



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2017 – 03:13 AM EST

PDB ID : 4TUD  
Title : Crystal structure of ASL-SufJ bound to Codon ACC-C on the Ribosome  
Authors : Fagan, C.E.; Dunham, C.M.  
Deposited on : unknown  
Resolution : 3.60 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

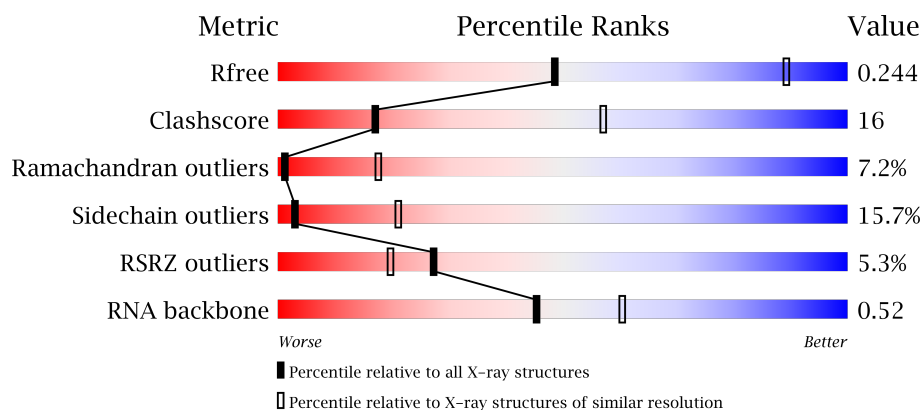
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)
RNA backbone	2435	1002 (4.30-2.90)

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	
1	XA	1522	
2	QB	256	
2	XB	256	







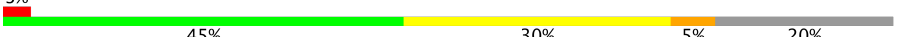
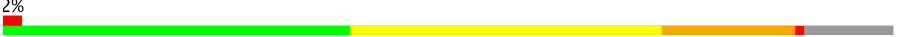
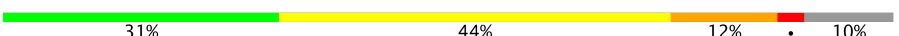

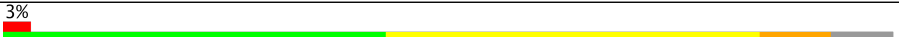
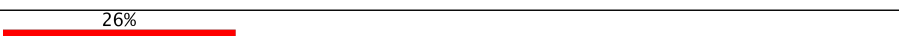

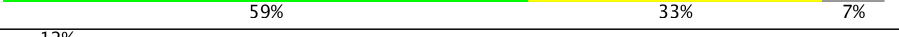






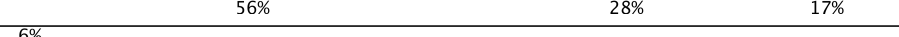




*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

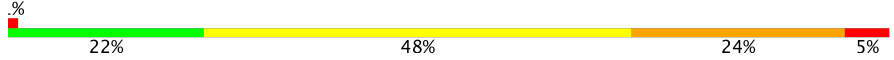
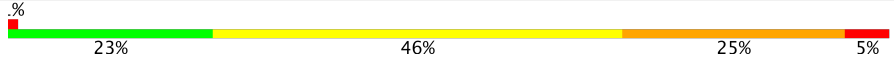

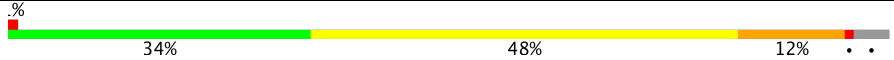
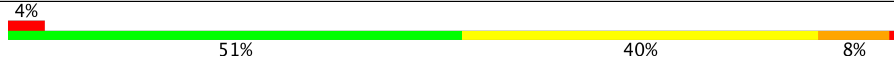
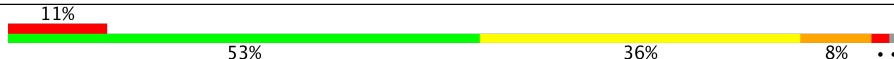
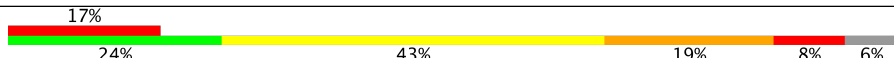
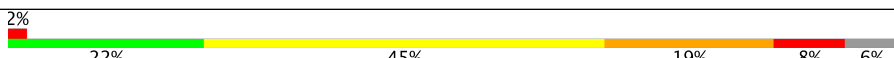
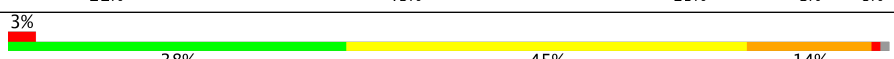
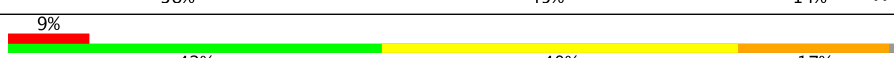


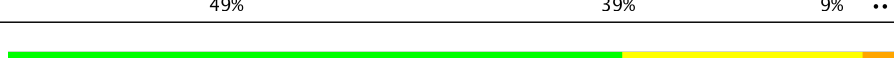
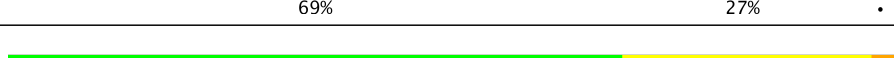



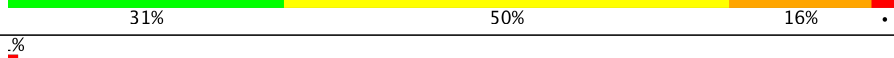
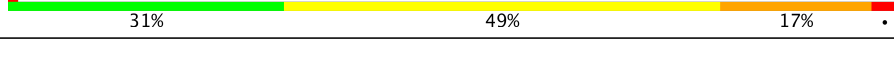


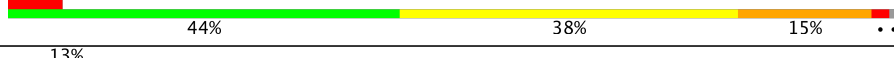
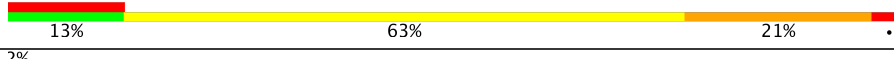
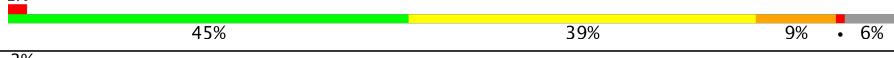
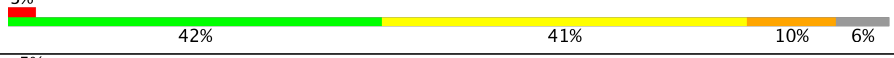
Continued from previous page...

Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

Continued on next page...



Continued from previous page...

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

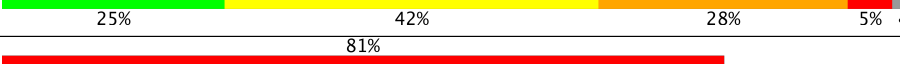
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z5	3	
56	Z6	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	1605	-	-	-	X
57	MG	QA	1613	-	-	-	X
57	MG	QA	1614	-	-	-	X
57	MG	QA	1615	-	-	-	X
57	MG	QA	1620	-	-	-	X
57	MG	QA	1622	-	-	-	X
57	MG	QA	1639	-	-	-	X
57	MG	QA	1645	-	-	-	X
57	MG	QA	1658	-	-	-	X
57	MG	QA	1660	-	-	-	X
57	MG	QA	1662	-	-	-	X
57	MG	QA	1665	-	-	-	X
57	MG	QA	1666	-	-	-	X
57	MG	QA	1669	-	-	-	X
57	MG	QA	1674	-	-	-	X
57	MG	QA	1676	-	-	-	X
57	MG	QA	1682	-	-	-	X
57	MG	QA	1684	-	-	-	X
57	MG	QA	1689	-	-	-	X
57	MG	R8	101	-	-	-	X
57	MG	RA	3002	-	-	-	X
57	MG	RA	3004	-	-	-	X
57	MG	RA	3006	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3011	-	-	-	X
57	MG	RA	3014	-	-	-	X
57	MG	RA	3018	-	-	-	X
57	MG	RA	3020	-	-	-	X
57	MG	RA	3023	-	-	-	X
57	MG	RA	3025	-	-	-	X
57	MG	RA	3032	-	-	-	X
57	MG	RA	3033	-	-	-	X
57	MG	RA	3035	-	-	-	X
57	MG	RA	3037	-	-	-	X
57	MG	RA	3039	-	-	-	X
57	MG	RA	3048	-	-	-	X
57	MG	RA	3051	-	-	-	X
57	MG	RA	3055	-	-	-	X
57	MG	RA	3056	-	-	-	X
57	MG	RA	3057	-	-	-	X
57	MG	RA	3058	-	-	-	X
57	MG	RA	3061	-	-	-	X
57	MG	RA	3062	-	-	-	X
57	MG	RA	3067	-	-	-	X
57	MG	RA	3073	-	-	-	X
57	MG	RA	3075	-	-	-	X
57	MG	RA	3077	-	-	-	X
57	MG	RA	3079	-	-	-	X
57	MG	RA	3083	-	-	-	X
57	MG	RA	3086	-	-	-	X
57	MG	RA	3087	-	-	-	X
57	MG	RA	3092	-	-	-	X
57	MG	RA	3093	-	-	-	X
57	MG	RA	3095	-	-	-	X
57	MG	RA	3096	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3100	-	-	-	X
57	MG	RA	3103	-	-	-	X
57	MG	RA	3108	-	-	-	X
57	MG	RA	3112	-	-	-	X
57	MG	RA	3116	-	-	-	X
57	MG	RA	3117	-	-	-	X
57	MG	RA	3121	-	-	-	X
57	MG	RA	3126	-	-	-	X
57	MG	RA	3132	-	-	-	X
57	MG	RA	3147	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3150	-	-	-	X
57	MG	RA	3152	-	-	-	X
57	MG	RA	3154	-	-	-	X
57	MG	RA	3161	-	-	-	X
57	MG	RA	3162	-	-	-	X
57	MG	RA	3166	-	-	-	X
57	MG	RA	3170	-	-	-	X
57	MG	RA	3175	-	-	-	X
57	MG	RA	3187	-	-	-	X
57	MG	RA	3188	-	-	-	X
57	MG	RA	3197	-	-	-	X
57	MG	RA	3198	-	-	-	X
57	MG	RA	3200	-	-	-	X
57	MG	RA	3217	-	-	-	X
57	MG	RA	3220	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3227	-	-	-	X
57	MG	RA	3232	-	-	-	X
57	MG	RA	3237	-	-	-	X
57	MG	RA	3257	-	-	-	X
57	MG	RA	3268	-	-	-	X
57	MG	RA	3274	-	-	-	X
57	MG	RA	3277	-	-	-	X
57	MG	RA	3283	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RR	201	-	-	-	X
57	MG	XA	1602	-	-	-	X
57	MG	XA	1603	-	-	-	X
57	MG	XA	1606	-	-	-	X
57	MG	XA	1616	-	-	-	X
57	MG	XA	1617	-	-	-	X
57	MG	XA	1618	-	-	-	X
57	MG	XA	1619	-	-	-	X
57	MG	XA	1621	-	-	-	X
57	MG	XA	1623	-	-	-	X
57	MG	XA	1626	-	-	-	X
57	MG	XA	1631	-	-	-	X
57	MG	XA	1632	-	-	-	X
57	MG	XA	1633	-	-	-	X
57	MG	XA	1640	-	-	-	X
57	MG	XA	1641	-	-	-	X
57	MG	XA	1650	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1663	-	-	-	X
57	MG	XA	1671	-	-	-	X
57	MG	XA	1675	-	-	-	X
57	MG	XA	1680	-	-	-	X
57	MG	XA	1689	-	-	-	X
57	MG	XA	1691	-	-	-	X
57	MG	XA	1695	-	-	-	X
57	MG	XD	302	-	-	-	X
57	MG	XV	102	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3006	-	-	-	X
57	MG	YA	3008	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3015	-	-	-	X
57	MG	YA	3017	-	-	-	X
57	MG	YA	3023	-	-	-	X
57	MG	YA	3025	-	-	-	X
57	MG	YA	3026	-	-	-	X
57	MG	YA	3027	-	-	-	X
57	MG	YA	3028	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3032	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3034	-	-	-	X
57	MG	YA	3035	-	-	-	X
57	MG	YA	3036	-	-	-	X
57	MG	YA	3037	-	-	-	X
57	MG	YA	3038	-	-	-	X
57	MG	YA	3041	-	-	-	X
57	MG	YA	3042	-	-	-	X
57	MG	YA	3047	-	-	-	X
57	MG	YA	3048	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3068	-	-	-	X
57	MG	YA	3071	-	-	-	X
57	MG	YA	3072	-	-	-	X
57	MG	YA	3078	-	-	-	X
57	MG	YA	3080	-	-	-	X
57	MG	YA	3084	-	-	-	X
57	MG	YA	3087	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3088	-	-	-	X
57	MG	YA	3096	-	-	-	X
57	MG	YA	3097	-	-	-	X
57	MG	YA	3098	-	-	-	X
57	MG	YA	3105	-	-	-	X
57	MG	YA	3106	-	-	-	X
57	MG	YA	3110	-	-	-	X
57	MG	YA	3112	-	-	-	X
57	MG	YA	3115	-	-	-	X
57	MG	YA	3121	-	-	-	X
57	MG	YA	3122	-	-	-	X
57	MG	YA	3132	-	-	-	X
57	MG	YA	3135	-	-	-	X
57	MG	YA	3137	-	-	-	X
57	MG	YA	3141	-	-	-	X
57	MG	YA	3154	-	-	-	X
57	MG	YA	3155	-	-	-	X
57	MG	YA	3161	-	-	-	X
57	MG	YA	3162	-	-	-	X
57	MG	YA	3164	-	-	-	X
57	MG	YA	3168	-	-	-	X
57	MG	YA	3170	-	-	-	X
57	MG	YA	3172	-	-	-	X
57	MG	YA	3176	-	-	-	X
57	MG	YA	3178	-	-	-	X
57	MG	YA	3185	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3192	-	-	-	X
57	MG	YA	3199	-	-	-	X
57	MG	YA	3200	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3213	-	-	-	X
57	MG	YA	3215	-	-	-	X
57	MG	YA	3227	-	-	-	X
57	MG	YA	3231	-	-	-	X
57	MG	YA	3233	-	-	-	X
57	MG	YA	3235	-	-	-	X
57	MG	YA	3237	-	-	-	X
57	MG	YA	3241	-	-	-	X
57	MG	YA	3242	-	-	-	X
57	MG	YA	3244	-	-	-	X
57	MG	YA	3246	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3259	-	-	-	X
57	MG	YA	3262	-	-	-	X
57	MG	YA	3269	-	-	-	X
57	MG	YA	3273	-	-	-	X
57	MG	YA	3277	-	-	-	X
57	MG	YA	3278	-	-	-	X
57	MG	YA	3280	-	-	-	X
57	MG	YA	3283	-	-	-	X
57	MG	YA	3292	-	-	-	X
57	MG	YD	301	-	-	-	X
57	MG	YR	202	-	-	-	X
58	PAR	QA	1691	-	-	-	X
60	PPU	Z6	101	-	-	-	X



## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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 Thx.

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	QX	9	Total	C	N	O	P	0	0	0
			173	76	31	57	9			
23	XX	9	Total	C	N	O	P	0	0	0
			173	76	31	57	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			
24	XY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			

- 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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*



*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	58	Total	C	N	O	S	0	0	0
			454	285	89	75	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 CC-Puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z5	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			
56	Z6	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	92	Total	Mg	0	0
			92	92		
57	YA	294	Total	Mg	0	0
			294	294		
57	Y5	1	Total	Mg	0	0
			1	1		
57	YR	2	Total	Mg	0	0
			2	2		
57	Y1	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

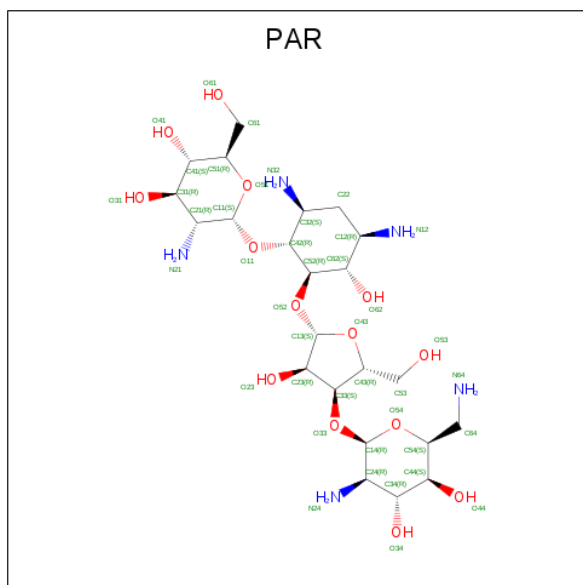
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YD	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	QV	3	Total 3	Mg 3	0	0
57	XA	104	Total 104	Mg 104	0	0
57	YY	1	Total 1	Mg 1	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	XY	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	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	RA	284	Total 284	Mg 284	0	0
57	YP	2	Total 2	Mg 2	0	0
57	RE	1	Total 1	Mg 1	0	0
57	YB	3	Total 3	Mg 3	0	0
57	QT	1	Total 1	Mg 1	0	0
57	QY	1	Total 1	Mg 1	0	0
57	XV	4	Total 4	Mg 4	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RB	3	Total	Mg	0	0
			3	3		
57	XD	1	Total	Mg	0	0
			1	1		
57	YE	1	Total	Mg	0	0
			1	1		

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



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

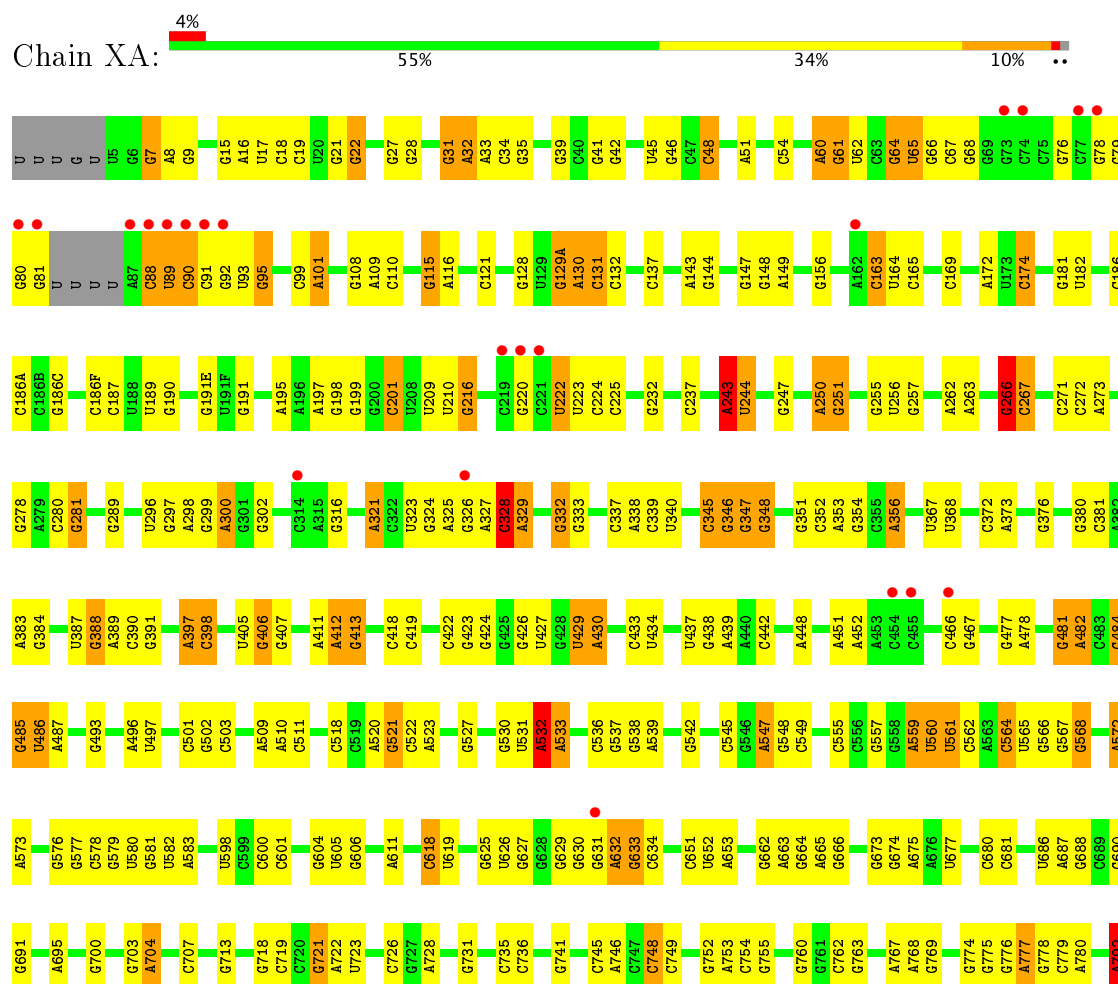
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

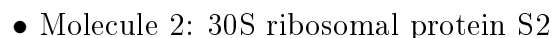
- 

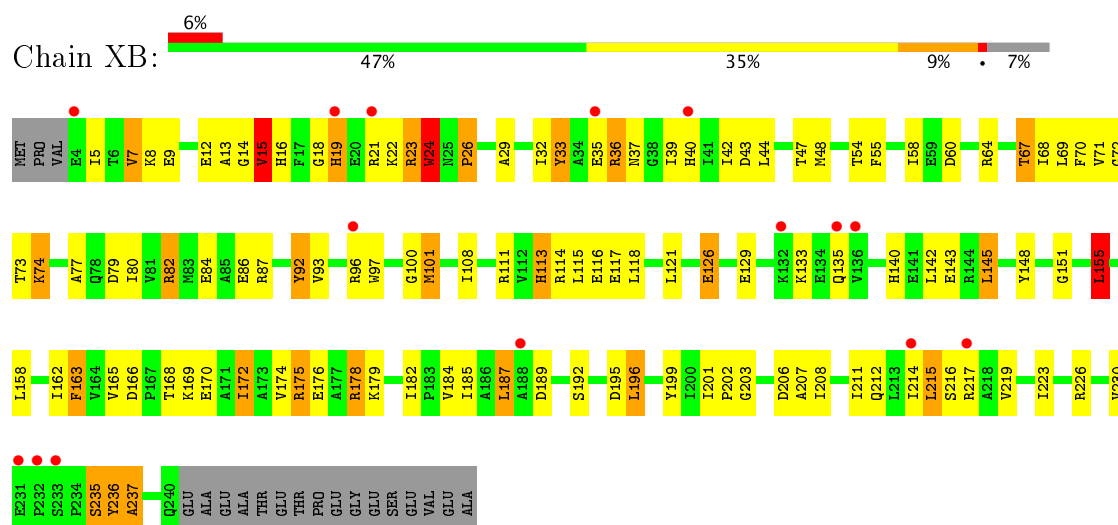
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	Z5	1	Total 37	C 22	N 7	O 7	P 1	0	0
60	Z6	1	Total 37	C 22	N 7	O 7	P 1	0	0



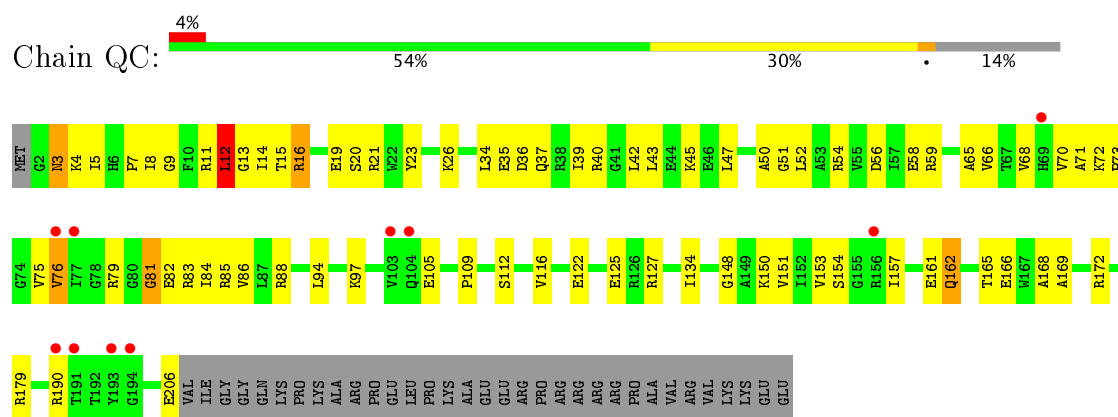




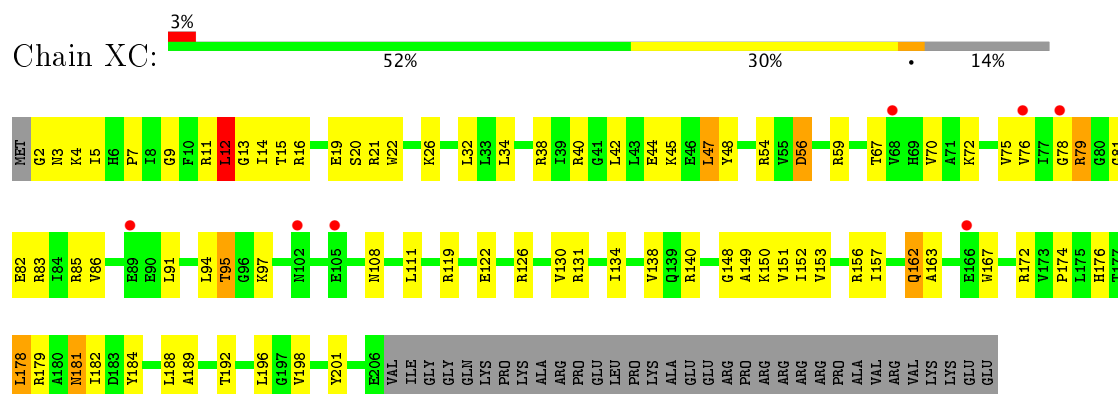




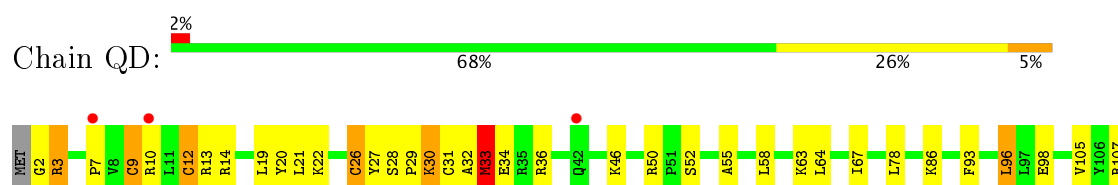
- Molecule 3: 30S ribosomal protein S3

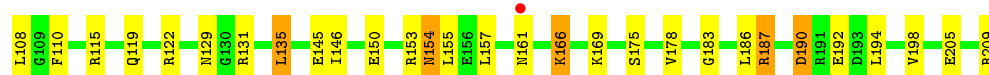


- Molecule 3: 30S ribosomal protein S3



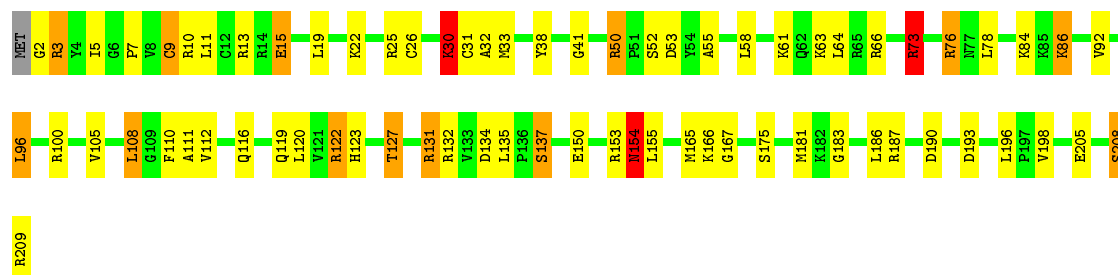
- Molecule 4: 30S ribosomal protein S4





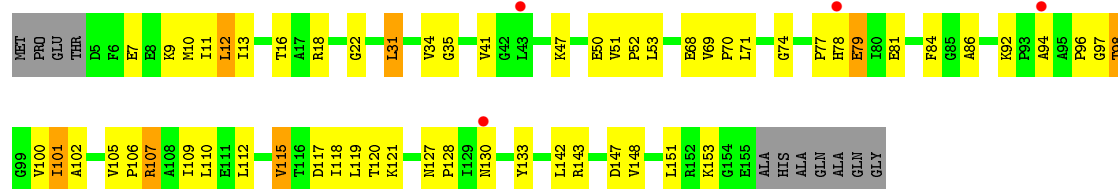
- Molecule 4: 30S ribosomal protein S4

Chain XD: 66% 26% 6% .



