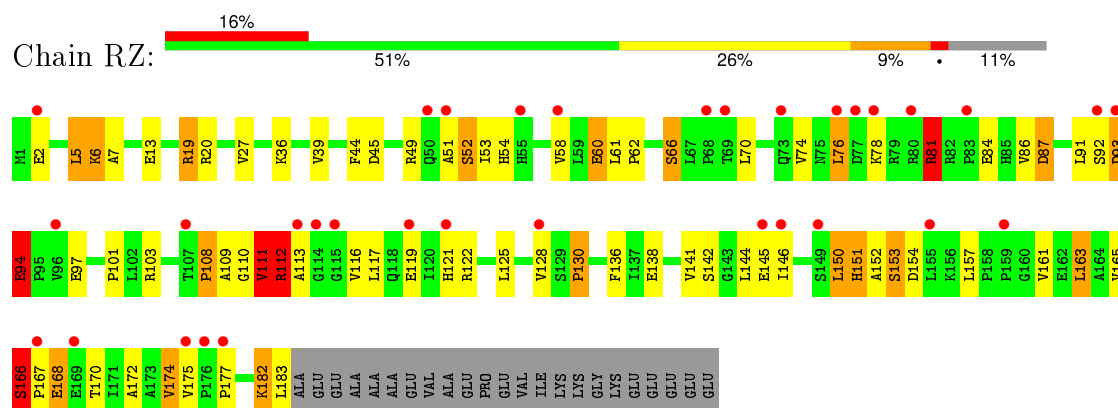
- | Met | R2  | R3  | R4  | R5  | R6  | R7  | R8  | R9  | G10 | D11 | T12 | V13 | L14 | V15 | A16 | S17 | G18 | K19 | Y20 | R21 | G22 | R23 | V24 | G25 | K26 | F27 | K28 | E29 | V30 | L31 | P32 | V35 | A36 | V37 | I38 | V39  | E40  | Q41  | V42  | M43 | T44 | V45 | K46 | T47 | A48 | V49 | R50 | S52 | P53 | V54 | V55 | P56 | S57 | S58 | S59 | F60 | T61 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| E62 | K63 | E64 | A65 | P66 | L67 | H68 | A69 | S70 | K71 | V72 | K73 | P74 | I75 | C76 | T77 | A78 | C79 | G80 | K81 |     | R84 | V85 | R86 | K87 | K88 | F89 | L90 | E91 | N92 | G93 | K94 | K95 | I96 | R97 | C99 | A100 | K101 | G102 | G103 | GLY | ALA | LEU | ASP | THR | GLU | GLU |     |     |     |     |     |     |     |     |     |     |     |



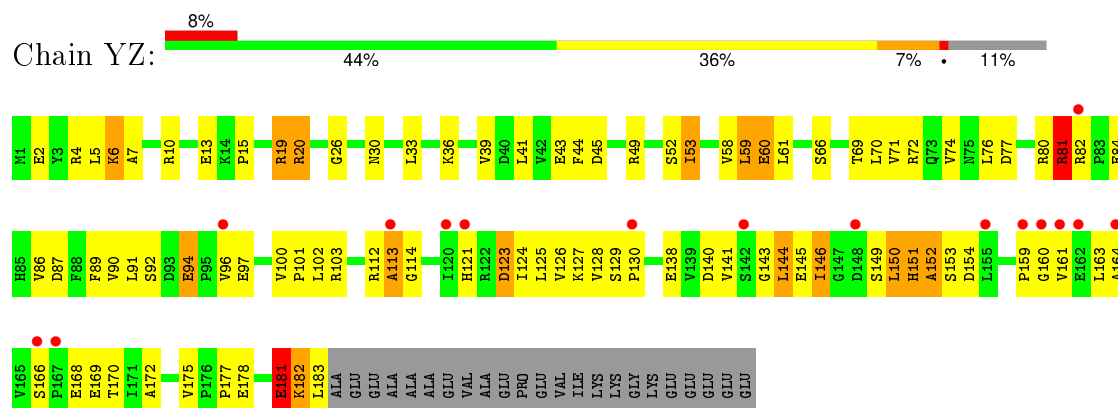
- Molecule 44: 50S ribosomal protein L23



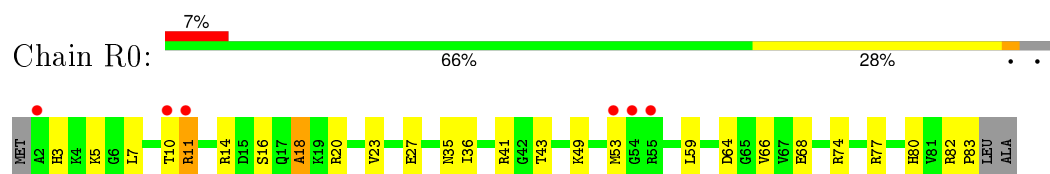
- Molecule 45: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L24



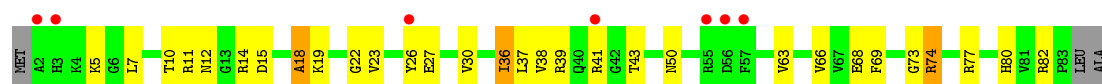
- Molecule 46: 50S ribosomal protein L25



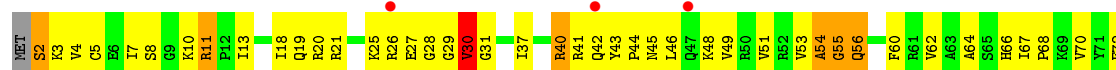
- Molecule 46: 50S ribosomal protein L25







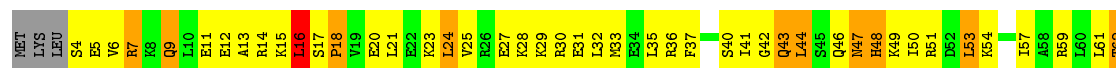
- Molecule 47: 50S ribosomal protein L27



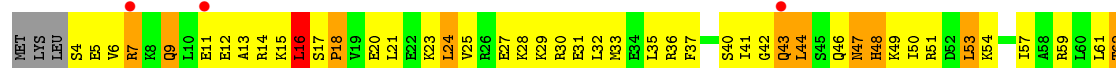
- Molecule 47: 50S ribosomal protein L27



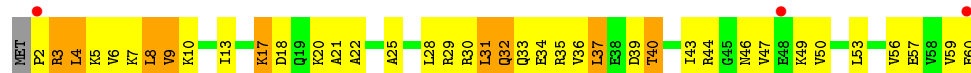
- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28

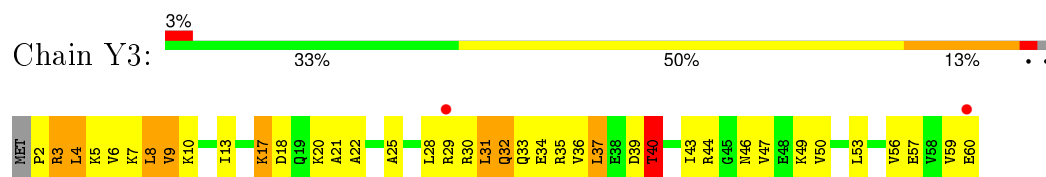


- Molecule 49: 50S ribosomal protein L29

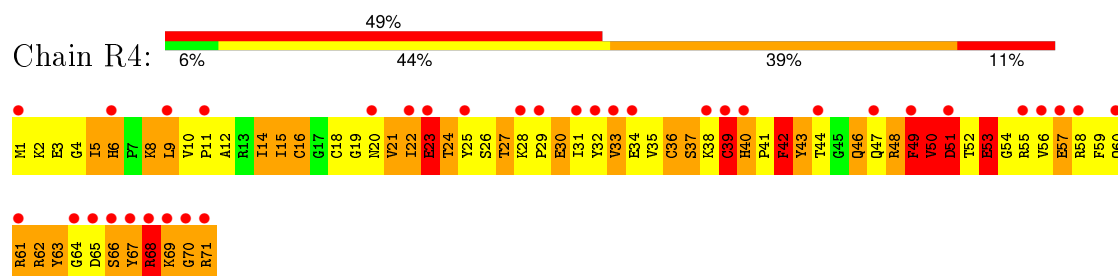




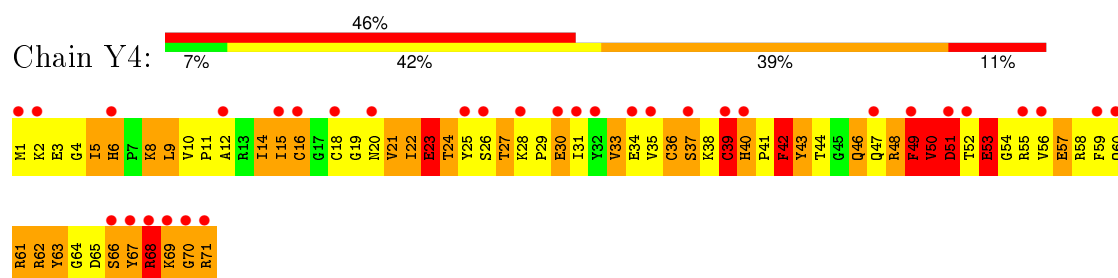
- Molecule 49: 50S ribosomal protein L29



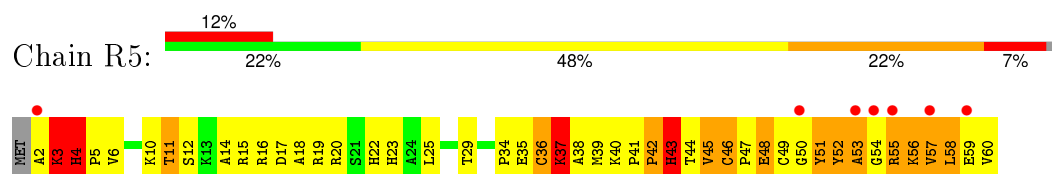
- Molecule 50: 50S ribosomal protein L30



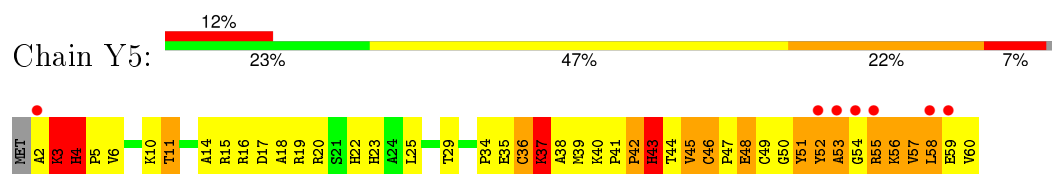
- Molecule 50: 50S ribosomal protein L30



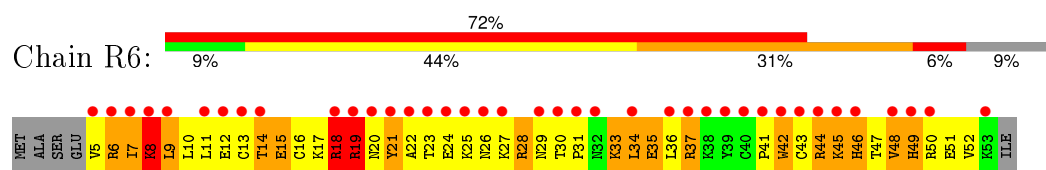
- Molecule 51: 50S ribosomal protein L32



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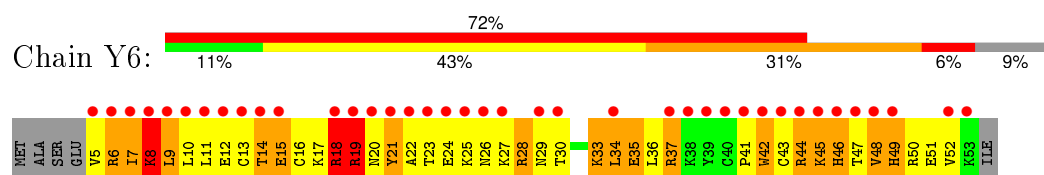


