wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 25, 2024 – 04:38 AM EST

PDB ID	:	4ZSN
Title	:	70S-wild-type HigB toxin complex bound to a AAA lysine codon
Authors	:	Schureck, M.A.; Dunham, C.M.
Deposited on	:	2015-05-13
Resolution	:	3.60 Å(reported)

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

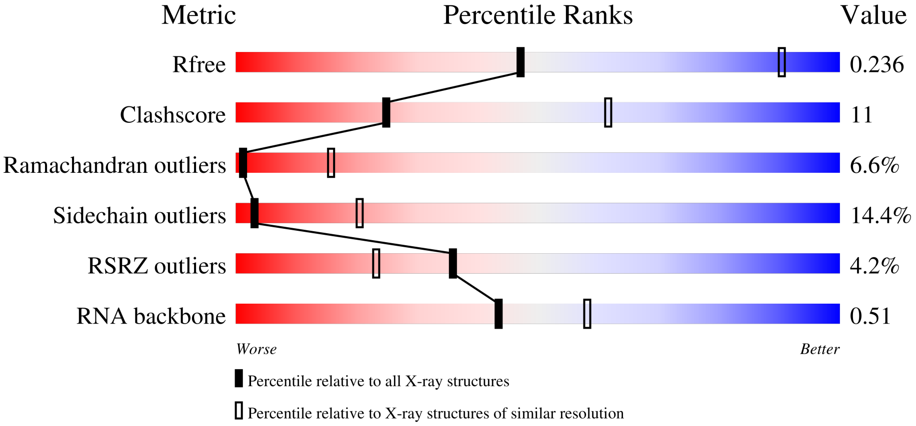
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

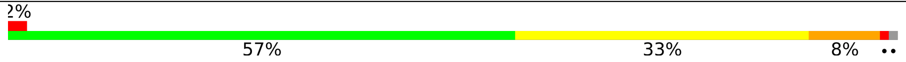
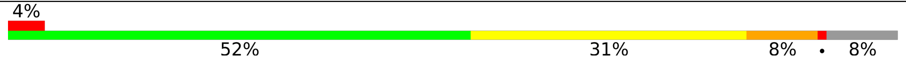
The reported resolution of this entry is 3.60 Å.

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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	

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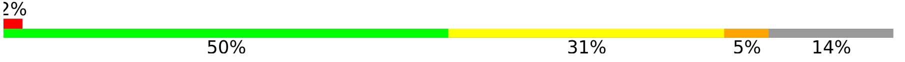
Mol	Chain	Length	Quality of chain
3	QC	239	
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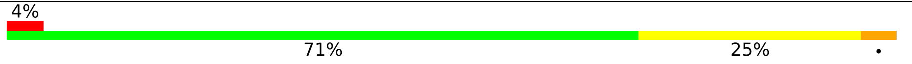
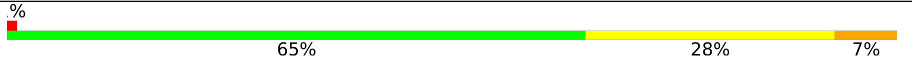
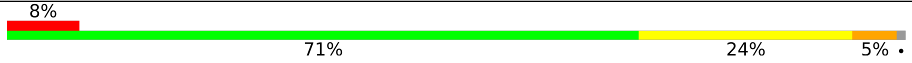
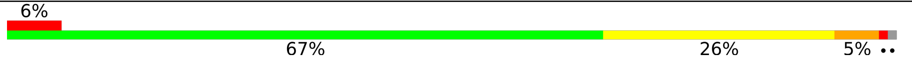
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
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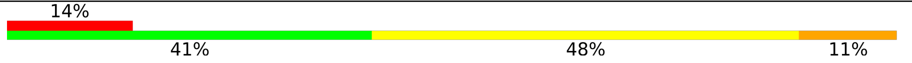
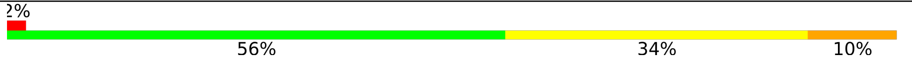
8	XH	138	
9	QI	128	
9	XI	128	
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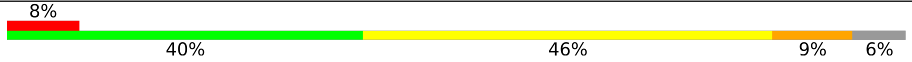
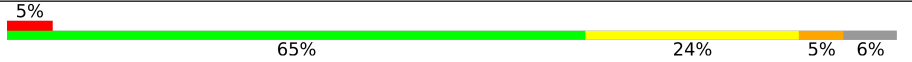
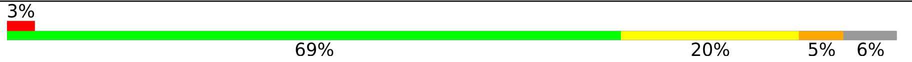
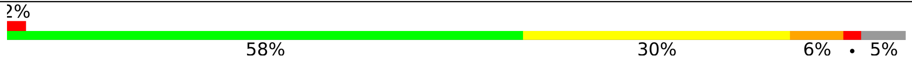
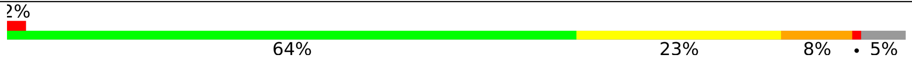
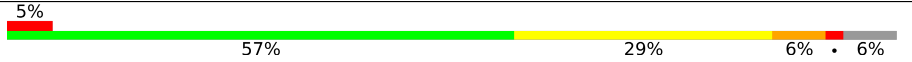
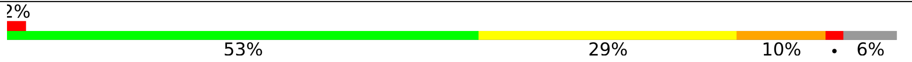
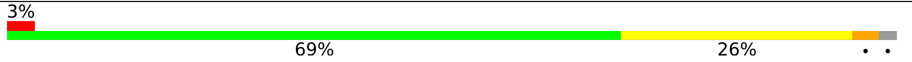
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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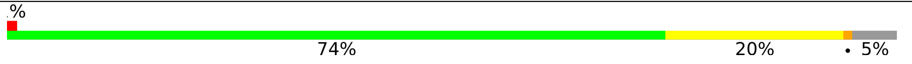
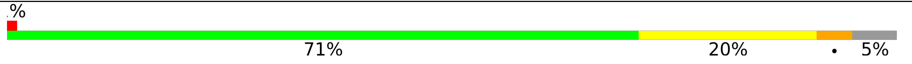
Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
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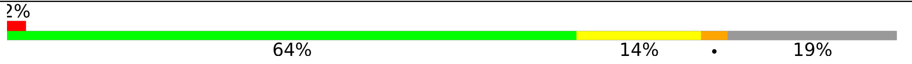
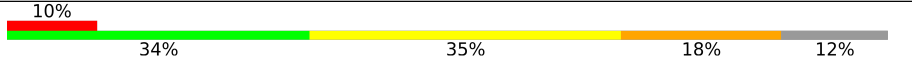
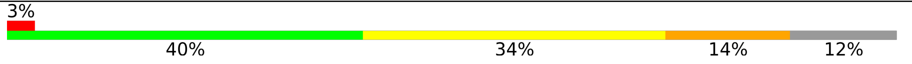
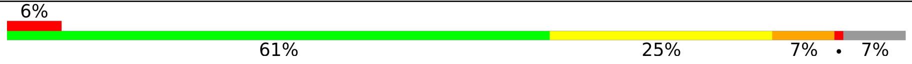
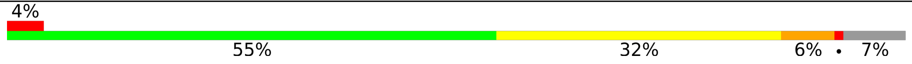
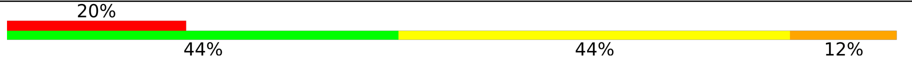
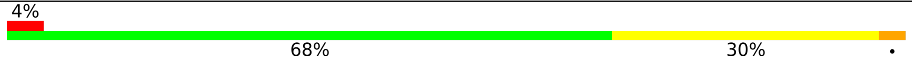
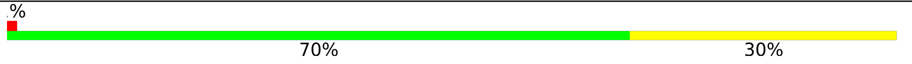
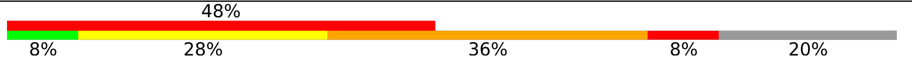
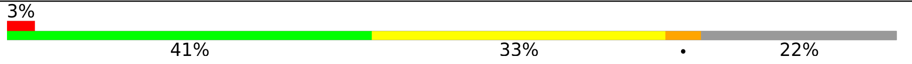
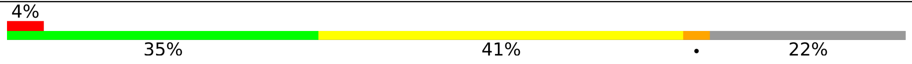
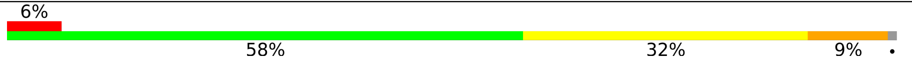
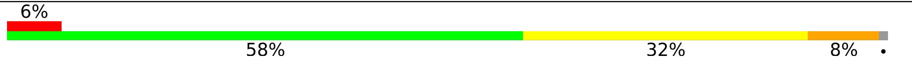
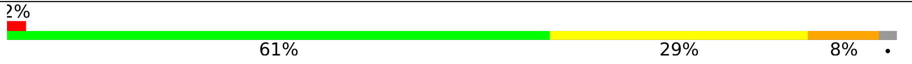
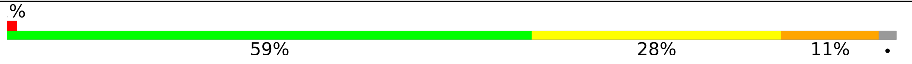
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	25	
21	XU	25	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	118	
24	XY	118	
25	RA	2916	
25	YA	2916	
26	RB	124	
26	YB	124	
27	RD	276	
27	YD	276	

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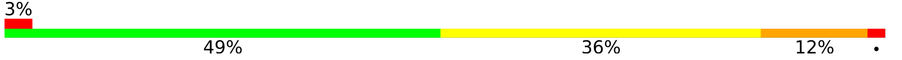
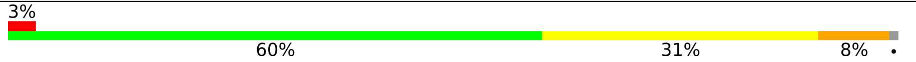
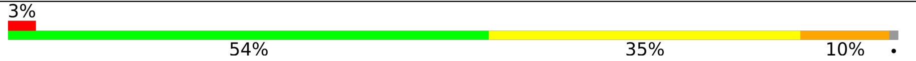
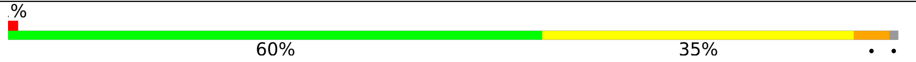
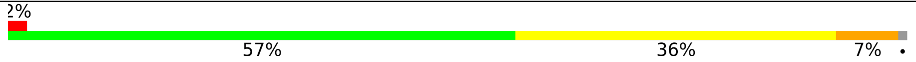
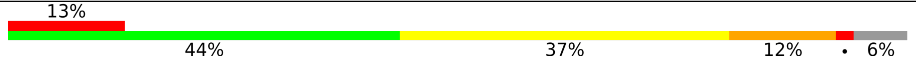
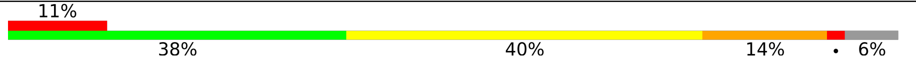
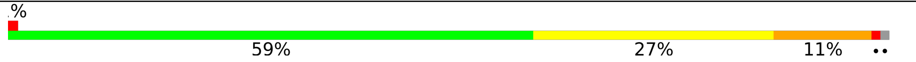
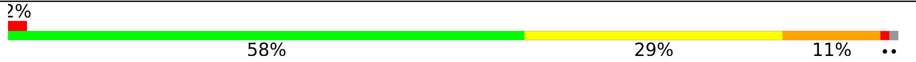
Mol	Chain	Length	Quality of chain
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
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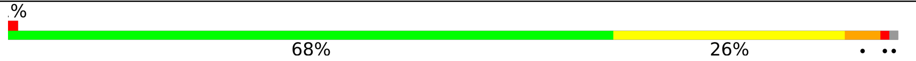
33	YN	140	
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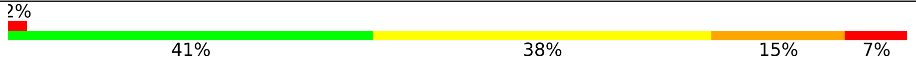
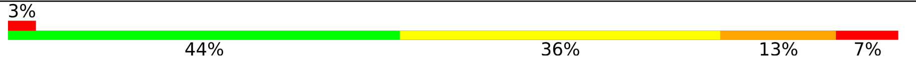
34	YO	122	
35	RP	150	
35	YP	150	
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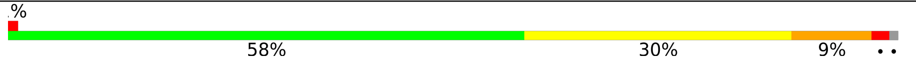
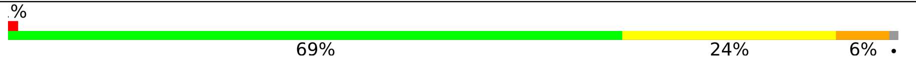
36	YQ	141	
37	RR	118	
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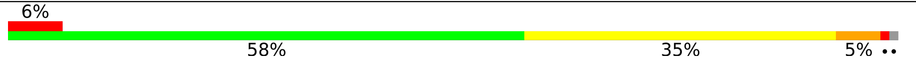
38	RS	112	
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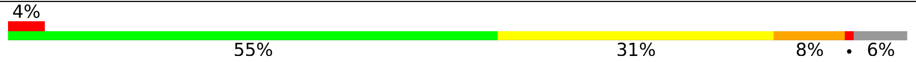
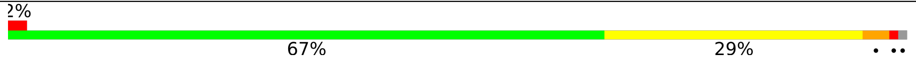
39	RT	146	
39	YT	146	
40	RU	118	