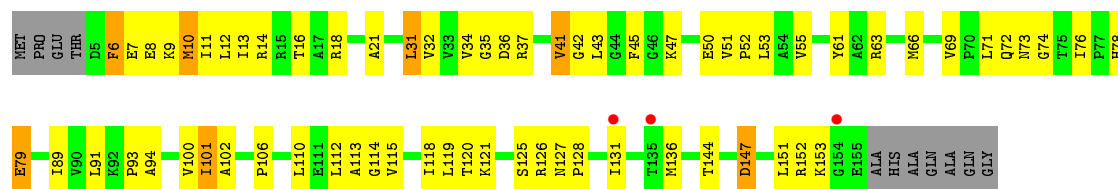
- Molecule 5: 30S ribosomal protein S5

Chain QE: 2% 57% 32% 7% .



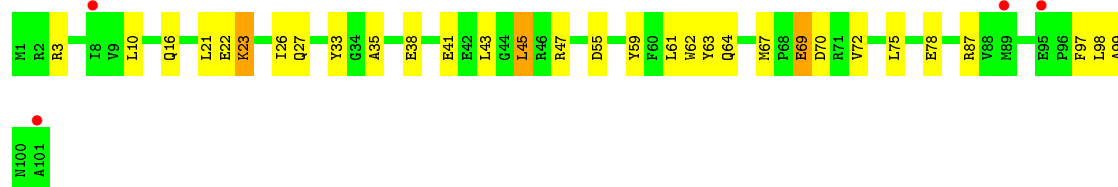
- Molecule 5: 30S ribosomal protein S5

Chain XE: 2% 52% 37% 7% .



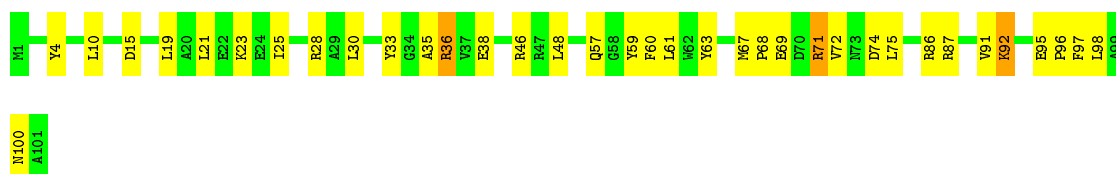
- Molecule 6: 30S ribosomal protein S6

Chain QF: 4% 69% 28% .

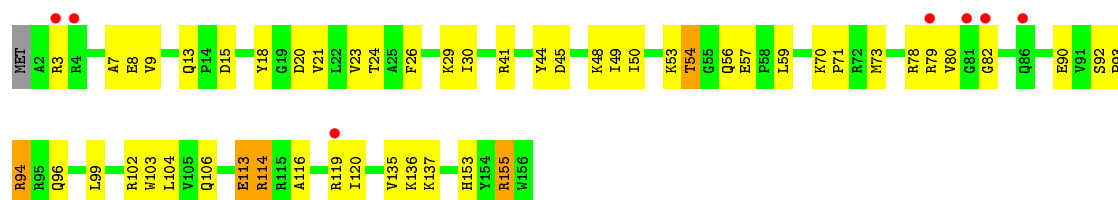


- Molecule 6: 30S ribosomal protein S6

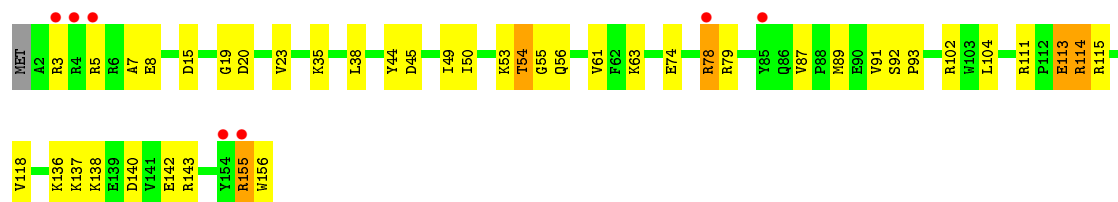
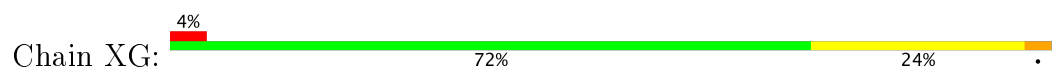
Chain XF: 64% 33% .



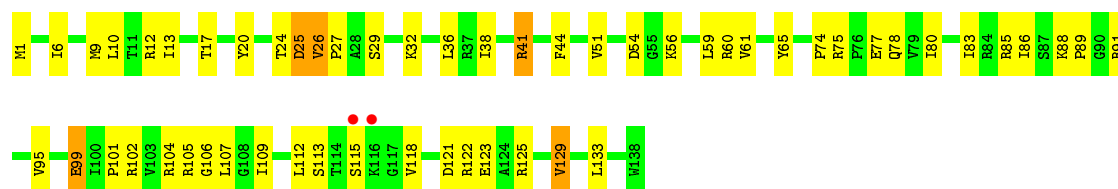
- Molecule 7: 30S ribosomal protein S7



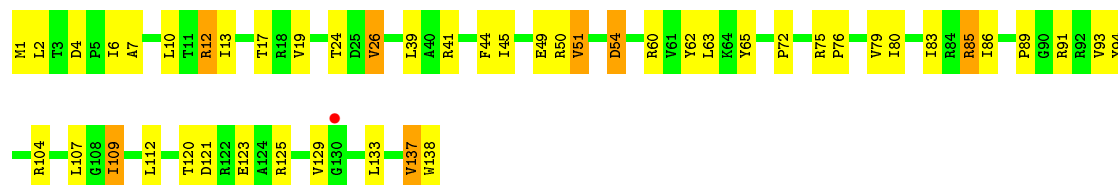
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

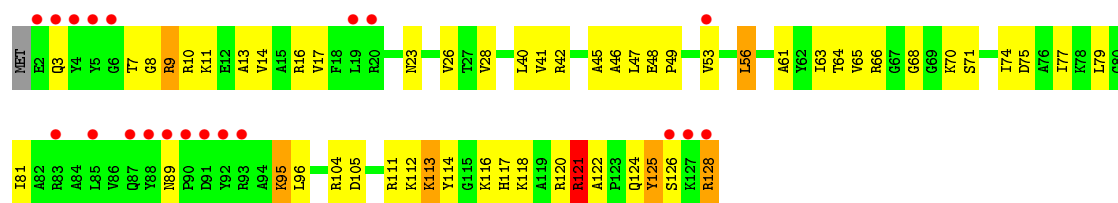


- Molecule 8: 30S ribosomal protein S8

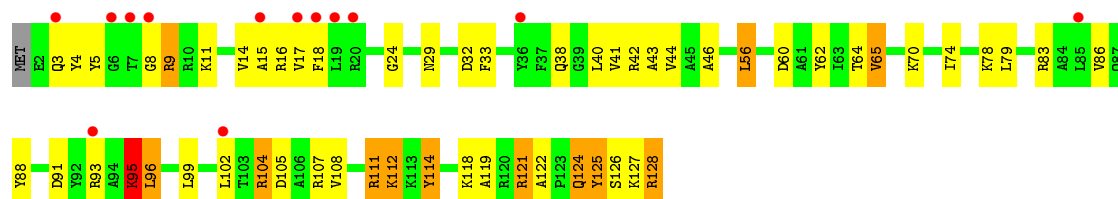


- Molecule 9: 30S ribosomal protein S9

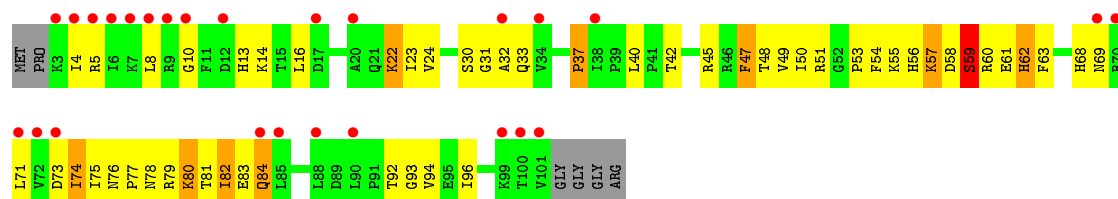
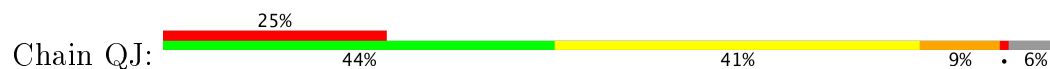




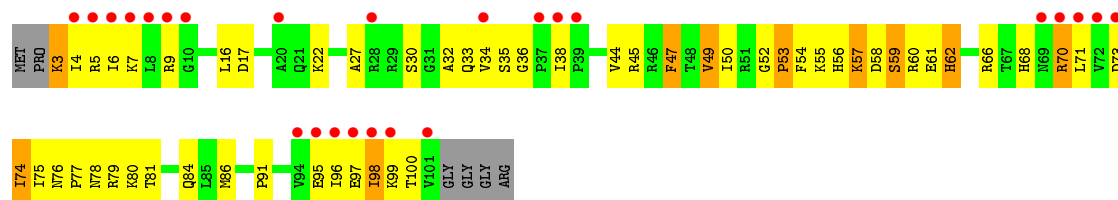
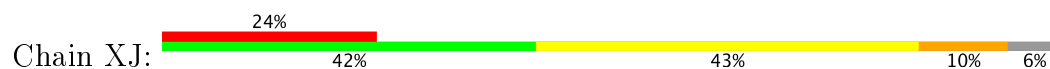
• Molecule 9: 30S ribosomal protein S9



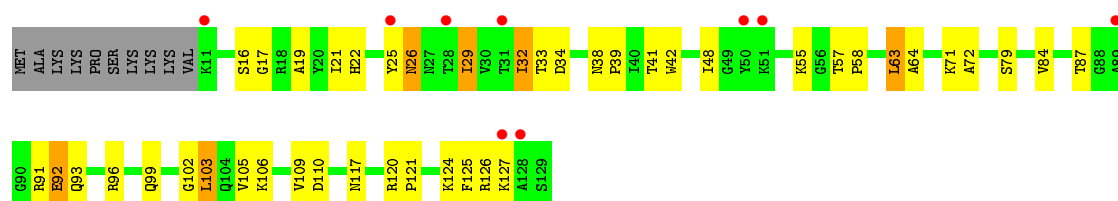
• Molecule 10: 30S ribosomal protein S10



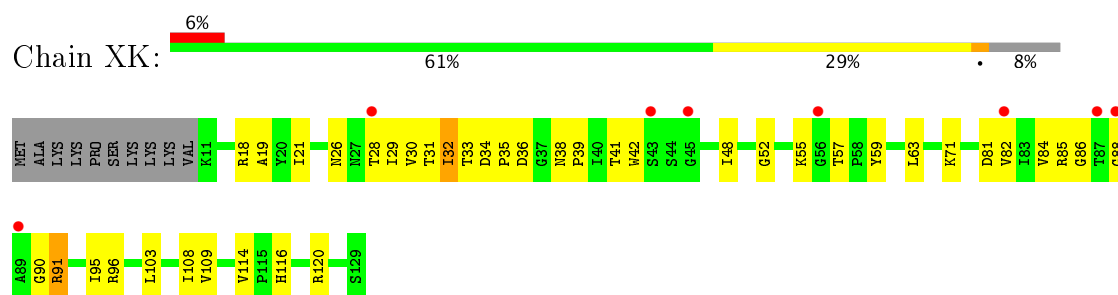
• Molecule 10: 30S ribosomal protein S10



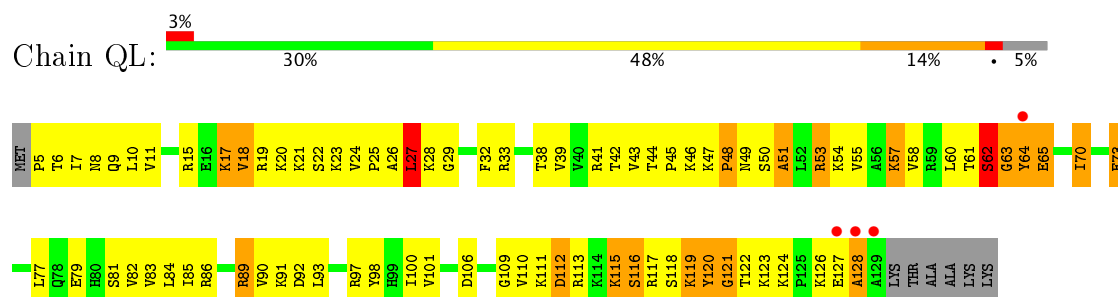
• Molecule 11: 30S ribosomal protein S11



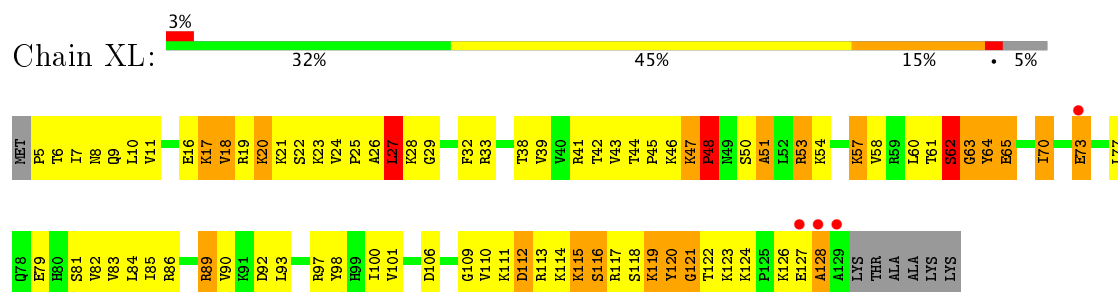
• Molecule 11: 30S ribosomal protein S11



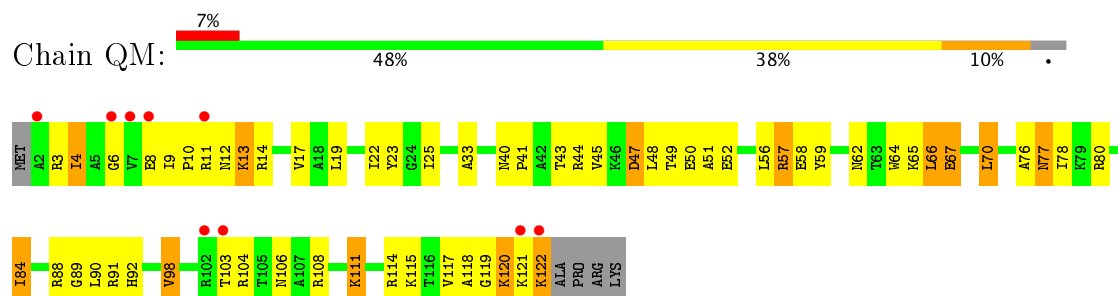
- Molecule 12: 30S ribosomal protein S12



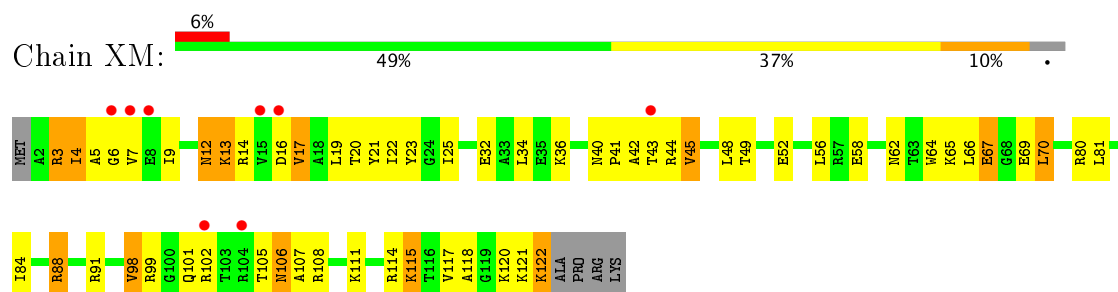
- Molecule 12: 30S ribosomal protein S12



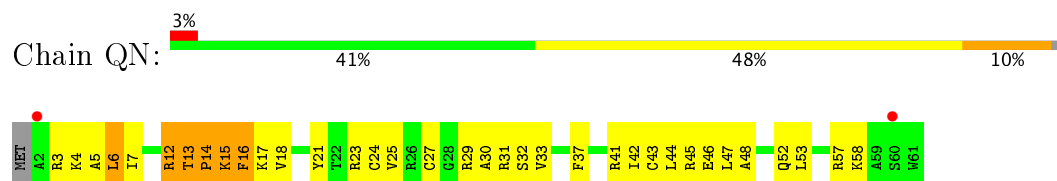
- Molecule 13: 30S ribosomal protein S13



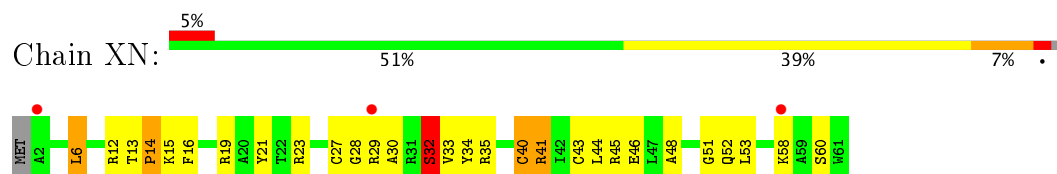
- Molecule 13: 30S ribosomal protein S13



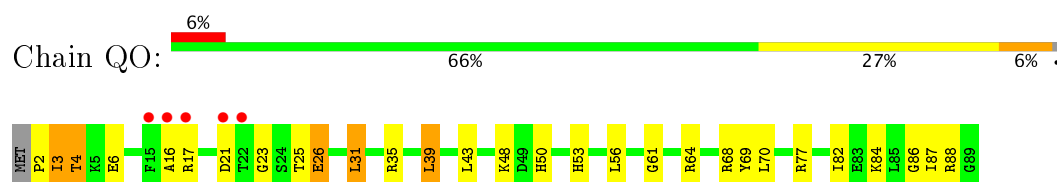
- Molecule 14: 30S ribosomal protein S14 type Z



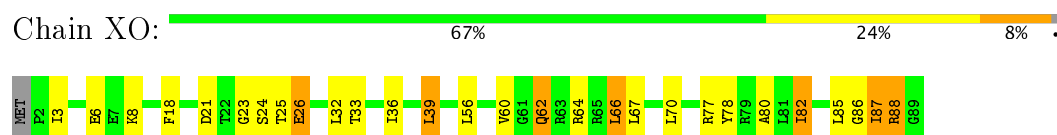
- Molecule 14: 30S ribosomal protein S14 type Z



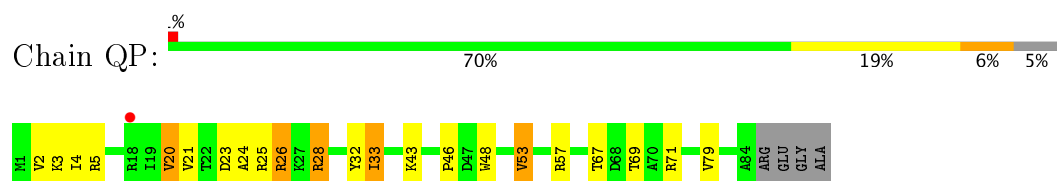
- Molecule 15: 30S ribosomal protein S15



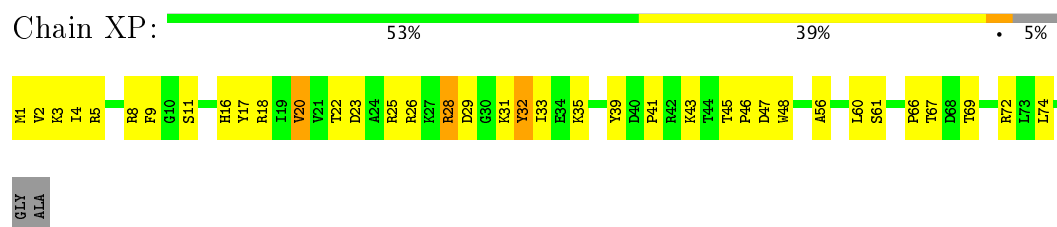
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

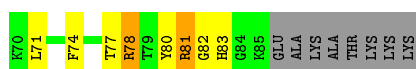


- Molecule 17: 30S ribosomal protein S17

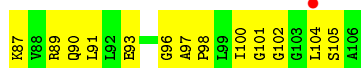




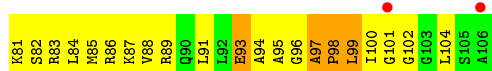
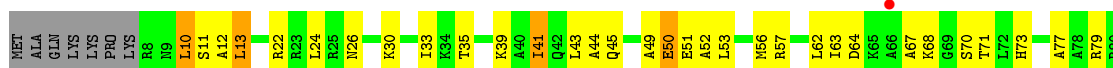
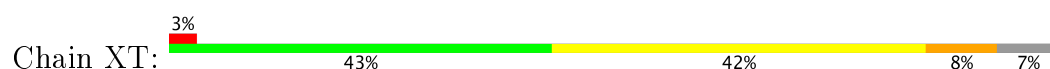




- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



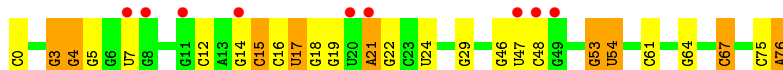
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

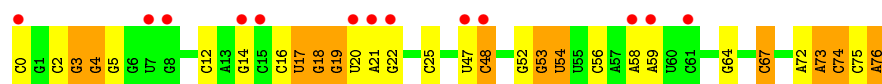


- Molecule 22: P-site tRNA-fMet



- Molecule 22: P-site tRNA-fMet





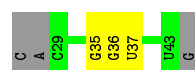
- Molecule 23: messenger RNA



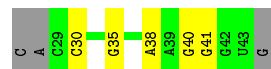
- Molecule 23: messenger RNA



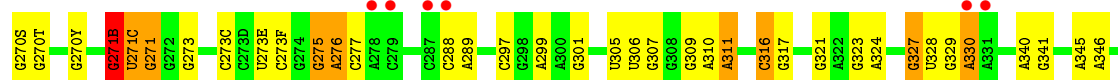
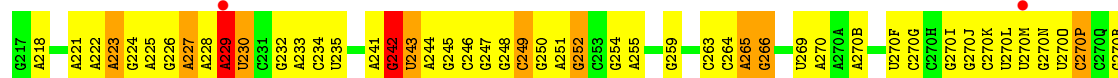
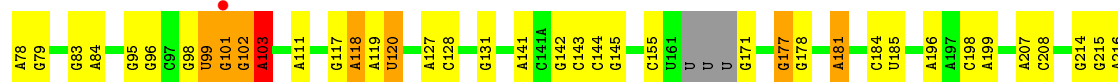
- Molecule 24: A-site ASL-SufJ