- Molecule 52: 50S ribosomal protein L33

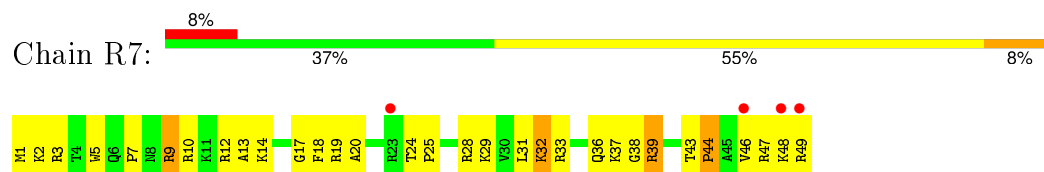


- Molecule 52: 50S ribosomal protein L33

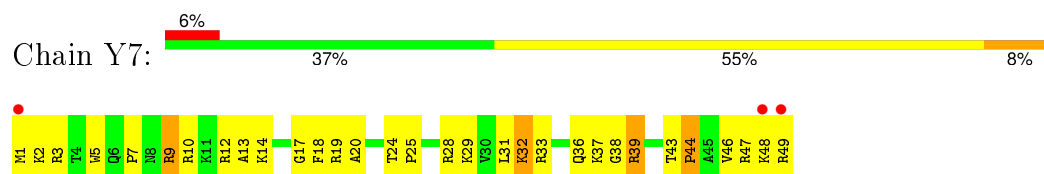




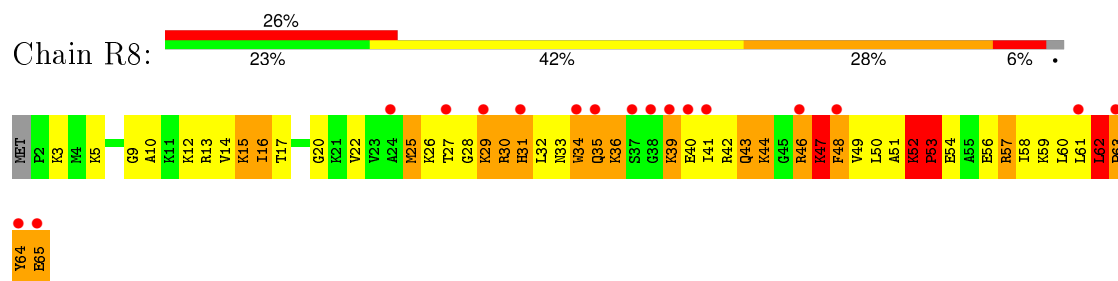
- Molecule 53: 50S ribosomal protein L34



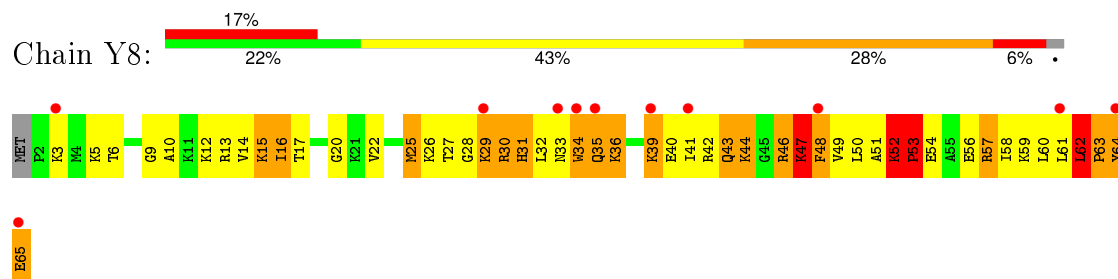
- Molecule 53: 50S ribosomal protein L34



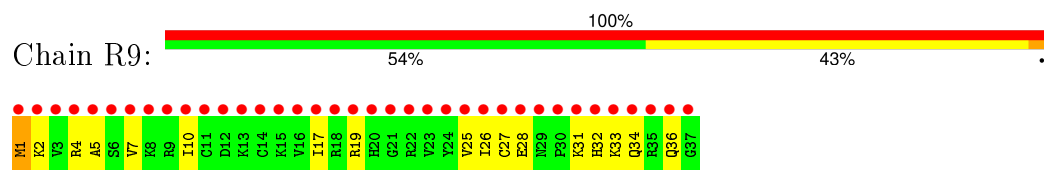
- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



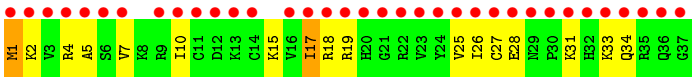
- Molecule 55: 50S ribosomal protein L36



- 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, $\alpha$ , $\beta$ , $\gamma$	209.21Å 448.45Å 619.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.60 – 3.14 189.60 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (189.60-3.14) 99.5 (189.60-3.09)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.230 , 0.262 0.239 , 0.265	Depositor DCC
$R_{free}$ test set	46777 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1047220 reflections	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	291998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

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

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.37	0/36098	0.89	48/56341 (0.1%)
1	XA	0.37	0/36101	0.89	50/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.61	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970



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



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

All (5) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

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

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

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

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

## 5.3 Torsion angles [i](#)

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

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

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



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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	2
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	2
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	0
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	0
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	0
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	0
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	0
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	0
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	8
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	8
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	4
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	4
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	2
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	2
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
32	RI	144/148 (97%)	102 (71%)	27 (19%)	15 (10%)	1	3
32	YI	144/148 (97%)	103 (72%)	25 (17%)	16 (11%)	0	3
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	0
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	0
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	7
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	7
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	4
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	4
37	RR	116/118 (98%)	83 (72%)	19 (16%)	14 (12%)	0	2
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	2
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	1
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	1
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	6
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	6
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	4
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	4
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	1
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	1
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	13
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	13
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
45	RZ	181/206 (88%)	126 (70%)	35 (19%)	20 (11%)	0	3
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	1	4
46	R0	80/85 (94%)	71 (89%)	7 (9%)	2 (2%)	7	34
46	Y0	80/85 (94%)	72 (90%)	6 (8%)	2 (2%)	7	34
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	2
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	2
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	1
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	1
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	15
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	15
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%)	2	10
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	10

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

5 of 1483 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	7	27
2	XB	205/220 (93%)	181 (88%)	24 (12%)	7	27
3	QC	159/188 (85%)	143 (90%)	16 (10%)	9	33
3	XC	159/188 (85%)	143 (90%)	16 (10%)	9	33
4	QD	180/181 (99%)	160 (89%)	20 (11%)	8	30
4	XD	180/181 (99%)	165 (92%)	15 (8%)	14	46
5	QE	116/123 (94%)	108 (93%)	8 (7%)	19	54
5	XE	116/123 (94%)	107 (92%)	9 (8%)	16	49
6	QF	90/90 (100%)	76 (84%)	14 (16%)	3	14
6	XF	90/90 (100%)	76 (84%)	14 (16%)	3	14
7	QG	126/127 (99%)	114 (90%)	12 (10%)	11	38
7	XG	126/127 (99%)	115 (91%)	11 (9%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	106 (89%)	13 (11%)	8	30
8	XH	119/119 (100%)	106 (89%)	13 (11%)	8	30
9	QI	98/99 (99%)	87 (89%)	11 (11%)	7	29
9	XI	98/99 (99%)	87 (89%)	11 (11%)	7	29
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	12	41
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	12	41
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	34
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9	34
12	QL	104/109 (95%)	90 (86%)	14 (14%)	5	20
12	XL	104/109 (95%)	90 (86%)	14 (14%)	5	20
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	12
13	XM	97/101 (96%)	81 (84%)	16 (16%)	3	12
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	9
14	XN	49/50 (98%)	44 (90%)	5 (10%)	9	33
15	QO	79/80 (99%)	73 (92%)	6 (8%)	16	50
15	XO	79/80 (99%)	73 (92%)	6 (8%)	16	50
16	QP	72/74 (97%)	63 (88%)	9 (12%)	6	23
16	XP	72/74 (97%)	63 (88%)	9 (12%)	6	23
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	22	58
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	22	58
18	QR	61/77 (79%)	54 (88%)	7 (12%)	7	27
18	XR	61/77 (79%)	54 (88%)	7 (12%)	7	27
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%)	8	32
20	XT	76/82 (93%)	68 (90%)	8 (10%)	8	32
21	QU	20/22 (91%)	19 (95%)	1 (5%)	30	67
21	XU	20/22 (91%)	19 (95%)	1 (5%)	30	67
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	11
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	11
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	4
29	RF	161/166 (97%)	140 (87%)	21 (13%)	5	21
29	YF	161/166 (97%)	140 (87%)	21 (13%)	5	21
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	12
30	YG	155/156 (99%)	130 (84%)	25 (16%)	3	12
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	7
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	7
32	RI	122/124 (98%)	100 (82%)	22 (18%)	2	9
32	YI	122/124 (98%)	98 (80%)	24 (20%)	1	7
33	RN	117/119 (98%)	98 (84%)	19 (16%)	3	12
33	YN	117/119 (98%)	98 (84%)	19 (16%)	3	12
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9	34
34	YO	100/100 (100%)	90 (90%)	10 (10%)	9	34
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	4
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	4
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	12
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	3	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%)	4	16
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	16
39	RT	120/127 (94%)	97 (81%)	23 (19%)	2	8
39	YT	120/127 (94%)	97 (81%)	23 (19%)	2	8
40	RU	93/94 (99%)	80 (86%)	13 (14%)	4	19
40	YU	93/94 (99%)	80 (86%)	13 (14%)	4	19
41	RV	82/82 (100%)	71 (87%)	11 (13%)	5	20
41	YV	82/82 (100%)	71 (87%)	11 (13%)	5	20
42	RW	92/92 (100%)	77 (84%)	15 (16%)	3	12
42	YW	92/92 (100%)	77 (84%)	15 (16%)	3	12
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	16
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	10
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	10
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	4	16
45	YZ	162/179 (90%)	142 (88%)	20 (12%)	6	24
46	R0	65/67 (97%)	58 (89%)	7 (11%)	8	31
46	Y0	65/67 (97%)	63 (97%)	2 (3%)	47	80
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	9
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	9
48	R2	64/67 (96%)	57 (89%)	7 (11%)	8	30
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	8	30
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	6
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	6
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	1
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	1
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	4
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	4
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	6
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	6
53	R7	42/42 (100%)	39 (93%)	3 (7%)	18	54
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	18	54
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	1
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	1
55	R9	34/34 (100%)	32 (94%)	2 (6%)	24	60
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	24	60
All	All	9702/10066 (96%)	8299 (86%)	1403 (14%)	4	17

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

Mol	Chain	Res	Type
48	R2	53	LEU
6	XF	97	PHE
45	YZ	76	LEU
50	R4	39	CYS
2	XB	23	ARG



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

Mol	Chain	Res	Type
47	R1	56	GLN
5	XE	78	HIS
43	YX	87	GLN
48	R2	47	ASN
2	XB	95	GLN

### 5.3.3 RNA ⓘ

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

5 of 1932 RNA backbone outliers are listed below:

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

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2566	A
1	XA	345	C
25	YA	1955	U

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Mol	Chain	Res	Type
25	RA	2723	C
1	XA	60	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
23	1MG	QY	37	23	16,26,27	2.92	3 (18%)	19,39,42	1.46	3 (15%)
23	1MG	XY	37	23	16,26,27	2.86	3 (18%)	19,39,42	1.42	2 (10%)
56	PPU	Z6	76	25,56	30,40,41	2.58	5 (16%)	37,57,60	3.25	11 (29%)
56	PPU	Z8	76	25,56	30,40,41	2.57	6 (20%)	37,57,60	3.24	11 (29%)

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

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	C9-N6	-5.62	1.32	1.45
56	Z8	76	PPU	C9-N6	-5.61	1.32	1.45
56	Z6	76	PPU	C10-N6	-5.30	1.32	1.45
56	Z8	76	PPU	C10-N6	-5.30	1.32	1.45
56	Z8	76	PPU	C5-N7	-2.00	1.32	1.39



The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C2'-C1'-N9	-10.33	98.50	114.29
56	Z8	76	PPU	C2'-C1'-N9	-10.32	98.52	114.29
56	Z8	76	PPU	N3-C2-N1	-9.79	121.40	128.89
56	Z6	76	PPU	N3-C2-N1	-9.73	121.45	128.89
56	Z6	76	PPU	C3'-N3'-C	-8.25	110.18	123.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PAR	QA	1670	-	45,45,45	1.30	7 (15%)	59,67,67	1.41	7 (11%)
58	PAR	XA	1675	-	45,45,45	1.34	7 (15%)	59,67,67	1.34	5 (8%)