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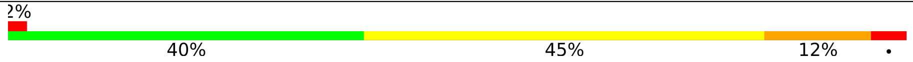
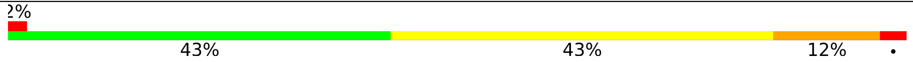
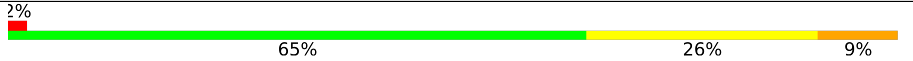
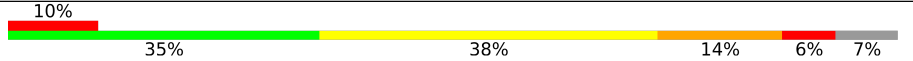
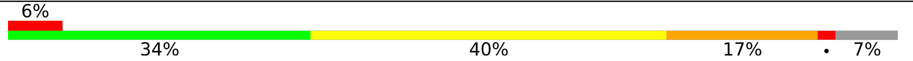
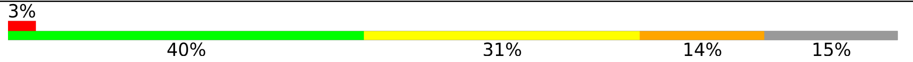
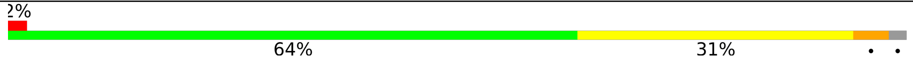
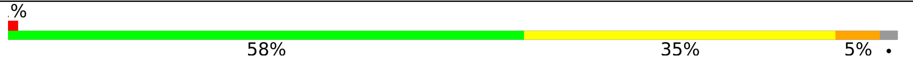
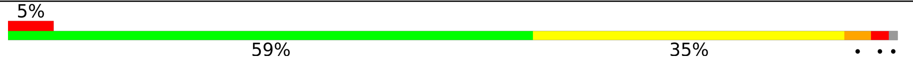
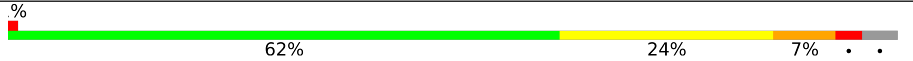
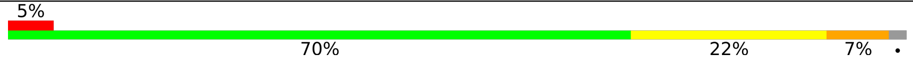
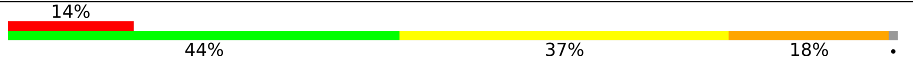
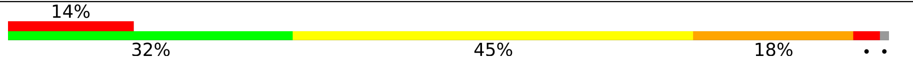
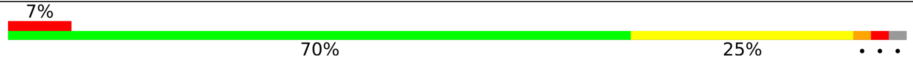
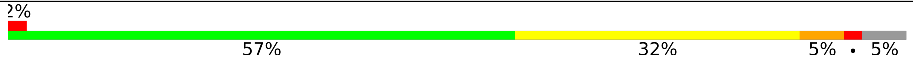
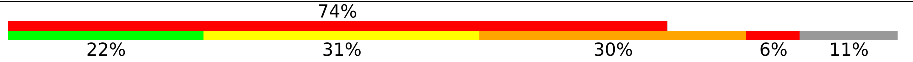
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	

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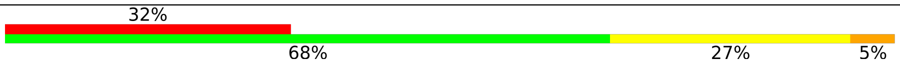
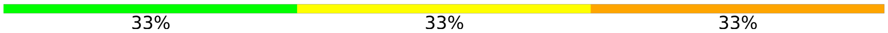
Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	Z7	3	

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	1613	-	-	-	X
57	MG	QA	1629	-	-	-	X
57	MG	QA	1637	-	-	-	X
57	MG	QA	1658	-	-	-	X
57	MG	QA	1663	-	-	-	X
57	MG	QA	1671	-	-	-	X
57	MG	QA	1672	-	-	-	X
57	MG	QA	1683	-	-	-	X
57	MG	QA	1696	-	-	-	X
57	MG	QA	1707	-	-	-	X
57	MG	QA	1710	-	-	-	X
57	MG	QA	1711	-	-	-	X
57	MG	QA	1716	-	-	-	X
57	MG	QA	1718	-	-	-	X
57	MG	QA	1719	-	-	-	X
57	MG	QA	1740	-	-	-	X
57	MG	QA	1742	-	-	-	X
57	MG	QA	1744	-	-	-	X
57	MG	QA	1747	-	-	-	X
57	MG	QD	302	-	-	-	X
57	MG	R0	102	-	-	-	X
57	MG	RA	3001	-	-	-	X
57	MG	RA	3048	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3089	-	-	-	X
57	MG	RA	3102	-	-	-	X
57	MG	RA	3142	-	-	-	X
57	MG	RA	3173	-	-	-	X
57	MG	RA	3176	-	-	-	X
57	MG	RA	3177	-	-	-	X
57	MG	RA	3182	-	-	-	X
57	MG	RA	3186	-	-	-	X
57	MG	RA	3187	-	-	-	X
57	MG	RA	3204	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3234	-	-	-	X
57	MG	RA	3262	-	-	-	X
57	MG	RA	3266	-	-	-	X
57	MG	RA	3269	-	-	-	X
57	MG	RA	3270	-	-	-	X
57	MG	RA	3275	-	-	-	X
57	MG	RA	3278	-	-	-	X
57	MG	RA	3284	-	-	-	X
57	MG	RA	3292	-	-	-	X
57	MG	RA	3298	-	-	-	X
57	MG	RA	3300	-	-	-	X
57	MG	RA	3302	-	-	-	X
57	MG	RA	3311	-	-	-	X
57	MG	RA	3316	-	-	-	X
57	MG	RA	3325	-	-	-	X
57	MG	RA	3326	-	-	-	X
57	MG	RA	3327	-	-	-	X
57	MG	RA	3333	-	-	-	X
57	MG	RA	3334	-	-	-	X
57	MG	RA	3335	-	-	-	X
57	MG	RA	3338	-	-	-	X
57	MG	RA	3340	-	-	-	X
57	MG	RA	3342	-	-	-	X
57	MG	RA	3347	-	-	-	X
57	MG	RA	3370	-	-	-	X
57	MG	RA	3372	-	-	-	X
57	MG	RA	3394	-	-	-	X
57	MG	RA	3400	-	-	-	X
57	MG	RA	3421	-	-	-	X
57	MG	RA	3425	-	-	-	X
57	MG	RA	3428	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3431	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RY	202	-	-	-	X
57	MG	XA	1630	-	-	-	X
57	MG	XA	1652	-	-	-	X
57	MG	XA	1676	-	-	-	X
57	MG	XA	1686	-	-	-	X
57	MG	XA	1688	-	-	-	X
57	MG	XA	1689	-	-	-	X
57	MG	XA	1700	-	-	-	X
57	MG	XA	1709	-	-	-	X
57	MG	XA	1710	-	-	-	X
57	MG	XA	1714	-	-	-	X
57	MG	XA	1718	-	-	-	X
57	MG	XA	1720	-	-	-	X
57	MG	XA	1722	-	-	-	X
57	MG	XA	1725	-	-	-	X
57	MG	XA	1729	-	-	-	X
57	MG	XA	1735	-	-	-	X
57	MG	XA	1742	-	-	-	X
57	MG	XA	1755	-	-	-	X
57	MG	XA	1756	-	-	-	X
57	MG	XV	103	-	-	-	X
57	MG	Y5	103	-	-	-	X
57	MG	YA	3113	-	-	-	X
57	MG	YA	3135	-	-	-	X
57	MG	YA	3146	-	-	-	X
57	MG	YA	3167	-	-	-	X
57	MG	YA	3168	-	-	-	X
57	MG	YA	3169	-	-	-	X
57	MG	YA	3179	-	-	-	X
57	MG	YA	3184	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3202	-	-	-	X
57	MG	YA	3222	-	-	-	X
57	MG	YA	3226	-	-	-	X
57	MG	YA	3228	-	-	-	X
57	MG	YA	3237	-	-	-	X
57	MG	YA	3264	-	-	-	X
57	MG	YA	3265	-	-	-	X
57	MG	YA	3278	-	-	-	X
57	MG	YA	3286	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3301	-	-	-	X
57	MG	YA	3303	-	-	-	X
57	MG	YA	3306	-	-	-	X
57	MG	YA	3309	-	-	-	X
57	MG	YA	3316	-	-	-	X
57	MG	YA	3318	-	-	-	X
57	MG	YA	3322	-	-	-	X
57	MG	YA	3325	-	-	-	X
57	MG	YA	3333	-	-	-	X
57	MG	YA	3338	-	-	-	X
57	MG	YA	3342	-	-	-	X
57	MG	YA	3343	-	-	-	X
57	MG	YA	3349	-	-	-	X
57	MG	YA	3351	-	-	-	X
57	MG	YA	3352	-	-	-	X
57	MG	YA	3353	-	-	-	X
57	MG	YA	3354	-	-	-	X
57	MG	YA	3357	-	-	-	X
57	MG	YA	3368	-	-	-	X
57	MG	YA	3372	-	-	-	X
57	MG	YA	3373	-	-	-	X
57	MG	YA	3377	-	-	-	X
57	MG	YA	3399	-	-	-	X
57	MG	YA	3400	-	-	-	X
57	MG	YA	3405	-	-	-	X
57	MG	YA	3409	-	-	-	X
57	MG	YA	3423	-	-	-	X
57	MG	YA	3425	-	-	-	X
57	MG	YA	3451	-	-	-	X
57	MG	YA	3459	-	-	-	X
57	MG	YA	3461	-	-	-	X
57	MG	YA	3471	-	-	-	X
57	MG	YD	301	-	-	-	X
57	MG	YQ	202	-	-	-	X
57	MG	YU	201	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294410 atoms, of which 18 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1511	32472	14453	6011	10497	1511	0	0	0
1	XA	1508	32409	14425	6001	10475	1508	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	236	1915	1223	343	344	5	0	0	0
2	XB	236	1915	1223	343	344	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	QC	206	1612	1016	314	281	1	0	0	0
3	XC	206	1612	1016	314	281	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	154	Total 1178	C 743	N 221	O 210	S 4	0	0	0
5	XE	154	Total 1178	C 743	N 221	O 210	S 4	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	128	Total 1018	C 644	N 198	O 175	S 1	0	0	0
9	XI	128	Total 1018	C 644	N 198	O 175	S 1	0	0	0

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	QK	121	901	560	171	167	3	0	0	0
11	XK	121	901	560	171	167	3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	QM	118	937	579	193	163	2	0	0	0
13	XM	118	937	579	193	163	2	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	71	Total	C	N	O	0	0	0
			585	373	116	96			
18	XR	71	Total	C	N	O	0	0	0
			585	373	116	96			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	82	Total	C	N	O	S	0	0	0
			656	419	121	114	2			
19	XS	82	Total	C	N	O	S	0	0	0
			656	419	121	114	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 217 134 52 31	0	0	0
21	XU	25	Total C N O 217 134 52 31	0	0	0