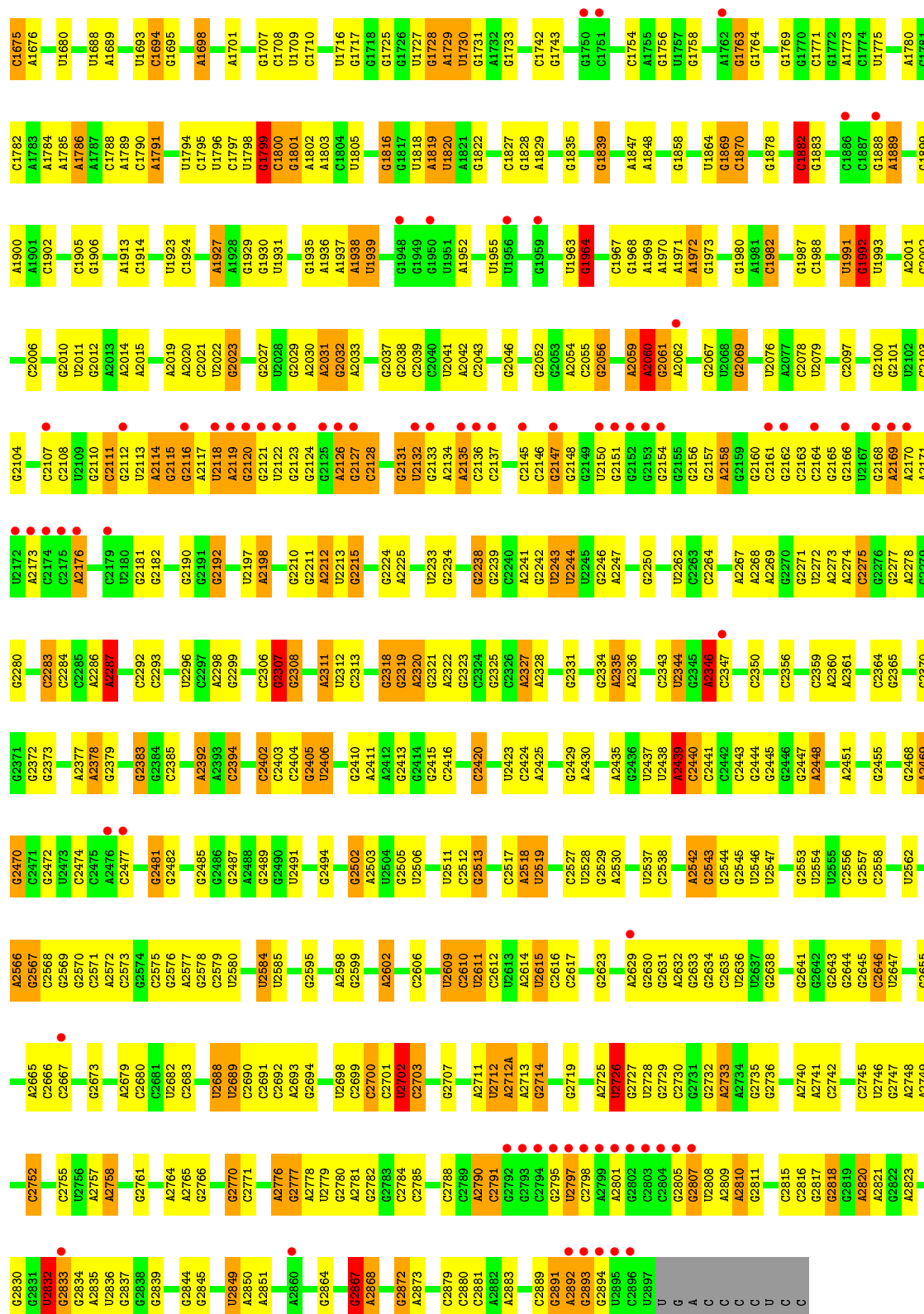
- Molecule 24: A-site ASL-SufJ



- Molecule 25: 23S rRNA



C1585	G1480	U1394	U1300	G1201	U1108	A1048	C967	G881	A793	G686	G636	G550	C455	G352
U1482	U1482	A1395	A1300	C1202	C1109	C1049	A973	G882	G794	G690	A637	G551	C486	G352
A1586	G1483	U1396	A1301	G1203	A1110	A1050	A974	G883	C795	G690	G638	G551	C486	G352
A1587	G1484	U1397	A1302	A1204	A1111	G1051	G974	G884	C796	G691	U639	U554	G458	G363B
C1588	G1485	U1400	G1303	U1205	U1112	C1052	C974A	C885	C797	G696	C640	U557	U459	G363C
C1589	A1490	G1401	A1308	U1206	U1113	C1053	A981	C886	A802	G697	A643	U558	A460	A363F
G1593	C1493	C1402	G1309	G1209	C1116	G1055	A982	C888	A802	G702	A644	G561	G467	C364
G1594	A1494	C1403	G1310	U1211	G1122	A1056	A983	C889	G805	G702	A645	U562	G468	A371
G1595	A1495	C1407	U1311	U1211	G1122	A1057	A987	A890	C806	A705	A646	G563	A470	U372
C1598	A1496	C1411	U1312	A1213	G1125	G1058	A987	G892	U807	A706	U650	U566	G476	U383
C1599	U1497	C1411	U1313	A1214	G1126	G1059	A990	C893	G808	G707	G651	U567	U384	U384
C1600	C1505	G1416	U1316	G1215	A1127	U1061	A991	U895	G809	C708	C652	U568	C385	G385
C1607	C1506	G1417	U1317	A1220	A1128	G1062	C992	A896	C812	U709	A653	U569	A479	U386
A1608	A1507	G1418	A1310	C1221	A1129	G1063	G993	A897	C812	G707	A654	U570	A480	C386
A1609	A1508	A1419	C1320	G1226	G1131	U1065	C994	C897	C817	G717	G654A	G570	A482	G389
A1610	C1509	U1420	A1321	G1226	A1132	U1066	A996	A900	G818	A722	G654B	G573	A483	C392
G1613	U1510	G1421	A1322	G1226	U1133	U1067	G997	A901	G819	G723	G	G	G495	G396
A1614	C1515	A1427	U1316	G1236	C1135	G1068	A1000	C904	U826	G729	G	G	A496	G396
C1617	C1515	A1428	C1330	A1237	G1136	A1069	A1000	U907	U827	C730	C	C	A497	G396
A1618	U1520	C1431	A1331	G1238	G1137	A1070	A1000	U907	U828	G730	C	C	A497	G396
G1622	G1522	G1436	G1338	A1247	G1138	G1071	G1003	A910	G830	U740	G	A586	G498	A401
G1630	G1530	G1441	U1340	A1262	G1139	C1072	C1004	A910	G831	G741	A	C587	A502	A402
C1636	C1533	G1442	U1341	A1263	C1140	A1073	C1005	G916	U839	G744	C	A590	A503	U403
A1637	G1534	G1443	U1342	A1263	U1141	C1074	C1006	A917	C940	G745	C	A591	U504	U404
G1638	U1535	G1444	G1337	G1264	U1142	C1075	C1007	A918	G845	A746	G	G592	A505	A406
U1639	A1536	A1444A	G1338	A1267	G1150	A1077	A1010	G919	G846	U747	G	G593	G506	G407
C1640	C1537	C1445	U1349	G1267	G1151	C1079	G1012	G921	C946	C	C	U594	A507	G408
G1641	G1538	C1446	A1348	G1267	C1152	U1081	G1013	U922	U847	A751	C	G	G508	C409
G1645	G1539	G1447	U1357	C1261	G1154	U1082	G1015	C923	G848	C753	C	A603	G512	G411
C1646	C1542	A1449	G1358	A1262	G1164	A1084	G1016	G932	G854	A764	A654J	H606	A514	C413
G1647	A1543	G1449A	A1399	U1263	U1165	A1085	G1017	A933	G855	G765	A654V	U607	A515	C414
C1648	C1544	A1453	C1363	U1264	U1169	A1086	A1020	G938	C856	G769	U657	A608	C516	C419
C1649	A1545	A1454	A1364	A1265	G1173	G1088	A1021	A941	U858	G770	C658	A609	U519	U421
G1650	C1547	U1454	A1365	U1267	A1174	U1090	U1023	G942	U860	G771	C659	U614	G520	U427
A1651	C1548	C1455	A1366	A1268	U1175	C1091	G1024	G944	A861	A774	C660	G615	G521	U427
A1652	A1554	C1458	A1367	A1269	U1176	C1092	G1025	A945	G862	G775	C661	G616	G522	A428
G1653	C1554	G1459	G1368	G1270	G1177	U1093	U1026	G946	A863	G776	C662	G617	C527	C435
A1654	A1554	G1461	C1370	A1271	C1177	U1094	A1027	G947	G864	G780	C663	G620	A528	G439
G1655	C1554	C1462	G1371	A1272	C1178	A1095	A1029	G948	U868	A781	C664	A621	A529	G439
C1657	G1559	C1467	U1372	A1278	C1179	A1096	A1029	G952	G869	A782	C665	A622	G530	G440
C1658	A1566	C1467	A1373	G1279	C1180	U1097	G1030	A953	U870	A784	C666	G624	A532	U441
A1665	C1566	C1468	A1378	A1286	G1183	A1098	U1033	G954	A871	G785	C667	A627	A443	G442
C1666	A1569	A1469	A1379	A1287	G1184	G1099	U1033	G954	U872	A786	C668	G627	C537	C444
G1667	G1470	A1470	C1185	U1287	C1185	U1101	G1039	A957	G873	C786	C671	G630	G539	A447
A1668	C1577	A1471	A1384	C1289	G1186	C1102	U1039	U958	C876	A788	C672	G631	G540	U448
C1672	U1578	A1477	G1385	C1290	G1187	A1103	C1043	A959	U877	A789	C674	A632	A449	A449
U1673	A1579	G1477	C1396	C1291	U1188	C1104	G1044	A960	U878	C790	C675	A633	G450	G450
A1580	U1292	A1478	C1387	U1292	G1195	U1105	A1045	C961	A878	C791	A676	C634	C546	G454
G1674	G1581	G1479	C1387	C1293	G1195	G1107	G1047	G966	G880	G792		C635	G549	A454

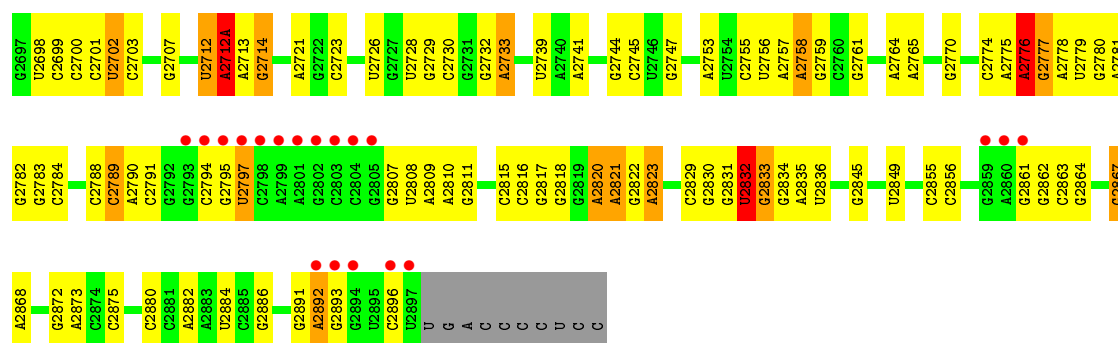


• Molecule 25: 23S rRNA

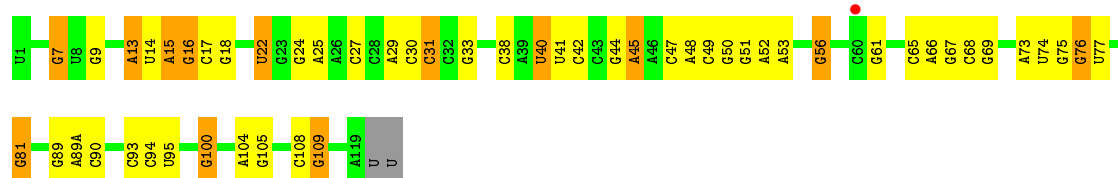


G1252	A1156	C1005	A917	G830	A752	C	C591	A513	A412	G274	A225	G101	G
A1253	G1464	C1006	A918	G831	C753	G	G592	A514	C413	G275	G226	G102	U
G1256	U1465	C1007	G919	G832	C754	G	G593	A515	C414	A227	A227	A103	C
C1257	C1466	A1010	G920	U833	C755	C	U594	G518	A415	C277	A228	A111	A
C1258	G1169	A1011	G921	C834	A764	C	G595	C523	U421	A278	A229	U112	G7
U1263	G1170	U1012	G923	U839	G765		U597	C527	U427	C279	C231	A118	A8
G1264	G1171	C1013	G924	C840	G769		G602	A526	A428	A286	G232	A119	U9
A1265	A1173	G1018	G925	C846	G770		A603	C527	A428	C287	A233	U120	G10
G1266	A1174	A1086	G932	G848	G771		A604	C528	C436	C288	A234	A127	G11
A1267	U1175	G1087	A933	G849	A774		C505	A529	G438	C297	C236	A128	A14
U1268	G1176	A1020	A934	A849	G775		U606	G530	G442	A298	C237		G15
A1269	A1177	A1021	A941	G855	G776		U607	C531	G443	A299			
C1270	C1178	G1022	G942	G856	A777		U613	A532	A443	A311	A241	G131	G26
G1271	C1179	U1023	U943	C857	A777		U614	G533	C444	A312	G242		G27
A1272	C1180	G1024	G944	G858	G780		G615	C534	C445	G323	U243	G138	A28
U1273	G1183	G1025	A945	U858	G781		A616	A535	G446	A324	A244	A141	U29
	G1184	U1026	G946	U859	A782		G617	C537	U447	G327	G247	C1414	G30
A1278	G1185	A1027	G952	U860	A783		G620	A538	U448	G328	G248	G142	C31
G1283	G1186	G1030	A953	A861	A784		G621	G539	A449	U328			C32
A1284	G1187	U1031	G954	G862	G785		A622	G540	C451	G329	G252	C153	U33
G1285	U1188	U1033	G955	G863	G786		G623	C546	G457	A330	C253	G154	G35
A1286	A1189	G1036	A957	G864	U787		G624	A547	C458	A331	G254	C155	G36
A1287	G1194	A1037	A958	G865	A788		G625	C548	U459	A332	A255	U161	
	G1195	G1042	U959	U877	A789		A627	A549	A460	A340		U	G43
U1292	C1201	C1043	A960	A878	C790		G628	G550	G341	G341	G260	U	A44
C1293	G1104	C1044	C961	A879	G791		G629	G551	G342	G342	G261	G45	G45
U1300	G1105	A1045	U969	G881	A792		A631	G552	U464	G345	G262	G171	C46
A1301	G1203	A1046	G970	G882	G796		A632	U553	G465	A345	A263	G172	A49
A1302	U1205	G1047	G971	G883	C797		A633	U554	A466	A346	C263	G173	
G1303	G1206	A1048	G972	C884	C797		C534	G556	G467	A347	C264	C174	
	A1210	A1050	A973	C885	G704		C635	G559	G468	G347	A265	A181	G55
G1309	U1211	G1053	G974	C886	A705		G636	C560	A470	G348	G266		G61
G1310	U1214	A1054	C974A	A887	G710		A637	G561	A478		U269	U185	
G1311	G1215	G1055	G975	C888	G711		U638	G562	A479		U270F	A190	U67
U1312	G1216	A1056	A980	C889	G717		U639	U563	A480		C270G		G70
U1313	A1220	A1057	A983	G892	A722		A643	A566	G481		G270J	A195	A71
A1321	C1221	G1058	G984	C893	G723		C644	A567	A482		C270K	A196	U72
U1329	G1224	U1060	C985	U895	G724		A646	A571	A483		U270L	A199	A73
C1330	G1230	G1061	A990	A896	G725		G651	A572	G488		U270M		A74
G1332	G1231	G1062	G991	C897	A727		A654	C574	A492		G270N	A207	C76
A1336	G1237	G1063	C992	C898	G728		G654A	A575	G498		C270P	C208	C77
G1337	G1238	U1064	G993	A900	G729		C654B	G579	A503		G270Q	A213	G78
G1338	A1237	U1065	G994	A901	C730		G	C580	U504		G270S	G215	G83
G1339	G1238	A1067	G995	C902	A734		G	C581	A505		G270T	A216	A84
A1342	A1241	G1068	A996	C903	G738		G	G582	G506		C271A	G217	G85
C1345	A1247	A1069	G997	U907	G739		C	G583	A507		G271B	G219	G86
		G1071	U999	A910	A824		C	A586	G508		G271C	G220	G94
G1348	G1250	C1072	G1002	U826	U747		C	C587	C509		G272	A221	G96
A1349	C1251	A1073	G1003	U827	G748		A	U588	G510		G273	A222	C97
		C1075	C1004	U828	A751		G	C589	U511			A223	G98
				A829				A590	G512			G224	U99

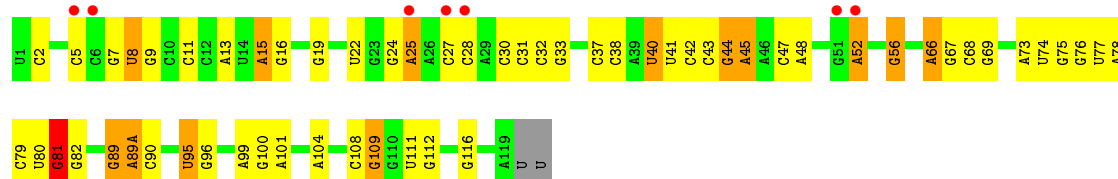




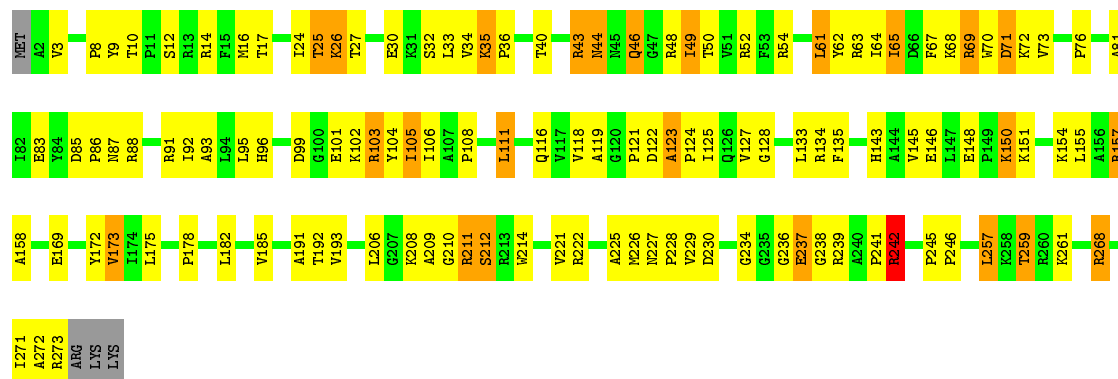
- Molecule 26: 5S rRNA



- Molecule 26: 5S rRNA

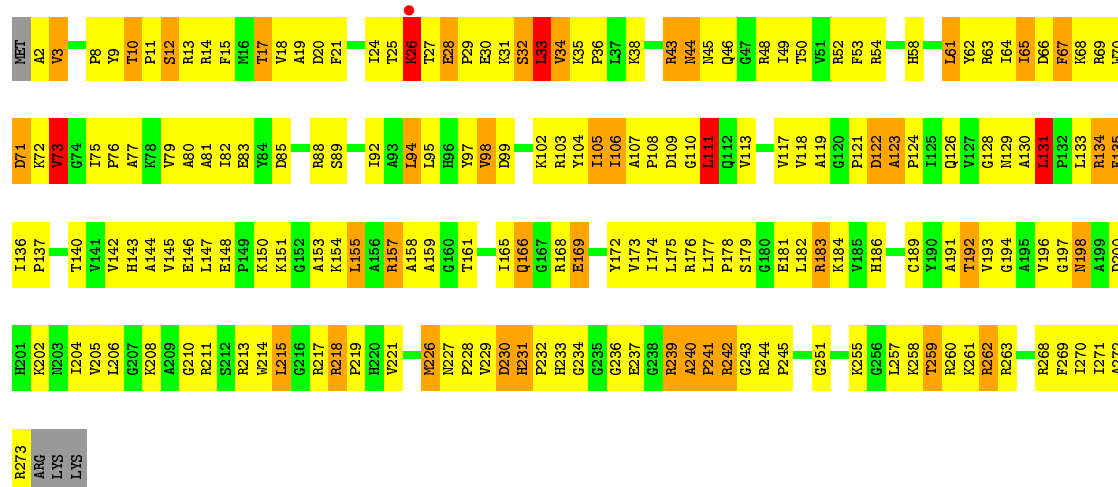


- Molecule 27: 50S ribosomal protein L2



- Molecule 27: 50S ribosomal protein L2

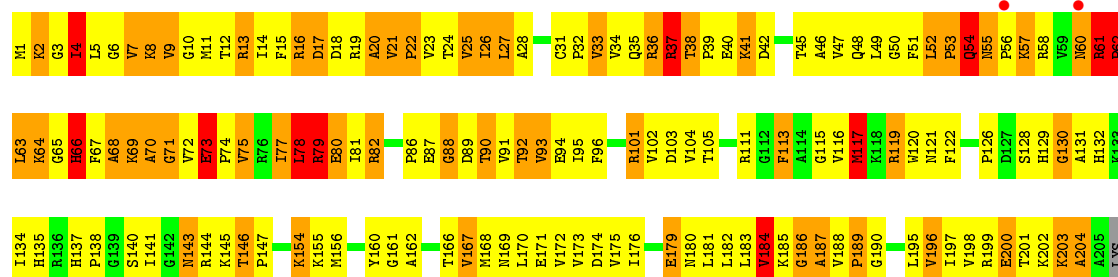




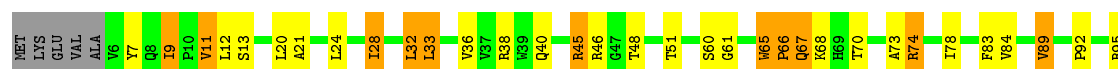
• Molecule 28: 50S ribosomal protein L3



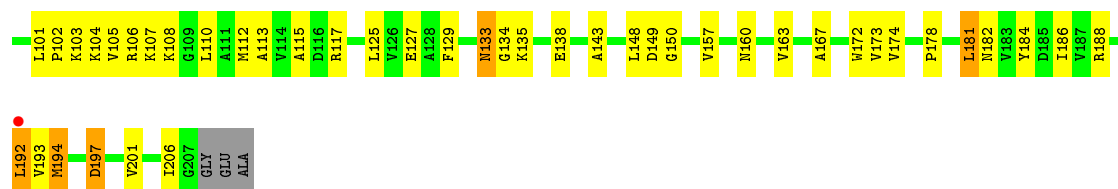
• Molecule 28: 50S ribosomal protein L3



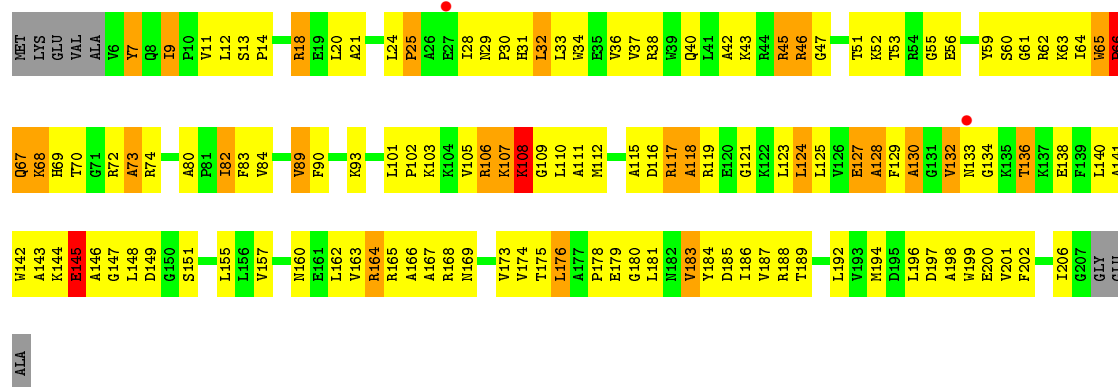
• Molecule 29: 50S ribosomal protein L4



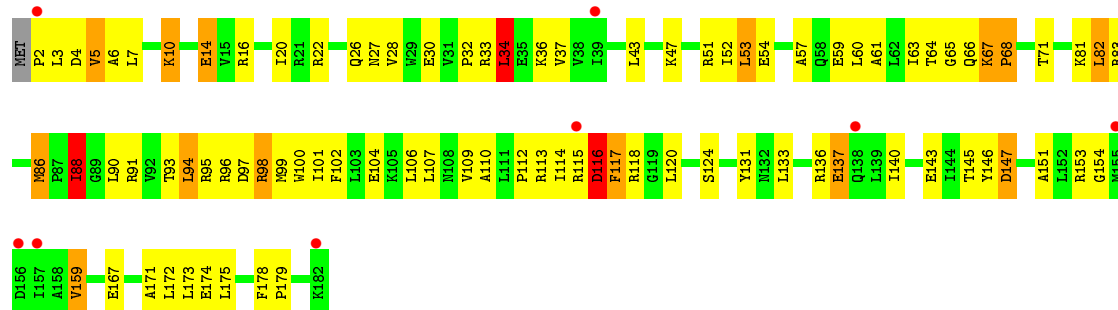




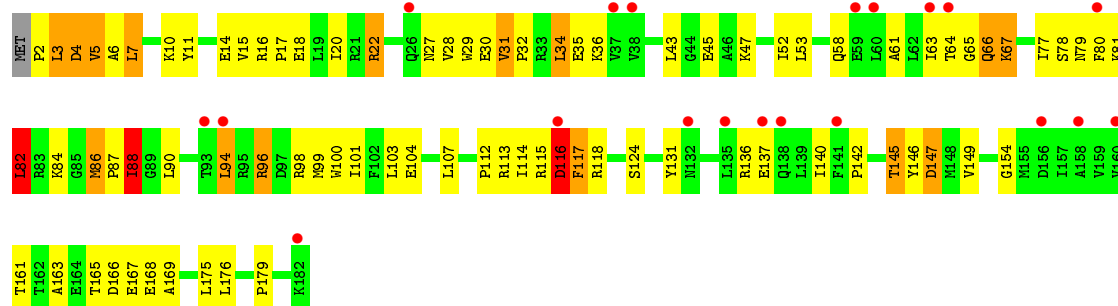
• Molecule 29: 50S ribosomal protein L4



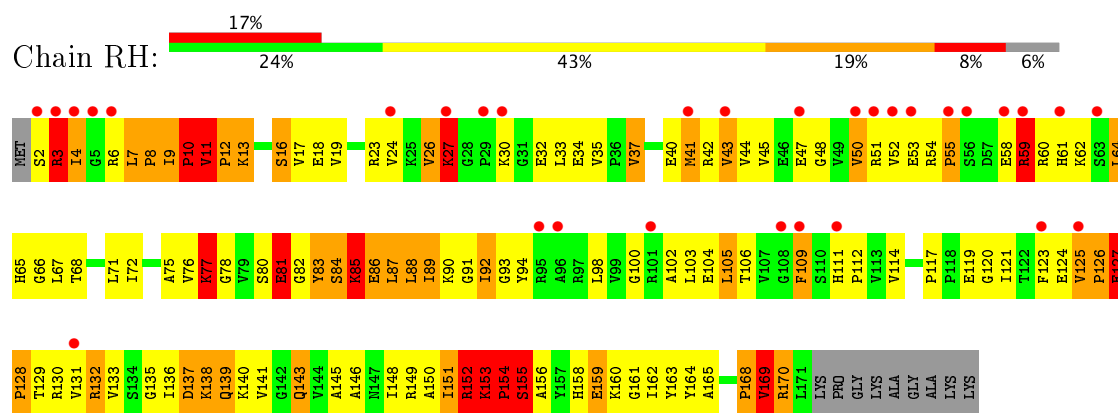
• Molecule 30: 50S ribosomal protein L5



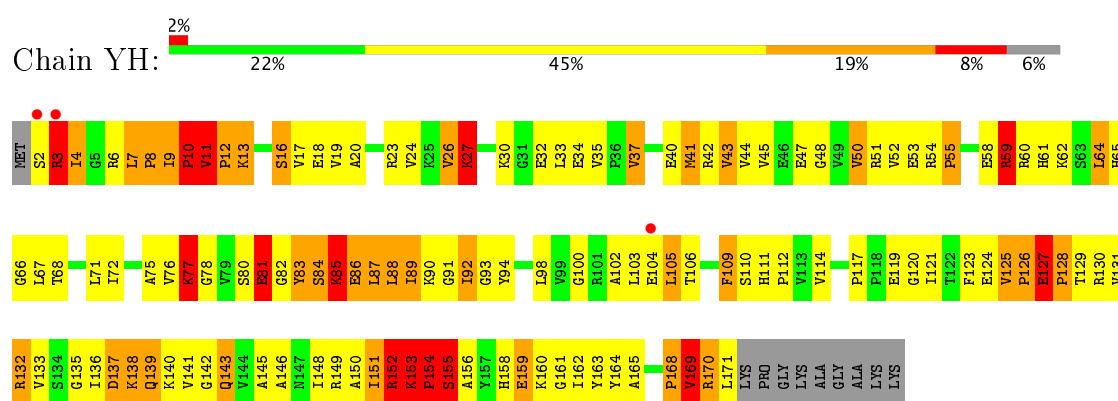
• Molecule 30: 50S ribosomal protein L5



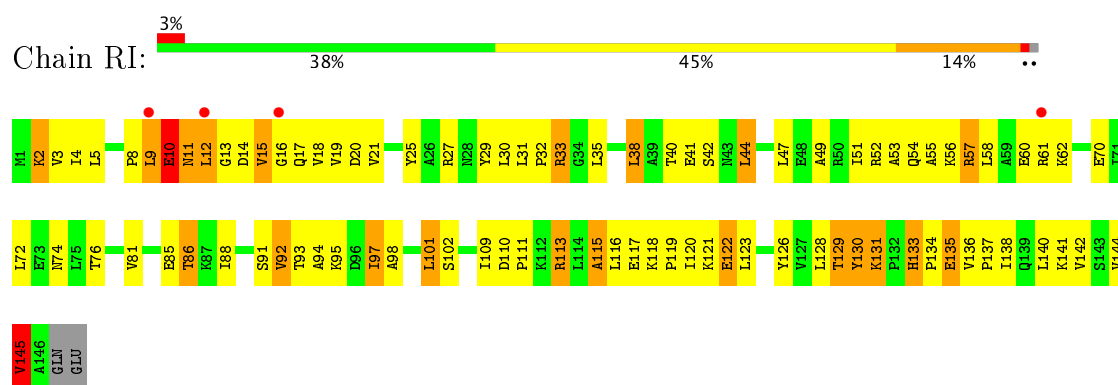
- Molecule 31: 50S ribosomal protein L6



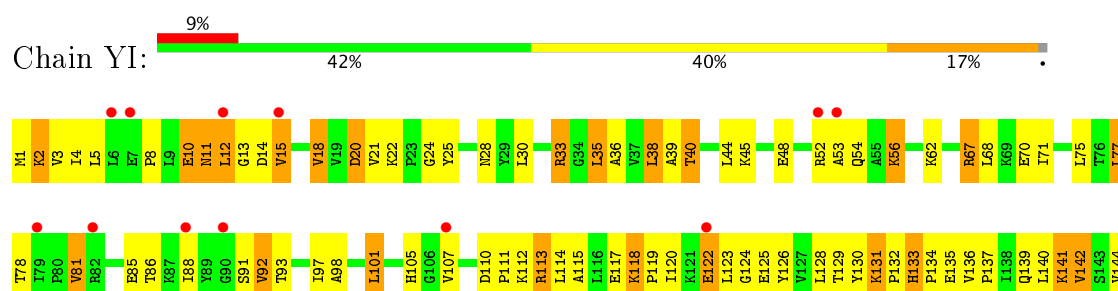
- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9



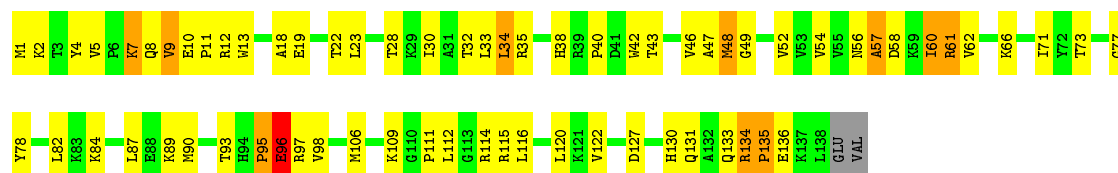
- Molecule 32: 50S ribosomal protein L9





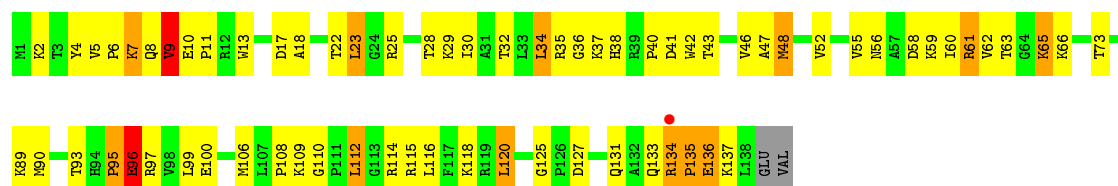
- Molecule 33: 50S ribosomal protein L13

Chain RN: 50% 41% 7% ..