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	QA	1670	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1675	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1670	PAR	C14-C24	2.00	1.56	1.52
58	XA	1675	PAR	C31-C21	2.01	1.56	1.53
58	QA	1670	PAR	C31-C21	2.12	1.56	1.53
58	QA	1670	PAR	C11-C21	2.16	1.56	1.52
58	XA	1675	PAR	C14-C24	2.19	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1670	PAR	O11-C42-C32	-2.96	101.76	108.92
58	QA	1670	PAR	O54-C54-C44	-2.05	105.83	109.68
58	XA	1675	PAR	C11-O51-C51	2.56	118.72	113.75
58	XA	1675	PAR	O54-C54-C64	2.70	111.37	106.10
58	QA	1670	PAR	O54-C54-C64	2.82	111.60	106.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.23	292 (19%) 1 1	27, 67, 148, 352	0
1	XA	1500/1522 (98%)	1.34	304 (20%) 1 0	18, 55, 149, 326	0
2	QB	237/256 (92%)	1.08	47 (19%) 1 0	54, 126, 215, 288	0
2	XB	237/256 (92%)	0.74	23 (9%) 10 3	43, 102, 177, 293	0
3	QC	205/239 (85%)	0.72	27 (13%) 4 2	56, 108, 175, 255	0
3	XC	205/239 (85%)	0.50	10 (4%) 33 14	30, 78, 132, 181	0
4	QD	208/209 (99%)	1.28	54 (25%) 1 0	41, 79, 136, 185	0
4	XD	208/209 (99%)	0.94	30 (14%) 3 1	30, 74, 134, 231	0
5	QE	151/162 (93%)	0.86	20 (13%) 4 2	42, 85, 148, 260	0
5	XE	151/162 (93%)	0.67	13 (8%) 13 4	23, 61, 121, 196	0
6	QF	101/101 (100%)	0.37	0 100 100	30, 74, 112, 155	0
6	XF	101/101 (100%)	0.50	6 (5%) 26 10	26, 69, 110, 146	0
7	QG	155/156 (99%)	0.92	24 (15%) 3 1	46, 97, 158, 302	0
7	XG	155/156 (99%)	0.76	18 (11%) 6 2	35, 82, 149, 230	0
8	QH	138/138 (100%)	0.78	11 (7%) 15 5	39, 83, 130, 174	0
8	XH	138/138 (100%)	0.77	13 (9%) 11 4	34, 68, 117, 169	0
9	QI	127/128 (99%)	2.36	61 (48%) 0 0	48, 117, 170, 243	0
9	XI	127/128 (99%)	1.30	36 (28%) 1 0	33, 91, 152, 203	0
10	QJ	99/105 (94%)	2.61	53 (53%) 0 0	53, 140, 243, 283	0
10	XJ	99/105 (94%)	1.94	44 (44%) 0 0	21, 100, 169, 213	0
11	QK	119/129 (92%)	0.98	15 (12%) 5 2	42, 77, 149, 228	0
11	XK	119/129 (92%)	1.28	25 (21%) 1 0	28, 70, 134, 196	0
12	QL	125/132 (94%)	1.24	30 (24%) 1 0	35, 69, 140, 262	0
12	XL	125/132 (94%)	0.88	13 (10%) 8 3	22, 51, 113, 282	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	2.15	46 (38%)	0	0	43, 108, 185, 410	0
13	XM	121/126 (96%)	1.42	30 (24%)	1	0	36, 86, 141, 273	0
14	QN	60/61 (98%)	2.14	28 (46%)	0	0	59, 101, 150, 166	0
14	XN	60/61 (98%)	1.20	16 (26%)	1	0	36, 67, 127, 143	0
15	QO	88/89 (98%)	0.79	10 (11%)	7	2	32, 78, 150, 180	0
15	XO	88/89 (98%)	0.83	13 (14%)	3	1	27, 62, 111, 129	0
16	QP	84/88 (95%)	1.12	15 (17%)	2	1	38, 71, 115, 186	0
16	XP	84/88 (95%)	1.43	25 (29%)	1	0	39, 73, 119, 211	0
17	QQ	100/105 (95%)	0.91	12 (12%)	6	2	44, 79, 131, 161	0
17	XQ	100/105 (95%)	1.40	25 (25%)	1	0	35, 75, 127, 166	0
18	QR	70/88 (79%)	0.58	2 (2%)	55	32	28, 73, 141, 149	0
18	XR	70/88 (79%)	0.42	3 (4%)	39	18	27, 66, 118, 171	0
19	QS	84/93 (90%)	2.67	54 (64%)	0	0	80, 119, 195, 275	0
19	XS	84/93 (90%)	1.51	24 (28%)	1	0	47, 88, 168, 219	0
20	QT	99/106 (93%)	1.59	33 (33%)	0	0	37, 82, 140, 220	0
20	XT	99/106 (93%)	1.85	44 (44%)	0	0	28, 86, 149, 177	0
21	QU	25/27 (92%)	5.80	24 (96%)	0	0	45, 98, 150, 185	0
21	XU	25/27 (92%)	3.22	17 (68%)	0	0	43, 69, 139, 153	0
22	QV	77/77 (100%)	1.00	13 (16%)	2	1	27, 73, 146, 212	0
22	XV	77/77 (100%)	0.77	8 (10%)	8	3	17, 59, 103, 207	0
23	QY	14/17 (82%)	1.49	3 (21%)	1	0	69, 116, 169, 189	0
23	XY	14/17 (82%)	1.58	3 (21%)	1	0	41, 102, 143, 157	0
24	QX	8/25 (32%)	1.28	2 (25%)	1	0	49, 58, 151, 164	0
24	XX	8/25 (32%)	2.24	2 (25%)	1	0	32, 38, 89, 104	0
25	RA	2882/2916 (98%)	1.18	366 (12%)	5	2	13, 44, 212, 472	0
25	YA	2883/2916 (98%)	1.04	250 (8%)	13	4	7, 35, 201, 461	0
26	RB	120/122 (98%)	1.04	18 (15%)	3	1	43, 69, 105, 120	0
26	YB	120/122 (98%)	0.42	0	100	100	29, 51, 71, 110	0
27	RD	272/276 (98%)	0.57	11 (4%)	42	21	9, 42, 81, 176	0
27	YD	272/276 (98%)	0.56	11 (4%)	42	21	5, 35, 71, 188	0
28	RE	205/206 (99%)	0.79	15 (7%)	18	7	11, 56, 123, 335	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YE	205/206 (99%)	0.66	10 (4%) 33 14	2, 52, 123, 250	0
29	RF	202/210 (96%)	0.54	11 (5%) 29 12	15, 62, 132, 185	0
29	YF	202/210 (96%)	0.53	8 (3%) 42 21	8, 45, 121, 194	0
30	RG	181/182 (99%)	3.26	114 (62%) 0 0	79, 156, 284, 386	0
30	YG	181/182 (99%)	1.58	61 (33%) 0 0	30, 89, 155, 309	0
31	RH	170/180 (94%)	2.80	108 (63%) 0 0	79, 145, 235, 306	0
31	YH	170/180 (94%)	0.85	13 (7%) 17 6	31, 79, 122, 167	0
32	RI	146/148 (98%)	0.45	9 (6%) 24 9	25, 87, 178, 297	0
32	YI	146/148 (98%)	0.55	10 (6%) 20 7	22, 83, 152, 183	0
33	RN	138/140 (98%)	0.43	3 (2%) 65 44	26, 64, 124, 179	0
33	YN	138/140 (98%)	0.43	2 (1%) 78 61	16, 54, 108, 166	0
34	RO	122/122 (100%)	0.49	3 (2%) 61 39	22, 55, 103, 142	0
34	YO	122/122 (100%)	0.59	2 (1%) 74 56	16, 48, 78, 126	0
35	RP	150/150 (100%)	1.23	38 (25%) 1 0	18, 68, 154, 247	0
35	YP	150/150 (100%)	0.85	18 (12%) 6 2	9, 53, 126, 253	0
36	RQ	141/141 (100%)	1.28	31 (21%) 1 0	28, 67, 128, 178	0
36	YQ	141/141 (100%)	0.55	9 (6%) 23 8	14, 47, 124, 154	0
37	RR	118/118 (100%)	0.65	10 (8%) 13 4	18, 48, 81, 170	0
37	YR	118/118 (100%)	0.59	6 (5%) 32 13	20, 46, 85, 137	0
38	RS	111/112 (99%)	1.10	22 (19%) 1 0	38, 76, 131, 184	0
38	YS	111/112 (99%)	0.65	3 (2%) 58 36	28, 58, 106, 195	0
39	RT	137/146 (93%)	0.89	14 (10%) 9 3	29, 67, 161, 259	0
39	YT	137/146 (93%)	0.79	13 (9%) 10 3	27, 61, 152, 303	0
40	RU	117/118 (99%)	1.01	19 (16%) 3 1	20, 54, 114, 221	0
40	YU	117/118 (99%)	0.67	4 (3%) 49 25	19, 39, 97, 221	0
41	RV	101/101 (100%)	0.63	4 (3%) 42 21	21, 77, 140, 320	0
41	YV	101/101 (100%)	0.58	4 (3%) 42 21	13, 63, 124, 304	0
42	RW	113/113 (100%)	0.37	4 (3%) 48 24	19, 41, 99, 220	0
42	YW	113/113 (100%)	0.17	1 (0%) 85 73	15, 41, 95, 193	0
43	RX	92/96 (95%)	0.50	0 100 100	26, 53, 87, 135	0
43	YX	92/96 (95%)	0.47	2 (2%) 65 44	12, 39, 76, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RY	102/110 (92%)	1.42	24 (23%) 1 0	40, 99, 177, 285	0
44	YY	102/110 (92%)	0.90	12 (11%) 6 2	31, 73, 155, 210	0
45	RZ	183/206 (88%)	1.16	33 (18%) 2 1	41, 93, 178, 292	0
45	YZ	183/206 (88%)	0.67	16 (8%) 13 4	32, 71, 179, 271	0
46	R0	82/85 (96%)	0.67	6 (7%) 18 7	18, 49, 71, 179	0
46	Y0	82/85 (96%)	0.50	7 (8%) 13 4	11, 34, 60, 87	0
47	R1	97/98 (98%)	0.84	6 (6%) 24 9	21, 51, 160, 335	0
47	Y1	97/98 (98%)	0.87	11 (11%) 7 2	16, 49, 139, 210	0
48	R2	69/72 (95%)	0.39	0 100 100	28, 69, 143, 169	0
48	Y2	69/72 (95%)	0.65	3 (4%) 39 18	19, 59, 119, 177	0
49	R3	59/60 (98%)	0.67	3 (5%) 32 13	31, 71, 112, 169	0
49	Y3	59/60 (98%)	0.40	2 (3%) 49 25	22, 49, 91, 198	0
50	R4	71/71 (100%)	3.11	35 (49%) 0 0	107, 211, 311, 396	0
50	Y4	71/71 (100%)	2.51	33 (46%) 0 0	66, 156, 274, 384	0
51	R5	59/60 (98%)	0.94	7 (11%) 6 2	8, 49, 223, 238	0
51	Y5	59/60 (98%)	0.77	7 (11%) 6 2	11, 49, 223, 335	0
52	R6	49/54 (90%)	5.70	39 (79%) 0 0	86, 175, 268, 291	0
52	Y6	49/54 (90%)	4.75	39 (79%) 0 0	76, 163, 229, 312	0
53	R7	49/49 (100%)	0.53	4 (8%) 14 5	16, 29, 87, 168	0
53	Y7	49/49 (100%)	0.38	3 (6%) 25 10	8, 23, 87, 176	0
54	R8	64/65 (98%)	1.50	17 (26%) 1 0	20, 53, 102, 208	0
54	Y8	64/65 (98%)	1.21	11 (17%) 2 1	16, 44, 97, 214	0
55	R9	37/37 (100%)	8.50	37 (100%) 0 0	82, 138, 203, 344	0
55	Y9	37/37 (100%)	6.09	35 (94%) 0 0	57, 119, 223, 246	0
56	Z6	2/3 (66%)	1.50	0 100 100	33, 33, 33, 47	0
56	Z8	2/3 (66%)	1.79	1 (50%) 0 0	24, 24, 24, 36	0
All	All	20873/21492 (97%)	1.12	3239 (15%) 3 1	2, 61, 174, 472	0