- 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 1640 732 297 535 76	0	0	0
22	XV	77	Total C N O P 1640 732 297 535 76	0	0	0

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	QX	20	Total C H N O P 449 199 9 89 132 20	0	0	0
23	XX	20	Total C H N O P 449 199 9 89 132 20	0	0	0

- Molecule 24 is a protein called Killer protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	QY	92	Total C N O 756 484 134 138	0	0	0
24	XY	92	Total C N O 756 484 134 138	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QY	0	MET	-	initiating methionine	UNP Q7A225
QY	1	GLY	-	expression tag	UNP Q7A225
QY	93	LYS	-	expression tag	UNP Q7A225
QY	94	LEU	-	expression tag	UNP Q7A225
QY	95	GLY	-	expression tag	UNP Q7A225
QY	96	PRO	-	expression tag	UNP Q7A225
QY	97	GLU	-	expression tag	UNP Q7A225
QY	98	GLN	-	expression tag	UNP Q7A225
QY	99	LYS	-	expression tag	UNP Q7A225
QY	100	LEU	-	expression tag	UNP Q7A225
QY	101	ILE	-	expression tag	UNP Q7A225

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Chain	Residue	Modelled	Actual	Comment	Reference
QY	102	SER	-	expression tag	UNP Q7A225
QY	103	GLU	-	expression tag	UNP Q7A225
QY	104	GLU	-	expression tag	UNP Q7A225
QY	105	ASP	-	expression tag	UNP Q7A225
QY	106	LEU	-	expression tag	UNP Q7A225
QY	107	ASN	-	expression tag	UNP Q7A225
QY	108	SER	-	expression tag	UNP Q7A225
QY	109	ALA	-	expression tag	UNP Q7A225
QY	110	VAL	-	expression tag	UNP Q7A225
QY	111	ASP	-	expression tag	UNP Q7A225
QY	112	HIS	-	expression tag	UNP Q7A225
QY	113	HIS	-	expression tag	UNP Q7A225
QY	114	HIS	-	expression tag	UNP Q7A225
QY	115	HIS	-	expression tag	UNP Q7A225
QY	116	HIS	-	expression tag	UNP Q7A225
QY	117	HIS	-	expression tag	UNP Q7A225
XY	0	MET	-	initiating methionine	UNP Q7A225
XY	1	GLY	-	expression tag	UNP Q7A225
XY	93	LYS	-	expression tag	UNP Q7A225
XY	94	LEU	-	expression tag	UNP Q7A225
XY	95	GLY	-	expression tag	UNP Q7A225
XY	96	PRO	-	expression tag	UNP Q7A225
XY	97	GLU	-	expression tag	UNP Q7A225
XY	98	GLN	-	expression tag	UNP Q7A225
XY	99	LYS	-	expression tag	UNP Q7A225
XY	100	LEU	-	expression tag	UNP Q7A225
XY	101	ILE	-	expression tag	UNP Q7A225
XY	102	SER	-	expression tag	UNP Q7A225
XY	103	GLU	-	expression tag	UNP Q7A225
XY	104	GLU	-	expression tag	UNP Q7A225
XY	105	ASP	-	expression tag	UNP Q7A225
XY	106	LEU	-	expression tag	UNP Q7A225
XY	107	ASN	-	expression tag	UNP Q7A225
XY	108	SER	-	expression tag	UNP Q7A225
XY	109	ALA	-	expression tag	UNP Q7A225
XY	110	VAL	-	expression tag	UNP Q7A225
XY	111	ASP	-	expression tag	UNP Q7A225
XY	112	HIS	-	expression tag	UNP Q7A225
XY	113	HIS	-	expression tag	UNP Q7A225
XY	114	HIS	-	expression tag	UNP Q7A225
XY	115	HIS	-	expression tag	UNP Q7A225
XY	116	HIS	-	expression tag	UNP Q7A225

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Chain	Residue	Modelled	Actual	Comment	Reference
XY	117	HIS	-	expression tag	UNP Q7A225

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2891	Total 62269	C 27713	N 11649	O 20016	P 2891	0	0	0
25	YA	2875	Total 61924	C 27560	N 11583	O 19906	P 2875	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RB	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0
26	YB	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	RF	208	Total 1627	C 1037	N 304	O 283	S 3	0	0	0
29	YF	208	Total 1627	C 1037	N 304	O 283	S 3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RQ	140	Total 1112	C 710	N 210	O 185	S 7	0	0	0
36	YQ	139	Total 1107	C 707	N 209	O 184	S 7	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	RR	117	Total 960	C 599	N 202	O 159	0	0	0
37	YR	117	Total 960	C 599	N 202	O 159	0	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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	176	Total	C	N	O	S	0	0	0
			1404	897	252	252	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
			Total	C	N	O	S			
46	R0	83	657	407	139	110	1	0	0	0
46	Y0	83	657	407	139	110	1	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	R4	70	573	359	107	103	4	0	0	0
50	Y4	70	573	359	107	103	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total 459	C 288	N 90	O 76	S 5	0	0	0
51	Y5	57	Total 442	C 278	N 88	O 71	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	48	Total 417	C 259	N 86	O 68	S 4	0	0	0
52	Y6	48	Total 417	C 259	N 86	O 68	S 4	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	R9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0
55	Y9	36	Total 299	C 183	N 67	O 46	S 3	0	0	0

- Molecule 56 is a RNA chain called CC-puromycin.

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	Z7	3	Total C N O P 74 40 13 19 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QA	147	Total Mg 147 147	0	0
57	QD	1	Total Mg 1 1	0	0
57	QE	1	Total Mg 1 1	0	0
57	QL	1	Total Mg 1 1	0	0
57	QV	5	Total Mg 5 5	0	0
57	RA	431	Total Mg 431 431	0	0
57	RB	5	Total Mg 5 5	0	0
57	RD	2	Total Mg 2 2	0	0
57	RE	2	Total Mg 2 2	0	0
57	RF	1	Total Mg 1 1	0	0
57	RP	2	Total Mg 2 2	0	0
57	RQ	2	Total Mg 2 2	0	0
57	RR	1	Total Mg 1 1	0	0
57	RY	2	Total Mg 2 2	0	0
57	R0	3	Total Mg 3 3	0	0
57	R2	1	Total Mg 1 1	0	0
57	R5	3	Total Mg 3 3	0	0
57	XA	161	Total Mg 161 161	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	XD	1	Total Mg 1 1	0	0
57	XF	1	Total Mg 1 1	0	0
57	XL	1	Total Mg 1 1	0	0
57	XN	1	Total Mg 1 1	0	0
57	XV	4	Total Mg 4 4	0	0
57	YA	473	Total Mg 473 473	0	0
57	YB	6	Total Mg 6 6	0	0
57	YD	1	Total Mg 1 1	0	0
57	YE	1	Total Mg 1 1	0	0
57	YF	1	Total Mg 1 1	0	0
57	YG	1	Total Mg 1 1	0	0
57	YH	2	Total Mg 2 2	0	0
57	YN	1	Total Mg 1 1	0	0
57	YP	2	Total Mg 2 2	0	0
57	YQ	2	Total Mg 2 2	0	0
57	YR	1	Total Mg 1 1	0	0
57	YU	1	Total Mg 1 1	0	0
57	YV	1	Total Mg 1 1	0	0
57	YY	1	Total Mg 1 1	0	0
57	Y0	3	Total Mg 3 3	0	0
57	Y1	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	Y5	3	Total Mg 3 3	0	0
57	Y7	1	Total Mg 1 1	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

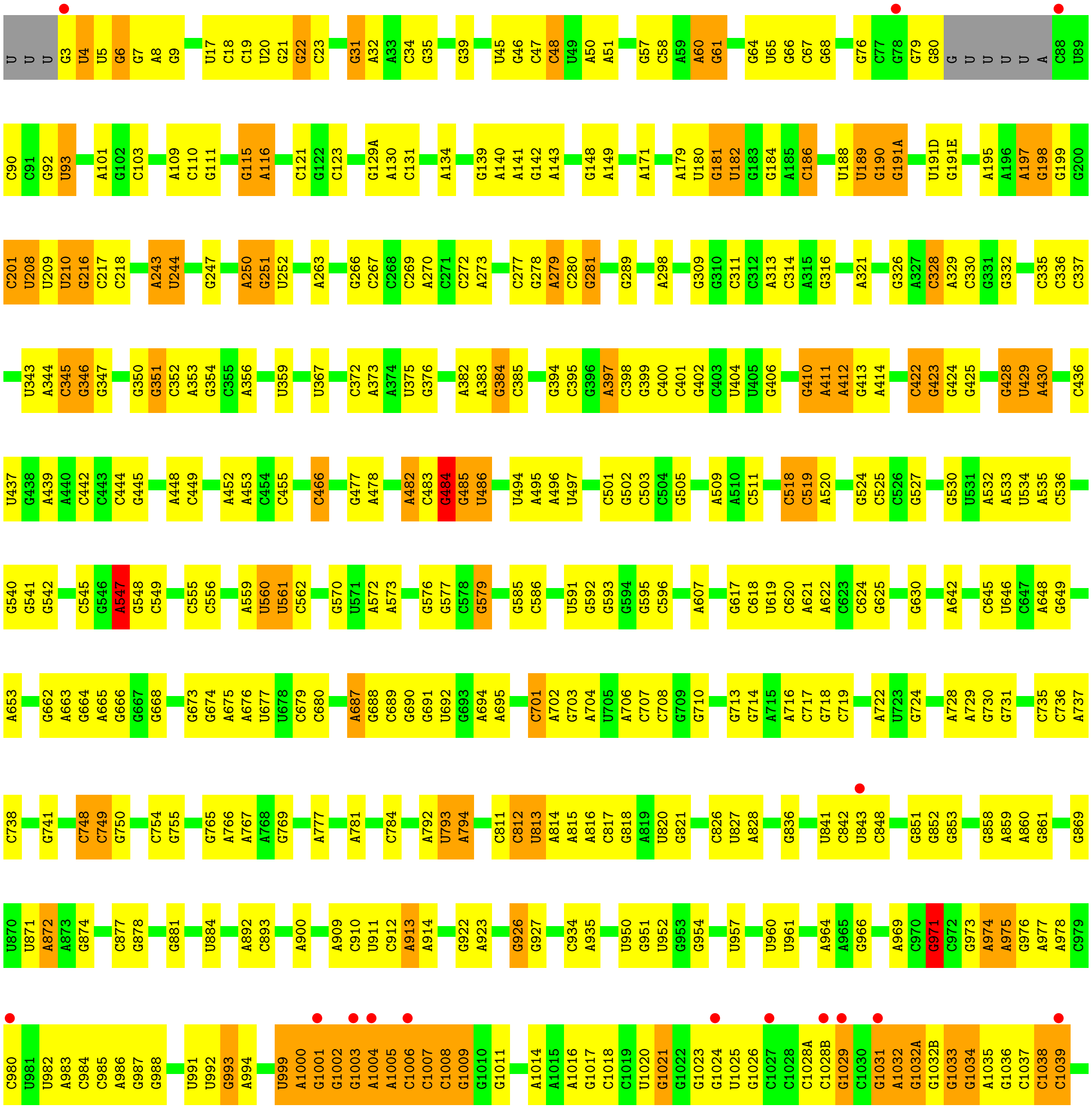
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	QD	1	Total Zn 1 1	0	0
58	QN	1	Total Zn 1 1	0	0
58	XD	1	Total Zn 1 1	0	0
58	XN	1	Total Zn 1 1	0	0