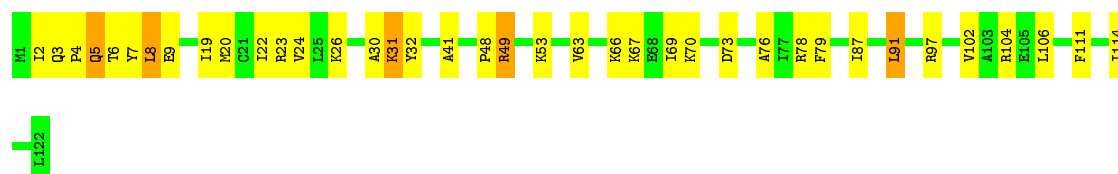
- Molecule 33: 50S ribosomal protein L13

Chain YN: 49% 39% 9% ..



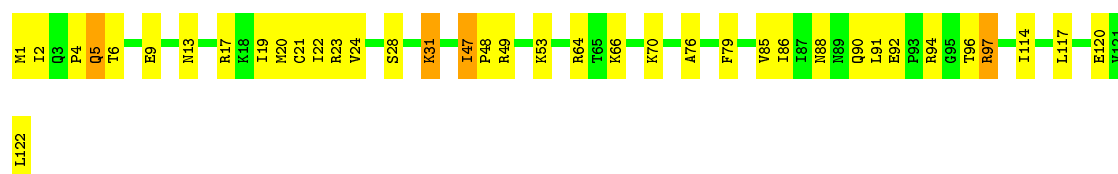
- Molecule 34: 50S ribosomal protein L14

Chain RO: 69% 27% .



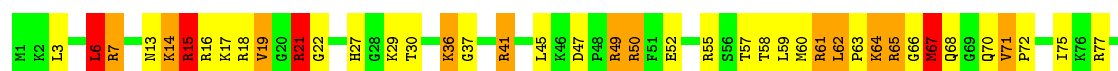
- Molecule 34: 50S ribosomal protein L14

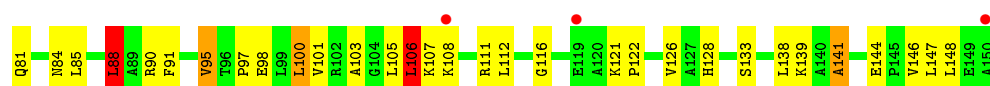
Chain YO: 69% 28% .



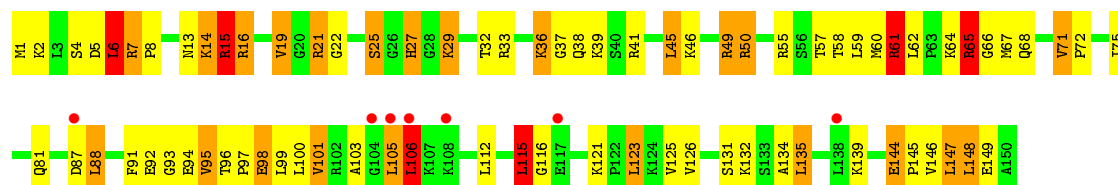
- Molecule 35: 50S ribosomal protein L15

Chain RP: 52% 34% 10% .

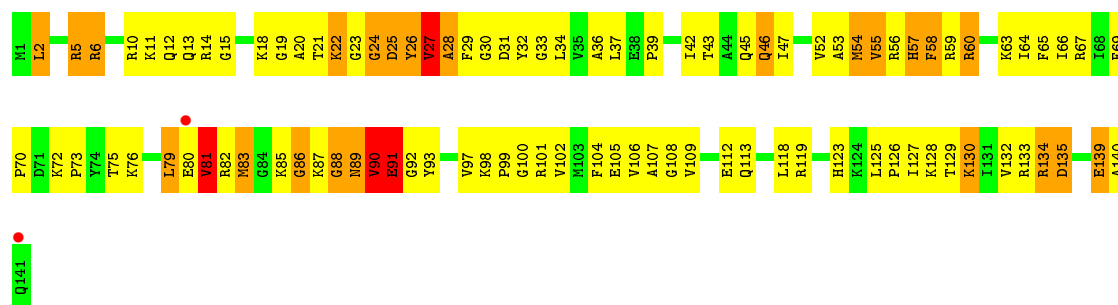




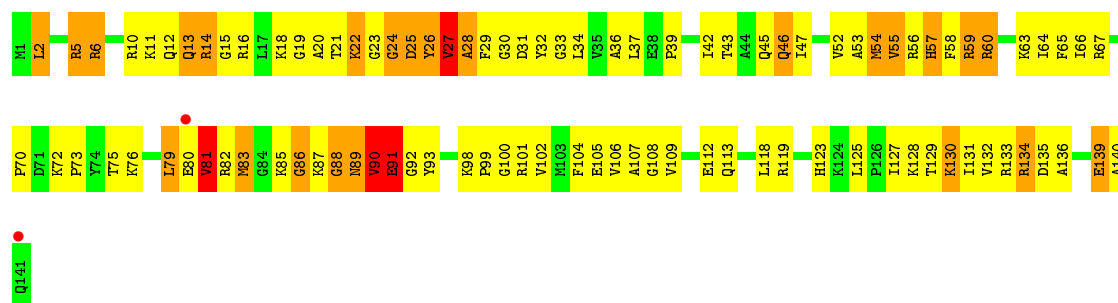
- Molecule 35: 50S ribosomal protein L15



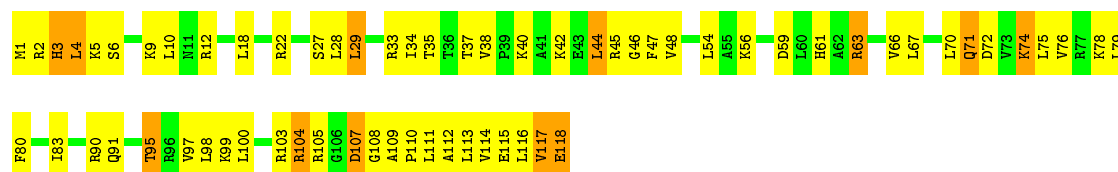
- Molecule 36: 50S ribosomal protein L16



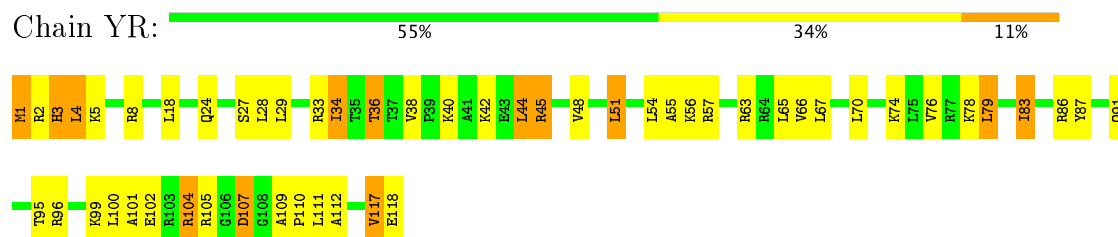
- Molecule 36: 50S ribosomal protein L16



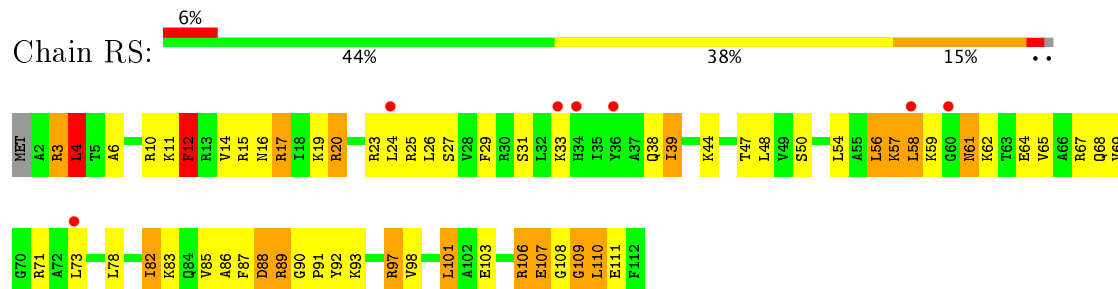
- Molecule 37: 50S ribosomal protein L17



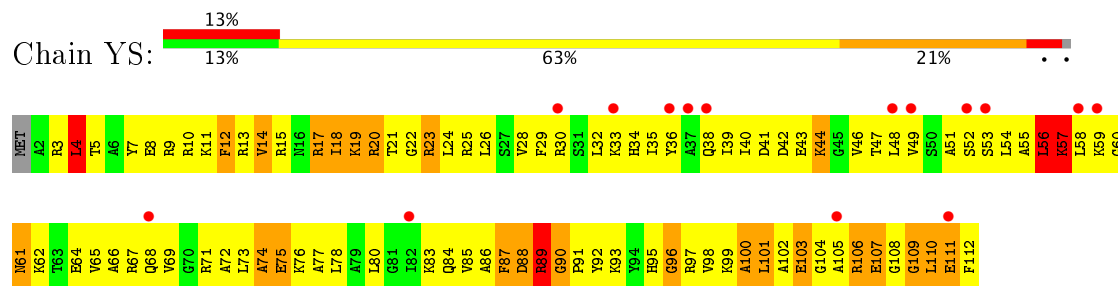
- Molecule 37: 50S ribosomal protein L17



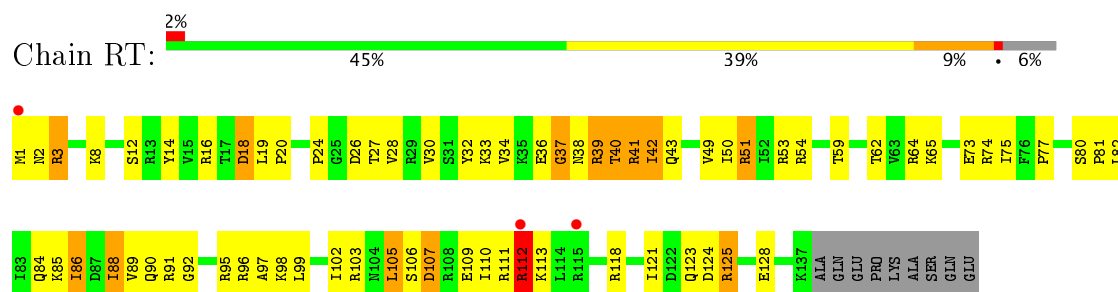
- Molecule 38: 50S ribosomal protein L18



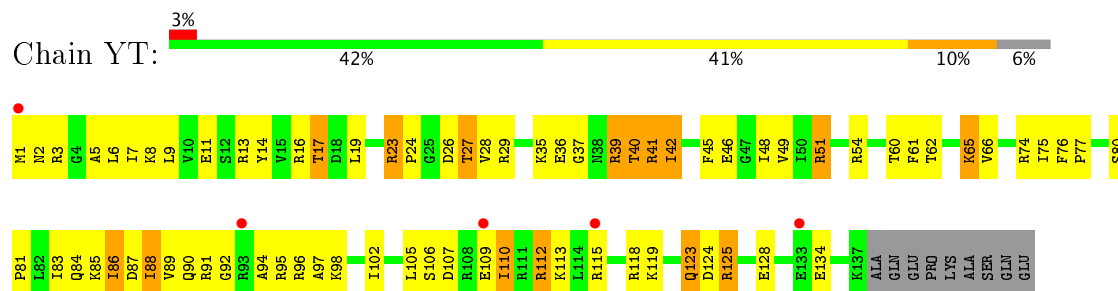
- Molecule 38: 50S ribosomal protein L18



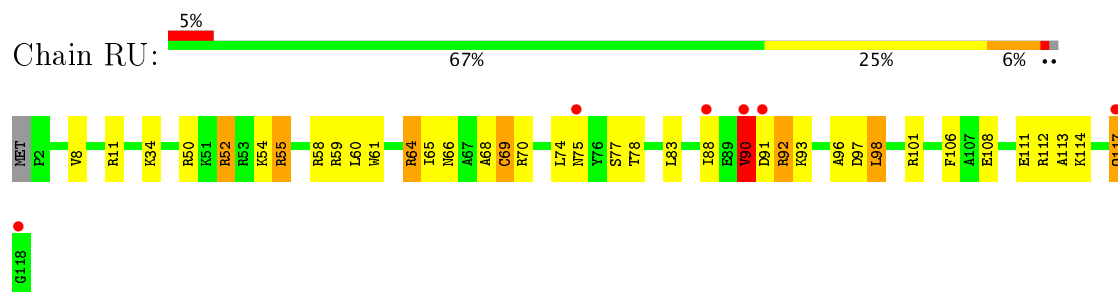
- Molecule 39: 50S ribosomal protein L19



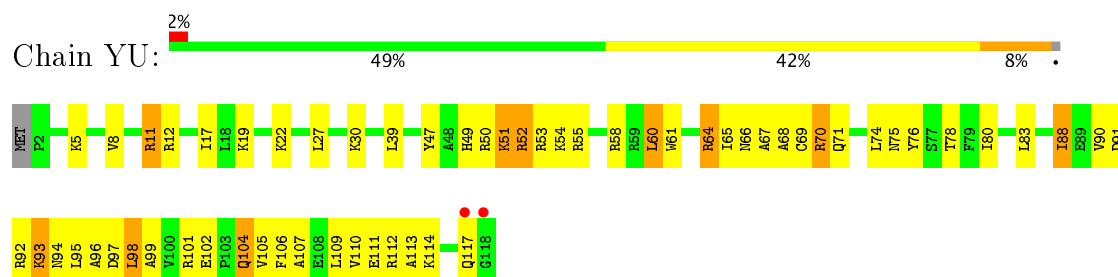
- Molecule 39: 50S ribosomal protein L19



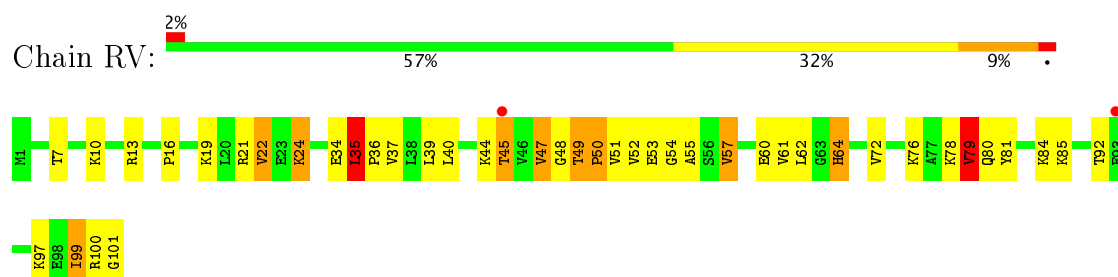
- Molecule 40: 50S ribosomal protein L20



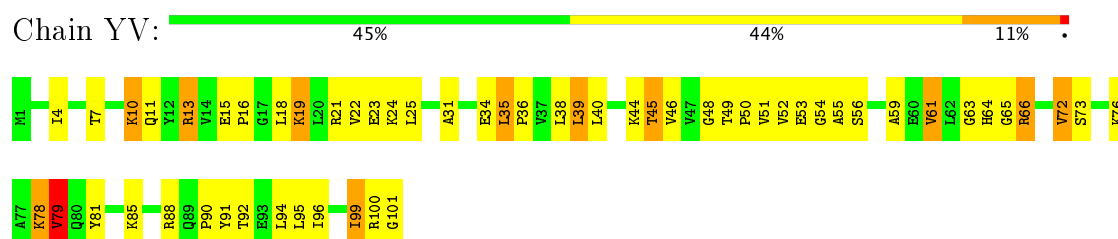
- Molecule 40: 50S ribosomal protein L20



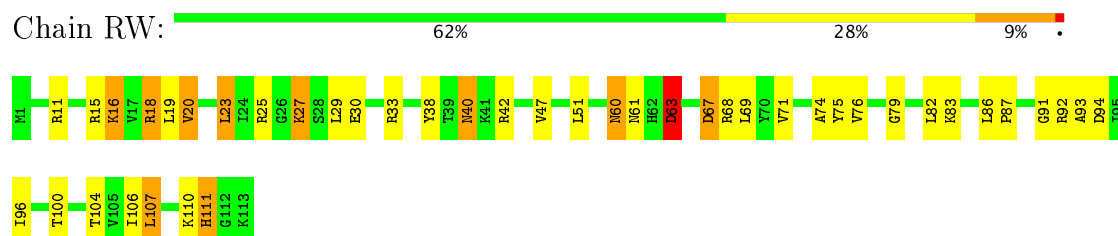
- Molecule 41: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L21

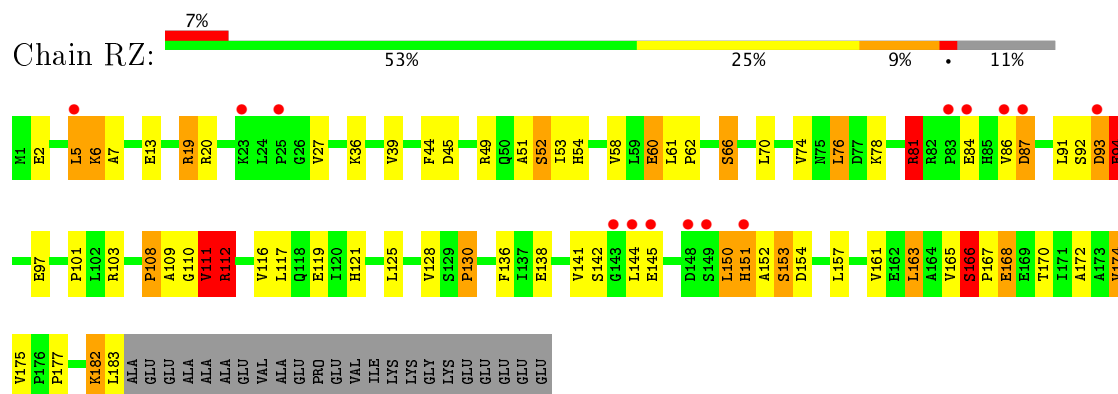


- Molecule 42: 50S ribosomal protein L22

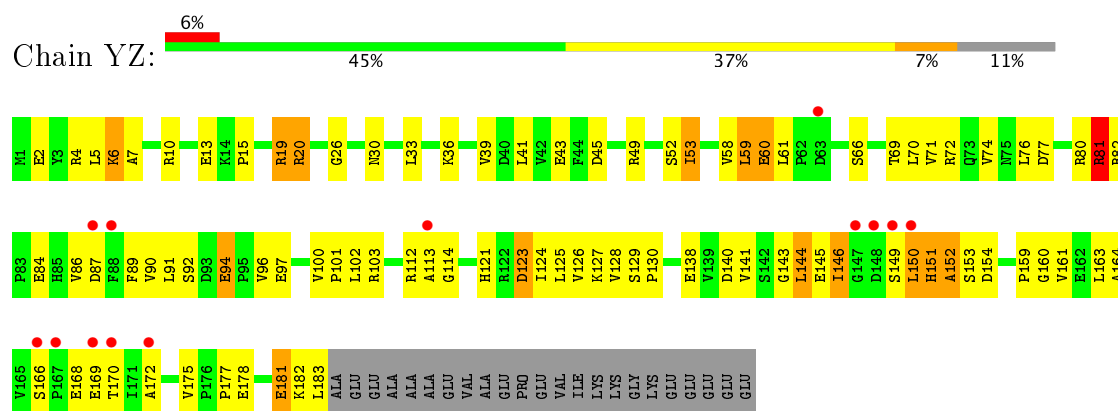


-

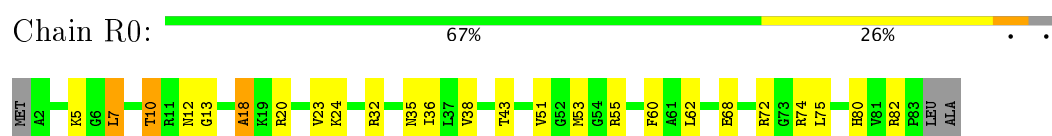
- Molecule 45: 50S ribosomal protein L25



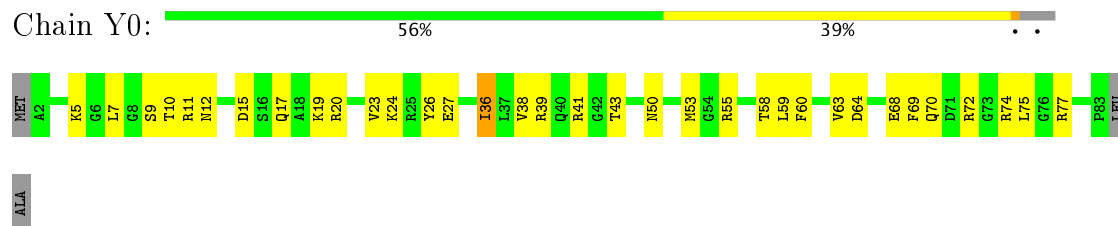
- Molecule 45: 50S ribosomal protein L25



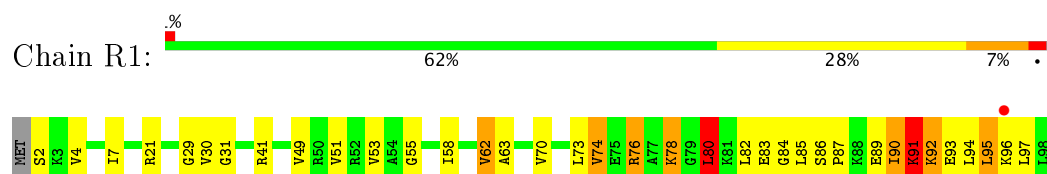
- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27

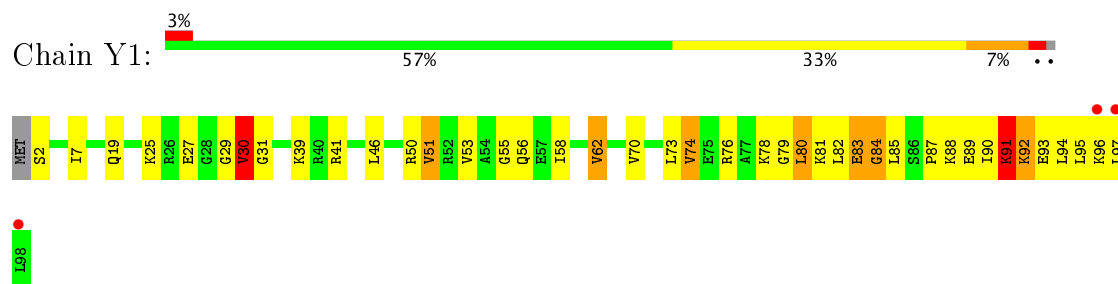


- Molecule 47: 50S ribosomal protein L28

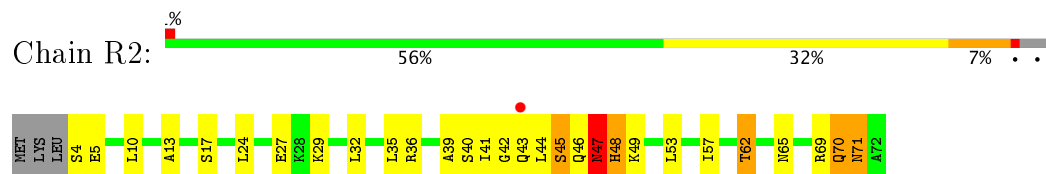




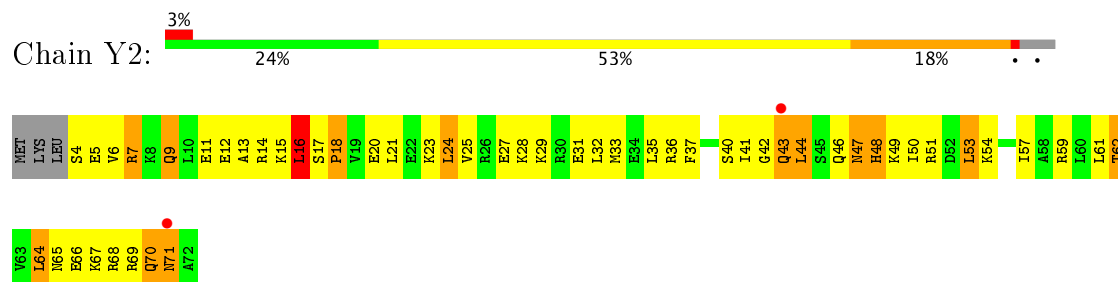
- Molecule 47: 50S ribosomal protein L28



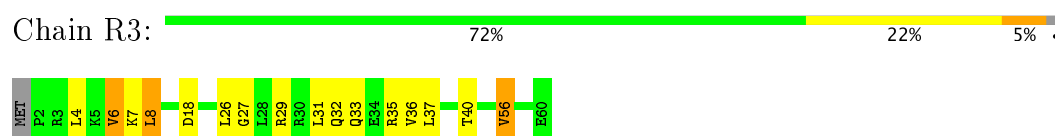
- Molecule 48: 50S ribosomal protein L29



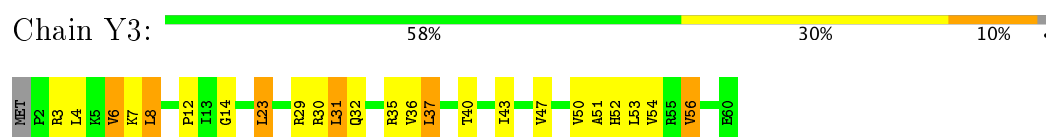
- Molecule 48: 50S ribosomal protein L29