The worst 5 of 3239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	2117	A	24.6
25	YA	1061	U	20.8

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Mol	Chain	Res	Type	RSRZ
25	YA	2112	G	20.7
13	QM	7	VAL	20.6
25	YA	2136	C	19.5

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	PPU	Z8	76	37/38	0.88	0.42	-	37,37,37,37	0
56	PPU	Z6	76	37/38	0.89	0.43	-	41,41,41,41	0
23	1MG	QY	37	24/25	0.93	0.27	-	63,63,63,63	0
23	1MG	XY	37	24/25	0.95	0.25	-	45,45,45,45	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	RA	3131	1/1	0.85	0.39	20.99	41,41,41,41	0
57	MG	YA	3207	1/1	0.64	0.69	18.24	80,80,80,80	0
57	MG	YA	3020	1/1	0.97	0.37	17.78	7,7,7,7	0
57	MG	YA	3240	1/1	0.93	0.43	15.83	43,43,43,43	0
57	MG	YA	3219	1/1	0.93	0.90	15.33	52,52,52,52	0
57	MG	YA	3050	1/1	0.98	0.33	11.54	9,9,9,9	0
57	MG	YA	3259	1/1	0.80	0.43	10.90	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3255	1/1	0.88	0.31	10.13	13,13,13,13	0
57	MG	Y7	101	1/1	0.87	0.40	9.84	38,38,38,38	0
57	MG	RA	3053	1/1	0.97	0.37	7.26	16,16,16,16	0
57	MG	RA	3063	1/1	0.97	0.41	6.46	6,6,6,6	0
57	MG	RA	3230	1/1	0.97	0.32	6.45	18,18,18,18	0
57	MG	RA	3126	1/1	0.91	0.34	6.12	33,33,33,33	0
57	MG	YA	3023	1/1	0.97	0.26	5.75	16,16,16,16	0
57	MG	RA	3099	1/1	0.94	0.34	5.69	24,24,24,24	0
57	MG	YA	3099	1/1	0.95	0.35	5.27	7,7,7,7	0
57	MG	RA	3221	1/1	0.52	0.40	5.08	62,62,62,62	0
57	MG	RA	3204	1/1	0.48	0.37	4.72	82,82,82,82	0
57	MG	RA	3088	1/1	0.88	0.33	4.65	19,19,19,19	0
57	MG	RA	3200	1/1	0.68	0.27	4.55	38,38,38,38	0
57	MG	RA	3005	1/1	0.98	0.37	4.39	13,13,13,13	0
57	MG	QA	1657	1/1	0.60	0.30	4.38	58,58,58,58	0
57	MG	YA	3258	1/1	0.95	0.37	4.16	11,11,11,11	0
57	MG	YA	3015	1/1	0.97	0.32	3.98	8,8,8,8	0
57	MG	RA	3029	1/1	0.98	0.31	3.94	2,2,2,2	0
57	MG	YA	3144	1/1	0.79	0.24	3.93	35,35,35,35	0
57	MG	YA	3100	1/1	0.97	0.31	3.75	13,13,13,13	0
57	MG	YA	3171	1/1	0.87	0.37	3.70	32,32,32,32	0
57	MG	QA	1615	1/1	0.91	0.25	3.68	23,23,23,23	0
57	MG	RA	3238	1/1	0.89	0.32	3.49	32,32,32,32	0
57	MG	RA	3035	1/1	0.95	0.31	3.40	11,11,11,11	0
57	MG	YA	3034	1/1	0.97	0.34	3.29	9,9,9,9	0
57	MG	YA	3027	1/1	0.98	0.28	3.06	0,0,0,0	0
57	MG	RA	3039	1/1	0.97	0.24	2.99	2,2,2,2	0
58	PAR	QA	1670	42/42	0.88	0.39	2.80	56,56,56,56	0
58	PAR	XA	1675	42/42	0.91	0.32	2.64	49,49,49,49	0
57	MG	RA	3060	1/1	0.96	0.29	2.33	8,8,8,8	0
57	MG	RA	3056	1/1	0.93	0.31	2.26	17,17,17,17	0
57	MG	RA	3034	1/1	0.95	0.34	2.21	30,30,30,30	0
57	MG	RA	3220	1/1	0.78	0.27	2.18	56,56,56,56	0
57	MG	RA	3125	1/1	0.98	0.24	2.18	28,28,28,28	0
57	MG	RA	3192	1/1	0.44	0.34	2.06	79,79,79,79	0
57	MG	RA	3076	1/1	0.95	0.25	1.93	15,15,15,15	0
57	MG	XA	1673	1/1	0.88	0.32	1.91	26,26,26,26	0
57	MG	YA	3109	1/1	0.98	0.30	1.88	10,10,10,10	0
57	MG	XA	1667	1/1	0.97	0.32	1.86	32,32,32,32	0
57	MG	RA	3057	1/1	0.97	0.27	1.78	11,11,11,11	0
57	MG	YA	3235	1/1	0.77	0.26	1.77	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3261	1/1	0.98	0.29	1.76	8,8,8,8	0
57	MG	RA	3132	1/1	0.95	0.31	1.75	22,22,22,22	0
57	MG	XA	1623	1/1	0.97	0.27	1.73	40,40,40,40	0
57	MG	QA	1631	1/1	0.85	0.52	1.62	46,46,46,46	0
57	MG	YA	3239	1/1	0.87	0.28	1.54	46,46,46,46	0
57	MG	YA	3011	1/1	0.97	0.27	1.47	20,20,20,20	0
57	MG	RA	3219	1/1	0.86	0.27	1.43	63,63,63,63	0
57	MG	YA	3105	1/1	0.12	0.25	1.37	21,21,21,21	0
57	MG	RA	3013	1/1	0.89	0.29	1.33	20,20,20,20	0
57	MG	RA	3226	1/1	0.48	0.27	1.29	48,48,48,48	0
57	MG	RA	3193	1/1	0.84	0.30	1.26	51,51,51,51	0
57	MG	RA	3100	1/1	0.98	0.34	1.11	9,9,9,9	0
57	MG	YA	3211	1/1	0.93	0.27	1.10	14,14,14,14	0
57	MG	RA	3155	1/1	0.76	0.30	1.07	24,24,24,24	0
57	MG	YA	3253	1/1	0.95	0.30	1.05	18,18,18,18	0
57	MG	RA	3229	1/1	0.98	0.29	1.04	5,5,5,5	0
57	MG	YA	3006	1/1	0.98	0.28	0.95	9,9,9,9	0
57	MG	YA	3101	1/1	0.93	0.30	0.94	8,8,8,8	0
57	MG	YA	3026	1/1	0.97	0.29	0.91	8,8,8,8	0
57	MG	RP	201	1/1	0.97	0.29	0.83	30,30,30,30	0
57	MG	RA	3206	1/1	0.96	0.33	0.80	15,15,15,15	0
57	MG	XA	1613	1/1	0.93	0.27	0.76	13,13,13,13	0
57	MG	YA	3044	1/1	0.97	0.29	0.75	7,7,7,7	0
57	MG	YA	3256	1/1	0.99	0.28	0.70	7,7,7,7	0
57	MG	RA	3185	1/1	0.92	0.33	0.67	25,25,25,25	0
57	MG	YA	3009	1/1	0.98	0.27	0.61	12,12,12,12	0
57	MG	RA	3050	1/1	0.74	0.26	0.60	31,31,31,31	0
57	MG	QA	1644	1/1	0.83	0.33	0.55	40,40,40,40	0
57	MG	XA	1640	1/1	0.94	0.29	0.44	31,31,31,31	0
57	MG	RA	3020	1/1	0.97	0.24	0.43	1,1,1,1	0
57	MG	YA	3180	1/1	0.95	0.25	0.41	49,49,49,49	0
57	MG	RA	3157	1/1	0.95	0.23	0.39	49,49,49,49	0
57	MG	YA	3071	1/1	0.84	0.25	0.33	10,10,10,10	0
57	MG	YA	3215	1/1	0.90	0.31	0.29	25,25,25,25	0
57	MG	YA	3049	1/1	0.95	0.28	0.26	14,14,14,14	0
57	MG	RA	3003	1/1	0.97	0.30	0.20	14,14,14,14	0
57	MG	YA	3087	1/1	0.98	0.27	0.18	15,15,15,15	0
57	MG	XA	1646	1/1	0.95	0.25	0.17	45,45,45,45	0
57	MG	RA	3016	1/1	0.98	0.24	0.17	1,1,1,1	0
57	MG	RA	3098	1/1	0.94	0.25	0.16	10,10,10,10	0
59	ZN	XD	301	1/1	0.81	0.36	0.06	45,45,45,45	0
57	MG	YA	3033	1/1	0.94	0.28	0.01	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1610	1/1	0.76	0.23	-0.01	42,42,42,42	0
57	MG	RA	3010	1/1	0.87	0.26	-0.01	78,78,78,78	0
57	MG	QA	1604	1/1	0.98	0.25	-0.05	12,12,12,12	0
57	MG	XA	1637	1/1	0.93	0.34	-0.07	24,24,24,24	0
57	MG	YA	3090	1/1	0.97	0.23	-0.13	5,5,5,5	0
57	MG	XA	1658	1/1	0.94	0.24	-0.13	46,46,46,46	0
57	MG	XA	1631	1/1	0.80	0.19	-0.16	35,35,35,35	0
57	MG	RA	3095	1/1	0.98	0.26	-0.17	14,14,14,14	0
57	MG	RA	3160	1/1	0.90	0.21	-0.17	51,51,51,51	0
57	MG	RA	3022	1/1	0.98	0.22	-0.18	16,16,16,16	0
57	MG	XA	1652	1/1	0.84	0.25	-0.20	32,32,32,32	0
57	MG	YA	3184	1/1	0.98	0.20	-0.31	20,20,20,20	0
57	MG	RE	302	1/1	0.97	0.26	-0.33	23,23,23,23	0
57	MG	YA	3002	1/1	0.98	0.27	-0.36	9,9,9,9	0
57	MG	RA	3179	1/1	0.85	0.23	-0.37	15,15,15,15	0
57	MG	RA	3133	1/1	0.93	0.18	-0.46	28,28,28,28	0
59	ZN	XN	101	1/1	0.74	0.23	-0.48	65,65,65,65	0
57	MG	RR	201	1/1	0.98	0.22	-0.49	7,7,7,7	0
57	MG	RD	301	1/1	0.89	0.23	-0.52	41,41,41,41	0
57	MG	XA	1605	1/1	0.97	0.21	-0.59	16,16,16,16	0
57	MG	YA	3047	1/1	0.96	0.28	-0.59	6,6,6,6	0
57	MG	YA	3041	1/1	0.93	0.23	-0.61	5,5,5,5	0
57	MG	RA	3086	1/1	0.91	0.23	-0.64	14,14,14,14	0
57	MG	RA	3032	1/1	0.96	0.26	-0.64	15,15,15,15	0
57	MG	RA	3142	1/1	0.86	0.24	-0.66	39,39,39,39	0
57	MG	YA	3068	1/1	0.94	0.23	-0.66	17,17,17,17	0
57	MG	QA	1611	1/1	0.96	0.25	-0.70	14,14,14,14	0
57	MG	XA	1606	1/1	0.95	0.25	-0.75	17,17,17,17	0
57	MG	RA	3078	1/1	0.95	0.21	-0.75	22,22,22,22	0
57	MG	YA	3032	1/1	0.94	0.21	-0.77	4,4,4,4	0
57	MG	YA	3048	1/1	0.95	0.22	-0.81	10,10,10,10	0
57	MG	RA	3037	1/1	0.98	0.21	-0.81	11,11,11,11	0
57	MG	QA	1617	1/1	0.92	0.16	-0.82	19,19,19,19	0