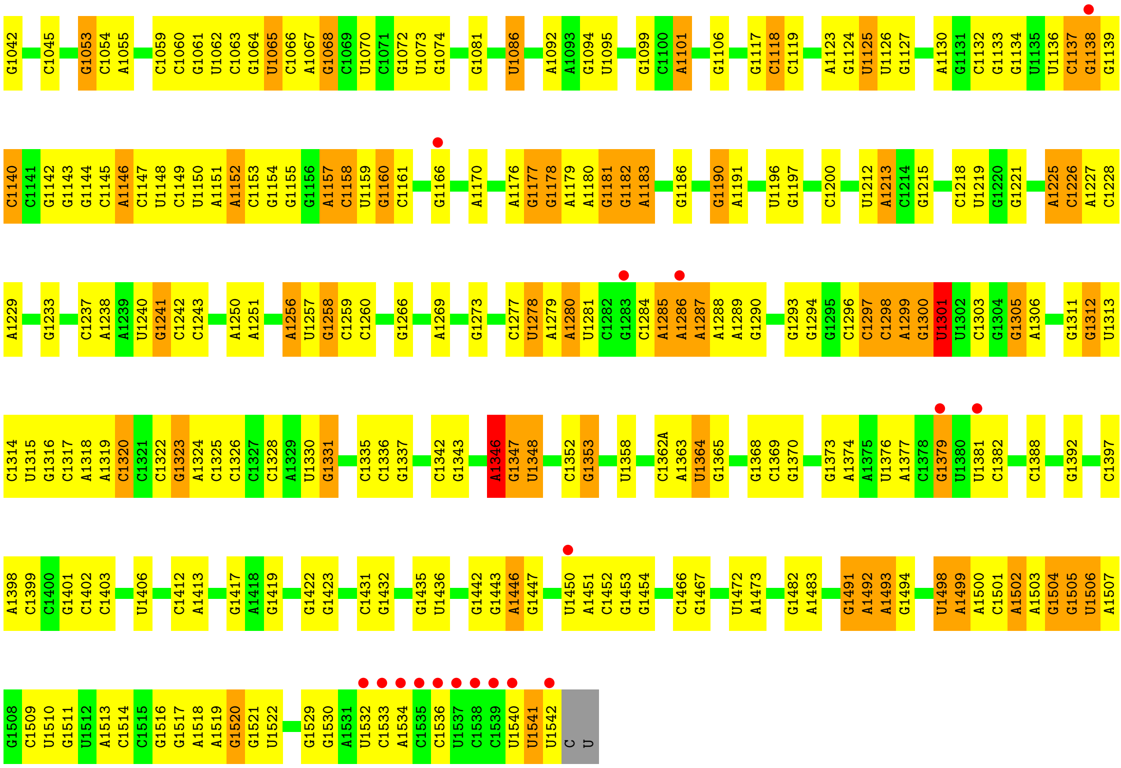
3 Residue-property plots ⓘ

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

- Molecule 1: 16S rRNA

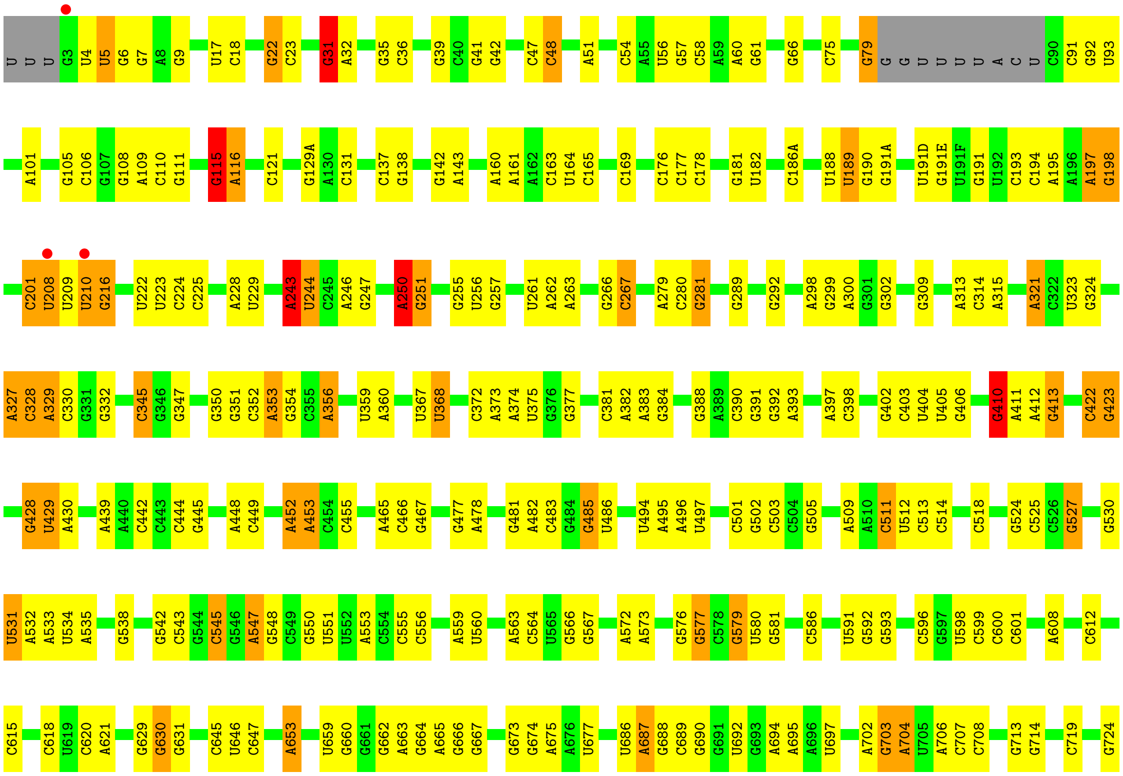
Chain QA:

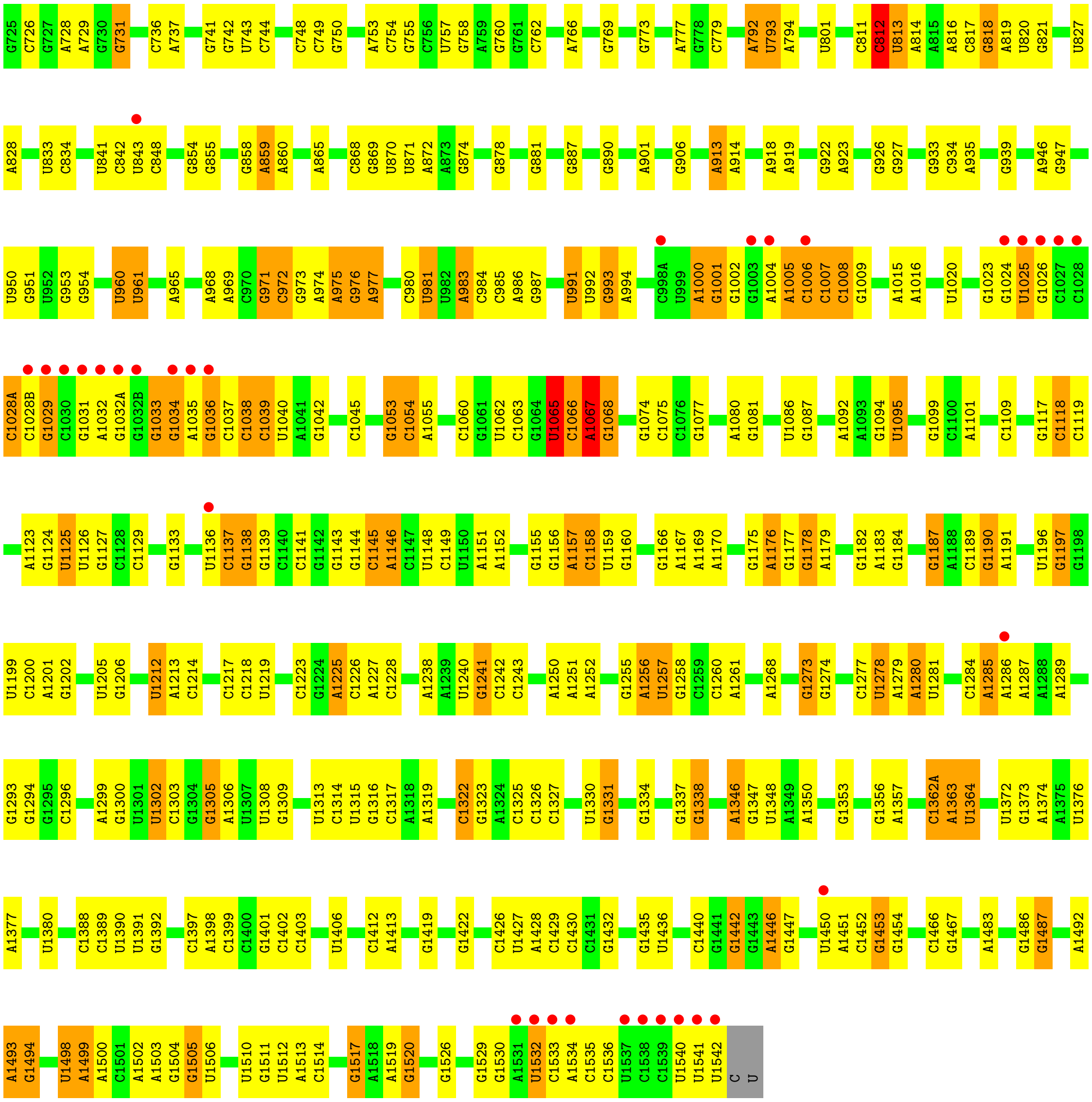




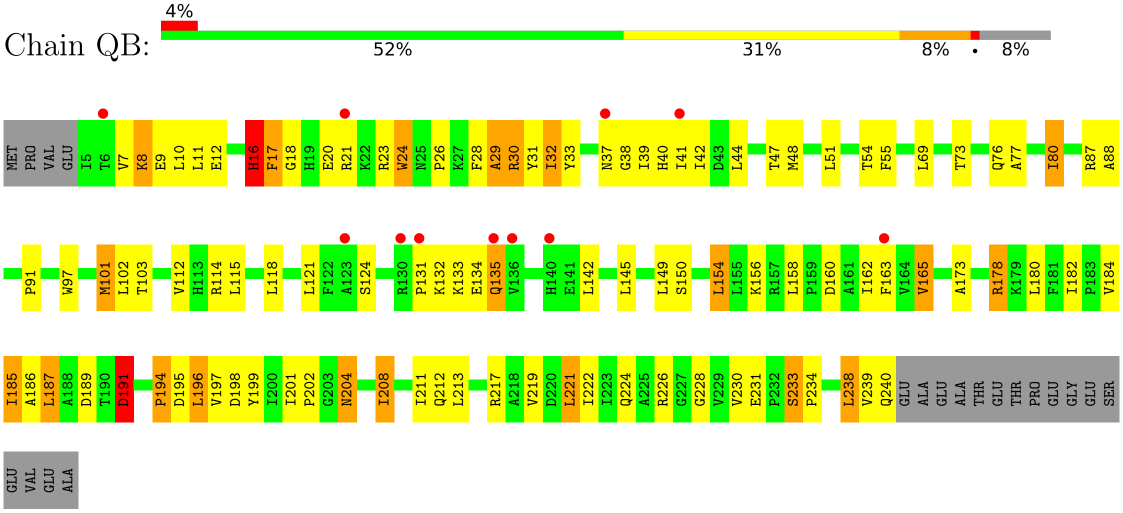
- Molecule 1: 16S rRNA

Chain XA:



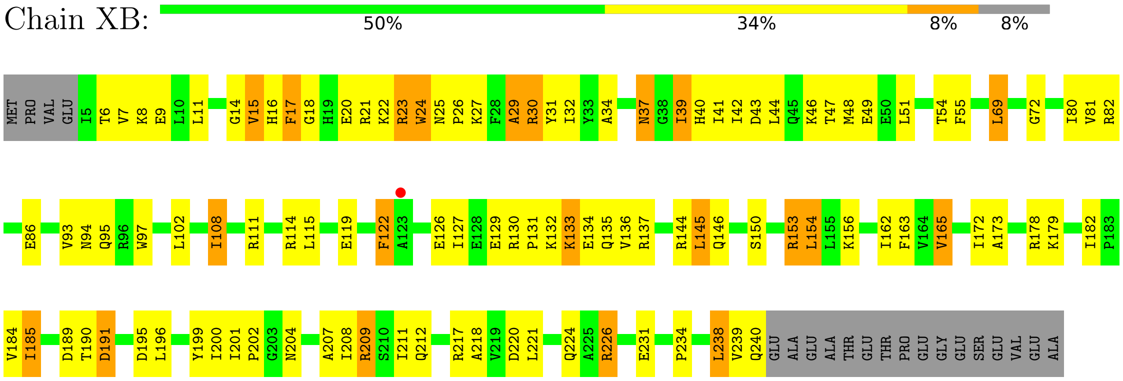


- Molecule 2: 30S ribosomal protein S2



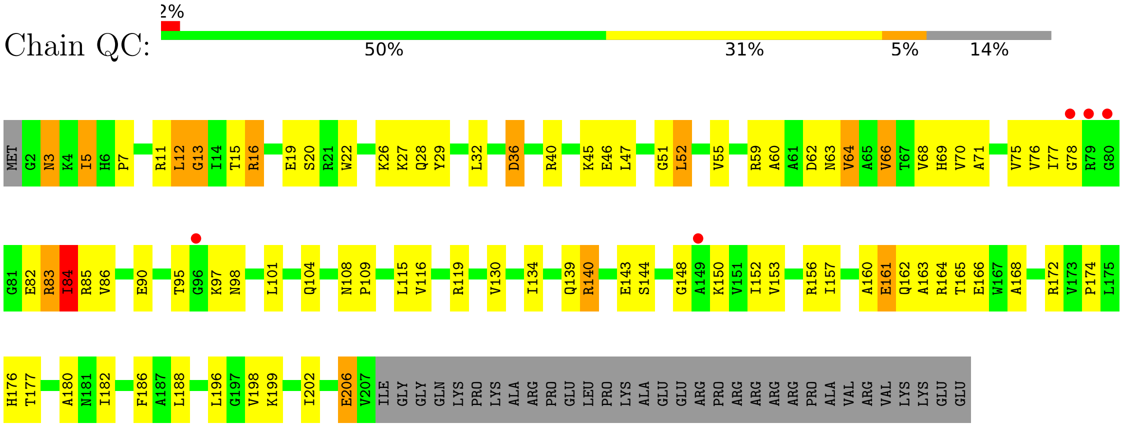
- Molecule 2: 30S ribosomal protein S2

Chain XB:



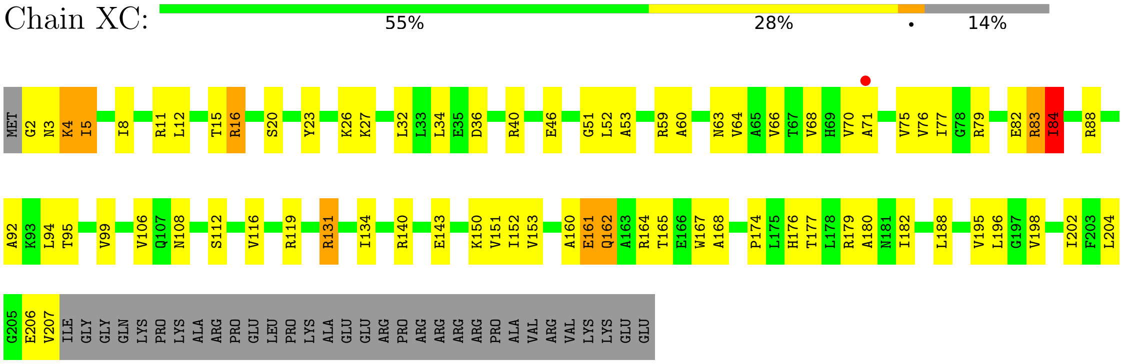
- Molecule 3: 30S ribosomal protein S3

Chain QC:



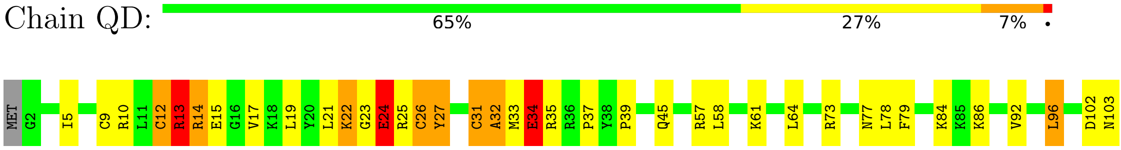
- Molecule 3: 30S ribosomal protein S3

Chain XC:



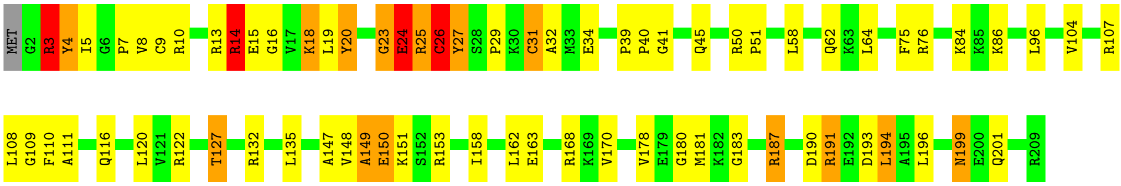
- Molecule 4: 30S ribosomal protein S4

Chain QD:



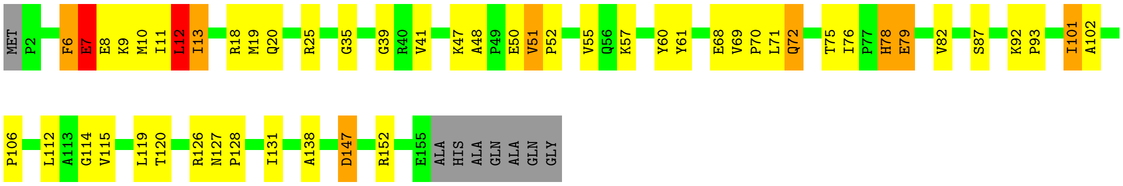
- Molecule 4: 30S ribosomal protein S4

Chain XD:



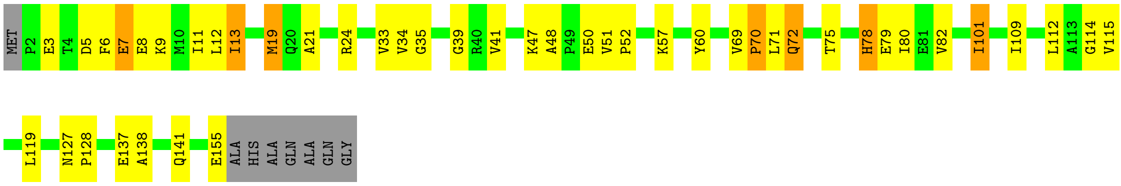
- Molecule 5: 30S ribosomal protein S5

Chain QE:



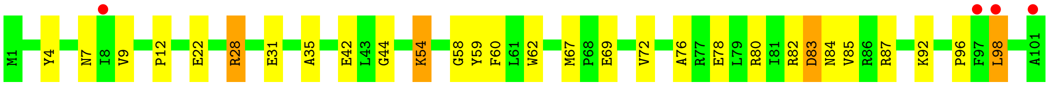
- Molecule 5: 30S ribosomal protein S5

Chain XE:



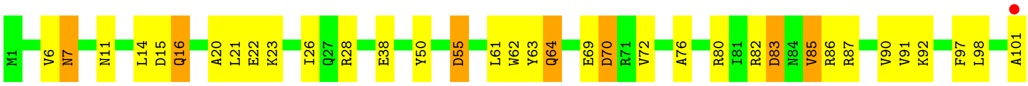
- Molecule 6: 30S ribosomal protein S6

Chain QF:

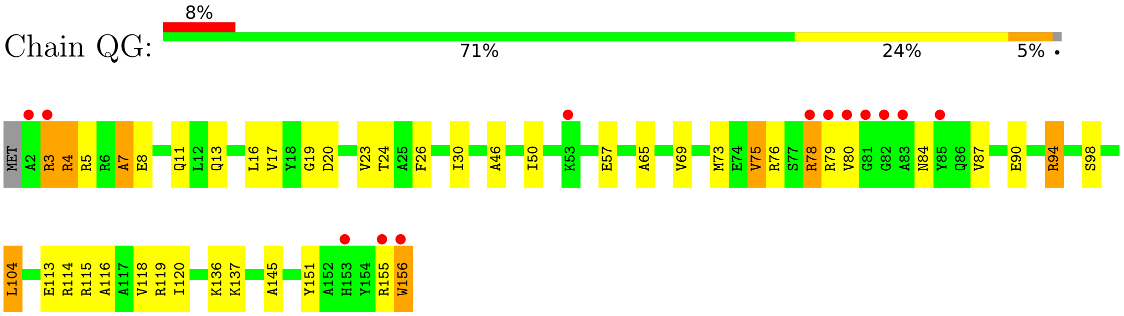


- Molecule 6: 30S ribosomal protein S6

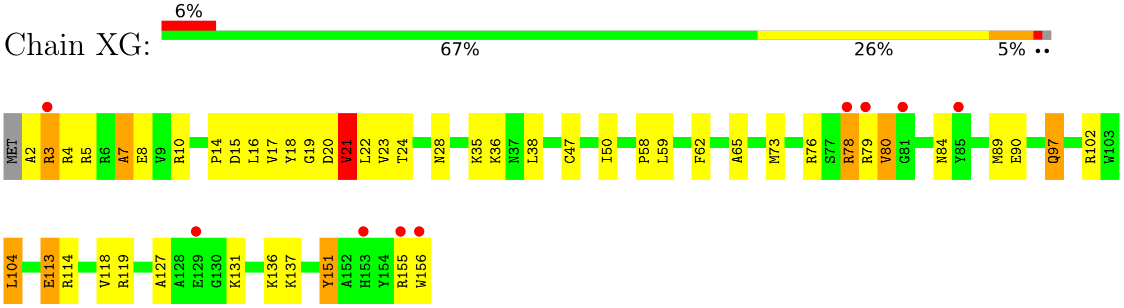
Chain XF:



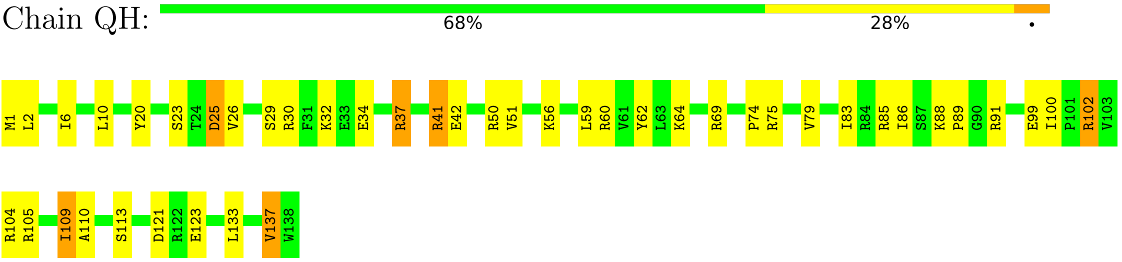
- Molecule 7: 30S ribosomal protein S7



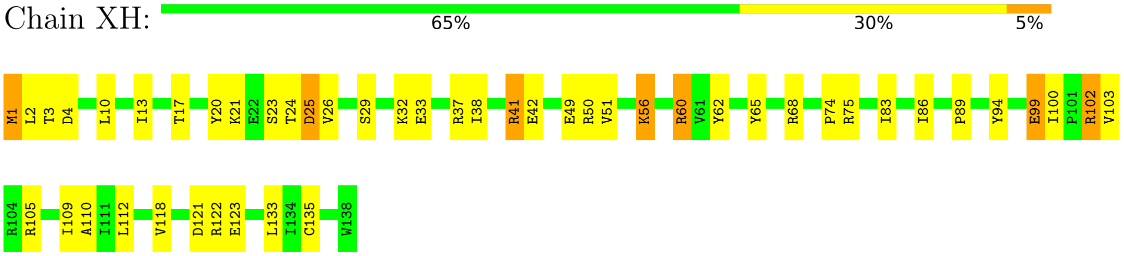
- Molecule 7: 30S ribosomal protein S7



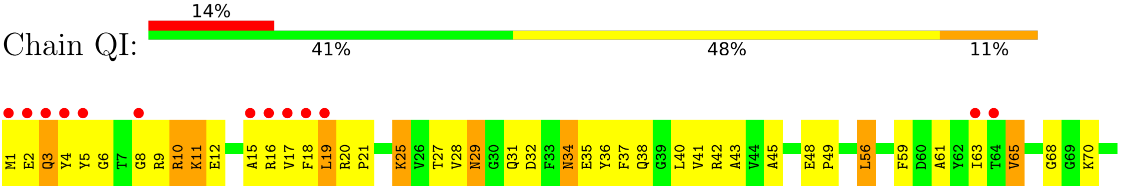
- Molecule 8: 30S ribosomal protein S8

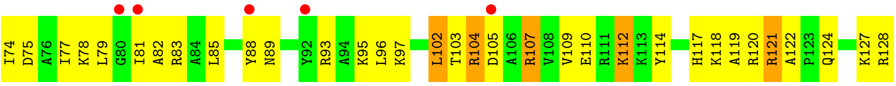


- Molecule 8: 30S ribosomal protein S8



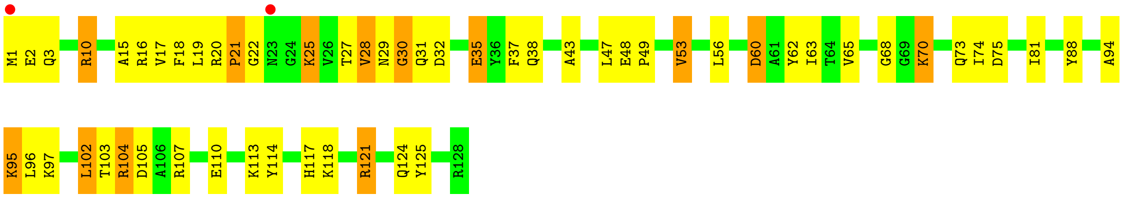
- Molecule 9: 30S ribosomal protein S9





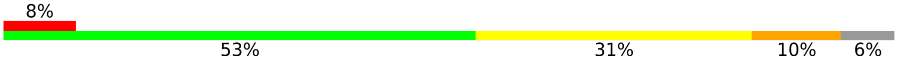
- Molecule 9: 30S ribosomal protein S9

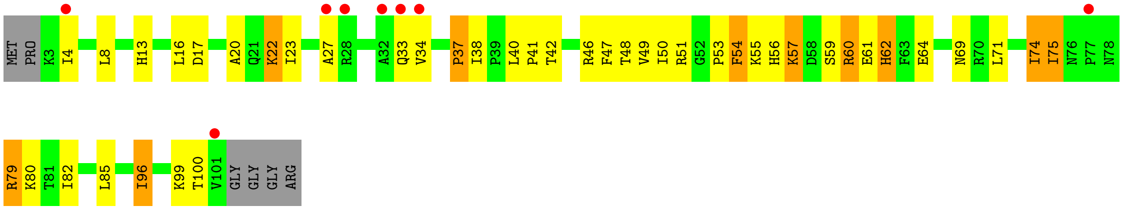
Chain XI:



- Molecule 10: 30S ribosomal protein S10

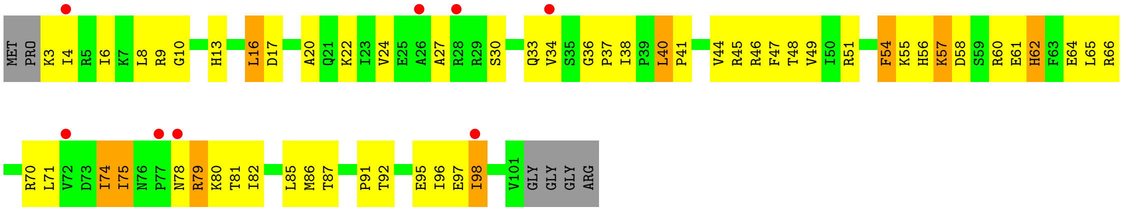
Chain QJ:





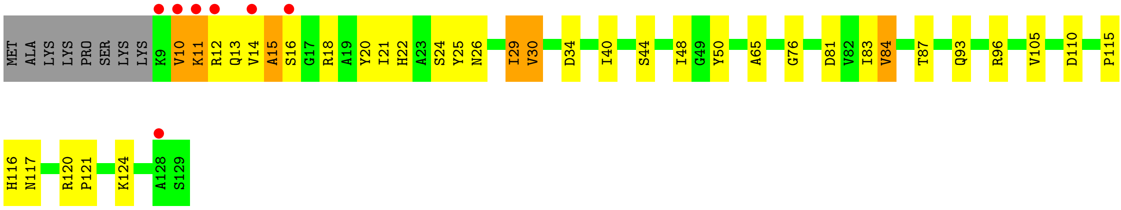
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



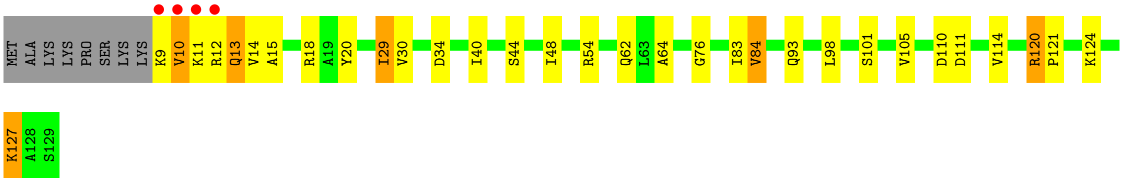
- Molecule 11: 30S ribosomal protein S11

Chain QK:



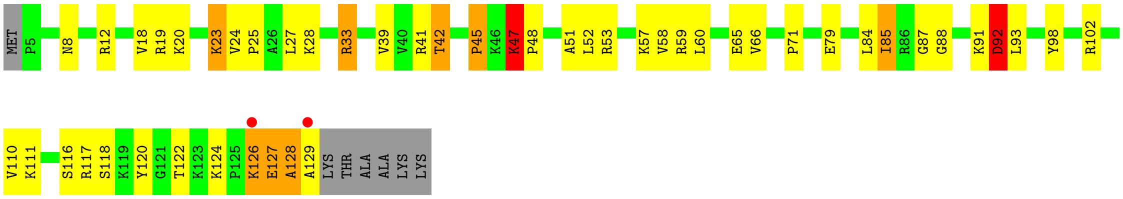
- Molecule 11: 30S ribosomal protein S11

Chain XK:



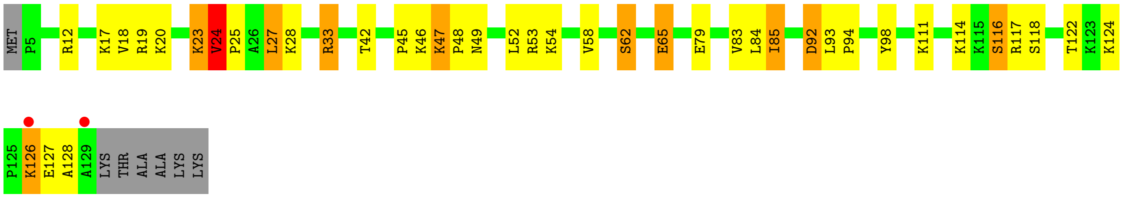
- Molecule 12: 30S ribosomal protein S12

Chain QL:



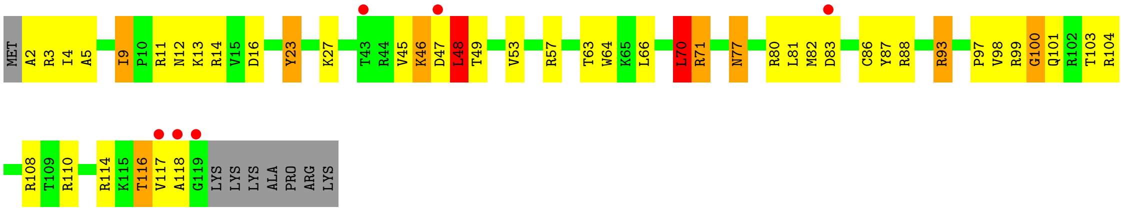
- Molecule 12: 30S ribosomal protein S12

Chain XL:



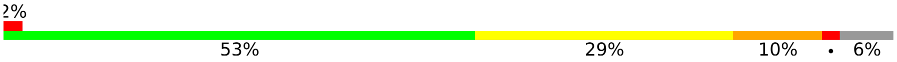
- Molecule 13: 30S ribosomal protein S13

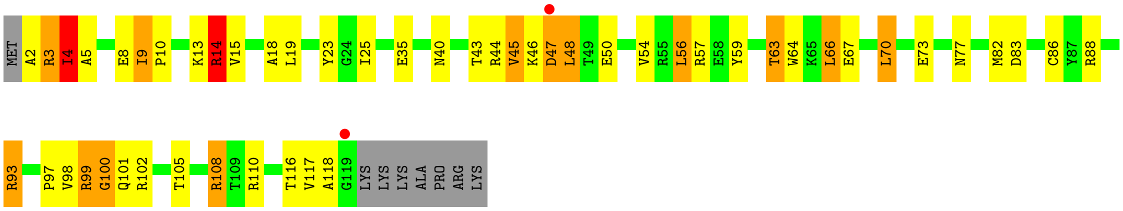
Chain QM:



- Molecule 13: 30S ribosomal protein S13

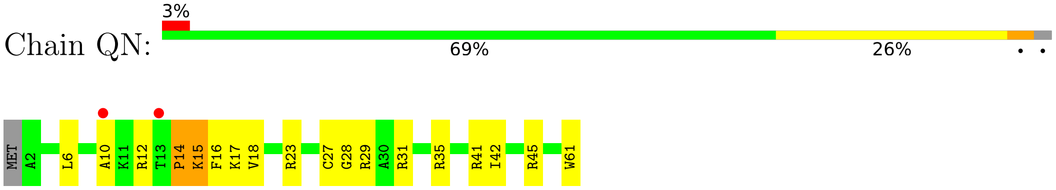
Chain XM:





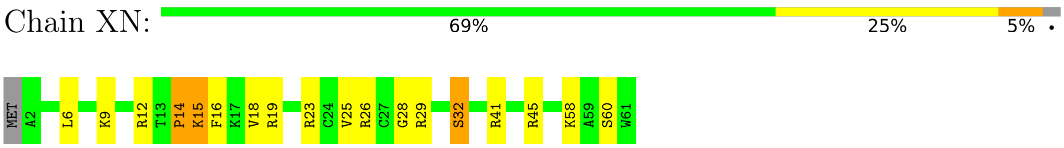
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



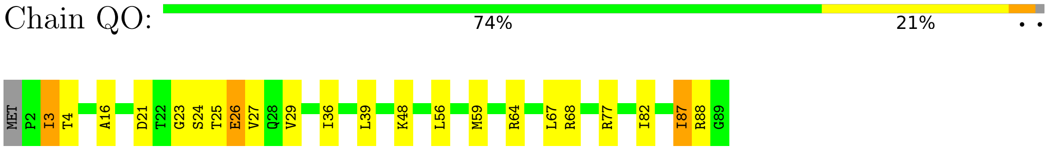
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



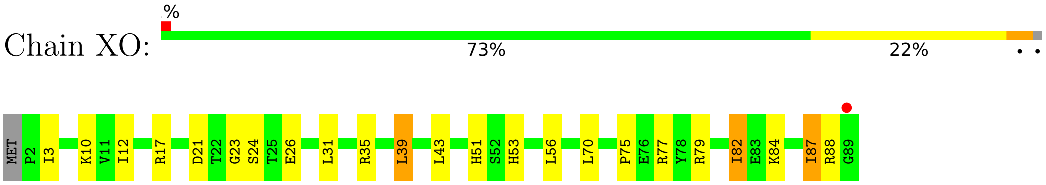
- Molecule 15: 30S ribosomal protein S15

Chain QO:



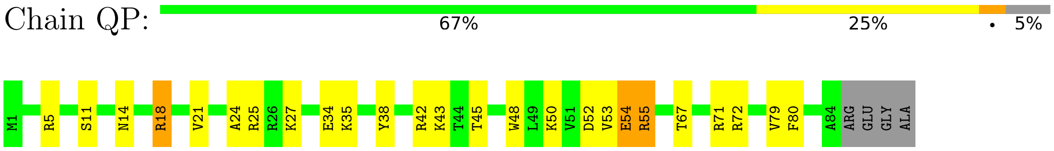
- Molecule 15: 30S ribosomal protein S15

Chain XO:



- Molecule 16: 30S ribosomal protein S16

Chain QP:



- Molecule 16: 30S ribosomal protein S16

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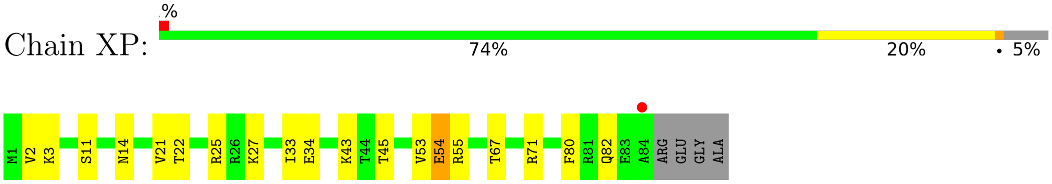

- Molecule 17: 30S ribosomal protein S17

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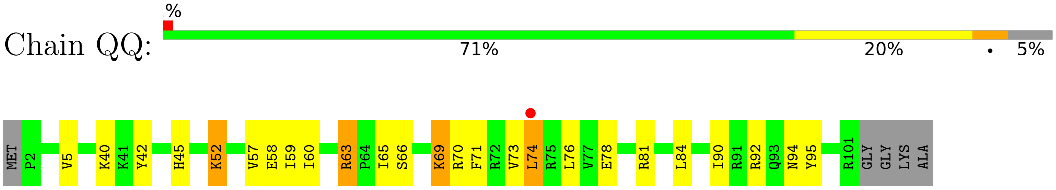

- Molecule 17: 30S ribosomal protein S17

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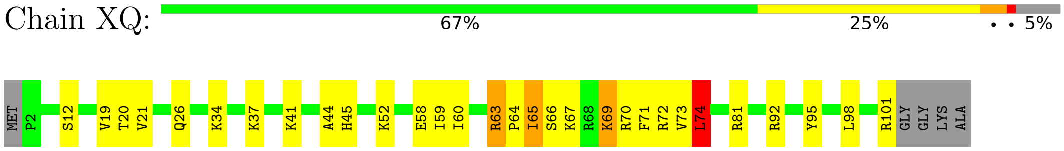

- Molecule 18: 30S ribosomal protein S18

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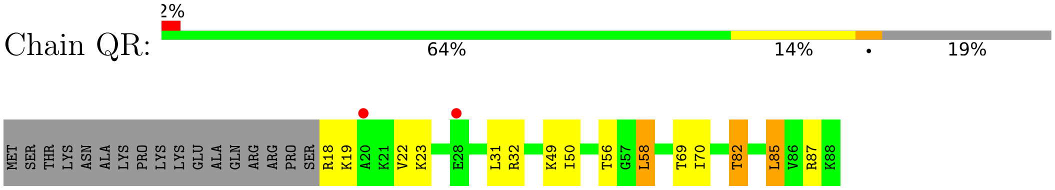

- Molecule 18: 30S ribosomal protein S18

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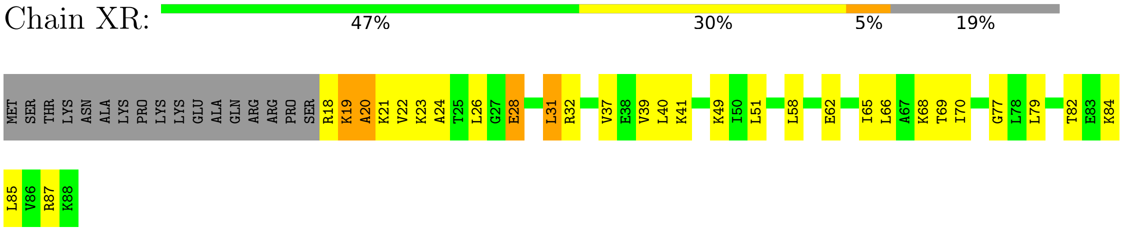

- Molecule 19: 30S ribosomal protein S19

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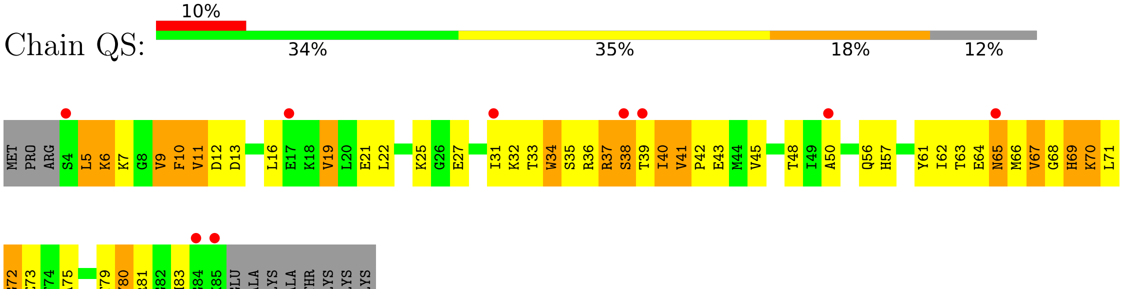