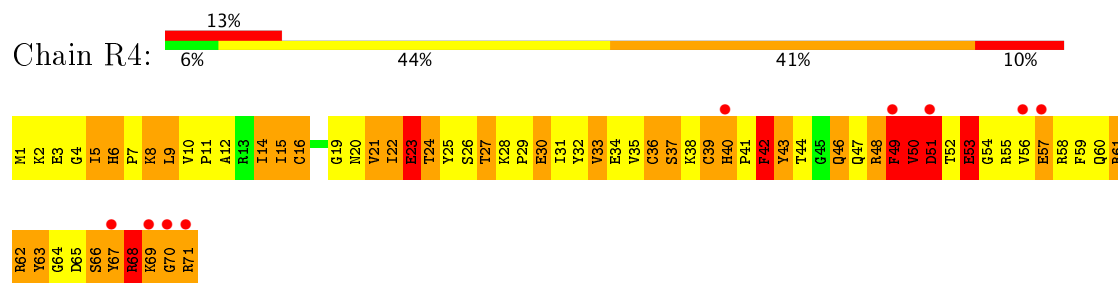
- Molecule 49: 50S ribosomal protein L30



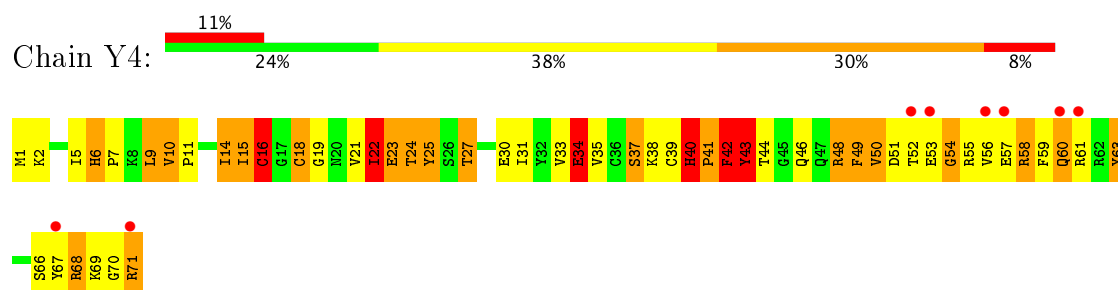
- Molecule 49: 50S ribosomal protein L30



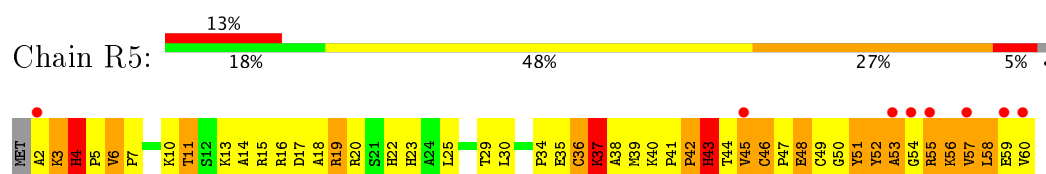
- Molecule 50: 50S ribosomal protein L31



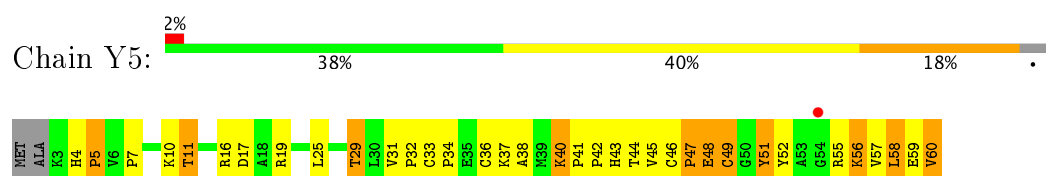
- Molecule 50: 50S ribosomal protein L31



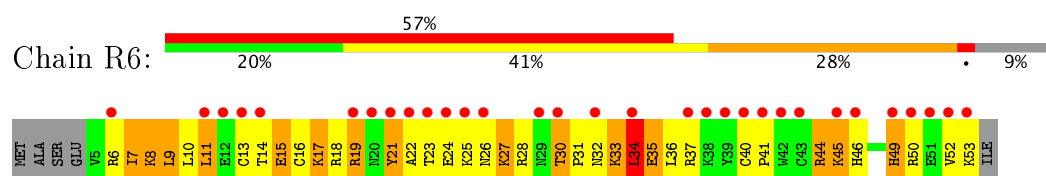
- Molecule 51: 50S ribosomal protein L32



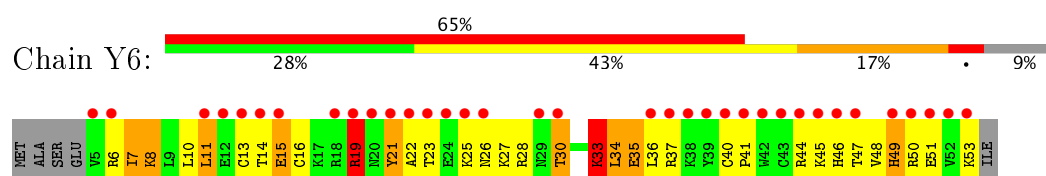
- Molecule 51: 50S ribosomal protein L32



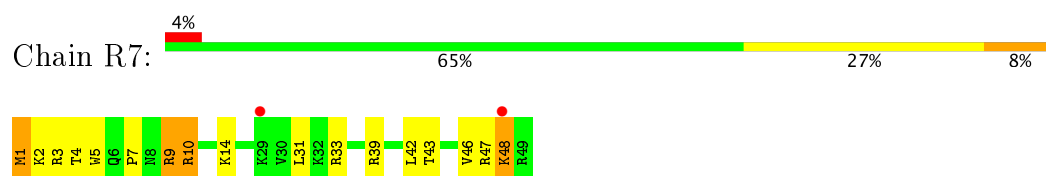
- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

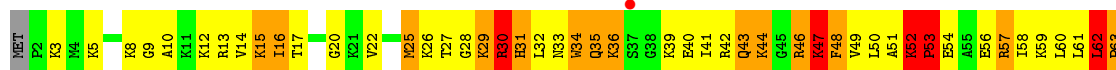
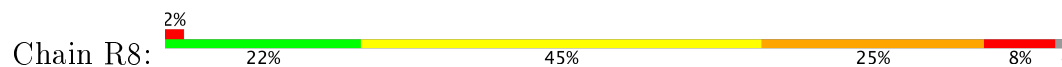


- Molecule 53: 50S ribosomal protein L34

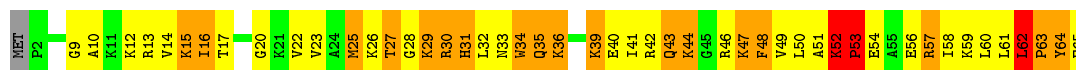




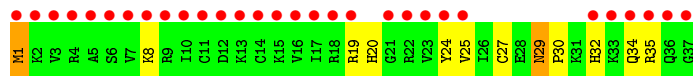
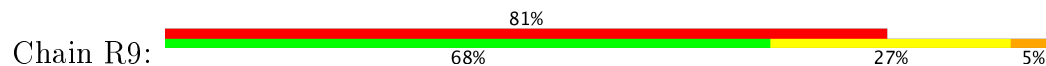
- Molecule 54: 50S ribosomal protein L35



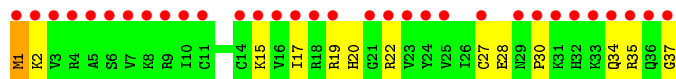
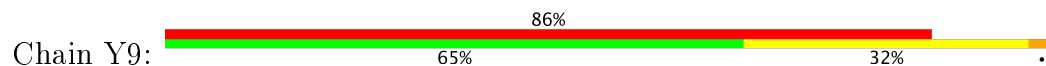
- Molecule 54: 50S ribosomal protein L35



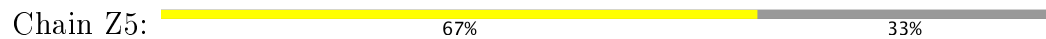
- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-Puro



- Molecule 56: CC-Puro



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.46Å 450.70Å 621.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 3.60 49.85 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.85-3.60) 97.8 (49.85-3.40)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.205 , 0.244 0.205 , 0.244	Depositor DCC
$R_{free}$ test set	30556 reflections (4.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 101.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	292106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 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	0.32	0/36098	0.86	40/56341 (0.1%)
1	XA	0.33	0/36101	0.87	28/56346 (0.0%)
2	QB	0.31	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.54	0/2195
3	XC	0.37	0/1629	0.57	0/2195
4	QD	0.27	0/1733	0.45	0/2318
4	XD	0.40	0/1733	0.60	0/2318
5	QE	0.40	1/1171 (0.1%)	0.60	0/1576
5	XE	0.39	0/1171	0.60	0/1576
6	QF	0.39	0/856	0.55	0/1154
6	XF	0.39	0/856	0.58	0/1154
7	QG	0.34	0/1276	0.50	0/1709
7	XG	0.35	0/1276	0.51	0/1709
8	QH	0.34	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.37	0/814	0.62	2/1095 (0.2%)
10	XJ	0.39	1/814 (0.1%)	0.63	1/1095 (0.1%)
11	QK	0.39	0/900	0.59	1/1213 (0.1%)
11	XK	0.39	0/900	0.59	0/1213
12	QL	0.49	1/991 (0.1%)	0.80	1/1327 (0.1%)
12	XL	0.49	0/991	0.83	3/1327 (0.2%)
13	QM	0.32	0/974	0.58	0/1303
13	XM	0.37	0/974	0.62	0/1303
14	QN	0.37	0/501	0.63	0/664
14	XN	0.43	0/501	0.66	0/664
15	QO	0.36	0/745	0.54	0/992
15	XO	0.40	0/745	0.55	0/992
16	QP	0.37	0/721	0.57	0/970
16	XP	0.36	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.36	0/847	0.54	0/1131
18	QR	0.36	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.60	0/768
19	QS	0.34	0/689	0.61	0/926
19	XS	0.39	0/689	0.69	1/926 (0.1%)
20	QT	0.39	0/765	0.67	0/1007
20	XT	0.32	0/765	0.62	0/1007
21	QU	0.31	0/221	0.55	0/288
21	XU	0.31	0/221	0.62	0/288
22	QV	0.42	1/1836 (0.1%)	0.87	0/2859
22	XV	0.41	1/1836 (0.1%)	0.85	0/2859
23	QX	0.26	0/192	0.68	0/297
23	XX	0.32	0/192	0.77	0/297
24	QY	0.21	0/355	0.74	0/551
24	XY	0.29	0/355	0.89	0/551
25	RA	0.40	1/69521 (0.0%)	0.92	86/108529 (0.1%)
25	YA	0.43	1/69521 (0.0%)	0.94	81/108529 (0.1%)
26	RB	0.36	0/2878	0.95	6/4490 (0.1%)
26	YB	0.36	0/2878	0.99	12/4490 (0.3%)
27	RD	0.51	0/2165	0.70	0/2919
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	0.30	0/1620	0.48	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.32	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	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	0.27	0/1151	0.56	0/1558
32	YI	0.29	0/1151	0.56	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.43	0/1131	0.63	0/1525
34	RO	0.42	0/943	0.62	1/1269 (0.1%)
34	YO	0.50	0/943	0.65	0/1269
35	RP	0.29	0/1162	0.60	1/1544 (0.1%)
35	YP	0.32	0/1162	0.64	0/1544
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	0.43	0/982	0.69	0/1312
37	YR	0.45	0/982	0.73	0/1312
38	RS	0.36	0/892	0.64	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YS	0.46	0/892	0.82	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.44	0/1155	0.66	0/1542
40	RU	0.40	0/982	0.65	0/1306
40	YU	0.51	0/982	0.70	0/1306
41	RV	0.38	0/790	0.62	1/1057 (0.1%)
41	YV	0.46	0/790	0.73	1/1057 (0.1%)
42	RW	0.50	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.48	0/739	0.65	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.46	0/798	0.69	0/1064
45	RZ	0.26	0/1493	0.52	0/2026
45	YZ	0.28	0/1493	0.55	0/2026
46	R0	0.47	0/657	0.68	0/874
46	Y0	0.49	0/657	0.70	0/874
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.38	0/583	0.64	0/771
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.35	0/474	0.56	0/635
49	Y3	0.42	0/474	0.59	0/635
50	R4	0.39	0/594	0.78	1/795 (0.1%)
50	Y4	0.44	0/594	0.73	1/795 (0.1%)
51	R5	0.49	0/473	0.74	0/639
51	Y5	0.49	0/468	0.72	0/632
52	R6	0.35	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.67	0/575
53	Y7	0.56	0/438	0.71	0/575
54	R8	0.61	0/525	0.92	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.27	0/310	0.46	0/407
55	Y9	0.32	0/310	0.48	0/407
56	Z5	0.79	0/40	1.80	1/60 (1.7%)
56	Z6	0.79	0/40	1.79	1/60 (1.7%)
All	All	0.39	7/316398 (0.0%)	0.85	297/473030 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.47	1.48	1.61
22	XV	0	C	OP3-P	-10.29	1.48	1.61
25	YA	1021	A	N9-C4	-5.52	1.34	1.37
12	QL	48	PRO	N-CD	5.45	1.55	1.47
5	QE	70	PRO	N-CD	5.40	1.55	1.47

The worst 5 of 297 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	YE	21	VAL	C-N-CD	-10.10	98.37	120.60
28	RE	21	VAL	C-N-CD	-10.09	98.40	120.60
26	YB	95	U	C5-C4-O4	9.62	131.67	125.90
26	YB	81	G	C5-C6-O6	-9.09	123.15	128.60
1	XA	1495	U	N1-C2-O2	8.95	129.07	122.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	450	0
1	XA	32249	0	16279	446	1
2	QB	1924	0	1975	62	0
2	XB	1924	0	1975	83	0
3	QC	1605	0	1668	50	0
3	XC	1605	0	1668	61	0
4	QD	1703	0	1764	57	0
4	XD	1703	0	1762	51	0
5	QE	1155	0	1213	49	0
5	XE	1155	0	1213	52	0
6	QF	843	0	857	16	0
6	XF	843	0	857	25	0
7	QG	1257	0	1296	37	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	24	0
8	QH	1116	0	1177	40	0
8	XH	1116	0	1177	28	0
9	QI	1010	0	1037	37	0
9	XI	1010	0	1037	43	0
10	QJ	801	0	849	66	0
10	XJ	801	0	849	57	0
11	QK	885	0	903	28	0
11	XK	885	0	904	25	0
12	QL	975	0	1062	91	0
12	XL	975	0	1062	99	0
13	QM	964	0	1034	47	0
13	XM	964	0	1034	44	0
14	QN	492	0	529	25	0
14	XN	492	0	529	22	0
15	QO	734	0	771	20	0
15	XO	734	0	771	16	0
16	QP	705	0	725	13	0
16	XP	705	0	725	24	0
17	QQ	834	0	904	21	0
17	XQ	834	0	904	19	0
18	QR	574	0	644	11	0
18	XR	574	0	644	20	0
19	QS	674	0	699	76	0
19	XS	674	0	699	54	0
20	QT	763	0	861	36	0
20	XT	763	0	861	62	0
21	QU	217	0	234	11	0
21	XU	217	0	234	6	0
22	QV	1644	0	836	13	0
22	XV	1644	0	836	20	0
23	QX	173	0	87	0	0
23	XX	173	0	87	1	0
24	QY	319	0	162	1	0
24	XY	319	0	162	3	0
25	RA	62071	0	31287	845	0
25	YA	62071	0	31287	863	0
26	RB	2573	0	1306	38	0
26	YB	2573	0	1306	46	0
27	RD	2115	0	2195	99	0
27	YD	2115	0	2195	318	0
28	RE	1568	0	1634	273	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	287	0
29	RF	1585	0	1632	57	0
29	YF	1585	0	1632	175	0
30	RG	1474	0	1535	99	0
30	YG	1474	0	1535	69	0
31	RH	1307	0	1382	224	0
31	YH	1307	0	1382	232	0
32	RI	1136	0	1223	63	1
32	YI	1136	0	1223	51	0
33	RN	1104	0	1180	39	0
33	YN	1104	0	1180	57	0
34	RO	933	0	996	27	0
34	YO	933	0	996	30	0
35	RP	1145	0	1228	71	0
35	YP	1145	0	1227	80	0
36	RQ	1122	0	1179	162	0
36	YQ	1122	0	1179	162	0
37	RR	968	0	1033	47	0
37	YR	968	0	1033	33	0
38	RS	882	0	943	50	0
38	YS	882	0	943	163	0
39	RT	1141	0	1202	62	0
39	YT	1141	0	1202	55	0
40	RU	964	0	1022	29	0
40	YU	964	0	1022	60	0
41	RV	779	0	852	22	0
41	YV	779	0	852	46	0
42	RW	900	0	964	25	0
42	YW	900	0	964	27	0
43	RX	725	0	778	28	0
43	YX	725	0	778	24	0
44	RY	785	0	878	52	0
44	YY	785	0	878	43	0
45	RZ	1461	0	1493	43	0
45	YZ	1461	0	1493	59	0
46	R0	648	0	672	25	0
46	Y0	648	0	672	36	0
47	R1	763	0	848	24	0
47	Y1	763	0	848	30	0
48	R2	581	0	629	21	0
48	Y2	581	0	629	78	0
49	R3	469	0	518	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	16	0
50	R4	581	0	575	211	0
50	Y4	581	0	577	100	0
51	R5	459	0	480	79	0
51	Y5	454	0	475	40	0
52	R6	424	0	450	29	0
52	Y6	424	0	450	29	0
53	R7	430	0	480	19	0
53	Y7	430	0	480	21	0
54	R8	517	0	582	94	0
54	Y8	517	0	582	107	0
55	R9	307	0	338	10	0
55	Y9	307	0	338	12	0
56	Z5	37	0	23	1	0
56	Z6	37	0	23	3	0
57	QA	92	0	0	0	0
57	QF	1	0	0	0	0
57	QT	1	0	0	0	0
57	QV	3	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	284	0	0	0	0
57	RB	3	0	0	0	0
57	RD	1	0	0	0	0
57	RE	1	0	0	0	0
57	RQ	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	104	0	0	0	0
57	XD	1	0	0	0	0
57	XV	4	0	0	0	0
57	XX	1	0	0	0	0
57	XY	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y1	1	0	0	0	0
57	Y5	1	0	0	0	0
57	YA	294	0	0	0	0
57	YB	3	0	0	0	0
57	YD	1	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YR	2	0	0	0	0
57	YY	1	0	0	0	0
58	QA	42	0	45	1	0
58	XA	42	0	45	0	0
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
60	Z5	37	0	28	6	0
60	Z6	37	0	28	10	0
All	All	292106	0	198346	7612	1

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 16.

The worst 5 of 7612 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)
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.54
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
30:RG:112:PRO:HB3	50:R4:37:SER:CB	1.45	1.45
30:RG:112:PRO:CB	50:R4:37:SER:HB2	1.46	1.42
19:QS:68:GLY:CA	50:R4:68:ARG:HG2	1.51	1.38

All (1) 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)
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.13	0.07

## 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%)	174 (74%)	44 (19%)	17 (7%)	1	17
2	XB	235/256 (92%)	177 (75%)	43 (18%)	15 (6%)	1	21
3	QC	203/239 (85%)	164 (81%)	33 (16%)	6 (3%)	5	40
3	XC	203/239 (85%)	172 (85%)	28 (14%)	3 (2%)	12	55
4	QD	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	12	55
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	7	45
5	QE	149/162 (92%)	136 (91%)	9 (6%)	4 (3%)	6	42
5	XE	149/162 (92%)	134 (90%)	13 (9%)	2 (1%)	14	57
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	14	57
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	14	57
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	25	68
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	5	41
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	32
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	5	38
10	QJ	97/105 (92%)	77 (79%)	16 (16%)	4 (4%)	3	32
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	25
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11	52
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11	52
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	8
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	8
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	15
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	15
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	19
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	10
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	15	59
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	7	46
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	15	59
16	XP	82/88 (93%)	72 (88%)	9 (11%)	1 (1%)	15	59
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	9	49
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	3	30
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	12	55
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	5
19	XS	82/93 (88%)	54 (66%)	18 (22%)	10 (12%)	0	7
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	2	22
20	XT	97/106 (92%)	77 (79%)	16 (16%)	4 (4%)	3	32
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3	30
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	3	30
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	3	30
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	18
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
29	RF	200/210 (95%)	181 (90%)	13 (6%)	6 (3%)	5	40
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	10
30	RG	179/182 (98%)	139 (78%)	25 (14%)	15 (8%)	1	13
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	20
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	109 (76%)	24 (17%)	11 (8%)	1	15
32	YI	144/148 (97%)	108 (75%)	23 (16%)	13 (9%)	1	12
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	12
33	YN	136/140 (97%)	107 (79%)	16 (12%)	13 (10%)	1	11
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	11	52
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	11	52
35	RP	148/150 (99%)	109 (74%)	26 (18%)	13 (9%)	1	12
35	YP	148/150 (99%)	101 (68%)	35 (24%)	12 (8%)	1	14
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	10
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	10
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	3	30
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	25
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	1	10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	4
39	RT	135/146 (92%)	108 (80%)	15 (11%)	12 (9%)	1	12
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	16
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	4	37
40	YU	115/118 (98%)	102 (89%)	11 (10%)	2 (2%)	11	52
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	22
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	14
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	4	36
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	10	51
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	8	47
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	8	47
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	4
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	7
45	RZ	181/206 (88%)	127 (70%)	34 (19%)	20 (11%)	0	8
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	1	10
46	R0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	14	57
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	1	11
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	21
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	2	22
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	5
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	4	37
49	Y3	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	10	51
50	R4	69/71 (97%)	22 (32%)	21 (30%)	26 (38%)	0	0
50	Y4	69/71 (97%)	34 (49%)	14 (20%)	21 (30%)	0	0
51	R5	57/60 (95%)	33 (58%)	10 (18%)	14 (25%)	0	1
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	4	36
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	1
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	3
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	8	48
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	8	48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2
54	Y8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	5
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11469/12128 (95%)	9030 (79%)	1608 (14%)	831 (7%)	1	17

5 of 831 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	33	MET
12	QL	18	VAL

### 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%)	172 (84%)	33 (16%)	3	19
2	XB	205/220 (93%)	180 (88%)	25 (12%)	6	31
3	QC	159/188 (85%)	145 (91%)	14 (9%)	12	47
3	XC	159/188 (85%)	145 (91%)	14 (9%)	12	47
4	QD	180/181 (99%)	161 (89%)	19 (11%)	8	38
4	XD	180/181 (99%)	154 (86%)	26 (14%)	4	25
5	QE	116/123 (94%)	103 (89%)	13 (11%)	7	36
5	XE	116/123 (94%)	104 (90%)	12 (10%)	8	40
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4	28
6	XF	90/90 (100%)	82 (91%)	8 (9%)	11	46
7	QG	126/127 (99%)	114 (90%)	12 (10%)	10	44
7	XG	126/127 (99%)	114 (90%)	12 (10%)	10	44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	109 (92%)	10 (8%)	13	49
8	XH	119/119 (100%)	106 (89%)	13 (11%)	7	37
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2	15
9	XI	98/99 (99%)	79 (81%)	19 (19%)	1	11
10	QJ	89/92 (97%)	79 (89%)	10 (11%)	7	36
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	3	21
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	41
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9	41
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	28
12	XL	104/109 (95%)	89 (86%)	15 (14%)	4	25
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	5
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	11
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	12
14	XN	49/50 (98%)	42 (86%)	7 (14%)	4	26
15	QO	79/80 (99%)	72 (91%)	7 (9%)	11	46
15	XO	79/80 (99%)	69 (87%)	10 (13%)	5	30
16	QP	72/74 (97%)	63 (88%)	9 (12%)	5	31
16	XP	72/74 (97%)	64 (89%)	8 (11%)	7	37
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	13	49
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	21	60
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	13
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	24
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	11
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	7
20	QT	76/82 (93%)	67 (88%)	9 (12%)	6	33
20	XT	76/82 (93%)	68 (90%)	8 (10%)	8	39
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	28	66
27	RD	214/218 (98%)	175 (82%)	39 (18%)	2	13
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	15
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	7
29	RF	161/166 (97%)	142 (88%)	19 (12%)	6	33
29	YF	161/166 (97%)	140 (87%)	21 (13%)	5	29
30	RG	155/156 (99%)	135 (87%)	20 (13%)	5	29
30	YG	155/156 (99%)	133 (86%)	22 (14%)	4	26
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	10
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	10
32	RI	122/124 (98%)	99 (81%)	23 (19%)	2	11
32	YI	122/124 (98%)	97 (80%)	25 (20%)	1	10
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	16
33	YN	117/119 (98%)	96 (82%)	21 (18%)	2	13
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9	41
34	YO	100/100 (100%)	88 (88%)	12 (12%)	6	32
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0	5
35	YP	116/116 (100%)	79 (68%)	37 (32%)	0	2
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	19
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	16
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	14
37	YR	101/101 (100%)	80 (79%)	21 (21%)	1	9
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	9
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	23
39	RT	120/127 (94%)	101 (84%)	19 (16%)	3	21
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	15
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	23
40	YU	93/94 (99%)	78 (84%)	15 (16%)	3	19
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	11
41	YV	82/82 (100%)	67 (82%)	15 (18%)	2	12
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	9
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	15
43	RX	74/78 (95%)	64 (86%)	10 (14%)	4	28
43	YX	74/78 (95%)	60 (81%)	14 (19%)	2	11

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	5
44	YY	85/91 (93%)	64 (75%)	21 (25%)	1	5
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	3	24
45	YZ	162/179 (90%)	144 (89%)	18 (11%)	7	37
46	R0	65/67 (97%)	60 (92%)	5 (8%)	15	52
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	11	45
47	R1	82/83 (99%)	73 (89%)	9 (11%)	7	37
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	24
48	R2	64/67 (96%)	55 (86%)	9 (14%)	4	26
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	7	37
49	R3	51/52 (98%)	45 (88%)	6 (12%)	6	33
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	3	21
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0	4
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	3
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	6
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	6
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	4
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	9
53	R7	42/42 (100%)	34 (81%)	8 (19%)	2	11
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	17
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	38 (70%)	16 (30%)	0	3
55	R9	34/34 (100%)	32 (94%)	2 (6%)	23	62
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	23	62
All	All	9702/10066 (96%)	8183 (84%)	1519 (16%)	3	21

5 of 1519 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	56	VAL
7	XG	137	LYS
45	YZ	4	ARG
51	R5	6	VAL
2	XB	163	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
55	R9	32	HIS
5	XE	72	GLN
46	Y0	29	GLN
2	XB	212	GLN
9	XI	3	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	260 (17%)	40 (2%)
1	XA	1498/1522 (98%)	283 (18%)	33 (2%)
22	QV	76/77 (98%)	18 (23%)	1 (1%)
22	XV	76/77 (98%)	18 (23%)	1 (1%)
23	QX	7/25 (28%)	1 (14%)	0
23	XX	7/25 (28%)	1 (14%)	0
24	QY	14/18 (77%)	2 (14%)	0
24	XY	14/18 (77%)	1 (7%)	0
25	RA	2879/2915 (98%)	571 (19%)	49 (1%)
25	YA	2879/2915 (98%)	580 (20%)	49 (1%)
26	RB	119/122 (97%)	18 (15%)	1 (0%)
26	YB	119/122 (97%)	25 (21%)	1 (0%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9189/9364 (98%)	1778 (19%)	175 (1%)

5 of 1778 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	32	A
1	QA	39	G

5 of 175 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2126	A
1	XA	243	A
25	YA	1819	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
25	RA	2439	A
25	RA	2832	U