57	MG	YA	3159	1/1	0.93	0.21	-0.83	18,18,18,18	0
57	MG	RA	3073	1/1	0.96	0.21	-0.83	24,24,24,24	0
57	MG	RR	202	1/1	0.91	0.23	-0.84	19,19,19,19	0
57	MG	RA	3188	1/1	0.84	0.22	-0.85	39,39,39,39	0
57	MG	YA	3036	1/1	0.95	0.22	-0.86	5,5,5,5	0
57	MG	YA	3154	1/1	0.93	0.22	-0.87	9,9,9,9	0
57	MG	RA	3080	1/1	0.95	0.23	-0.91	19,19,19,19	0
57	MG	RA	3036	1/1	0.95	0.21	-0.92	4,4,4,4	0
57	MG	YA	3119	1/1	0.94	0.23	-0.93	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3095	1/1	0.96	0.21	-0.97	7,7,7,7	0
57	MG	RA	3119	1/1	0.86	0.24	-0.98	56,56,56,56	0
57	MG	XA	1657	1/1	0.92	0.19	-0.99	31,31,31,31	0
57	MG	YA	3031	1/1	0.98	0.22	-1.03	2,2,2,2	0
57	MG	XA	1622	1/1	0.92	0.16	-1.04	26,26,26,26	0
57	MG	RA	3212	1/1	0.81	0.19	-1.05	42,42,42,42	0
57	MG	YA	3035	1/1	0.97	0.20	-1.09	5,5,5,5	0
57	MG	RA	3027	1/1	0.99	0.23	-1.09	3,3,3,3	0
59	ZN	QD	301	1/1	0.95	0.26	-1.10	47,47,47,47	0
57	MG	YA	3107	1/1	0.87	0.22	-1.10	11,11,11,11	0
57	MG	QA	1654	1/1	0.95	0.11	-1.11	79,79,79,79	0
57	MG	YA	3181	1/1	0.93	0.21	-1.12	34,34,34,34	0
57	MG	XA	1661	1/1	0.88	0.22	-1.13	48,48,48,48	0
57	MG	RA	3041	1/1	0.97	0.21	-1.13	2,2,2,2	0
57	MG	RA	3144	1/1	0.95	0.26	-1.15	17,17,17,17	0
57	MG	YA	3008	1/1	0.91	0.22	-1.16	9,9,9,9	0
57	MG	RA	3184	1/1	0.91	0.24	-1.17	13,13,13,13	0
57	MG	QA	1632	1/1	0.87	0.22	-1.21	35,35,35,35	0
57	MG	YA	3057	1/1	0.99	0.22	-1.27	6,6,6,6	0
57	MG	XA	1668	1/1	0.93	0.33	-1.27	19,19,19,19	0
57	MG	RA	3239	1/1	0.96	0.23	-1.30	19,19,19,19	0
57	MG	YA	3227	1/1	0.90	0.18	-1.31	13,13,13,13	0
57	MG	YA	3037	1/1	0.97	0.19	-1.33	1,1,1,1	0
57	MG	QA	1669	1/1	0.91	0.23	-1.33	45,45,45,45	0
57	MG	RA	3210	1/1	0.83	0.18	-1.34	30,30,30,30	0
57	MG	RA	3121	1/1	0.95	0.20	-1.37	29,29,29,29	0
57	MG	YA	3170	1/1	0.77	0.15	-1.41	38,38,38,38	0
57	MG	YA	3260	1/1	0.97	0.17	-1.45	14,14,14,14	0
57	MG	YA	3114	1/1	0.97	0.19	-1.45	8,8,8,8	0
57	MG	XA	1620	1/1	0.97	0.23	-1.46	17,17,17,17	0
57	MG	YA	3092	1/1	0.99	0.18	-1.47	30,30,30,30	0
57	MG	YA	3042	1/1	0.98	0.19	-1.47	19,19,19,19	0
57	MG	QA	1620	1/1	0.87	0.17	-1.47	28,28,28,28	0
57	MG	XA	1653	1/1	0.79	0.15	-1.50	60,60,60,60	0
59	ZN	QN	101	1/1	0.91	0.12	-1.51	80,80,80,80	0
57	MG	YA	3197	1/1	0.96	0.13	-1.52	44,44,44,44	0
57	MG	RA	3064	1/1	0.94	0.24	-1.54	5,5,5,5	0
57	MG	YA	3178	1/1	0.94	0.19	-1.54	35,35,35,35	0
57	MG	RA	3122	1/1	0.96	0.15	-1.55	29,29,29,29	0
57	MG	YA	3129	1/1	0.89	0.19	-1.59	27,27,27,27	0
57	MG	YA	3025	1/1	0.96	0.19	-1.59	8,8,8,8	0
57	MG	YA	3072	1/1	0.89	0.23	-1.61	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3163	1/1	0.88	0.16	-1.61	38,38,38,38	0
57	MG	QA	1618	1/1	0.89	0.19	-1.61	42,42,42,42	0
57	MG	RA	3171	1/1	0.86	0.18	-1.65	33,33,33,33	0
57	MG	YA	3246	1/1	0.94	0.24	-1.68	21,21,21,21	0
57	MG	RA	3066	1/1	0.94	0.20	-1.73	24,24,24,24	0
57	MG	QA	1609	1/1	0.78	0.15	-1.74	34,34,34,34	0
57	MG	YA	3091	1/1	0.98	0.19	-1.74	21,21,21,21	0
57	MG	YA	3111	1/1	0.96	0.15	-1.75	34,34,34,34	0
57	MG	RA	3117	1/1	0.95	0.19	-1.76	3,3,3,3	0
57	MG	RA	3175	1/1	0.91	0.20	-1.78	21,21,21,21	0
57	MG	XV	101	1/1	0.94	0.19	-1.81	9,9,9,9	0
57	MG	RA	3208	1/1	0.90	0.15	-1.82	19,19,19,19	0
57	MG	YA	3058	1/1	0.96	0.18	-1.82	12,12,12,12	0
57	MG	YA	3004	1/1	0.95	0.17	-1.84	5,5,5,5	0
57	MG	YA	3073	1/1	0.97	0.21	-1.86	7,7,7,7	0
57	MG	RA	3051	1/1	0.93	0.16	-1.87	3,3,3,3	0
57	MG	XA	1614	1/1	0.97	0.17	-1.91	7,7,7,7	0
57	MG	XA	1609	1/1	0.76	0.21	-1.91	22,22,22,22	0
57	MG	YA	3125	1/1	0.96	0.18	-1.92	11,11,11,11	0
57	MG	RA	3015	1/1	0.97	0.17	-1.95	2,2,2,2	0
57	MG	QA	1655	1/1	0.88	0.14	-1.96	51,51,51,51	0
57	MG	QA	1650	1/1	0.61	0.18	-1.96	49,49,49,49	0
57	MG	YA	3014	1/1	0.96	0.17	-1.97	3,3,3,3	0
57	MG	QA	1621	1/1	0.95	0.08	-1.97	14,14,14,14	0
57	MG	RB	201	1/1	0.95	0.12	-1.99	59,59,59,59	0
57	MG	RA	3124	1/1	0.85	0.18	-1.99	23,23,23,23	0
57	MG	YA	3135	1/1	0.92	0.13	-2.02	21,21,21,21	0
57	MG	YE	302	1/1	0.87	0.20	-2.03	10,10,10,10	0
57	MG	QA	1639	1/1	0.93	0.11	-2.06	36,36,36,36	0
57	MG	YA	3070	1/1	0.96	0.19	-2.09	8,8,8,8	0
57	MG	XA	1616	1/1	0.93	0.11	-2.18	17,17,17,17	0
57	MG	XA	1647	1/1	0.81	0.15	-2.19	49,49,49,49	0
57	MG	YA	3115	1/1	0.96	0.16	-2.20	17,17,17,17	0
57	MG	YA	3024	1/1	0.93	0.19	-2.21	16,16,16,16	0
57	MG	RA	3023	1/1	0.94	0.21	-2.24	14,14,14,14	0
57	MG	RA	3043	1/1	0.83	0.16	-2.25	4,4,4,4	0
57	MG	RA	3106	1/1	0.97	0.16	-2.30	11,11,11,11	0
57	MG	XA	1645	1/1	0.90	0.13	-2.38	29,29,29,29	0
57	MG	XA	1617	1/1	0.96	0.16	-2.39	14,14,14,14	0
57	MG	YA	3132	1/1	0.94	0.14	-2.42	18,18,18,18	0
57	MG	RF	301	1/1	0.95	0.10	-2.44	40,40,40,40	0
57	MG	YA	3185	1/1	0.94	0.14	-2.47	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3059	1/1	0.93	0.16	-2.49	2,2,2,2	0
57	MG	QA	1647	1/1	0.89	0.10	-2.49	23,23,23,23	0
57	MG	RA	3137	1/1	0.85	0.20	-2.50	10,10,10,10	0
57	MG	YA	3175	1/1	0.95	0.21	-2.53	37,37,37,37	0
57	MG	YA	3228	1/1	0.91	0.19	-2.54	22,22,22,22	0
57	MG	YA	3209	1/1	0.91	0.17	-2.55	27,27,27,27	0
57	MG	YA	3217	1/1	0.89	0.15	-2.55	29,29,29,29	0
57	MG	XA	1628	1/1	0.97	0.16	-2.56	27,27,27,27	0
57	MG	RA	3147	1/1	0.98	0.18	-2.57	21,21,21,21	0
57	MG	QA	1667	1/1	0.94	0.13	-2.59	32,32,32,32	0
57	MG	QM	201	1/1	0.99	0.04	-2.59	55,55,55,55	0
57	MG	QA	1630	1/1	0.96	0.17	-2.68	48,48,48,48	0
57	MG	YA	3238	1/1	0.93	0.12	-2.68	24,24,24,24	0
57	MG	RA	3223	1/1	0.93	0.17	-2.75	23,23,23,23	0
57	MG	YA	3028	1/1	0.98	0.19	-2.76	9,9,9,9	0
57	MG	XA	1625	1/1	0.92	0.12	-2.76	16,16,16,16	0
57	MG	YA	3205	1/1	0.89	0.18	-2.78	38,38,38,38	0
57	MG	RA	3087	1/1	0.95	0.14	-2.81	34,34,34,34	0
57	MG	RA	3082	1/1	0.94	0.18	-2.82	42,42,42,42	0
57	MG	RA	3113	1/1	0.96	0.11	-2.84	32,32,32,32	0
57	MG	QA	1640	1/1	0.89	0.14	-2.85	51,51,51,51	0
57	MG	YA	3153	1/1	0.76	0.15	-2.86	21,21,21,21	0
57	MG	RA	3234	1/1	0.93	0.17	-2.90	48,48,48,48	0
57	MG	RA	3159	1/1	0.90	0.17	-2.93	30,30,30,30	0
57	MG	QA	1606	1/1	0.97	0.10	-2.95	22,22,22,22	0
57	MG	XA	1650	1/1	0.94	0.09	-2.96	26,26,26,26	0
57	MG	RA	3191	1/1	0.91	0.10	-2.98	21,21,21,21	0
57	MG	RA	3065	1/1	0.99	0.14	-3.08	16,16,16,16	0
57	MG	YB	203	1/1	0.86	0.17	-3.11	37,37,37,37	0
57	MG	RA	3123	1/1	0.97	0.19	-3.18	28,28,28,28	0
57	MG	YA	3113	1/1	0.95	0.19	-3.20	19,19,19,19	0
57	MG	QA	1614	1/1	0.93	0.12	-3.22	26,26,26,26	0
57	MG	RA	3055	1/1	0.82	0.17	-3.25	7,7,7,7	0
57	MG	YA	3081	1/1	0.98	0.19	-3.26	5,5,5,5	0
57	MG	RA	3069	1/1	0.86	0.11	-3.29	21,21,21,21	0
57	MG	QA	1636	1/1	0.99	0.09	-3.38	16,16,16,16	0
57	MG	XA	1630	1/1	0.80	0.15	-3.44	16,16,16,16	0
57	MG	XA	1621	1/1	0.82	0.15	-3.47	29,29,29,29	0
57	MG	QA	1622	1/1	0.94	0.07	-3.48	32,32,32,32	0
57	MG	YA	3224	1/1	0.93	0.15	-3.54	24,24,24,24	0
57	MG	YA	3080	1/1	0.98	0.18	-3.55	10,10,10,10	0
57	MG	YA	3142	1/1	0.93	0.22	-3.63	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1616	1/1	0.91	0.07	-3.65	40,40,40,40	0
57	MG	YA	3117	1/1	0.94	0.12	-3.79	18,18,18,18	0
57	MG	RA	3103	1/1	0.93	0.12	-3.82	8,8,8,8	0
57	MG	QA	1665	1/1	0.86	0.14	-3.83	18,18,18,18	0
57	MG	YA	3147	1/1	0.96	0.14	-3.92	8,8,8,8	0
57	MG	YA	3059	1/1	0.98	0.12	-3.95	6,6,6,6	0
57	MG	YA	3017	1/1	0.97	0.18	-3.96	2,2,2,2	0
57	MG	XA	1663	1/1	0.88	0.09	-3.97	44,44,44,44	0
57	MG	QV	101	1/1	0.99	0.15	-3.98	26,26,26,26	0
57	MG	YA	3016	1/1	0.84	0.13	-4.02	8,8,8,8	0
57	MG	YA	3108	1/1	0.99	0.17	-4.02	3,3,3,3	0
57	MG	YA	3137	1/1	0.90	0.15	-4.20	6,6,6,6	0
57	MG	RA	3089	1/1	0.98	0.15	-4.23	8,8,8,8	0
57	MG	YA	3262	1/1	0.91	0.17	-4.27	38,38,38,38	0
57	MG	QA	1659	1/1	0.94	0.11	-4.33	39,39,39,39	0
57	MG	RA	3151	1/1	0.91	0.11	-4.41	18,18,18,18	0
57	MG	YA	3168	1/1	0.96	0.08	-4.42	13,13,13,13	0
57	MG	YA	3138	1/1	0.96	0.10	-4.48	10,10,10,10	0
57	MG	YA	3082	1/1	0.92	0.14	-4.50	8,8,8,8	0
57	MG	YA	3242	1/1	0.93	0.17	-4.64	72,72,72,72	0
57	MG	QA	1646	1/1	0.91	0.09	-4.64	39,39,39,39	0
57	MG	XA	1638	1/1	0.91	0.11	-4.66	16,16,16,16	0
57	MG	XA	1624	1/1	0.93	0.10	-4.71	55,55,55,55	0
57	MG	YA	3079	1/1	0.94	0.13	-4.81	12,12,12,12	0
57	MG	YA	3176	1/1	0.98	0.16	-4.90	6,6,6,6	0
57	MG	XA	1662	1/1	0.97	0.08	-4.92	11,11,11,11	0
57	MG	YA	3056	1/1	0.96	0.14	-4.96	8,8,8,8	0
57	MG	YA	3263	1/1	0.94	0.17	-4.98	33,33,33,33	0
57	MG	YA	3038	1/1	0.95	0.12	-4.99	6,6,6,6	0
57	MG	YA	3206	1/1	0.89	0.14	-5.11	15,15,15,15	0
57	MG	YA	3065	1/1	0.94	0.14	-5.14	8,8,8,8	0
57	MG	RA	3108	1/1	0.96	0.14	-5.16	24,24,24,24	0
57	MG	RA	3165	1/1	0.89	0.09	-5.17	19,19,19,19	0
57	MG	RA	3081	1/1	0.89	0.07	-5.19	30,30,30,30	0
57	MG	YA	3190	1/1	0.99	0.07	-5.23	2,2,2,2	0
57	MG	YA	3234	1/1	0.92	0.14	-5.40	21,21,21,21	0
57	MG	QA	1610	1/1	0.98	0.13	-5.63	11,11,11,11	0
57	MG	XA	1636	1/1	0.91	0.13	-5.66	5,5,5,5	0
57	MG	QA	1613	1/1	0.93	0.19	-5.72	21,21,21,21	0
57	MG	RA	3025	1/1	0.98	0.17	-5.79	15,15,15,15	0
57	MG	YA	3112	1/1	0.98	0.06	-6.22	15,15,15,15	0
57	MG	RA	3161	1/1	0.90	0.15	-6.49	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3177	1/1	0.86	0.10	-6.63	20,20,20,20	0
57	MG	YA	3167	1/1	0.98	0.09	-6.88	21,21,21,21	0
57	MG	RA	3018	1/1	0.97	0.12	-6.90	9,9,9,9	0
57	MG	YA	3005	1/1	0.98	0.06	-7.08	1,1,1,1	0
57	MG	QA	1607	1/1	0.96	0.10	-7.23	40,40,40,40	0
57	MG	YP	201	1/1	0.92	0.12	-7.27	23,23,23,23	0
57	MG	YA	3061	1/1	0.95	0.11	-7.48	15,15,15,15	0
57	MG	RA	3150	1/1	0.90	0.13	-8.12	25,25,25,25	0
57	MG	RA	3198	1/1	0.89	0.12	-8.15	20,20,20,20	0
57	MG	RA	3162	1/1	0.93	0.14	-8.19	18,18,18,18	0
57	MG	RA	3136	1/1	0.96	0.10	-8.67	9,9,9,9	0
57	MG	YA	3218	1/1	0.92	0.10	-8.82	10,10,10,10	0
57	MG	RA	3186	1/1	0.98	0.07	-10.49	20,20,20,20	0
57	MG	RA	3075	1/1	0.97	0.09	-10.64	15,15,15,15	0
57	MG	XA	1627	1/1	0.97	0.09	-11.00	7,7,7,7	0
57	MG	XA	1612	1/1	0.97	0.12	-11.78	13,13,13,13	0
57	MG	YA	3074	1/1	0.87	0.09	-12.57	6,6,6,6	0
57	MG	YA	3201	1/1	0.89	0.13	-	14,14,14,14	0
57	MG	RA	3102	1/1	0.95	0.23	-	14,14,14,14	0
57	MG	RA	3190	1/1	0.89	0.17	-	38,38,38,38	0
57	MG	YA	3122	1/1	0.99	0.17	-	9,9,9,9	0
57	MG	RA	3201	1/1	0.84	0.20	-	24,24,24,24	0
57	MG	RA	3116	1/1	0.98	0.22	-	1,1,1,1	0
57	MG	YA	3152	1/1	0.88	0.23	-	51,51,51,51	0
57	MG	RA	3084	1/1	0.74	0.16	-	9,9,9,9	0
57	MG	XA	1656	1/1	0.73	0.12	-	31,31,31,31	0
57	MG	YA	3120	1/1	0.45	0.62	-	63,63,63,63	0
57	MG	RA	3052	1/1	0.93	0.25	-	4,4,4,4	0
57	MG	XA	1659	1/1	0.91	0.30	-	34,34,34,34	0
57	MG	YA	3013	1/1	0.96	0.22	-	1,1,1,1	0
57	MG	YA	3131	1/1	0.94	0.14	-	35,35,35,35	0
57	MG	RA	3213	1/1	0.90	0.29	-	29,29,29,29	0
57	MG	XA	1633	1/1	0.86	0.16	-	37,37,37,37	0
57	MG	YA	3001	1/1	0.96	0.22	-	9,9,9,9	0
57	MG	QA	1664	1/1	0.84	0.15	-	40,40,40,40	0
57	MG	QA	1661	1/1	0.93	0.09	-	38,38,38,38	0
57	MG	RA	3079	1/1	0.98	0.20	-	17,17,17,17	0
57	MG	YA	3194	1/1	0.86	0.23	-	41,41,41,41	0
57	MG	RA	3209	1/1	0.79	0.32	-	50,50,50,50	0
57	MG	YA	3039	1/1	0.88	0.12	-	19,19,19,19	0
57	MG	YA	3098	1/1	0.97	0.16	-	16,16,16,16	0
57	MG	YA	3247	1/1	0.92	0.13	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3086	1/1	0.97	0.22	-	6,6,6,6	0
57	MG	RA	3141	1/1	0.89	0.16	-	33,33,33,33	0
57	MG	XA	1654	1/1	0.86	0.26	-	53,53,53,53	0
57	MG	YA	3075	1/1	0.94	0.25	-	28,28,28,28	0
57	MG	RA	3011	1/1	0.94	0.49	-	32,32,32,32	0
57	MG	XA	1660	1/1	0.90	0.12	-	30,30,30,30	0
57	MG	QA	1633	1/1	0.90	0.26	-	44,44,44,44	0
57	MG	RA	3145	1/1	0.87	0.15	-	27,27,27,27	0
57	MG	YA	3019	1/1	0.98	0.25	-	1,1,1,1	0
57	MG	RA	3071	1/1	0.94	0.18	-	19,19,19,19	0
57	MG	QA	1634	1/1	0.95	0.23	-	20,20,20,20	0
57	MG	RA	3118	1/1	0.92	0.10	-	33,33,33,33	0
57	MG	RB	202	1/1	0.75	0.09	-	54,54,54,54	0
57	MG	YA	3069	1/1	0.96	0.31	-	15,15,15,15	0
57	MG	YA	3222	1/1	0.78	0.17	-	34,34,34,34	0
57	MG	QA	1658	1/1	0.92	0.20	-	63,63,63,63	0
57	MG	YA	3192	1/1	0.83	0.25	-	30,30,30,30	0
57	MG	YA	3225	1/1	0.96	0.19	-	9,9,9,9	0
57	MG	RA	3183	1/1	0.87	0.17	-	19,19,19,19	0
57	MG	YA	3063	1/1	0.87	0.14	-	13,13,13,13	0
57	MG	RA	3031	1/1	0.99	0.18	-	16,16,16,16	0
57	MG	XA	1601	1/1	0.95	0.20	-	4,4,4,4	0
57	MG	QA	1666	1/1	0.92	0.19	-	36,36,36,36	0
57	MG	YA	3158	1/1	0.73	0.18	-	24,24,24,24	0
57	MG	YQ	201	1/1	0.97	0.14	-	25,25,25,25	0
57	MG	YA	3127	1/1	0.67	0.30	-	26,26,26,26	0
57	MG	YA	3085	1/1	0.98	0.15	-	71,71,71,71	0
57	MG	XA	1603	1/1	0.96	0.14	-	38,38,38,38	0
57	MG	RA	3033	1/1	0.96	0.27	-	3,3,3,3	0
57	MG	YA	3066	1/1	0.99	0.22	-	16,16,16,16	0
57	MG	YA	3149	1/1	0.95	0.13	-	16,16,16,16	0
57	MG	QA	1656	1/1	0.68	0.26	-	52,52,52,52	0
57	MG	YA	3043	1/1	0.98	0.33	-	15,15,15,15	0
57	MG	RA	3038	1/1	0.99	0.31	-	9,9,9,9	0
57	MG	RA	3068	1/1	0.86	0.18	-	21,21,21,21	0
57	MG	XA	1615	1/1	0.98	0.08	-	15,15,15,15	0
57	MG	YA	3162	1/1	0.95	0.15	-	20,20,20,20	0
57	MG	RA	3048	1/1	0.96	0.16	-	1,1,1,1	0
57	MG	RA	3167	1/1	0.93	0.14	-	29,29,29,29	0
57	MG	YA	3045	1/1	0.83	0.18	-	2,2,2,2	0
57	MG	YA	3084	1/1	0.85	0.21	-	10,10,10,10	0
57	MG	YA	3124	1/1	0.98	0.27	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1608	1/1	0.96	0.06	-	13,13,13,13	0
57	MG	YA	3133	1/1	0.93	0.12	-	18,18,18,18	0
57	MG	XA	1639	1/1	0.91	0.09	-	35,35,35,35	0
57	MG	RA	3077	1/1	0.99	0.30	-	6,6,6,6	0
57	MG	XA	1619	1/1	0.98	0.11	-	18,18,18,18	0
57	MG	RA	3130	1/1	0.75	0.23	-	46,46,46,46	0
57	MG	QA	1625	1/1	0.92	0.09	-	36,36,36,36	0
57	MG	YA	3204	1/1	0.80	0.18	-	19,19,19,19	0
57	MG	RA	3217	1/1	0.82	0.10	-	28,28,28,28	0
57	MG	YA	3188	1/1	0.91	0.14	-	32,32,32,32	0
57	MG	RA	3128	1/1	0.96	0.25	-	31,31,31,31	0