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 819 ligands modelled in this entry, 815 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PAR	QA	1691	-	45,45,45	1.62	8 (17%)	60,67,67	1.36	6 (10%)
58	PAR	XA	1705	-	45,45,45	1.61	7 (15%)	60,67,67	1.30	7 (11%)
60	PPU	Z5	101	56	31,40,41	2.57	6 (19%)	34,57,60	2.57	6 (17%)
60	PPU	Z6	101	56	31,40,41	2.57	6 (19%)	34,57,60	2.54	6 (17%)

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	1691	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1705	-	-	0/18/94/94	0/4/4/4
60	PPU	Z5	101	56	-	0/21/43/44	0/4/4/4
60	PPU	Z6	101	56	-	0/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Z6	101	PPU	C9-N6	-5.79	1.31	1.45
60	Z5	101	PPU	C9-N6	-5.76	1.31	1.45
60	Z5	101	PPU	C10-N6	-5.41	1.32	1.45
60	Z6	101	PPU	C10-N6	-5.37	1.32	1.45
60	Z5	101	PPU	C5-N7	-2.03	1.32	1.39

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Z5	101	PPU	C3'-N3'-C	-8.65	110.16	123.21
60	Z6	101	PPU	C3'-N3'-C	-8.56	110.30	123.21
60	Z5	101	PPU	N3-C2-N1	-8.54	121.42	128.86
60	Z6	101	PPU	N3-C2-N1	-8.36	121.58	128.86
60	Z5	101	PPU	C4'-O4'-C1'	-4.21	105.29	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1691	PAR	1	0
60	Z5	101	PPU	6	0
60	Z6	101	PPU	10	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	QA	1500/1522 (98%)	0.28	56 (3%) 42 31	57, 104, 185, 383	0
1	XA	1500/1522 (98%)	0.40	66 (4%) 35 25	51, 103, 207, 434	0
2	QB	237/256 (92%)	0.49	26 (10%) 6 6	84, 155, 246, 386	0
2	XB	237/256 (92%)	0.30	15 (6%) 21 15	81, 153, 230, 296	0
3	QC	205/239 (85%)	0.27	10 (4%) 30 21	87, 140, 198, 246	0
3	XC	205/239 (85%)	0.20	7 (3%) 46 33	74, 125, 191, 265	0
4	QD	208/209 (99%)	-0.05	4 (1%) 67 53	67, 119, 174, 208	0
4	XD	208/209 (99%)	-0.16	0 100 100	59, 102, 153, 201	0
5	QE	151/162 (93%)	0.32	4 (2%) 56 42	67, 121, 174, 270	0
5	XE	151/162 (93%)	0.21	3 (1%) 65 51	64, 99, 154, 224	0
6	QF	101/101 (100%)	0.06	4 (3%) 39 28	61, 101, 141, 186	0
6	XF	101/101 (100%)	0.15	0 100 100	62, 117, 176, 247	0
7	QG	155/156 (99%)	0.25	7 (4%) 34 24	68, 122, 169, 283	0
7	XG	155/156 (99%)	0.19	7 (4%) 34 24	90, 141, 199, 237	0
8	QH	138/138 (100%)	-0.16	2 (1%) 75 62	79, 122, 158, 186	0
8	XH	138/138 (100%)	-0.19	1 (0%) 87 78	68, 110, 153, 210	0
9	QI	127/128 (99%)	0.55	20 (15%) 2 2	91, 148, 201, 230	0
9	XI	127/128 (99%)	0.78	13 (10%) 7 6	84, 175, 244, 299	0
10	QJ	99/105 (94%)	1.16	26 (26%) 1 1	82, 161, 241, 373	0
10	XJ	99/105 (94%)	1.19	25 (25%) 1 1	79, 163, 228, 273	0
11	QK	119/129 (92%)	0.36	9 (7%) 15 11	56, 101, 162, 256	0
11	XK	119/129 (92%)	0.48	8 (6%) 19 13	67, 110, 177, 274	0
12	QL	125/132 (94%)	0.10	4 (3%) 48 35	69, 104, 168, 283	0
12	XL	125/132 (94%)	0.15	4 (3%) 48 35	53, 84, 144, 324	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	0.14	9 (7%) 15 11	71, 128, 203, 279	0
13	XM	121/126 (96%)	0.22	8 (6%) 19 13	86, 136, 197, 303	0
14	QN	60/61 (98%)	0.14	2 (3%) 47 35	91, 134, 169, 183	0
14	XN	60/61 (98%)	0.25	3 (5%) 30 21	72, 118, 153, 169	0
15	QO	88/89 (98%)	0.19	5 (5%) 24 17	67, 104, 163, 177	0
15	XO	88/89 (98%)	-0.04	0 100 100	68, 104, 164, 190	0
16	QP	84/88 (95%)	0.47	1 (1%) 79 66	73, 105, 160, 205	0
16	XP	84/88 (95%)	0.35	0 100 100	82, 111, 164, 246	0
17	QQ	100/105 (95%)	0.25	5 (5%) 30 21	70, 112, 153, 202	0
17	XQ	100/105 (95%)	0.10	0 100 100	66, 107, 155, 172	0
18	QR	70/88 (79%)	0.41	3 (4%) 36 25	65, 103, 146, 201	0
18	XR	70/88 (79%)	0.47	3 (4%) 36 25	71, 117, 165, 215	0
19	QS	84/93 (90%)	0.31	2 (2%) 59 45	94, 147, 213, 259	0
19	XS	84/93 (90%)	0.22	0 100 100	78, 146, 191, 257	0
20	QT	99/106 (93%)	0.07	2 (2%) 65 51	74, 119, 177, 200	0
20	XT	99/106 (93%)	0.29	3 (3%) 51 37	77, 138, 193, 294	0
21	QU	25/27 (92%)	1.89	7 (28%) 1 1	75, 120, 182, 217	0
21	XU	25/27 (92%)	1.45	4 (16%) 2 2	87, 134, 191, 194	0
22	QV	77/77 (100%)	0.66	9 (11%) 5 5	55, 115, 175, 233	0
22	XV	77/77 (100%)	0.89	13 (16%) 2 2	49, 105, 172, 220	0
23	QX	9/25 (36%)	0.33	1 (11%) 6 5	75, 96, 133, 165	0
23	XX	9/25 (36%)	0.38	1 (11%) 6 5	71, 83, 133, 180	0
24	QY	15/18 (83%)	-0.12	0 100 100	95, 123, 212, 232	0
24	XY	15/18 (83%)	0.10	0 100 100	84, 117, 186, 205	0
25	RA	2882/2915 (98%)	0.35	165 (5%) 24 17	39, 80, 234, 425	0
25	YA	2882/2915 (98%)	0.35	175 (6%) 22 16	34, 77, 235, 417	0
26	RB	120/122 (98%)	0.03	1 (0%) 86 75	84, 112, 143, 194	0
26	YB	120/122 (98%)	0.27	7 (5%) 24 17	77, 126, 164, 215	0
27	RD	272/276 (98%)	-0.19	0 100 100	39, 71, 108, 261	0
27	YD	272/276 (98%)	-0.24	1 (0%) 92 87	35, 71, 111, 288	0
28	RE	205/206 (99%)	0.08	3 (1%) 74 61	52, 98, 171, 310	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YE	205/206 (99%)	0.15	2 (0%) 82 70	34, 95, 173, 258	0
29	RF	202/210 (96%)	0.01	1 (0%) 90 84	40, 88, 154, 206	0
29	YF	202/210 (96%)	-0.16	2 (0%) 82 70	29, 81, 144, 195	0
30	RG	181/182 (99%)	0.22	8 (4%) 35 25	72, 122, 179, 230	0
30	YG	181/182 (99%)	0.43	20 (11%) 6 6	89, 136, 196, 248	0
31	RH	170/180 (94%)	0.97	31 (18%) 1 1	106, 194, 282, 354	0
31	YH	170/180 (94%)	0.22	3 (1%) 69 55	73, 117, 176, 235	0
32	RI	146/148 (98%)	0.15	4 (2%) 55 41	60, 141, 186, 279	0
32	YI	146/148 (98%)	0.42	13 (8%) 10 8	83, 154, 200, 232	0
33	RN	138/140 (98%)	-0.31	0 100 100	67, 100, 163, 207	0
33	YN	138/140 (98%)	-0.27	1 (0%) 87 78	63, 99, 168, 191	0
34	RO	122/122 (100%)	-0.11	0 100 100	52, 95, 138, 173	0
34	YO	122/122 (100%)	-0.18	0 100 100	42, 74, 109, 166	0
35	RP	150/150 (100%)	0.10	3 (2%) 65 51	45, 96, 164, 244	0
35	YP	150/150 (100%)	0.24	7 (4%) 32 23	30, 89, 148, 315	0
36	RQ	141/141 (100%)	0.06	2 (1%) 75 62	57, 103, 163, 249	0
36	YQ	141/141 (100%)	-0.09	2 (1%) 75 62	51, 95, 157, 272	0
37	RR	118/118 (100%)	-0.32	0 100 100	54, 81, 120, 145	0
37	YR	118/118 (100%)	-0.17	0 100 100	51, 86, 126, 180	0
38	RS	111/112 (99%)	0.30	7 (6%) 21 15	67, 115, 168, 265	0
38	YS	111/112 (99%)	0.70	15 (13%) 3 3	85, 134, 190, 269	0
39	RT	137/146 (93%)	0.02	3 (2%) 62 48	64, 107, 210, 292	0
39	YT	137/146 (93%)	0.03	5 (3%) 43 32	60, 93, 177, 240	0
40	RU	117/118 (99%)	0.28	6 (5%) 29 20	48, 83, 146, 225	0
40	YU	117/118 (99%)	0.06	2 (1%) 70 57	43, 87, 148, 282	0
41	RV	101/101 (100%)	0.09	2 (1%) 65 51	51, 108, 171, 279	0
41	YV	101/101 (100%)	-0.04	0 100 100	55, 115, 179, 318	0
42	RW	113/113 (100%)	-0.34	0 100 100	42, 71, 130, 212	0
42	YW	113/113 (100%)	-0.26	2 (1%) 69 55	47, 74, 140, 251	0
43	RX	92/96 (95%)	-0.35	0 100 100	52, 83, 125, 147	0
43	YX	92/96 (95%)	-0.19	0 100 100	51, 78, 122, 171	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RY	102/110 (92%)	0.85	19 (18%) 1 1	55, 114, 227, 327	0
44	YY	102/110 (92%)	0.02	5 (4%) 30 21	59, 105, 184, 353	0
45	RZ	183/206 (88%)	0.58	14 (7%) 14 11	82, 141, 220, 276	0
45	YZ	183/206 (88%)	0.40	13 (7%) 17 12	77, 141, 224, 346	0
46	R0	82/85 (96%)	-0.04	0 100 100	62, 84, 115, 132	0
46	Y0	82/85 (96%)	0.06	0 100 100	57, 93, 121, 148	0
47	R1	97/98 (98%)	0.14	1 (1%) 82 70	44, 83, 188, 262	0
47	Y1	97/98 (98%)	0.15	3 (3%) 49 36	43, 85, 163, 203	0
48	R2	69/72 (95%)	0.11	1 (1%) 75 62	64, 110, 179, 234	0
48	Y2	69/72 (95%)	0.03	2 (2%) 52 38	51, 91, 147, 262	0
49	R3	59/60 (98%)	0.27	0 100 100	61, 99, 152, 191	0
49	Y3	59/60 (98%)	-0.17	0 100 100	56, 99, 165, 237	0
50	R4	71/71 (100%)	0.81	9 (12%) 4 4	114, 191, 338, 387	0
50	Y4	71/71 (100%)	0.40	8 (11%) 6 5	122, 190, 287, 387	0
51	R5	59/60 (98%)	0.68	8 (13%) 3 3	46, 92, 234, 303	0
51	Y5	58/60 (96%)	0.03	1 (1%) 70 57	43, 97, 261, 296	0
52	R6	49/54 (90%)	2.86	31 (63%) 0 0	109, 153, 219, 278	0
52	Y6	49/54 (90%)	3.45	35 (71%) 0 0	117, 165, 246, 359	0
53	R7	49/49 (100%)	0.31	2 (4%) 38 27	39, 61, 133, 189	0
53	Y7	49/49 (100%)	0.55	3 (6%) 22 16	34, 55, 138, 211	0
54	R8	64/65 (98%)	0.14	1 (1%) 72 59	49, 83, 154, 240	0
54	Y8	64/65 (98%)	0.02	0 100 100	53, 84, 145, 225	0
55	R9	37/37 (100%)	4.04	30 (81%) 0 0	152, 197, 266, 308	0
55	Y9	37/37 (100%)	4.37	32 (86%) 0 0	121, 172, 251, 289	0
56	Z5	2/3 (66%)	0.51	0 100 100	66, 66, 66, 77	0
56	Z6	2/3 (66%)	0.86	0 100 100	74, 74, 74, 74	0
All	All	20875/21492 (97%)	0.28	1113 (5%) 27 20	29, 102, 206, 434	0

The worst 5 of 1113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	2799	A	22.0
25	YA	1536	A	17.4

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
25	RA	2801	A	14.5
25	YA	1057	A	12.6
2	QB	4	GLU	11.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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	3277	1/1	0.72	0.98	64.81	69,69,69,69	0
57	MG	YA	3246	1/1	0.87	0.72	54.41	56,56,56,56	0
57	MG	YA	3084	1/1	0.97	0.64	52.61	39,39,39,39	0
57	MG	XA	1650	1/1	0.75	1.27	51.16	67,67,67,67	0
57	MG	YA	3172	1/1	0.88	0.51	41.80	46,46,46,46	0
57	MG	RA	3126	1/1	0.95	0.57	36.38	65,65,65,65	0
57	MG	YA	3278	1/1	0.97	0.56	34.34	65,65,65,65	0
57	MG	RA	3268	1/1	0.90	0.91	33.59	70,70,70,70	0
57	MG	RA	3154	1/1	0.81	0.55	32.31	46,46,46,46	0
57	MG	RA	3067	1/1	0.94	0.49	31.74	35,35,35,35	0
57	MG	XA	1675	1/1	0.74	0.52	29.86	56,56,56,56	0
57	MG	YA	3178	1/1	0.94	0.56	29.76	22,22,22,22	0
57	MG	YA	3141	1/1	0.63	0.60	28.44	56,56,56,56	0
57	MG	YA	3213	1/1	0.89	0.89	27.74	77,77,77,77	0
57	MG	YA	3110	1/1	0.95	0.63	26.34	45,45,45,45	0
57	MG	RA	3062	1/1	0.95	0.71	25.92	19,19,19,19	0
57	MG	RA	3161	1/1	0.81	0.55	24.49	62,62,62,62	0
57	MG	RA	3058	1/1	0.96	0.44	23.88	14,14,14,14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3087	1/1	0.92	0.70	23.70	49,49,49,49	0
57	MG	YA	3106	1/1	0.95	0.59	23.64	24,24,24,24	0
57	MG	R8	101	1/1	0.52	0.97	23.07	86,86,86,86	0
57	MG	RA	3093	1/1	0.97	0.66	22.77	30,30,30,30	0
57	MG	YA	3269	1/1	0.83	0.60	22.44	68,68,68,68	0
57	MG	YA	3047	1/1	0.95	0.53	21.03	23,23,23,23	0
57	MG	YA	3155	1/1	0.86	0.44	20.67	51,51,51,51	0
57	MG	YA	3026	1/1	0.96	0.80	20.33	31,31,31,31	0
57	MG	YA	3237	1/1	0.90	0.45	19.59	15,15,15,15	0
57	MG	RA	3095	1/1	0.99	0.58	19.57	33,33,33,33	0
57	MG	RA	3200	1/1	0.69	0.56	19.55	69,69,69,69	0
57	MG	RA	3051	1/1	0.97	0.55	19.48	29,29,29,29	0
57	MG	RA	3166	1/1	0.93	0.50	19.42	40,40,40,40	0
57	MG	YA	3033	1/1	0.98	0.50	18.74	20,20,20,20	0
57	MG	YA	3050	1/1	0.98	0.52	18.29	24,24,24,24	0
57	MG	YA	3170	1/1	0.64	0.54	18.15	55,55,55,55	0
57	MG	YA	3277	1/1	0.95	0.43	17.10	58,58,58,58	0
57	MG	YA	3009	1/1	0.96	0.55	17.02	40,40,40,40	0
57	MG	RA	3032	1/1	0.95	0.71	16.93	48,48,48,48	0
57	MG	RA	3048	1/1	0.87	0.51	16.70	47,47,47,47	0
57	MG	YA	3259	1/1	0.36	0.65	16.63	145,145,145,145	0
57	MG	YA	3105	1/1	1.00	0.38	16.37	13,13,13,13	0
57	MG	QA	1645	1/1	0.92	0.70	16.25	52,52,52,52	0
57	MG	RA	3077	1/1	0.97	0.54	16.04	30,30,30,30	0
57	MG	XA	1632	1/1	0.89	0.89	15.91	65,65,65,65	0
57	MG	YA	3192	1/1	0.80	0.33	15.47	44,44,44,44	0
57	MG	RA	3075	1/1	0.98	0.52	15.19	34,34,34,34	0
57	MG	YA	3227	1/1	0.98	0.59	15.13	17,17,17,17	0
57	MG	YA	3283	1/1	0.88	0.48	14.87	47,47,47,47	0
57	MG	YA	3164	1/1	0.96	0.61	14.42	38,38,38,38	0
57	MG	RA	3033	1/1	0.94	0.49	14.37	31,31,31,31	0
57	MG	YA	3215	1/1	0.66	0.61	14.01	77,77,77,77	0
57	MG	RA	3220	1/1	0.91	0.46	13.76	20,20,20,20	0
57	MG	YA	3097	1/1	0.96	0.55	13.63	45,45,45,45	0
57	MG	RA	3056	1/1	0.95	0.44	13.32	32,32,32,32	0
57	MG	RA	3162	1/1	0.90	0.54	13.22	39,39,39,39	0
57	MG	QA	1665	1/1	0.93	0.86	12.87	55,55,55,55	0
57	MG	YA	3013	1/1	0.99	0.54	12.76	18,18,18,18	0
57	MG	YA	3017	1/1	0.99	0.41	12.66	42,42,42,42	0
57	MG	RA	3150	1/1	0.97	0.36	12.36	36,36,36,36	0
57	MG	YA	3098	1/1	0.99	0.41	12.24	13,13,13,13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1619	1/1	0.94	0.52	12.10	43,43,43,43	0
57	MG	RA	3257	1/1	0.85	0.57	12.09	60,60,60,60	0
57	MG	YA	3088	1/1	0.95	0.50	11.92	54,54,54,54	0
57	MG	YA	3031	1/1	0.98	0.50	11.92	11,11,11,11	0
57	MG	RA	3035	1/1	0.98	0.47	11.91	32,32,32,32	0
57	MG	YA	3162	1/1	0.97	0.39	11.56	59,59,59,59	0
57	MG	RA	3188	1/1	0.71	0.44	11.45	75,75,75,75	0
57	MG	YA	3244	1/1	0.98	0.31	11.41	26,26,26,26	0
57	MG	XA	1680	1/1	0.89	0.83	11.36	61,61,61,61	0
57	MG	YA	3049	1/1	0.97	0.55	11.32	23,23,23,23	0
57	MG	YA	3168	1/1	0.91	0.58	11.27	39,39,39,39	0
57	MG	YA	3200	1/1	0.92	0.47	11.23	79,79,79,79	0
57	MG	RA	3061	1/1	0.95	0.45	11.16	12,12,12,12	0
57	MG	YA	3034	1/1	0.98	0.33	11.01	20,20,20,20	0
57	MG	QA	1666	1/1	0.96	0.54	10.98	71,71,71,71	0
57	MG	RA	3227	1/1	0.97	0.37	10.89	46,46,46,46	0
57	MG	YD	301	1/1	0.70	0.57	10.72	52,52,52,52	0
57	MG	XA	1641	1/1	0.96	0.67	10.67	68,68,68,68	0
57	MG	YA	3096	1/1	0.96	0.36	10.14	36,36,36,36	0
57	MG	RA	3096	1/1	0.97	0.44	10.05	24,24,24,24	0
57	MG	XA	1691	1/1	0.97	0.32	10.05	66,66,66,66	0
57	MG	YA	3023	1/1	0.98	0.42	10.03	31,31,31,31	0
57	MG	QA	1613	1/1	0.96	0.42	9.91	40,40,40,40	0
57	MG	YA	3176	1/1	0.77	0.37	9.84	54,54,54,54	0
57	MG	YA	3112	1/1	0.99	0.43	9.82	35,35,35,35	0
57	MG	RA	3037	1/1	0.96	0.38	9.53	33,33,33,33	0
57	MG	RA	3221	1/1	0.95	0.48	9.31	23,23,23,23	0
57	MG	QA	1662	1/1	0.97	0.45	8.71	34,34,34,34	0
57	MG	YA	3025	1/1	0.98	0.34	8.46	17,17,17,17	0
57	MG	RA	3011	1/1	0.96	0.47	8.19	24,24,24,24	0
57	MG	YA	3235	1/1	0.92	0.43	8.07	29,29,29,29	0
57	MG	RA	3198	1/1	0.91	0.41	8.05	64,64,64,64	0
57	MG	YA	3233	1/1	0.98	0.46	8.05	39,39,39,39	0
57	MG	YA	3078	1/1	0.98	0.37	7.99	21,21,21,21	0
57	MG	RA	3055	1/1	0.98	0.41	7.95	29,29,29,29	0
57	MG	YA	3032	1/1	0.96	0.34	7.86	18,18,18,18	0
57	MG	YA	3006	1/1	0.79	0.47	7.74	62,62,62,62	0
57	MG	YA	3087	1/1	0.96	0.39	7.60	21,21,21,21	0
57	MG	YA	3080	1/1	0.85	0.27	7.57	47,47,47,47	0
57	MG	YA	3231	1/1	0.88	0.44	7.52	46,46,46,46	0
57	MG	YA	3154	1/1	0.65	0.39	7.37	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3132	1/1	0.90	0.33	7.33	21,21,21,21	0
57	MG	XA	1671	1/1	0.95	0.73	7.16	54,54,54,54	0
57	MG	QA	1639	1/1	0.76	0.38	7.11	62,62,62,62	0
57	MG	RA	3187	1/1	0.94	0.42	6.99	34,34,34,34	0
57	MG	YA	3068	1/1	0.99	0.48	6.97	36,36,36,36	0
57	MG	RA	3112	1/1	0.91	0.32	6.94	34,34,34,34	0
57	MG	RA	3237	1/1	0.94	0.47	6.79	55,55,55,55	0
57	MG	RA	3018	1/1	0.99	0.42	6.72	22,22,22,22	0
57	MG	YR	202	1/1	0.93	0.60	6.67	46,46,46,46	0
57	MG	RA	3025	1/1	0.94	0.35	6.60	16,16,16,16	0
57	MG	YA	3121	1/1	0.93	0.49	6.53	26,26,26,26	0
57	MG	XA	1633	1/1	0.92	0.39	6.51	47,47,47,47	0
57	MG	RA	3152	1/1	0.89	0.39	6.38	59,59,59,59	0
57	MG	YA	3038	1/1	0.97	0.33	6.25	28,28,28,28	0
57	MG	YA	3137	1/1	0.85	0.61	6.09	50,50,50,50	0
57	MG	YA	3036	1/1	0.97	0.31	6.01	30,30,30,30	0
57	MG	QA	1682	1/1	0.84	0.70	5.91	67,67,67,67	0
57	MG	QA	1660	1/1	0.95	0.53	5.86	30,30,30,30	0
57	MG	RA	3039	1/1	0.97	0.39	5.74	29,29,29,29	0
57	MG	XV	102	1/1	0.97	0.41	5.74	47,47,47,47	0
57	MG	RA	3006	1/1	0.97	0.43	5.68	20,20,20,20	0
57	MG	YA	3273	1/1	0.96	0.29	5.68	44,44,44,44	0
57	MG	XA	1618	1/1	0.91	0.61	5.59	52,52,52,52	0
57	MG	YA	3262	1/1	0.94	0.42	5.59	53,53,53,53	0
57	MG	YA	3122	1/1	0.87	0.31	5.46	34,34,34,34	0
57	MG	RA	3175	1/1	0.81	0.43	5.39	58,58,58,58	0
57	MG	RA	3274	1/1	0.96	0.27	5.28	58,58,58,58	0
57	MG	XA	1616	1/1	0.95	0.43	5.28	47,47,47,47	0
57	MG	QA	1674	1/1	0.96	0.50	5.16	55,55,55,55	0
57	MG	YA	3161	1/1	0.81	0.29	5.09	64,64,64,64	0
57	MG	RA	3092	1/1	0.98	0.52	5.03	39,39,39,39	0
57	MG	YA	3002	1/1	0.98	0.42	5.03	26,26,26,26	0
57	MG	XA	1689	1/1	0.92	0.39	5.02	55,55,55,55	0
57	MG	RA	3020	1/1	0.98	0.30	5.01	23,23,23,23	0
57	MG	QA	1615	1/1	0.90	0.33	5.01	58,58,58,58	0
57	MG	RA	3023	1/1	0.98	0.28	4.92	27,27,27,27	0
57	MG	XA	1603	1/1	0.94	0.53	4.90	31,31,31,31	0
57	MG	RA	3014	1/1	0.97	0.38	4.86	17,17,17,17	0
57	MG	YA	3241	1/1	0.97	0.43	4.83	27,27,27,27	0
57	MG	YA	3135	1/1	0.95	0.32	4.83	17,17,17,17	0
57	MG	RA	3117	1/1	0.92	0.46	4.83	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1669	1/1	0.99	0.28	4.71	41,41,41,41	0
57	MG	XA	1623	1/1	0.98	0.29	4.71	54,54,54,54	0
57	MG	QA	1605	1/1	0.96	0.49	4.63	30,30,30,30	0
57	MG	YA	3027	1/1	0.96	0.27	4.53	22,22,22,22	0
57	MG	RA	3283	1/1	0.96	0.33	4.32	50,50,50,50	0
57	MG	YA	3072	1/1	0.95	0.25	4.28	38,38,38,38	0
57	MG	RA	3147	1/1	0.96	0.29	4.22	37,37,37,37	0
57	MG	XA	1606	1/1	0.82	0.40	4.16	42,42,42,42	0
57	MG	RA	3121	1/1	0.89	0.24	4.11	33,33,33,33	0
57	MG	RA	3217	1/1	0.98	0.48	4.06	32,32,32,32	0
57	MG	RA	3108	1/1	0.86	0.34	4.06	48,48,48,48	0
57	MG	YA	3042	1/1	0.96	0.46	4.02	42,42,42,42	0
57	MG	RA	3004	1/1	0.98	0.33	3.95	20,20,20,20	0
57	MG	RA	3100	1/1	0.05	0.40	3.94	53,53,53,53	0
57	MG	XA	1631	1/1	0.97	0.30	3.94	49,49,49,49	0
57	MG	RA	3116	1/1	0.95	0.34	3.93	64,64,64,64	0
57	MG	RA	3083	1/1	0.98	0.31	3.86	28,28,28,28	0
57	MG	RR	201	1/1	0.88	0.57	3.86	30,30,30,30	0
57	MG	XA	1640	1/1	0.98	0.26	3.77	60,60,60,60	0
57	MG	XA	1695	1/1	0.96	0.33	3.72	57,57,57,57	0
57	MG	XD	302	1/1	0.84	0.37	3.66	90,90,90,90	0
57	MG	RA	3232	1/1	0.94	0.28	3.65	77,77,77,77	0
57	MG	YA	3048	1/1	0.97	0.28	3.63	18,18,18,18	0
57	MG	XA	1626	1/1	0.90	0.26	3.60	38,38,38,38	0
57	MG	YA	3071	1/1	0.98	0.36	3.59	21,21,21,21	0
57	MG	YA	3015	1/1	0.98	0.39	3.58	28,28,28,28	0
57	MG	RA	3170	1/1	0.85	0.30	3.55	50,50,50,50	0
57	MG	YA	3035	1/1	0.97	0.39	3.45	16,16,16,16	0
57	MG	XA	1602	1/1	0.97	0.29	3.41	19,19,19,19	0
57	MG	YA	3132	1/1	0.73	0.30	3.41	48,48,48,48	0
57	MG	YA	3191	1/1	0.78	0.27	3.39	66,66,66,66	0
57	MG	XA	1617	1/1	0.94	0.25	3.38	21,21,21,21	0
57	MG	QA	1620	1/1	0.92	0.24	3.31	62,62,62,62	0
57	MG	RA	3073	1/1	0.98	0.25	3.26	39,39,39,39	0
57	MG	RA	3197	1/1	0.97	0.25	3.26	21,21,21,21	0
57	MG	QA	1658	1/1	0.97	0.23	3.16	50,50,50,50	0
57	MG	YA	3041	1/1	0.94	0.36	3.15	9,9,9,9	0
57	MG	XA	1663	1/1	0.96	0.23	3.13	35,35,35,35	0
57	MG	YA	3199	1/1	0.83	0.27	3.10	93,93,93,93	0
57	MG	XA	1621	1/1	0.98	0.27	3.09	39,39,39,39	0
57	MG	QA	1614	1/1	0.98	0.29	3.07	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1622	1/1	0.96	0.25	2.87	80,80,80,80	0
57	MG	YA	3037	1/1	0.96	0.30	2.82	21,21,21,21	0
57	MG	YA	3242	1/1	0.99	0.33	2.73	47,47,47,47	0
57	MG	YA	3207	1/1	0.73	0.27	2.71	48,48,48,48	0
57	MG	RA	3086	1/1	0.95	0.31	2.67	30,30,30,30	0
57	MG	RA	3079	1/1	0.99	0.31	2.63	34,34,34,34	0
57	MG	RA	3103	1/1	0.94	0.30	2.61	49,49,49,49	0
57	MG	QA	1689	1/1	0.97	0.26	2.52	80,80,80,80	0
57	MG	YA	3185	1/1	0.93	0.32	2.50	52,52,52,52	0
57	MG	YA	3115	1/1	0.86	0.27	2.50	43,43,43,43	0
57	MG	RD	301	1/1	0.89	0.27	2.47	66,66,66,66	0
57	MG	QA	1676	1/1	0.87	0.30	2.44	66,66,66,66	0
57	MG	YA	3028	1/1	0.99	0.28	2.42	18,18,18,18	0
57	MG	RA	3057	1/1	0.91	0.25	2.39	21,21,21,21	0
57	MG	QA	1684	1/1	0.85	0.34	2.38	76,76,76,76	0
57	MG	RA	3002	1/1	0.96	0.39	2.23	27,27,27,27	0
60	PPU	Z6	101	37/38	0.94	0.30	2.22	54,60,68,70	0
57	MG	YA	3292	1/1	0.86	0.34	2.20	66,66,66,66	0
57	MG	RA	3097	1/1	0.93	0.33	2.17	52,52,52,52	0
57	MG	YA	3008	1/1	0.99	0.26	2.10	21,21,21,21	0
58	PAR	QA	1691	42/42	0.93	0.23	2.04	82,82,83,83	0
57	MG	RA	3127	1/1	0.97	0.27	2.00	30,30,30,30	0
57	MG	QA	1657	1/1	0.83	0.37	1.98	64,64,64,64	0
57	MG	RA	3118	1/1	0.95	0.26	1.97	40,40,40,40	0
57	MG	RA	3078	1/1	0.98	0.28	1.83	42,42,42,42	0
57	MG	YP	201	1/1	0.86	0.32	1.83	48,48,48,48	0
57	MG	YA	3070	1/1	0.60	0.26	1.82	39,39,39,39	0
57	MG	YA	3069	1/1	0.96	0.21	1.80	19,19,19,19	0
57	MG	RA	3105	1/1	0.97	0.27	1.71	24,24,24,24	0
57	MG	YA	3044	1/1	0.92	0.29	1.67	14,14,14,14	0
57	MG	YA	3092	1/1	0.95	0.32	1.67	40,40,40,40	0
57	MG	RA	3084	1/1	0.98	0.30	1.62	53,53,53,53	0
57	MG	RA	3024	1/1	0.54	0.25	1.56	50,50,50,50	0
57	MG	YA	3280	1/1	0.89	0.57	1.56	72,72,72,72	0
57	MG	YA	3236	1/1	0.89	0.29	1.49	76,76,76,76	0
57	MG	YA	3011	1/1	0.97	0.26	1.38	22,22,22,22	0
57	MG	RA	3030	1/1	0.94	0.34	1.38	50,50,50,50	0
57	MG	YA	3058	1/1	0.97	0.23	1.32	20,20,20,20	0
57	MG	XA	1612	1/1	0.94	0.25	1.30	54,54,54,54	0
57	MG	RA	3085	1/1	0.95	0.31	1.25	37,37,37,37	0
57	MG	RA	3128	1/1	0.85	0.17	1.22	69,69,69,69	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3004	1/1	0.97	0.26	1.21	14,14,14,14	0
57	MG	QV	102	1/1	0.93	0.27	1.19	43,43,43,43	0
57	MG	YA	3291	1/1	0.98	0.28	1.19	37,37,37,37	0
57	MG	RA	3034	1/1	0.96	0.28	1.16	21,21,21,21	0
57	MG	QA	1611	1/1	0.99	0.27	1.13	29,29,29,29	0
57	MG	QA	1617	1/1	0.98	0.31	1.11	39,39,39,39	0
57	MG	YA	3195	1/1	0.63	0.36	1.03	65,65,65,65	0
57	MG	QA	1652	1/1	0.97	0.24	1.02	44,44,44,44	0
57	MG	XA	1704	1/1	0.90	0.26	1.02	68,68,68,68	0
57	MG	XA	1608	1/1	0.98	0.22	0.99	23,23,23,23	0
57	MG	RA	3016	1/1	0.99	0.23	0.99	27,27,27,27	0
57	MG	YA	3139	1/1	0.94	0.24	0.92	52,52,52,52	0
57	MG	QA	1632	1/1	0.78	0.23	0.90	50,50,50,50	0
57	MG	RA	3282	1/1	0.62	0.35	0.87	86,86,86,86	0
57	MG	RA	3243	1/1	0.95	0.22	0.81	41,41,41,41	0
57	MG	RA	3137	1/1	0.83	0.22	0.78	59,59,59,59	0
58	PAR	XA	1705	42/42	0.95	0.23	0.78	68,68,69,69	0
60	PPU	Z5	101	37/38	0.95	0.27	0.77	68,69,69,69	0
57	MG	QA	1621	1/1	0.90	0.29	0.65	62,62,62,62	0
57	MG	QA	1683	1/1	0.79	0.27	0.63	96,96,96,96	0
57	MG	RA	3124	1/1	0.98	0.24	0.59	51,51,51,51	0
57	MG	RA	3164	1/1	0.90	0.19	0.52	37,37,37,37	0
57	MG	YA	3111	1/1	0.94	0.24	0.48	62,62,62,62	0
57	MG	Y1	101	1/1	0.94	0.30	0.45	37,37,37,37	0
57	MG	YA	3167	1/1	0.92	0.21	0.42	52,52,52,52	0
57	MG	RA	3098	1/1	0.46	0.23	0.39	40,40,40,40	0
57	MG	RA	3021	1/1	0.87	0.25	0.32	36,36,36,36	0
57	MG	YA	3065	1/1	0.82	0.21	0.31	26,26,26,26	0
57	MG	RA	3041	1/1	0.99	0.22	0.30	34,34,34,34	0
59	ZN	QD	301	1/1	0.97	0.29	0.26	74,74,74,74	0
57	MG	YA	3014	1/1	0.97	0.27	0.24	12,12,12,12	0
57	MG	RA	3195	1/1	0.95	0.18	0.23	43,43,43,43	0
57	MG	YA	3217	1/1	0.90	0.23	0.22	50,50,50,50	0
57	MG	RA	3148	1/1	0.61	0.25	0.20	41,41,41,41	0
57	MG	RA	3064	1/1	0.90	0.28	0.12	17,17,17,17	0
59	ZN	XD	301	1/1	0.97	0.29	-0.03	65,65,65,65	0
57	MG	RA	3223	1/1	0.92	0.22	-0.16	57,57,57,57	0
57	MG	YA	3243	1/1	0.87	0.22	-0.25	35,35,35,35	0
57	MG	YA	3230	1/1	0.99	0.29	-0.30	18,18,18,18	0
57	MG	YA	3294	1/1	0.79	0.25	-0.31	52,52,52,52	0
57	MG	RA	3179	1/1	0.85	0.21	-0.33	75,75,75,75	0
57	MG	RA	3141	1/1	0.96	0.20	-0.37	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3117	1/1	0.92	0.24	-0.40	66,66,66,66	0
57	MG	QF	201	1/1	0.93	0.24	-0.44	70,70,70,70	0
57	MG	XA	1613	1/1	0.97	0.22	-0.46	26,26,26,26	0
57	MG	YA	3177	1/1	0.82	0.19	-0.49	55,55,55,55	0
57	MG	RA	3072	1/1	0.78	0.16	-0.54	61,61,61,61	0
57	MG	YA	3005	1/1	0.96	0.16	-0.66	18,18,18,18	0
57	MG	XA	1646	1/1	0.84	0.15	-0.67	49,49,49,49	0
57	MG	XA	1644	1/1	0.44	0.20	-0.73	100,100,100,100	0
57	MG	XA	1610	1/1	0.95	0.16	-0.79	30,30,30,30	0
57	MG	YA	3169	1/1	0.96	0.16	-0.82	63,63,63,63	0
59	ZN	XN	101	1/1	0.97	0.18	-0.83	122,122,122,122	0
57	MG	XA	1635	1/1	0.90	0.17	-0.86	36,36,36,36	0
57	MG	XA	1653	1/1	0.92	0.26	-0.86	48,48,48,48	0
57	MG	YA	3129	1/1	0.82	0.15	-0.94	57,57,57,57	0
57	MG	YA	3284	1/1	0.93	0.18	-0.97	66,66,66,66	0
57	MG	YA	3109	1/1	0.99	0.16	-1.00	49,49,49,49	0
57	MG	RA	3053	1/1	0.84	0.16	-1.01	51,51,51,51	0
57	MG	RA	3192	1/1	0.70	0.15	-1.02	35,35,35,35	0
57	MG	QA	1609	1/1	0.94	0.14	-1.02	55,55,55,55	0
57	MG	RA	3063	1/1	0.94	0.17	-1.05	19,19,19,19	0
57	MG	XA	1686	1/1	0.77	0.18	-1.06	69,69,69,69	0
57	MG	RA	3177	1/1	0.69	0.18	-1.09	60,60,60,60	0
57	MG	QA	1635	1/1	0.96	0.17	-1.10	51,51,51,51	0
57	MG	XA	1652	1/1	0.95	0.18	-1.13	70,70,70,70	0
57	MG	YA	3149	1/1	0.90	0.18	-1.18	69,69,69,69	0
57	MG	QA	1693	1/1	0.74	0.13	-1.21	87,87,87,87	0
57	MG	YA	3024	1/1	0.95	0.21	-1.22	22,22,22,22	0
57	MG	RA	3241	1/1	0.88	0.22	-1.23	58,58,58,58	0
57	MG	YA	3216	1/1	0.97	0.18	-1.23	34,34,34,34	0
57	MG	RA	3013	1/1	0.96	0.17	-1.27	20,20,20,20	0
57	MG	RA	3238	1/1	0.94	0.15	-1.29	54,54,54,54	0
57	MG	YA	3126	1/1	0.92	0.15	-1.31	58,58,58,58	0
57	MG	YA	3189	1/1	0.95	0.17	-1.37	70,70,70,70	0
57	MG	QA	1646	1/1	0.93	0.19	-1.56	80,80,80,80	0
59	ZN	QN	101	1/1	0.98	0.11	-1.57	104,104,104,104	0
57	MG	RA	3281	1/1	0.93	0.16	-1.57	26,26,26,26	0
57	MG	RA	3070	1/1	0.98	0.12	-1.65	29,29,29,29	0
57	MG	QA	1643	1/1	0.87	0.25	-1.65	50,50,50,50	0
57	MG	YA	3150	1/1	0.95	0.16	-1.70	44,44,44,44	0
57	MG	XA	1654	1/1	0.97	0.11	-1.73	84,84,84,84	0
57	MG	YA	3214	1/1	0.96	0.12	-1.75	36,36,36,36	0
57	MG	RA	3240	1/1	0.96	0.14	-1.89	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1607	1/1	0.98	0.13	-1.91	37,37,37,37	0
57	MG	YA	3056	1/1	0.97	0.15	-1.94	19,19,19,19	0
57	MG	RA	3120	1/1	0.93	0.13	-1.94	45,45,45,45	0
57	MG	QA	1692	1/1	0.93	0.13	-1.97	64,64,64,64	0
57	MG	YA	3134	1/1	0.90	0.14	-2.06	40,40,40,40	0
57	MG	XA	1694	1/1	0.85	0.16	-2.12	117,117,117,117	0
57	MG	RA	3144	1/1	0.95	0.12	-2.24	34,34,34,34	0
57	MG	XA	1660	1/1	0.95	0.15	-2.28	46,46,46,46	0
57	MG	RB	201	1/1	0.98	0.12	-2.32	71,71,71,71	0
57	MG	YA	3077	1/1	0.92	0.16	-2.36	40,40,40,40	0
57	MG	RA	3131	1/1	0.97	0.16	-2.37	43,43,43,43	0
57	MG	YA	3173	1/1	0.96	0.12	-2.59	53,53,53,53	0
57	MG	RA	3259	1/1	0.94	0.13	-2.60	63,63,63,63	0
57	MG	RA	3157	1/1	0.94	0.11	-2.68	47,47,47,47	0
57	MG	YA	3182	1/1	0.96	0.11	-2.75	58,58,58,58	0
57	MG	QA	1610	1/1	0.99	0.16	-2.78	31,31,31,31	0
57	MG	RA	3262	1/1	0.95	0.12	-3.02	70,70,70,70	0
57	MG	QA	1650	1/1	0.91	0.10	-3.22	72,72,72,72	0
57	MG	RA	3176	1/1	0.94	0.11	-3.28	40,40,40,40	0
57	MG	YB	202	1/1	0.96	0.12	-3.37	83,83,83,83	0
57	MG	YA	3059	1/1	0.97	0.11	-3.50	59,59,59,59	0
57	MG	XA	1677	1/1	0.95	0.09	-3.57	62,62,62,62	0
57	MG	RA	3205	1/1	0.86	0.09	-3.72	69,69,69,69	0
57	MG	QA	1631	1/1	0.89	0.14	-3.82	68,68,68,68	0
57	MG	YA	3102	1/1	0.78	0.14	-5.09	23,23,23,23	0
57	MG	XA	1624	1/1	0.98	0.09	-5.59	45,45,45,45	0
57	MG	YA	3253	1/1	0.97	0.14	-5.73	53,53,53,53	0
57	MG	XA	1620	1/1	0.97	0.07	-6.18	56,56,56,56	0
57	MG	RA	3059	1/1	0.98	0.32	-	17,17,17,17	0
57	MG	YA	3156	1/1	0.66	0.20	-	53,53,53,53	0
57	MG	YA	3290	1/1	0.92	0.13	-	57,57,57,57	0
57	MG	YA	3046	1/1	0.94	0.41	-	23,23,23,23	0
57	MG	RA	3167	1/1	0.92	0.34	-	40,40,40,40	0
57	MG	RA	3168	1/1	0.88	0.29	-	53,53,53,53	0
57	MG	RA	3134	1/1	0.68	0.19	-	79,79,79,79	0
57	MG	YA	3265	1/1	0.86	0.31	-	62,62,62,62	0
57	MG	YA	3119	1/1	0.95	0.24	-	36,36,36,36	0
57	MG	XA	1672	1/1	0.92	0.34	-	57,57,57,57	0
57	MG	YA	3057	1/1	0.96	0.41	-	19,19,19,19	0
57	MG	XA	1638	1/1	0.93	0.17	-	62,62,62,62	0
57	MG	RA	3270	1/1	0.66	0.45	-	47,47,47,47	0
57	MG	YA	3062	1/1	0.99	0.26	-	16,16,16,16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3251	1/1	0.77	0.34	-	66,66,66,66	0
57	MG	RA	3173	1/1	0.91	0.31	-	44,44,44,44	0
57	MG	YA	3086	1/1	0.98	0.41	-	24,24,24,24	0
57	MG	RA	3211	1/1	0.88	0.84	-	56,56,56,56	0
57	MG	QA	1668	1/1	0.70	0.73	-	75,75,75,75	0
57	MG	QA	1685	1/1	0.77	0.41	-	60,60,60,60	0
57	MG	RA	3136	1/1	0.63	0.66	-	45,45,45,45	0
57	MG	RA	3174	1/1	0.93	0.27	-	61,61,61,61	0
57	MG	YE	301	1/1	0.86	0.41	-	30,30,30,30	0
57	MG	YA	3083	1/1	0.97	0.41	-	32,32,32,32	0
57	MG	YA	3281	1/1	0.64	0.71	-	66,66,66,66	0
57	MG	YR	201	1/1	0.85	0.88	-	54,54,54,54	0
57	MG	RA	3005	1/1	0.87	0.43	-	29,29,29,29	0
57	MG	YA	3012	1/1	0.97	0.52	-	13,13,13,13	0
57	MG	RA	3246	1/1	0.89	0.80	-	59,59,59,59	0
57	MG	YA	3053	1/1	0.95	0.42	-	24,24,24,24	0
57	MG	YA	3022	1/1	0.96	0.50	-	20,20,20,20	0
57	MG	YA	3260	1/1	0.89	0.53	-	59,59,59,59	0
57	MG	YA	3124	1/1	0.94	1.04	-	60,60,60,60	0
57	MG	RA	3111	1/1	0.89	0.53	-	42,42,42,42	0
57	MG	YA	3101	1/1	0.97	0.49	-	25,25,25,25	0
57	MG	RA	3208	1/1	0.95	0.52	-	22,22,22,22	0
57	MG	RA	3206	1/1	0.78	0.28	-	70,70,70,70	0
57	MG	RA	3235	1/1	0.95	0.69	-	64,64,64,64	0
57	MG	XA	1702	1/1	0.77	0.80	-	75,75,75,75	0
57	MG	YA	3040	1/1	0.99	0.38	-	8,8,8,8	0
57	MG	YA	3181	1/1	0.70	0.29	-	63,63,63,63	0
57	MG	YA	3144	1/1	0.93	0.23	-	14,14,14,14	0
57	MG	XA	1683	1/1	0.93	0.21	-	74,74,74,74	0
57	MG	YA	3104	1/1	0.78	0.60	-	41,41,41,41	0
57	MG	RA	3269	1/1	0.86	0.69	-	62,62,62,62	0
57	MG	YA	3147	1/1	0.95	0.08	-	68,68,68,68	0
57	MG	QA	1655	1/1	0.96	0.10	-	120,120,120,120	0
57	MG	YA	3039	1/1	0.90	0.12	-	30,30,30,30	0
57	MG	YA	3186	1/1	0.92	0.22	-	60,60,60,60	0
57	MG	QA	1612	1/1	0.95	0.28	-	23,23,23,23	0
57	MG	YA	3063	1/1	0.72	0.18	-	42,42,42,42	0
57	MG	XA	1674	1/1	0.93	0.51	-	39,39,39,39	0
57	MG	RA	3219	1/1	0.88	0.42	-	44,44,44,44	0
57	MG	YA	3165	1/1	0.85	0.27	-	90,90,90,90	0
57	MG	YA	3075	1/1	0.98	0.34	-	21,21,21,21	0
57	MG	RA	3074	1/1	0.99	0.30	-	19,19,19,19	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3194	1/1	0.76	0.48	-	48,48,48,48	0
57	MG	QA	1619	1/1	0.87	0.65	-	58,58,58,58	0
57	MG	XA	1622	1/1	0.94	0.51	-	53,53,53,53	0