57	MG	YA	3089	1/1	0.97	0.28	-	8,8,8,8	0
57	MG	RA	3109	1/1	0.97	0.09	-	8,8,8,8	0
57	MG	YA	3088	1/1	0.93	0.18	-	1,1,1,1	0
57	MG	YA	3021	1/1	0.98	0.30	-	9,9,9,9	0
57	MG	RA	3236	1/1	0.96	0.28	-	33,33,33,33	0
57	MG	YA	3172	1/1	0.76	0.18	-	43,43,43,43	0
57	MG	RA	3047	1/1	0.96	0.34	-	9,9,9,9	0
57	MG	YA	3123	1/1	0.94	0.18	-	9,9,9,9	0
57	MG	YA	3067	1/1	0.99	0.20	-	22,22,22,22	0
57	MG	QA	1641	1/1	0.93	0.17	-	24,24,24,24	0
57	MG	YA	3130	1/1	0.81	0.24	-	17,17,17,17	0
57	MG	QA	1651	1/1	0.87	0.21	-	35,35,35,35	0
57	MG	RA	3074	1/1	0.96	0.18	-	4,4,4,4	0
57	MG	YA	3203	1/1	0.98	0.18	-	27,27,27,27	0
57	MG	QA	1626	1/1	0.15	0.20	-	59,59,59,59	0
57	MG	YA	3254	1/1	0.97	0.19	-	7,7,7,7	0
57	MG	RA	3195	1/1	0.78	0.37	-	31,31,31,31	0
57	MG	YA	3052	1/1	0.84	0.23	-	21,21,21,21	0
57	MG	RA	3019	1/1	0.96	0.31	-	19,19,19,19	0
57	MG	YA	3174	1/1	0.86	0.12	-	19,19,19,19	0
57	MG	RA	3222	1/1	0.37	0.42	-	93,93,93,93	0
57	MG	RA	3153	1/1	0.90	0.28	-	51,51,51,51	0
57	MG	YA	3232	1/1	0.97	0.13	-	23,23,23,23	0
57	MG	YA	3223	1/1	0.94	0.15	-	25,25,25,25	0
57	MG	QA	1668	1/1	0.88	0.14	-	42,42,42,42	0
57	MG	RA	3067	1/1	0.99	0.20	-	9,9,9,9	0
57	MG	Y0	101	1/1	0.87	0.22	-	7,7,7,7	0
57	MG	RA	3007	1/1	0.98	0.24	-	6,6,6,6	0
57	MG	RA	3168	1/1	0.93	0.26	-	22,22,22,22	0
57	MG	RA	3181	1/1	0.86	0.33	-	48,48,48,48	0
57	MG	XA	1644	1/1	0.96	0.19	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3116	1/1	0.84	0.19	-	36,36,36,36	0
57	MG	RA	3062	1/1	0.91	0.11	-	56,56,56,56	0
57	MG	YA	3018	1/1	0.89	0.32	-	13,13,13,13	0
57	MG	YA	3055	1/1	0.97	0.24	-	10,10,10,10	0
57	MG	RA	3017	1/1	0.99	0.28	-	8,8,8,8	0
57	MG	RA	3237	1/1	0.96	0.27	-	26,26,26,26	0
57	MG	YA	3214	1/1	0.93	0.16	-	35,35,35,35	0
57	MG	RA	3058	1/1	0.92	0.25	-	37,37,37,37	0
57	MG	R5	101	1/1	0.89	0.19	-	19,19,19,19	0
57	MG	QA	1662	1/1	0.91	0.11	-	53,53,53,53	0
57	MG	QA	1643	1/1	0.94	0.12	-	22,22,22,22	0
57	MG	YA	3157	1/1	0.95	0.10	-	30,30,30,30	0
57	MG	RA	3228	1/1	0.85	0.67	-	58,58,58,58	0
57	MG	RA	3107	1/1	0.96	0.17	-	25,25,25,25	0
57	MG	QA	1648	1/1	0.95	0.16	-	12,12,12,12	0
57	MG	RA	3211	1/1	0.84	0.40	-	43,43,43,43	0
57	MG	RA	3114	1/1	0.98	0.25	-	20,20,20,20	0
57	MG	YA	3046	1/1	0.91	0.25	-	8,8,8,8	0
57	MG	RA	3094	1/1	0.97	0.14	-	9,9,9,9	0
57	MG	YA	3182	1/1	0.88	0.21	-	24,24,24,24	0
57	MG	YA	3202	1/1	0.93	0.22	-	59,59,59,59	0
57	MG	RA	3154	1/1	0.97	0.20	-	22,22,22,22	0
57	MG	YA	3187	1/1	0.95	0.09	-	29,29,29,29	0
57	MG	RA	3134	1/1	0.82	0.27	-	44,44,44,44	0
57	MG	RA	3164	1/1	0.91	0.29	-	36,36,36,36	0
57	MG	YA	3128	1/1	0.89	0.27	-	26,26,26,26	0
57	MG	RA	3216	1/1	0.87	0.24	-	43,43,43,43	0
57	MG	YA	3165	1/1	0.30	0.32	-	54,54,54,54	0
57	MG	RA	3028	1/1	0.98	0.23	-	4,4,4,4	0
57	MG	YA	3229	1/1	0.85	0.16	-	24,24,24,24	0
57	MG	XA	1643	1/1	0.91	0.15	-	29,29,29,29	0
57	MG	RA	3146	1/1	0.95	0.14	-	33,33,33,33	0
57	MG	QA	1645	1/1	0.81	0.28	-	53,53,53,53	0
57	MG	R0	101	1/1	0.83	0.19	-	11,11,11,11	0
57	MG	XA	1608	1/1	0.97	0.34	-	23,23,23,23	0
57	MG	QA	1601	1/1	0.94	0.17	-	33,33,33,33	0
57	MG	RA	3096	1/1	0.95	0.28	-	23,23,23,23	0
57	MG	RA	3148	1/1	0.93	0.26	-	36,36,36,36	0
57	MG	YA	3210	1/1	0.86	0.21	-	37,37,37,37	0
57	MG	YA	3094	1/1	0.96	0.18	-	2,2,2,2	0
57	MG	YA	3143	1/1	0.91	0.18	-	17,17,17,17	0
57	MG	RA	3143	1/1	0.82	0.27	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3002	1/1	0.78	0.54	-	36,36,36,36	0
57	MG	RA	3203	1/1	0.95	0.14	-	35,35,35,35	0
57	MG	YA	3226	1/1	0.95	0.19	-	3,3,3,3	0
57	MG	YA	3140	1/1	0.94	0.28	-	20,20,20,20	0
57	MG	XA	1626	1/1	0.99	0.19	-	19,19,19,19	0
57	MG	QA	1619	1/1	0.95	0.11	-	33,33,33,33	0
57	MG	YA	3161	1/1	0.93	0.10	-	25,25,25,25	0
57	MG	YA	3096	1/1	0.97	0.21	-	10,10,10,10	0
57	MG	YA	3213	1/1	0.95	0.27	-	29,29,29,29	0
57	MG	RA	3111	1/1	0.97	0.35	-	22,22,22,22	0
57	MG	RA	3104	1/1	0.98	0.19	-	16,16,16,16	0
57	MG	RA	3152	1/1	0.97	0.17	-	14,14,14,14	0
57	MG	YA	3060	1/1	0.88	0.17	-	4,4,4,4	0
57	MG	YA	3151	1/1	0.94	0.18	-	25,25,25,25	0
57	MG	YA	3010	1/1	0.97	0.21	-	4,4,4,4	0
57	MG	RA	3174	1/1	0.93	0.10	-	38,38,38,38	0
57	MG	RA	3240	1/1	0.96	0.33	-	25,25,25,25	0
57	MG	QA	1638	1/1	0.83	0.25	-	27,27,27,27	0
57	MG	YB	202	1/1	0.92	0.23	-	20,20,20,20	0
57	MG	RA	3045	1/1	0.95	0.24	-	16,16,16,16	0
57	MG	YA	3191	1/1	0.88	0.25	-	24,24,24,24	0
57	MG	YA	3198	1/1	0.76	0.34	-	59,59,59,59	0
57	MG	RA	3214	1/1	0.92	0.17	-	18,18,18,18	0
57	MG	XA	1674	1/1	0.91	0.12	-	25,25,25,25	0
57	MG	RA	3014	1/1	0.98	0.30	-	9,9,9,9	0
57	MG	RA	3030	1/1	0.95	0.27	-	12,12,12,12	0
57	MG	RE	301	1/1	0.97	0.11	-	1,1,1,1	0
57	MG	YA	3150	1/1	0.89	0.23	-	61,61,61,61	0
57	MG	YA	3145	1/1	0.91	0.23	-	11,11,11,11	0
57	MG	XA	1642	1/1	0.96	0.19	-	23,23,23,23	0
57	MG	RA	3021	1/1	0.98	0.29	-	2,2,2,2	0
57	MG	YA	3163	1/1	0.94	0.14	-	28,28,28,28	0
57	MG	RA	3158	1/1	0.90	0.33	-	51,51,51,51	0
57	MG	RA	3233	1/1	0.97	0.27	-	24,24,24,24	0
57	MG	RA	3024	1/1	0.95	0.21	-	5,5,5,5	0
57	MG	RA	3112	1/1	0.96	0.10	-	25,25,25,25	0
57	MG	YA	3252	1/1	0.96	0.38	-	25,25,25,25	0
57	MG	YA	3139	1/1	0.36	0.26	-	70,70,70,70	0
57	MG	YA	3040	1/1	0.96	0.26	-	8,8,8,8	0
57	MG	RA	3182	1/1	0.93	0.18	-	10,10,10,10	0
57	MG	YA	3237	1/1	0.82	0.21	-	44,44,44,44	0
57	MG	YA	3083	1/1	0.94	0.20	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1637	1/1	0.77	0.23	-	57,57,57,57	0
57	MG	QA	1623	1/1	0.93	0.16	-	37,37,37,37	0
57	MG	RA	3205	1/1	0.89	0.24	-	46,46,46,46	0
57	MG	YA	3077	1/1	0.97	0.23	-	16,16,16,16	0
57	MG	RA	3001	1/1	0.93	0.24	-	11,11,11,11	0
57	MG	YA	3110	1/1	0.96	0.10	-	15,15,15,15	0
57	MG	RA	3101	1/1	0.76	0.22	-	7,7,7,7	0
57	MG	RA	3004	1/1	0.97	0.32	-	15,15,15,15	0
57	MG	RA	3026	1/1	0.81	0.16	-	8,8,8,8	0
57	MG	RA	3156	1/1	0.94	0.23	-	44,44,44,44	0
57	MG	RA	3199	1/1	0.77	0.14	-	29,29,29,29	0
57	MG	QA	1603	1/1	0.92	0.16	-	7,7,7,7	0
57	MG	RA	3231	1/1	0.96	0.37	-	9,9,9,9	0
57	MG	RA	3085	1/1	0.95	0.18	-	16,16,16,16	0
57	MG	YA	3241	1/1	0.59	0.25	-	46,46,46,46	0
57	MG	XA	1607	1/1	0.94	0.28	-	31,31,31,31	0
57	MG	YA	3003	1/1	0.98	0.22	-	10,10,10,10	0
57	MG	YA	3078	1/1	0.97	0.24	-	19,19,19,19	0
57	MG	QA	1663	1/1	0.94	0.10	-	82,82,82,82	0
57	MG	RA	3177	1/1	0.76	0.40	-	38,38,38,38	0
57	MG	YA	3251	1/1	0.92	0.29	-	20,20,20,20	0
57	MG	YA	3216	1/1	0.88	0.20	-	59,59,59,59	0
57	MG	YA	3166	1/1	0.89	0.30	-	58,58,58,58	0
57	MG	QA	1605	1/1	0.93	0.32	-	30,30,30,30	0
57	MG	QA	1627	1/1	0.93	0.10	-	26,26,26,26	0
57	MG	YA	3156	1/1	0.90	0.26	-	33,33,33,33	0
57	MG	YA	3186	1/1	0.94	0.16	-	39,39,39,39	0
57	MG	QA	1602	1/1	0.93	0.20	-	18,18,18,18	0
57	MG	RA	3180	1/1	0.84	0.17	-	34,34,34,34	0