57	MG	RA	3038	1/1	0.97	0.29	-	39,39,39,39	0
57	MG	YA	3257	1/1	0.89	0.67	-	52,52,52,52	0
57	MG	YA	3151	1/1	0.92	0.15	-	40,40,40,40	0
57	MG	XA	1601	1/1	0.96	0.69	-	43,43,43,43	0
57	MG	XA	1670	1/1	0.92	0.53	-	57,57,57,57	0
57	MG	RA	3214	1/1	0.85	0.65	-	41,41,41,41	0
57	MG	QA	1629	1/1	0.84	0.95	-	64,64,64,64	0
57	MG	QA	1677	1/1	0.93	0.48	-	45,45,45,45	0
57	MG	YA	3240	1/1	0.79	0.48	-	37,37,37,37	0
57	MG	YA	3219	1/1	0.91	0.28	-	45,45,45,45	0
57	MG	QA	1673	1/1	0.93	0.23	-	55,55,55,55	0
57	MG	YA	3206	1/1	0.98	0.41	-	16,16,16,16	0
57	MG	YA	3076	1/1	0.95	0.27	-	24,24,24,24	0
57	MG	YA	3289	1/1	0.97	0.86	-	52,52,52,52	0
57	MG	QA	1690	1/1	0.78	0.71	-	79,79,79,79	0
57	MG	YA	3138	1/1	0.93	0.41	-	40,40,40,40	0
57	MG	YA	3020	1/1	0.95	0.64	-	25,25,25,25	0
57	MG	RA	3229	1/1	0.99	0.18	-	94,94,94,94	0
57	MG	RA	3042	1/1	0.90	0.31	-	43,43,43,43	0
57	MG	QA	1659	1/1	0.88	0.61	-	50,50,50,50	0
57	MG	QA	1654	1/1	0.94	0.06	-	87,87,87,87	0
57	MG	YA	3095	1/1	0.98	0.41	-	44,44,44,44	0
57	MG	RA	3218	1/1	0.91	0.25	-	34,34,34,34	0
57	MG	RA	3145	1/1	0.97	0.49	-	50,50,50,50	0
57	MG	YA	3222	1/1	0.86	0.60	-	39,39,39,39	0
57	MG	XA	1647	1/1	0.95	0.57	-	74,74,74,74	0
57	MG	RA	3155	1/1	0.94	0.32	-	50,50,50,50	0
57	MG	YA	3261	1/1	0.91	0.55	-	63,63,63,63	0
57	MG	RA	3076	1/1	0.97	0.32	-	39,39,39,39	0
57	MG	RA	3233	1/1	0.81	0.95	-	63,63,63,63	0
57	MG	RA	3143	1/1	0.97	0.29	-	70,70,70,70	0
57	MG	R5	101	1/1	0.75	0.32	-	49,49,49,49	0
57	MG	YA	3116	1/1	0.97	0.48	-	23,23,23,23	0
57	MG	RA	3082	1/1	0.97	0.37	-	23,23,23,23	0
57	MG	RA	3267	1/1	0.85	0.64	-	57,57,57,57	0
57	MG	RA	3182	1/1	0.93	0.17	-	68,68,68,68	0
57	MG	RA	3203	1/1	0.82	0.66	-	76,76,76,76	0
57	MG	YA	3145	1/1	0.90	0.30	-	41,41,41,41	0
57	MG	YA	3166	1/1	0.90	0.17	-	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3128	1/1	0.90	0.07	-	58,58,58,58	0
57	MG	RA	3212	1/1	0.83	0.30	-	66,66,66,66	0
57	MG	XA	1701	1/1	0.87	0.35	-	67,67,67,67	0
57	MG	RA	3207	1/1	0.97	0.40	-	25,25,25,25	0
57	MG	XA	1659	1/1	0.79	0.18	-	89,89,89,89	0
57	MG	YP	202	1/1	0.86	0.94	-	53,53,53,53	0
57	MG	QA	1606	1/1	0.95	0.60	-	39,39,39,39	0
57	MG	RA	3247	1/1	0.70	0.33	-	52,52,52,52	0
57	MG	YA	3073	1/1	0.86	0.74	-	44,44,44,44	0
57	MG	RA	3261	1/1	0.89	0.65	-	57,57,57,57	0
57	MG	RA	3046	1/1	0.98	0.47	-	22,22,22,22	0
57	MG	YA	3157	1/1	0.93	0.29	-	50,50,50,50	0
57	MG	QA	1651	1/1	0.95	0.30	-	85,85,85,85	0
57	MG	YA	3052	1/1	0.94	0.23	-	23,23,23,23	0
57	MG	YA	3198	1/1	0.92	0.30	-	83,83,83,83	0
57	MG	YA	3001	1/1	0.96	0.54	-	22,22,22,22	0
57	MG	YA	3163	1/1	0.98	0.45	-	47,47,47,47	0
57	MG	RA	3049	1/1	0.97	0.37	-	22,22,22,22	0
57	MG	YB	203	1/1	0.82	0.46	-	61,61,61,61	0
57	MG	RA	3149	1/1	0.83	0.43	-	47,47,47,47	0
57	MG	RA	3193	1/1	0.73	0.34	-	45,45,45,45	0
57	MG	RA	3253	1/1	0.94	0.41	-	53,53,53,53	0
57	MG	YA	3010	1/1	0.98	0.26	-	21,21,21,21	0
57	MG	RA	3264	1/1	0.88	0.74	-	60,60,60,60	0
57	MG	YA	3203	1/1	0.84	0.40	-	75,75,75,75	0
57	MG	RA	3159	1/1	0.85	0.44	-	74,74,74,74	0
57	MG	RA	3052	1/1	0.98	0.32	-	17,17,17,17	0
57	MG	YA	3114	1/1	0.76	0.65	-	70,70,70,70	0
57	MG	RA	3244	1/1	0.79	0.50	-	55,55,55,55	0
57	MG	XA	1639	1/1	0.95	0.23	-	54,54,54,54	0
57	MG	RA	3263	1/1	0.90	0.88	-	43,43,43,43	0
57	MG	QA	1625	1/1	0.90	0.65	-	68,68,68,68	0
57	MG	RA	3028	1/1	0.97	0.31	-	22,22,22,22	0
57	MG	YA	3108	1/1	0.96	0.31	-	44,44,44,44	0
57	MG	QA	1680	1/1	0.88	0.49	-	54,54,54,54	0
57	MG	YA	3187	1/1	0.71	0.98	-	57,57,57,57	0
57	MG	RA	3133	1/1	0.77	0.29	-	68,68,68,68	0
57	MG	RA	3007	1/1	0.85	0.57	-	44,44,44,44	0
57	MG	YA	3293	1/1	0.94	0.49	-	35,35,35,35	0
57	MG	YA	3131	1/1	0.91	0.47	-	51,51,51,51	0
57	MG	YA	3051	1/1	0.97	0.27	-	28,28,28,28	0
57	MG	RA	3215	1/1	0.91	0.48	-	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3119	1/1	0.85	0.19	-	69,69,69,69	0
57	MG	YA	3275	1/1	0.94	0.29	-	65,65,65,65	0
57	MG	YA	3153	1/1	0.97	0.46	-	52,52,52,52	0
57	MG	RA	3216	1/1	0.93	0.45	-	48,48,48,48	0
57	MG	XA	1668	1/1	0.86	0.55	-	51,51,51,51	0
57	MG	RA	3001	1/1	0.88	0.63	-	41,41,41,41	0
57	MG	YA	3263	1/1	0.93	0.40	-	34,34,34,34	0
57	MG	QA	1624	1/1	0.52	0.74	-	76,76,76,76	0
57	MG	XA	1605	1/1	0.77	0.85	-	55,55,55,55	0
57	MG	RA	3250	1/1	0.85	0.45	-	65,65,65,65	0
57	MG	XA	1678	1/1	0.89	0.23	-	82,82,82,82	0
57	MG	RA	3088	1/1	0.81	0.34	-	70,70,70,70	0
57	MG	RA	3140	1/1	0.98	0.42	-	44,44,44,44	0
57	MG	RA	3284	1/1	0.89	0.52	-	49,49,49,49	0
57	MG	XA	1645	1/1	0.57	0.54	-	59,59,59,59	0
57	MG	YA	3066	1/1	0.95	0.73	-	34,34,34,34	0
57	MG	YA	3067	1/1	0.98	0.18	-	46,46,46,46	0
57	MG	RA	3091	1/1	0.99	0.20	-	27,27,27,27	0
57	MG	QA	1649	1/1	0.94	0.20	-	77,77,77,77	0
57	MG	QA	1633	1/1	0.94	0.36	-	35,35,35,35	0
57	MG	QT	201	1/1	0.65	0.32	-	70,70,70,70	0
57	MG	RA	3260	1/1	0.94	0.44	-	80,80,80,80	0
57	MG	QA	1672	1/1	0.98	0.19	-	61,61,61,61	0
57	MG	RA	3094	1/1	0.98	0.26	-	31,31,31,31	0
57	MG	XA	1614	1/1	0.98	0.24	-	25,25,25,25	0
57	MG	RA	3026	1/1	0.98	0.26	-	26,26,26,26	0
57	MG	XA	1684	1/1	0.83	0.23	-	52,52,52,52	0
57	MG	QA	1667	1/1	0.40	0.74	-	75,75,75,75	0
57	MG	RA	3183	1/1	0.80	0.22	-	102,102,102,102	0
57	MG	QA	1686	1/1	0.90	0.42	-	80,80,80,80	0
57	MG	YA	3136	1/1	0.78	0.17	-	64,64,64,64	0
57	MG	YA	3127	1/1	0.57	0.48	-	51,51,51,51	0
57	MG	YA	3099	1/1	0.94	0.79	-	48,48,48,48	0
57	MG	YA	3064	1/1	0.92	0.35	-	49,49,49,49	0
57	MG	YA	3188	1/1	0.95	0.30	-	39,39,39,39	0
57	MG	QA	1675	1/1	0.97	0.38	-	75,75,75,75	0
57	MG	YA	3055	1/1	0.95	0.24	-	29,29,29,29	0
57	MG	XA	1604	1/1	0.93	0.58	-	53,53,53,53	0
57	MG	RA	3228	1/1	0.99	0.30	-	38,38,38,38	0
57	MG	YA	3210	1/1	0.96	0.19	-	51,51,51,51	0
57	MG	YA	3194	1/1	0.84	0.53	-	44,44,44,44	0
57	MG	XA	1690	1/1	0.92	0.38	-	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1651	1/1	0.96	0.23	-	38,38,38,38	0
57	MG	RA	3189	1/1	0.88	0.41	-	45,45,45,45	0
57	MG	YA	3016	1/1	0.95	0.10	-	27,27,27,27	0
57	MG	YA	3118	1/1	0.64	0.39	-	46,46,46,46	0
57	MG	RA	3066	1/1	0.76	0.16	-	39,39,39,39	0
57	MG	RQ	201	1/1	0.73	1.53	-	91,91,91,91	0
57	MG	YA	3142	1/1	0.91	0.84	-	61,61,61,61	0
57	MG	YA	3030	1/1	0.92	0.34	-	29,29,29,29	0
57	MG	RA	3114	1/1	0.96	0.15	-	58,58,58,58	0
57	MG	RA	3142	1/1	0.97	0.55	-	55,55,55,55	0
57	MG	RA	3242	1/1	0.91	0.46	-	53,53,53,53	0
57	MG	YA	3258	1/1	0.76	0.39	-	71,71,71,71	0
57	MG	YA	3143	1/1	0.88	0.58	-	45,45,45,45	0
57	MG	RA	3010	1/1	0.98	0.29	-	22,22,22,22	0
57	MG	QA	1608	1/1	0.97	0.06	-	28,28,28,28	0
57	MG	YA	3220	1/1	0.94	0.34	-	41,41,41,41	0
57	MG	XA	1637	1/1	0.93	0.55	-	55,55,55,55	0
57	MG	YA	3196	1/1	0.95	0.15	-	30,30,30,30	0
57	MG	QA	1618	1/1	0.83	1.26	-	70,70,70,70	0
57	MG	RA	3044	1/1	0.95	0.20	-	17,17,17,17	0
57	MG	YA	3285	1/1	0.89	0.75	-	61,61,61,61	0
57	MG	RA	3104	1/1	0.99	0.07	-	24,24,24,24	0
57	MG	RA	3279	1/1	0.78	0.57	-	60,60,60,60	0
57	MG	RA	3090	1/1	0.95	0.42	-	27,27,27,27	0
57	MG	XA	1703	1/1	0.76	0.62	-	58,58,58,58	0
57	MG	XA	1615	1/1	0.94	0.13	-	33,33,33,33	0
57	MG	RA	3256	1/1	0.83	0.51	-	59,59,59,59	0
57	MG	RA	3278	1/1	0.67	0.40	-	48,48,48,48	0
57	MG	YA	3205	1/1	0.84	0.54	-	33,33,33,33	0
57	MG	YA	3238	1/1	0.90	0.64	-	48,48,48,48	0
57	MG	QA	1626	1/1	0.47	0.47	-	124,124,124,124	0
57	MG	RA	3230	1/1	0.98	0.35	-	58,58,58,58	0
57	MG	YA	3100	1/1	0.98	0.13	-	55,55,55,55	0
57	MG	YA	3113	1/1	0.97	0.18	-	45,45,45,45	0
57	MG	RA	3115	1/1	0.75	0.20	-	66,66,66,66	0
57	MG	RA	3160	1/1	0.98	0.53	-	38,38,38,38	0
57	MG	YA	3003	1/1	0.95	0.41	-	17,17,17,17	0
57	MG	YA	3061	1/1	0.95	0.42	-	31,31,31,31	0
57	MG	QA	1642	1/1	0.96	0.11	-	35,35,35,35	0
57	MG	XA	1699	1/1	0.86	1.22	-	64,64,64,64	0
57	MG	XA	1628	1/1	0.91	0.12	-	47,47,47,47	0
57	MG	RA	3106	1/1	0.92	0.36	-	37,37,37,37	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3255	1/1	0.98	0.42	-	37,37,37,37	0
57	MG	QA	1661	1/1	0.96	0.58	-	65,65,65,65	0
57	MG	RA	3122	1/1	0.66	0.28	-	52,52,52,52	0
57	MG	YA	3266	1/1	0.62	0.60	-	66,66,66,66	0
57	MG	YA	3197	1/1	0.96	1.00	-	72,72,72,72	0
57	MG	YA	3090	1/1	0.99	0.52	-	33,33,33,33	0
57	MG	Y0	101	1/1	0.35	0.59	-	72,72,72,72	0
57	MG	RA	3185	1/1	0.93	0.19	-	38,38,38,38	0
57	MG	YA	3267	1/1	0.94	0.90	-	103,103,103,103	0
57	MG	YA	3018	1/1	0.96	0.42	-	34,34,34,34	0
57	MG	XA	1636	1/1	0.96	0.16	-	82,82,82,82	0
57	MG	XA	1676	1/1	0.83	0.86	-	58,58,58,58	0
57	MG	RA	3027	1/1	0.94	0.34	-	20,20,20,20	0
57	MG	YA	3082	1/1	0.65	0.41	-	47,47,47,47	0
57	MG	YA	3223	1/1	0.82	0.69	-	56,56,56,56	0
57	MG	RA	3081	1/1	0.72	0.38	-	41,41,41,41	0
57	MG	RA	3080	1/1	0.98	0.36	-	44,44,44,44	0
57	MG	QA	1688	1/1	0.91	0.45	-	54,54,54,54	0
57	MG	RA	3172	1/1	0.89	0.85	-	84,84,84,84	0
57	MG	YA	3232	1/1	0.96	0.37	-	47,47,47,47	0
57	MG	RA	3275	1/1	0.87	1.06	-	68,68,68,68	0
57	MG	YA	3074	1/1	0.97	0.42	-	21,21,21,21	0
57	MG	RA	3054	1/1	0.96	0.52	-	29,29,29,29	0
57	MG	XA	1662	1/1	0.80	0.32	-	29,29,29,29	0
57	MG	YA	3180	1/1	0.96	0.37	-	26,26,26,26	0
57	MG	RB	202	1/1	0.99	0.18	-	63,63,63,63	0
57	MG	XV	104	1/1	0.93	0.22	-	23,23,23,23	0
57	MG	QA	1678	1/1	0.95	0.47	-	53,53,53,53	0
57	MG	RA	3099	1/1	0.95	0.70	-	45,45,45,45	0
57	MG	XA	1679	1/1	0.91	0.18	-	41,41,41,41	0
57	MG	RA	3190	1/1	0.97	0.59	-	57,57,57,57	0
57	MG	RA	3036	1/1	0.99	0.28	-	18,18,18,18	0
57	MG	QA	1630	1/1	0.95	0.18	-	64,64,64,64	0
57	MG	RA	3239	1/1	0.75	1.47	-	77,77,77,77	0
57	MG	QA	1640	1/1	0.88	0.47	-	51,51,51,51	0
57	MG	QA	1641	1/1	0.97	0.16	-	45,45,45,45	0
57	MG	RA	3153	1/1	0.79	0.93	-	60,60,60,60	0
57	MG	RA	3129	1/1	0.94	0.47	-	68,68,68,68	0
57	MG	YA	3103	1/1	0.96	0.33	-	47,47,47,47	0
57	MG	XA	1625	1/1	0.98	0.29	-	38,38,38,38	0
57	MG	RA	3071	1/1	0.99	0.31	-	26,26,26,26	0
57	MG	RA	3210	1/1	0.76	0.12	-	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3268	1/1	0.95	0.38	-	61,61,61,61	0
57	MG	XA	1609	1/1	0.95	0.32	-	39,39,39,39	0
57	MG	YY	201	1/1	0.92	0.24	-	67,67,67,67	0
57	MG	QA	1671	1/1	0.99	0.32	-	48,48,48,48	0
57	MG	YA	3208	1/1	0.90	0.18	-	64,64,64,64	0
57	MG	YA	3276	1/1	0.94	0.66	-	51,51,51,51	0
57	MG	YA	3159	1/1	0.96	0.68	-	48,48,48,48	0
57	MG	RA	3199	1/1	0.87	0.16	-	74,74,74,74	0
57	MG	RA	3156	1/1	0.72	0.90	-	41,41,41,41	0
57	MG	RA	3069	1/1	0.96	0.42	-	43,43,43,43	0
57	MG	XA	1627	1/1	0.91	0.11	-	36,36,36,36	0
57	MG	RA	3138	1/1	0.97	0.44	-	23,23,23,23	0
57	MG	RA	3151	1/1	0.90	0.23	-	32,32,32,32	0
57	MG	QA	1638	1/1	0.91	0.35	-	74,74,74,74	0
57	MG	YA	3256	1/1	0.97	0.30	-	38,38,38,38	0
57	MG	XA	1692	1/1	0.93	0.43	-	68,68,68,68	0
57	MG	YA	3079	1/1	0.97	0.28	-	25,25,25,25	0
57	MG	YA	3288	1/1	0.82	0.78	-	63,63,63,63	0
57	MG	RA	3204	1/1	0.96	0.33	-	51,51,51,51	0
57	MG	XX	101	1/1	0.95	0.55	-	68,68,68,68	0
57	MG	RA	3135	1/1	0.92	0.46	-	42,42,42,42	0
57	MG	RA	3113	1/1	0.84	0.31	-	55,55,55,55	0
57	MG	RA	3276	1/1	0.91	0.52	-	51,51,51,51	0
57	MG	XV	101	1/1	0.90	0.41	-	53,53,53,53	0
57	MG	RA	3258	1/1	0.84	0.80	-	52,52,52,52	0
57	MG	RA	3012	1/1	0.94	0.48	-	22,22,22,22	0
57	MG	RA	3271	1/1	0.92	0.61	-	61,61,61,61	0
57	MG	RA	3209	1/1	0.98	0.33	-	12,12,12,12	0
57	MG	XA	1642	1/1	0.92	0.23	-	40,40,40,40	0
57	MG	YA	3239	1/1	0.89	0.64	-	39,39,39,39	0
57	MG	XA	1697	1/1	0.78	0.22	-	68,68,68,68	0
57	MG	RA	3180	1/1	0.95	0.27	-	57,57,57,57	0
57	MG	RA	3226	1/1	0.88	0.54	-	41,41,41,41	0
57	MG	XA	1681	1/1	0.91	0.15	-	58,58,58,58	0
57	MG	RA	3213	1/1	0.81	0.85	-	64,64,64,64	0
57	MG	YA	3045	1/1	0.65	0.39	-	30,30,30,30	0
57	MG	YA	3248	1/1	0.94	0.46	-	52,52,52,52	0
57	MG	QA	1663	1/1	0.89	0.93	-	68,68,68,68	0
57	MG	QA	1644	1/1	0.96	0.63	-	62,62,62,62	0
57	MG	RA	3029	1/1	0.99	0.51	-	41,41,41,41	0
57	MG	YA	3250	1/1	0.96	0.54	-	25,25,25,25	0
57	MG	QA	1627	1/1	0.83	0.22	-	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1664	1/1	0.92	0.43	-	50,50,50,50	0
57	MG	YA	3107	1/1	0.98	0.29	-	23,23,23,23	0
57	MG	YA	3021	1/1	0.99	0.41	-	15,15,15,15	0
57	MG	XA	1643	1/1	0.96	0.45	-	42,42,42,42	0
57	MG	YA	3279	1/1	0.93	0.63	-	64,64,64,64	0
57	MG	XA	1611	1/1	0.96	0.10	-	32,32,32,32	0
57	MG	QA	1670	1/1	0.83	0.26	-	45,45,45,45	0
57	MG	YA	3211	1/1	0.97	0.40	-	49,49,49,49	0
57	MG	YA	3183	1/1	0.86	0.37	-	55,55,55,55	0
57	MG	RA	3040	1/1	0.98	0.39	-	40,40,40,40	0
57	MG	RA	3107	1/1	0.91	0.47	-	39,39,39,39	0
57	MG	QA	1604	1/1	0.91	0.96	-	64,64,64,64	0
57	MG	XA	1630	1/1	0.94	0.33	-	46,46,46,46	0
57	MG	YA	3229	1/1	0.93	0.66	-	23,23,23,23	0
57	MG	YA	3224	1/1	0.92	0.52	-	42,42,42,42	0
57	MG	YA	3007	1/1	0.92	0.18	-	17,17,17,17	0
57	MG	R0	102	1/1	0.81	0.53	-	64,64,64,64	0
57	MG	YA	3255	1/1	0.91	0.44	-	46,46,46,46	0
57	MG	QA	1603	1/1	0.83	1.27	-	83,83,83,83	0
57	MG	YA	3019	1/1	0.89	0.39	-	30,30,30,30	0
57	MG	RA	3201	1/1	0.91	0.70	-	46,46,46,46	0
57	MG	RA	3196	1/1	0.90	0.27	-	47,47,47,47	0
57	MG	YB	201	1/1	0.97	0.47	-	71,71,71,71	0
57	MG	RA	3231	1/1	0.94	0.86	-	59,59,59,59	0
57	MG	YA	3249	1/1	0.92	0.20	-	53,53,53,53	0
57	MG	YA	3287	1/1	0.82	0.77	-	54,54,54,54	0
57	MG	RA	3186	1/1	0.94	0.14	-	79,79,79,79	0
57	MG	QA	1653	1/1	0.97	0.69	-	69,69,69,69	0
57	MG	RA	3068	1/1	0.95	0.49	-	27,27,27,27	0
57	MG	YA	3029	1/1	0.98	0.31	-	21,21,21,21	0
57	MG	RA	3019	1/1	0.96	0.48	-	17,17,17,17	0
57	MG	YA	3193	1/1	0.80	0.29	-	85,85,85,85	0
57	MG	YA	3286	1/1	0.84	1.16	-	81,81,81,81	0
57	MG	RA	3009	1/1	0.90	0.49	-	48,48,48,48	0
57	MG	YA	3247	1/1	0.98	0.14	-	31,31,31,31	0
57	MG	RA	3089	1/1	0.98	0.23	-	33,33,33,33	0
57	MG	RE	301	1/1	0.88	0.28	-	41,41,41,41	0
57	MG	YA	3175	1/1	0.87	0.60	-	57,57,57,57	0
57	MG	RA	3254	1/1	0.91	0.44	-	64,64,64,64	0
57	MG	RA	3191	1/1	0.92	0.84	-	45,45,45,45	0
57	MG	R0	101	1/1	0.60	0.31	-	41,41,41,41	0
57	MG	YA	3179	1/1	0.97	0.09	-	62,62,62,62	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1693	1/1	0.89	0.36	-	62,62,62,62	0
57	MG	RA	3169	1/1	0.47	0.87	-	40,40,40,40	0
57	MG	XA	1634	1/1	0.97	0.27	-	92,92,92,92	0
57	MG	YA	3123	1/1	0.83	0.24	-	32,32,32,32	0
57	MG	YA	3043	1/1	0.96	0.46	-	13,13,13,13	0
57	MG	RA	3225	1/1	0.95	0.52	-	25,25,25,25	0
57	MG	RA	3125	1/1	0.84	0.25	-	84,84,84,84	0
57	MG	QA	1616	1/1	0.98	0.14	-	97,97,97,97	0
57	MG	YA	3202	1/1	0.97	0.12	-	76,76,76,76	0
57	MG	YA	3218	1/1	0.81	0.32	-	48,48,48,48	0
57	MG	QA	1681	1/1	0.94	0.34	-	50,50,50,50	0
57	MG	YA	3160	1/1	0.71	0.27	-	69,69,69,69	0
57	MG	YA	3130	1/1	0.84	0.48	-	65,65,65,65	0
57	MG	YA	3174	1/1	0.78	0.67	-	56,56,56,56	0
57	MG	YA	3251	1/1	0.95	0.55	-	51,51,51,51	0
57	MG	XA	1657	1/1	0.79	0.27	-	47,47,47,47	0
57	MG	XV	103	1/1	0.92	0.69	-	36,36,36,36	0
57	MG	YA	3234	1/1	0.85	1.22	-	52,52,52,52	0
57	MG	YA	3085	1/1	0.96	0.41	-	23,23,23,23	0
57	MG	YA	3060	1/1	0.98	0.23	-	24,24,24,24	0
57	MG	RA	3003	1/1	0.98	0.32	-	17,17,17,17	0
57	MG	RA	3184	1/1	0.61	0.48	-	45,45,45,45	0
57	MG	YA	3158	1/1	0.96	0.26	-	47,47,47,47	0
57	MG	YA	3125	1/1	0.93	0.39	-	26,26,26,26	0
57	MG	RA	3022	1/1	0.98	0.16	-	34,34,34,34	0
57	MG	YA	3209	1/1	0.97	0.11	-	53,53,53,53	0
57	MG	RA	3139	1/1	0.98	0.37	-	32,32,32,32	0
57	MG	RA	3008	1/1	0.93	0.23	-	45,45,45,45	0
57	MG	RA	3109	1/1	0.93	0.21	-	54,54,54,54	0
57	MG	YA	3282	1/1	0.77	0.81	-	75,75,75,75	0
57	MG	RA	3252	1/1	0.94	0.35	-	49,49,49,49	0
57	MG	RA	3178	1/1	0.81	0.50	-	61,61,61,61	0
57	MG	XA	1688	1/1	0.68	0.29	-	57,57,57,57	0
57	MG	YA	3274	1/1	0.93	0.18	-	82,82,82,82	0
57	MG	RA	3266	1/1	0.84	0.81	-	54,54,54,54	0
57	MG	RA	3265	1/1	0.80	0.45	-	48,48,48,48	0
57	MG	YA	3204	1/1	0.95	0.35	-	84,84,84,84	0
57	MG	QA	1601	1/1	0.95	0.54	-	55,55,55,55	0
57	MG	XA	1607	1/1	0.97	0.59	-	36,36,36,36	0
57	MG	YA	3133	1/1	0.96	0.52	-	31,31,31,31	0
57	MG	RA	3017	1/1	0.96	0.58	-	27,27,27,27	0
57	MG	QA	1679	1/1	0.96	0.35	-	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3089	1/1	0.97	0.26	-	54,54,54,54	0
57	MG	QA	1634	1/1	0.97	0.17	-	68,68,68,68	0
57	MG	RA	3165	1/1	0.61	0.56	-	93,93,93,93	0
57	MG	RA	3245	1/1	0.96	0.59	-	64,64,64,64	0
57	MG	YA	3184	1/1	0.56	0.38	-	84,84,84,84	0
57	MG	XA	1687	1/1	0.82	0.10	-	120,120,120,120	0
57	MG	RA	3222	1/1	0.79	0.69	-	46,46,46,46	0
57	MG	RA	3202	1/1	0.70	0.27	-	60,60,60,60	0
57	MG	QA	1623	1/1	0.93	0.51	-	64,64,64,64	0
57	MG	RA	3130	1/1	0.35	0.56	-	68,68,68,68	0
57	MG	RA	3060	1/1	0.50	0.26	-	81,81,81,81	0
57	MG	YA	3171	1/1	-0.09	0.73	-	151,151,151,151	0
57	MG	RA	3234	1/1	0.95	0.23	-	36,36,36,36	0
57	MG	YA	3093	1/1	0.98	0.49	-	43,43,43,43	0
57	MG	QY	101	1/1	0.95	0.15	-	61,61,61,61	0
57	MG	RA	3171	1/1	0.89	0.56	-	57,57,57,57	0
57	MG	Y5	101	1/1	0.98	0.19	-	28,28,28,28	0
57	MG	XA	1673	1/1	0.92	0.85	-	54,54,54,54	0
57	MG	XA	1700	1/1	0.96	0.66	-	61,61,61,61	0
57	MG	YA	3091	1/1	0.94	0.68	-	32,32,32,32	0
57	MG	XA	1649	1/1	0.76	0.60	-	77,77,77,77	0
57	MG	YA	3140	1/1	0.95	0.65	-	217,217,217,217	0
57	MG	YA	3270	1/1	0.86	0.61	-	63,63,63,63	0
57	MG	XA	1667	1/1	0.95	0.68	-	56,56,56,56	0
57	MG	QA	1628	1/1	0.91	0.36	-	55,55,55,55	0
57	MG	XA	1666	1/1	0.96	0.30	-	71,71,71,71	0
57	MG	YA	3252	1/1	0.88	0.10	-	87,87,87,87	0
57	MG	XA	1656	1/1	0.92	0.30	-	67,67,67,67	0
57	MG	RA	3236	1/1	0.80	0.59	-	72,72,72,72	0
57	MG	RA	3158	1/1	0.96	0.23	-	45,45,45,45	0
57	MG	YA	3264	1/1	0.89	0.87	-	44,44,44,44	0
57	MG	RA	3045	1/1	0.98	0.44	-	25,25,25,25	0
57	MG	XA	1682	1/1	0.58	1.16	-	68,68,68,68	0
57	MG	RA	3110	1/1	0.64	0.33	-	42,42,42,42	0
57	MG	YA	3190	1/1	0.83	0.70	-	38,38,38,38	0
57	MG	RA	3272	1/1	0.60	0.65	-	63,63,63,63	0
57	MG	QA	1648	1/1	0.99	0.32	-	42,42,42,42	0
57	MG	RA	3043	1/1	0.93	0.62	-	29,29,29,29	0
57	MG	RA	3146	1/1	0.90	0.15	-	57,57,57,57	0
57	MG	YA	3228	1/1	0.98	0.20	-	26,26,26,26	0
57	MG	RA	3123	1/1	0.96	0.36	-	39,39,39,39	0
57	MG	QA	1656	1/1	0.74	0.28	-	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3015	1/1	0.99	0.31	-	30,30,30,30	0
57	MG	XY	101	1/1	0.96	0.11	-	54,54,54,54	0
57	MG	RA	3249	1/1	0.92	0.57	-	47,47,47,47	0
57	MG	RA	3050	1/1	0.97	0.42	-	14,14,14,14	0
57	MG	RA	3181	1/1	0.98	0.10	-	53,53,53,53	0
57	MG	XA	1648	1/1	0.88	0.37	-	92,92,92,92	0
57	MG	QA	1637	1/1	0.74	0.78	-	92,92,92,92	0
57	MG	RA	3248	1/1	0.89	0.86	-	62,62,62,62	0
57	MG	RA	3031	1/1	0.96	0.47	-	16,16,16,16	0
57	MG	RA	3280	1/1	0.88	0.10	-	145,145,145,145	0
57	MG	YA	3081	1/1	0.98	0.30	-	47,47,47,47	0
57	MG	YA	3152	1/1	0.93	0.21	-	79,79,79,79	0
57	MG	QV	103	1/1	0.94	0.41	-	35,35,35,35	0
57	MG	YA	3221	1/1	0.92	0.76	-	54,54,54,54	0
57	MG	QA	1664	1/1	0.92	0.45	-	52,52,52,52	0
57	MG	RA	3065	1/1	0.98	0.40	-	29,29,29,29	0
57	MG	YA	3225	1/1	0.76	0.49	-	40,40,40,40	0
57	MG	YA	3054	1/1	0.93	0.53	-	63,63,63,63	0
57	MG	XA	1665	1/1	0.94	0.40	-	51,51,51,51	0
57	MG	YA	3148	1/1	0.84	0.50	-	36,36,36,36	0
57	MG	XA	1658	1/1	0.87	0.76	-	72,72,72,72	0
57	MG	XA	1698	1/1	0.95	0.29	-	77,77,77,77	0
57	MG	YA	3094	1/1	0.97	0.62	-	28,28,28,28	0
57	MG	QA	1647	1/1	0.73	0.21	-	39,39,39,39	0
57	MG	RA	3224	1/1	0.98	0.07	-	62,62,62,62	0
57	MG	QA	1636	1/1	0.77	0.21	-	87,87,87,87	0
57	MG	RA	3273	1/1	0.81	0.99	-	57,57,57,57	0
57	MG	RA	3047	1/1	0.90	0.17	-	30,30,30,30	0
57	MG	YA	3272	1/1	0.97	0.54	-	57,57,57,57	0
57	MG	YA	3226	1/1	0.95	0.52	-	20,20,20,20	0
57	MG	RA	3163	1/1	0.79	0.24	-	56,56,56,56	0
57	MG	YA	3271	1/1	0.84	0.55	-	43,43,43,43	0
57	MG	YA	3201	1/1	0.96	0.56	-	56,56,56,56	0
57	MG	XA	1685	1/1	0.99	0.50	-	60,60,60,60	0
57	MG	YA	3254	1/1	0.51	0.71	-	67,67,67,67	0
57	MG	YA	3146	1/1	0.95	0.17	-	65,65,65,65	0
57	MG	QA	1602	1/1	0.88	0.78	-	37,37,37,37	0
57	MG	XA	1655	1/1	0.96	0.33	-	62,62,62,62	0
57	MG	RA	3101	1/1	0.94	0.21	-	27,27,27,27	0
57	MG	XA	1629	1/1	0.86	0.17	-	62,62,62,62	0
57	MG	RA	3102	1/1	0.97	0.24	-	28,28,28,28	0
57	MG	YA	3120	1/1	0.95	0.30	-	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RB	203	1/1	0.96	0.39	-	46,46,46,46	0
57	MG	YA	3245	1/1	0.93	0.30	-	32,32,32,32	0
57	MG	XA	1669	1/1	0.93	0.26	-	55,55,55,55	0
57	MG	XA	1661	1/1	0.54	0.33	-	58,58,58,58	0
57	MG	QV	101	1/1	0.76	0.54	-	55,55,55,55	0
57	MG	QA	1687	1/1	0.82	1.02	-	59,59,59,59	0
57	MG	XA	1696	1/1	0.85	0.32	-	37,37,37,37	0
57	MG	YA	3212	1/1	0.96	0.85	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.