57	MG	RA	3012	1/1	0.98	0.26	-	8,8,8,8	0
57	MG	XA	1670	1/1	0.95	0.11	-	29,29,29,29	0
57	MG	RA	3070	1/1	0.93	0.24	-	26,26,26,26	0
57	MG	YA	3236	1/1	0.92	0.22	-	40,40,40,40	0
57	MG	RA	3139	1/1	0.73	0.20	-	49,49,49,49	0
57	MG	XA	1655	1/1	0.56	0.23	-	81,81,81,81	0
57	MG	RA	3061	1/1	0.97	0.28	-	9,9,9,9	0
57	MG	YA	3053	1/1	0.95	0.23	-	5,5,5,5	0
57	MG	RA	3092	1/1	0.94	0.12	-	9,9,9,9	0
57	MG	XA	1664	1/1	0.87	0.24	-	51,51,51,51	0
57	MG	YA	3121	1/1	0.97	0.11	-	18,18,18,18	0
57	MG	YA	3244	1/1	0.83	0.28	-	25,25,25,25	0
57	MG	YA	3243	1/1	0.90	0.21	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1628	1/1	0.95	0.28	-	25,25,25,25	0
57	MG	XA	1648	1/1	0.90	0.11	-	39,39,39,39	0
57	MG	YA	3155	1/1	0.86	0.17	-	53,53,53,53	0
57	MG	RA	3105	1/1	0.96	0.26	-	18,18,18,18	0
57	MG	YA	3164	1/1	0.59	0.41	-	36,36,36,36	0
57	MG	QH	201	1/1	0.77	0.09	-	58,58,58,58	0
57	MG	QA	1660	1/1	0.91	0.21	-	35,35,35,35	0
57	MG	YA	3146	1/1	0.84	0.32	-	57,57,57,57	0
57	MG	QA	1635	1/1	0.97	0.08	-	33,33,33,33	0
57	MG	YA	3220	1/1	0.81	0.32	-	52,52,52,52	0
57	MG	RA	3127	1/1	0.86	0.21	-	23,23,23,23	0
57	MG	XA	1604	1/1	0.97	0.14	-	15,15,15,15	0
57	MG	YA	3230	1/1	0.95	0.18	-	32,32,32,32	0
57	MG	RA	3187	1/1	0.86	0.24	-	63,63,63,63	0
57	MG	RA	3149	1/1	0.93	0.17	-	32,32,32,32	0
57	MG	YA	3200	1/1	0.88	0.19	-	26,26,26,26	0
57	MG	YA	3007	1/1	0.99	0.20	-	9,9,9,9	0
57	MG	RA	3232	1/1	0.79	0.18	-	30,30,30,30	0
57	MG	XV	102	1/1	0.97	0.21	-	0,0,0,0	0
57	MG	RA	3166	1/1	0.94	0.12	-	43,43,43,43	0
57	MG	RA	3042	1/1	0.98	0.24	-	3,3,3,3	0
57	MG	RA	3046	1/1	0.97	0.15	-	12,12,12,12	0
57	MG	QA	1624	1/1	0.96	0.19	-	27,27,27,27	0
57	MG	RA	3083	1/1	0.96	0.20	-	11,11,11,11	0
57	MG	YA	3126	1/1	0.92	0.15	-	22,22,22,22	0
57	MG	YA	3022	1/1	0.91	0.28	-	7,7,7,7	0
57	MG	XA	1629	1/1	0.96	0.19	-	29,29,29,29	0
57	MG	RA	3202	1/1	0.95	0.10	-	21,21,21,21	0
57	MG	RA	3040	1/1	0.97	0.30	-	21,21,21,21	0
57	MG	YA	3118	1/1	0.96	0.28	-	25,25,25,25	0
57	MG	YA	3097	1/1	0.97	0.21	-	19,19,19,19	0
57	MG	RA	3091	1/1	0.69	0.47	-	73,73,73,73	0
57	MG	YA	3183	1/1	0.87	0.18	-	30,30,30,30	0
57	MG	RA	3215	1/1	0.86	0.14	-	48,48,48,48	0
57	MG	RA	3218	1/1	0.91	0.18	-	29,29,29,29	0
57	MG	RA	3227	1/1	0.74	0.24	-	73,73,73,73	0
57	MG	XA	1669	1/1	0.97	0.16	-	41,41,41,41	0
57	MG	RA	3044	1/1	0.91	0.21	-	24,24,24,24	0
57	MG	XA	1672	1/1	0.65	0.20	-	40,40,40,40	0
57	MG	YA	3104	1/1	0.94	0.25	-	24,24,24,24	0
57	MG	RA	3120	1/1	0.21	0.34	-	60,60,60,60	0
57	MG	YA	3265	1/1	0.96	0.29	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3160	1/1	0.80	0.16	-	12,12,12,12	0
57	MG	YA	3102	1/1	0.95	0.26	-	12,12,12,12	0
57	MG	YB	201	1/1	0.93	0.32	-	35,35,35,35	0
57	MG	YA	3173	1/1	0.84	0.21	-	43,43,43,43	0
57	MG	XA	1602	1/1	0.98	0.12	-	30,30,30,30	0
57	MG	RA	3172	1/1	0.95	0.12	-	23,23,23,23	0
57	MG	RA	3140	1/1	0.95	0.38	-	26,26,26,26	0
57	MG	Y5	101	1/1	0.98	0.16	-	26,26,26,26	0
57	MG	RA	3196	1/1	0.92	0.20	-	15,15,15,15	0
57	MG	YA	3136	1/1	0.98	0.17	-	18,18,18,18	0
57	MG	YA	3189	1/1	0.76	0.27	-	23,23,23,23	0
57	MG	RA	3135	1/1	0.87	0.17	-	16,16,16,16	0
57	MG	RA	3072	1/1	0.94	0.24	-	13,13,13,13	0
57	MG	RA	3097	1/1	0.95	0.27	-	14,14,14,14	0
57	MG	YA	3051	1/1	0.99	0.18	-	2,2,2,2	0
57	MG	YA	3199	1/1	0.91	0.31	-	18,18,18,18	0
57	MG	YE	301	1/1	0.87	0.18	-	7,7,7,7	0
57	MG	QA	1629	1/1	0.38	0.33	-	43,43,43,43	0
57	MG	YA	3233	1/1	0.93	0.12	-	34,34,34,34	0
57	MG	RA	3115	1/1	0.75	0.20	-	7,7,7,7	0
57	MG	XA	1649	1/1	0.85	0.20	-	30,30,30,30	0
57	MG	YA	3062	1/1	0.96	0.12	-	9,9,9,9	0
57	MG	QA	1653	1/1	0.94	0.15	-	36,36,36,36	0
57	MG	QF	201	1/1	0.90	0.20	-	39,39,39,39	0
57	MG	RA	3207	1/1	0.76	0.36	-	47,47,47,47	0
57	MG	RA	3225	1/1	0.88	0.10	-	27,27,27,27	0
57	MG	QA	1612	1/1	0.96	0.21	-	13,13,13,13	0
57	MG	YA	3029	1/1	0.93	0.23	-	12,12,12,12	0
57	MG	YA	3134	1/1	0.93	0.18	-	21,21,21,21	0
57	MG	YA	3106	1/1	0.94	0.13	-	9,9,9,9	0
57	MG	YA	3245	1/1	0.97	0.14	-	38,38,38,38	0
57	MG	RA	3235	1/1	0.89	0.25	-	22,22,22,22	0
57	MG	XA	1634	1/1	0.96	0.10	-	15,15,15,15	0
57	MG	YA	3169	1/1	0.96	0.20	-	20,20,20,20	0
57	MG	XA	1641	1/1	0.95	0.10	-	40,40,40,40	0
57	MG	RA	3138	1/1	0.85	0.32	-	12,12,12,12	0
57	MG	RA	3054	1/1	0.94	0.11	-	0,0,0,0	0
57	MG	RA	3008	1/1	0.89	0.20	-	27,27,27,27	0
57	MG	RA	3009	1/1	0.91	0.10	-	9,9,9,9	0
57	MG	RA	3197	1/1	0.85	0.18	-	55,55,55,55	0
57	MG	YA	3195	1/1	0.89	0.20	-	35,35,35,35	0
57	MG	YA	3179	1/1	0.89	0.23	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3208	1/1	0.82	0.15	-	55,55,55,55	0
57	MG	YA	3076	1/1	0.98	0.34	-	7,7,7,7	0
57	MG	YA	3221	1/1	0.85	0.23	-	19,19,19,19	0
57	MG	RA	3176	1/1	0.81	0.14	-	24,24,24,24	0
57	MG	RA	3170	1/1	0.91	0.11	-	25,25,25,25	0
57	MG	XA	1671	1/1	0.86	0.16	-	71,71,71,71	0
57	MG	YA	3193	1/1	0.95	0.20	-	27,27,27,27	0
57	MG	YA	3012	1/1	0.96	0.38	-	9,9,9,9	0
57	MG	RA	3189	1/1	0.95	0.10	-	34,34,34,34	0
57	MG	RA	3129	1/1	0.97	0.12	-	21,21,21,21	0
57	MG	YA	3141	1/1	0.97	0.10	-	16,16,16,16	0
57	MG	YA	3196	1/1	0.78	0.30	-	28,28,28,28	0
57	MG	YA	3264	1/1	0.96	0.13	-	24,24,24,24	0
57	MG	YA	3064	1/1	0.97	0.08	-	39,39,39,39	0
57	MG	YA	3257	1/1	0.99	0.24	-	3,3,3,3	0
57	MG	XA	1651	1/1	0.97	0.14	-	12,12,12,12	0
57	MG	YA	3148	1/1	0.93	0.16	-	14,14,14,14	0
57	MG	QA	1652	1/1	0.96	0.20	-	37,37,37,37	0
57	MG	XA	1635	1/1	0.87	0.16	-	41,41,41,41	0
57	MG	YA	3103	1/1	0.94	0.22	-	31,31,31,31	0
57	MG	YA	3250	1/1	0.95	0.12	-	40,40,40,40	0
57	MG	RA	3224	1/1	0.98	0.11	-	52,52,52,52	0
57	MG	RA	3090	1/1	0.97	0.17	-	23,23,23,23	0
57	MG	RA	3110	1/1	0.92	0.21	-	9,9,9,9	0
57	MG	YA	3248	1/1	0.98	0.23	-	26,26,26,26	0
57	MG	RA	3093	1/1	0.95	0.26	-	9,9,9,9	0
57	MG	XA	1666	1/1	0.90	0.34	-	43,43,43,43	0
57	MG	RA	3178	1/1	0.92	0.16	-	22,22,22,22	0
57	MG	YA	3231	1/1	0.95	0.10	-	19,19,19,19	0
57	MG	YA	3212	1/1	0.98	0.11	-	9,9,9,9	0
57	MG	XX	101	1/1	0.95	0.18	-	22,22,22,22	0
57	MG	RA	3049	1/1	0.89	0.10	-	8,8,8,8	0
57	MG	YA	3249	1/1	0.95	0.18	-	26,26,26,26	0
57	MG	YA	3093	1/1	0.97	0.16	-	13,13,13,13	0
57	MG	XA	1665	1/1	0.83	0.21	-	44,44,44,44	0
57	MG	RA	3194	1/1	0.80	0.22	-	44,44,44,44	0
57	MG	YA	3054	1/1	0.94	0.22	-	49,49,49,49	0
57	MG	QA	1649	1/1	0.96	0.17	-	39,39,39,39	0
57	MG	RA	3173	1/1	0.88	0.16	-	15,15,15,15	0
57	MG	XA	1611	1/1	0.93	0.21	-	23,23,23,23	0
57	MG	XA	1632	1/1	0.91	0.18	-	17,17,17,17	0
57	MG	QA	1642	1/1	0.97	0.11	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1618	1/1	0.98	0.16	-	7,7,7,7	0
57	MG	RA	3006	1/1	0.95	0.34	-	18,18,18,18	0
57	MG	RA	3169	1/1	0.97	0.45	-	35,35,35,35	0
57	MG	YA	3030	1/1	0.94	0.38	-	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.