- Molecule 19: 30S ribosomal protein S19

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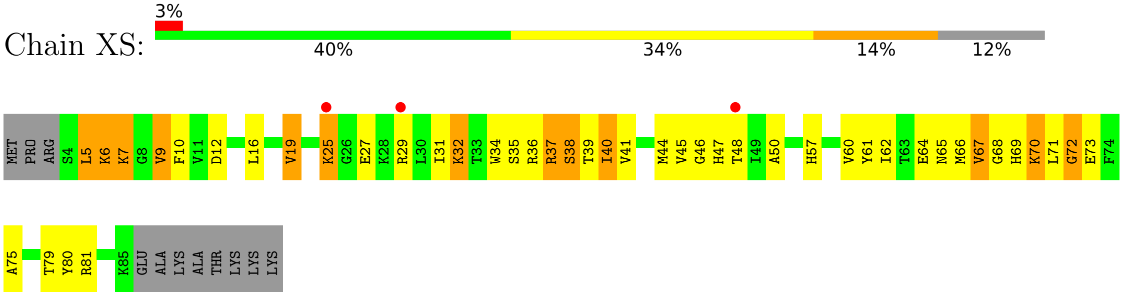

- Molecule 20: 30S ribosomal protein S20

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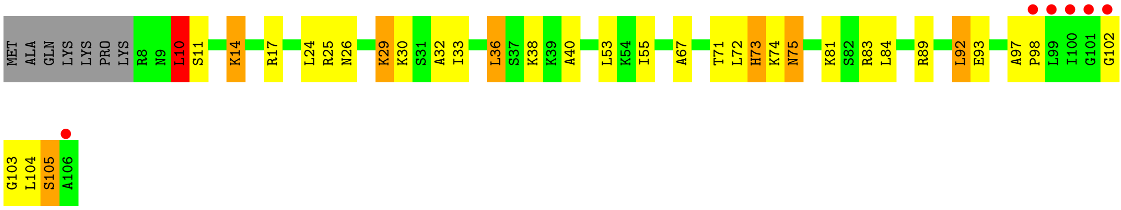

- Molecule 20: 30S ribosomal protein S20

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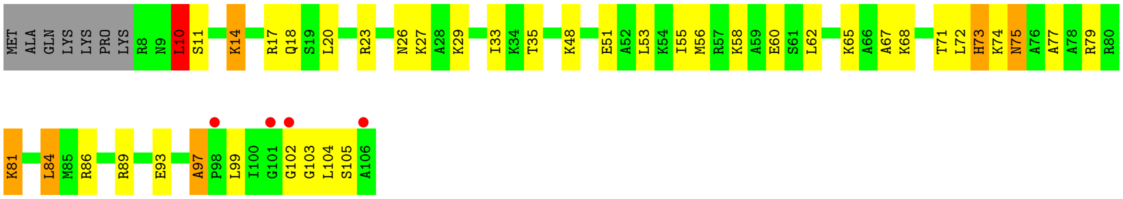
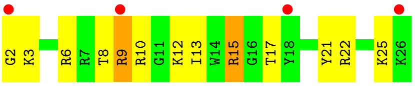


- Molecule 21: 30S ribosomal protein Thx

Chain QU:



- Molecule 21: 30S ribosomal protein Thx

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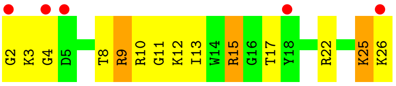
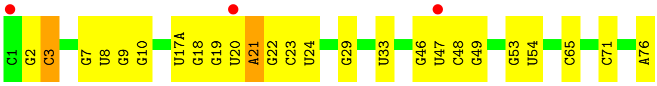


- Molecule 22: P-site tRNA-fMet

Chain QV:



- Molecule 22: P-site tRNA-fMet

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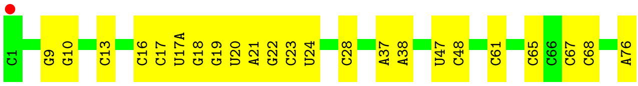
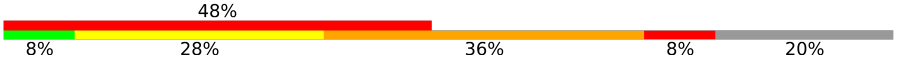
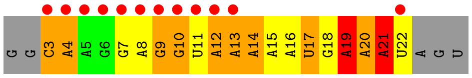


- Molecule 23: messenger RNA

Chain QX:





- Molecule 23: messenger RNA

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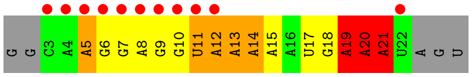

- Molecule 24: Killer protein

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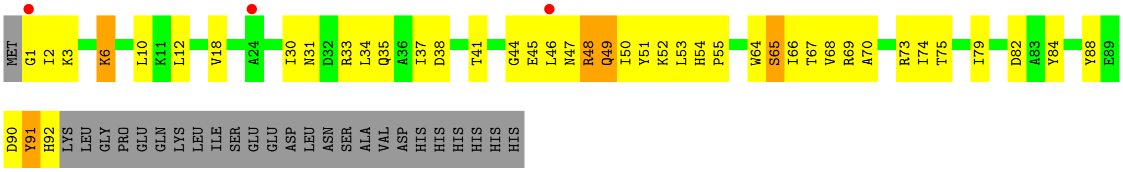
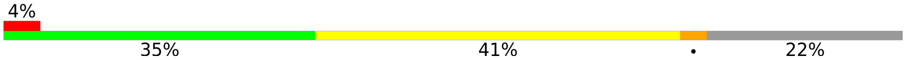
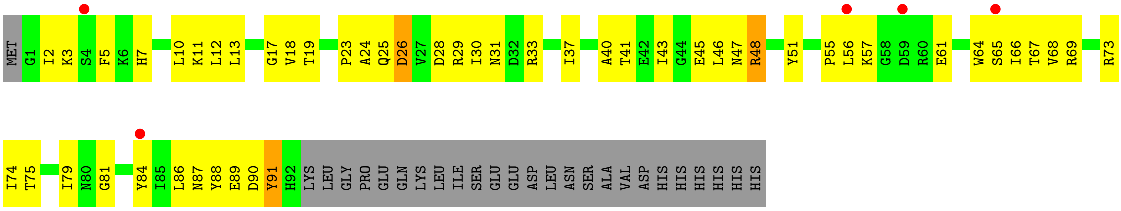


- Molecule 24: Killer protein

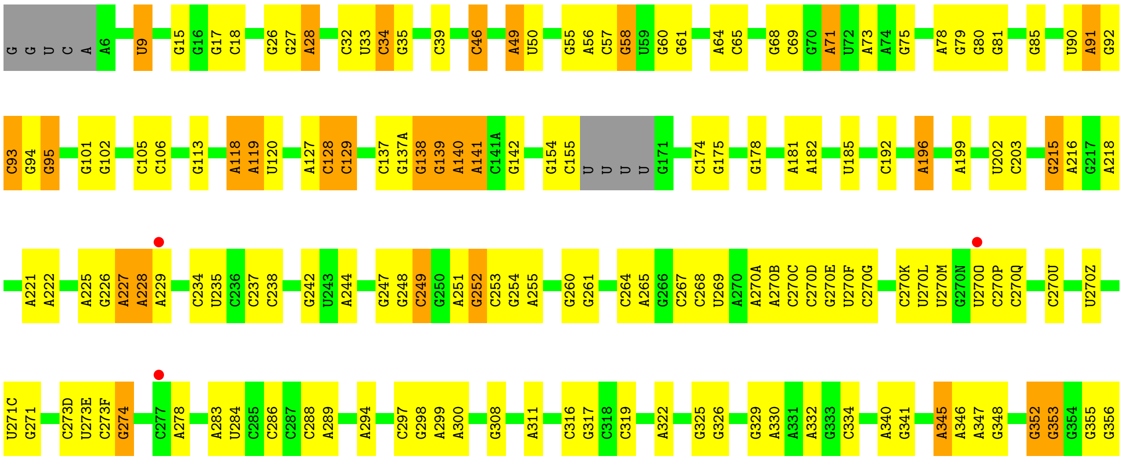
Chain XY:

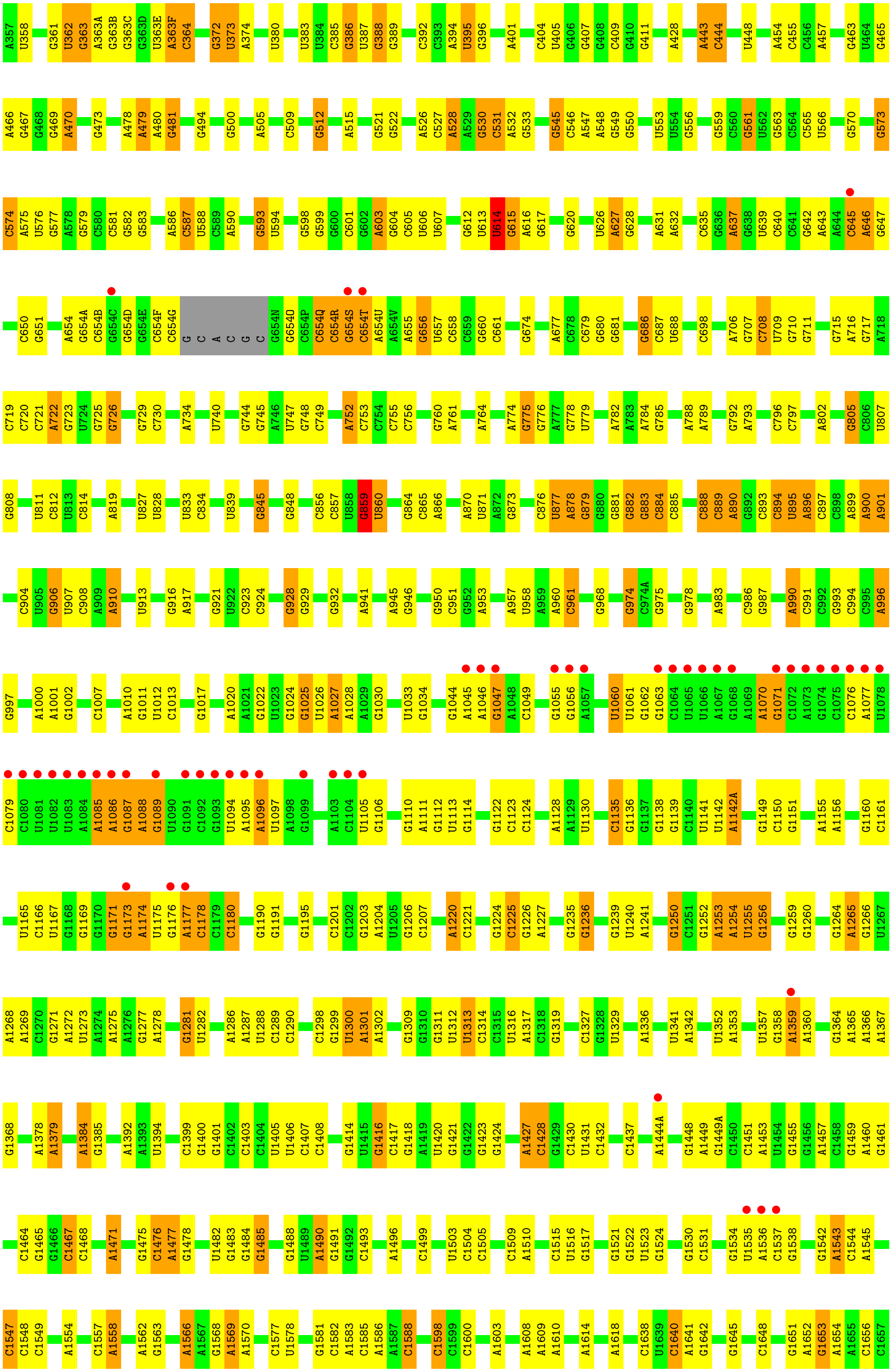




- Molecule 25: 23S rRNA

Chain RA:

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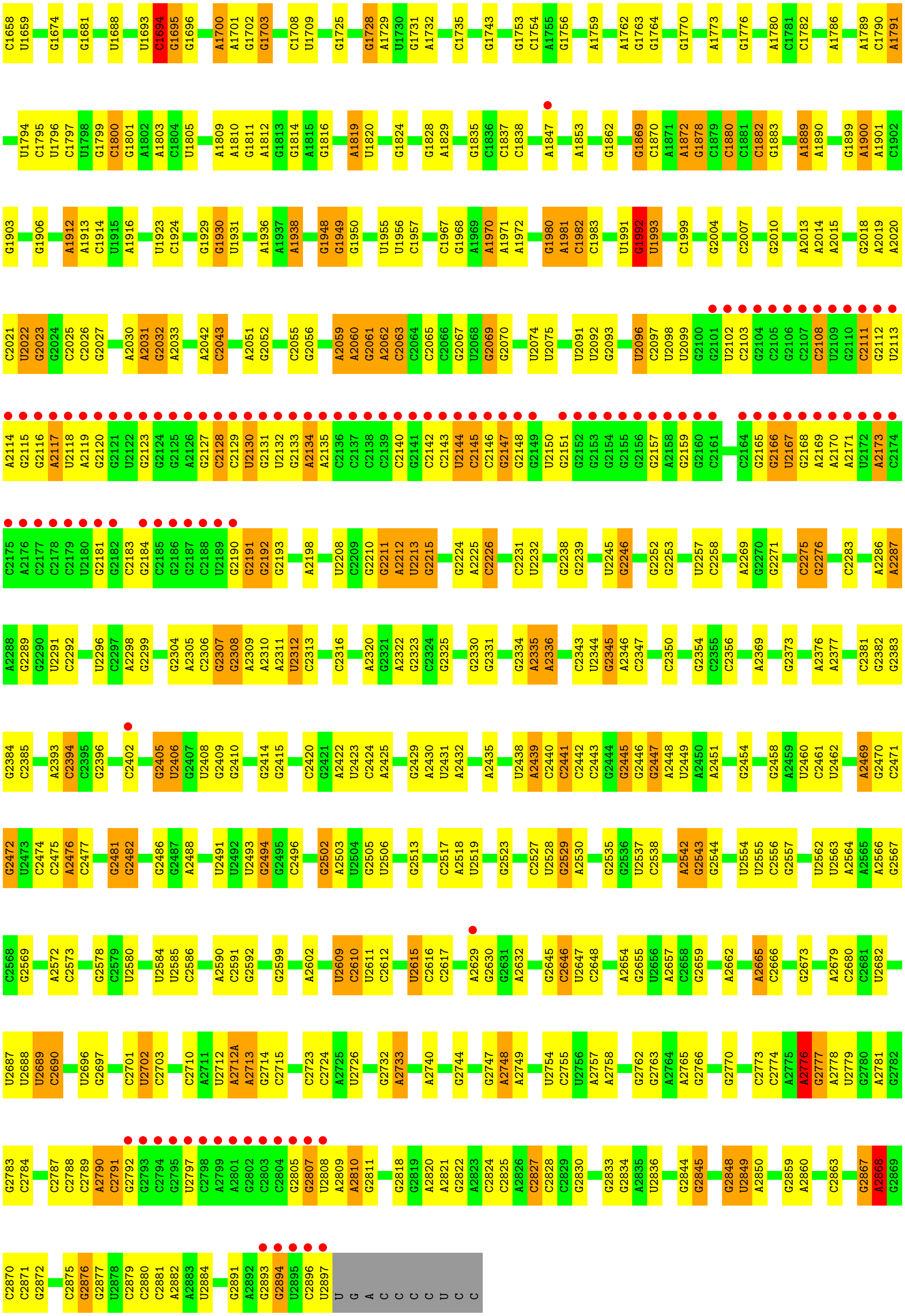
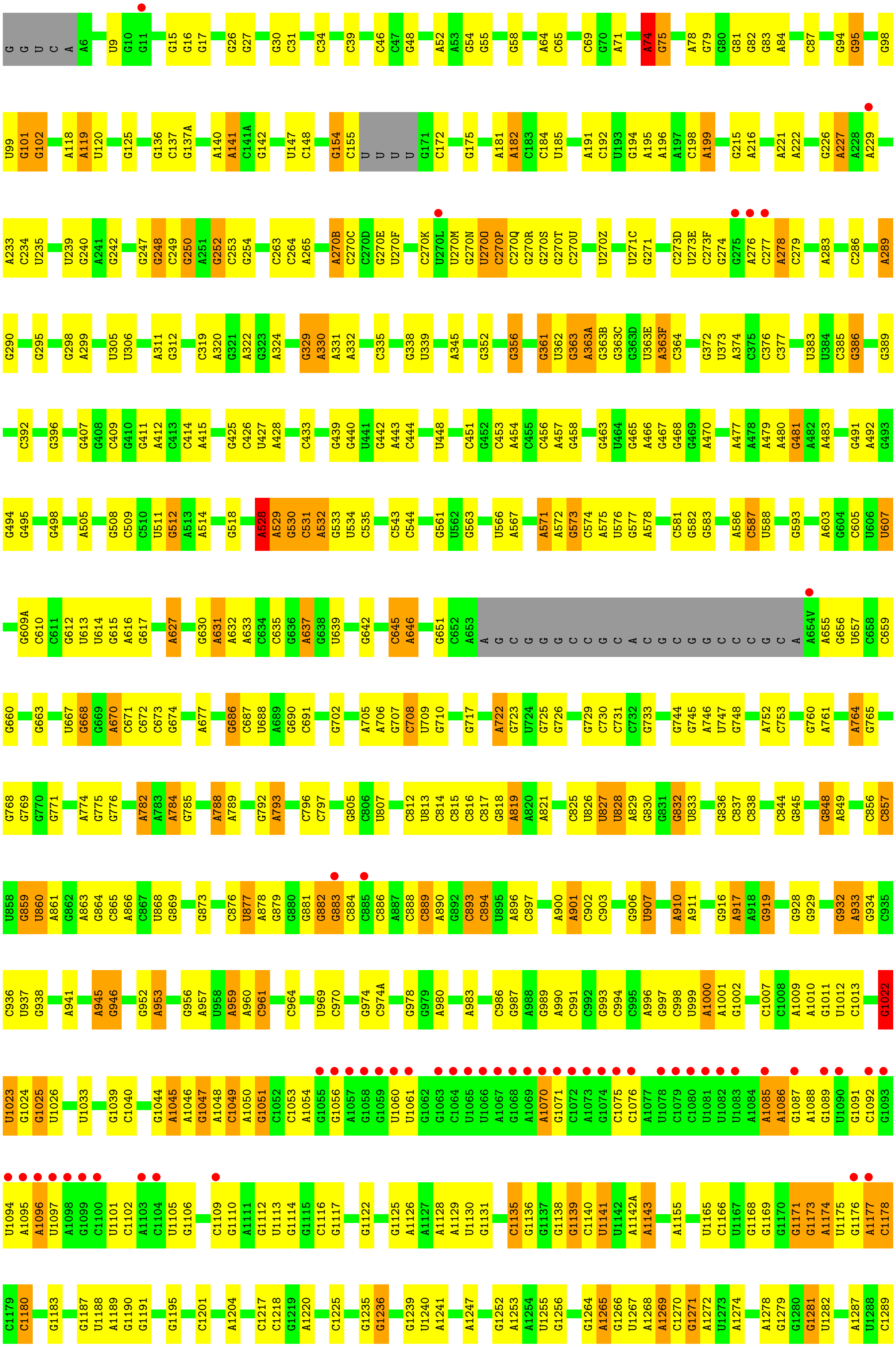


- Molecule 25: 23S rRNA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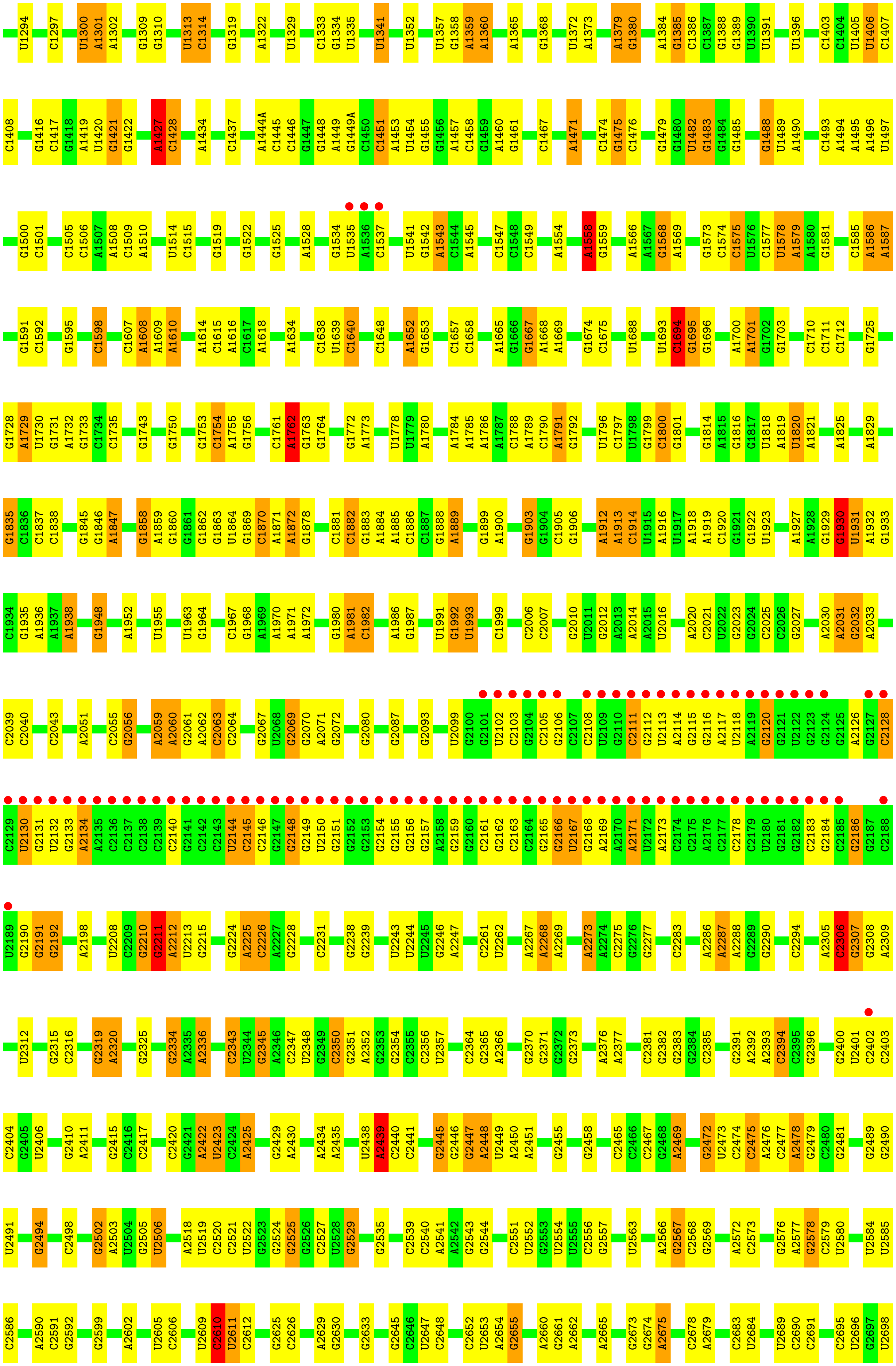
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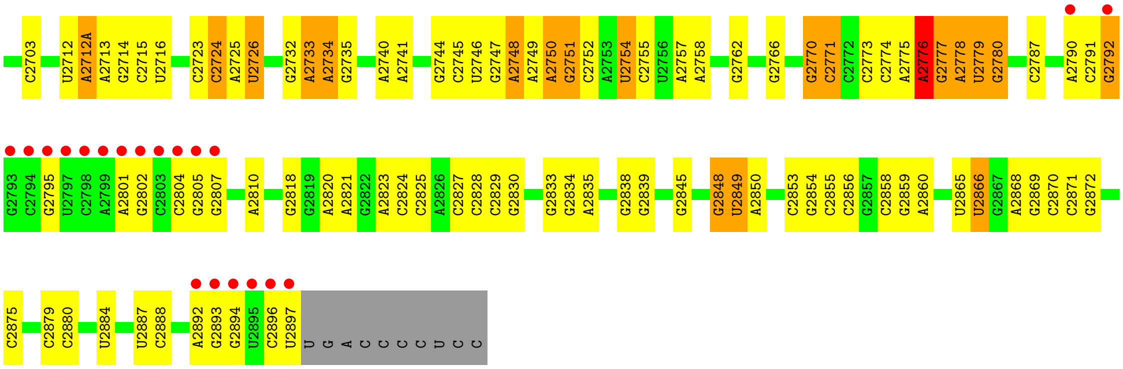
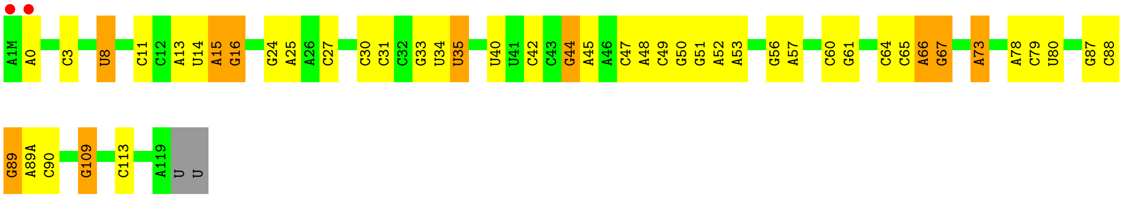
U2491 G2494 C2498 G2502 A2503 U2504 G2505 U2506 A2518 U2519 C2520 C2521 U2522 G2523 G2524 G2525 G2526 C2527 U2528 G2529 G2535 C2539 C2540 A2541 A2542 G2543 G2544 C2551 U2552 G2553 U2554 U2555 C2556 G2557 U2563 A2566 G2567 C2568 G2569 A2572 C2573 G2576 A2577 G2578 C2579 U2580 U2584 U2585
C2586 A2590 C2591 G2592 G2599 A2602 U2605 C2606 U2609 C2610 U2611 C2612 G2625 C2626 A2629 G2630 G2633 G2645 C2646 U2647 C2648 C2652 U2653 A2654 G2655 A2660 G2661 A2662 A2665 G2673 G2674 A2675 C2678 A2679 C2683 U2684 U2689 C2690 C2691 C2695 U2696 G2697 U2698



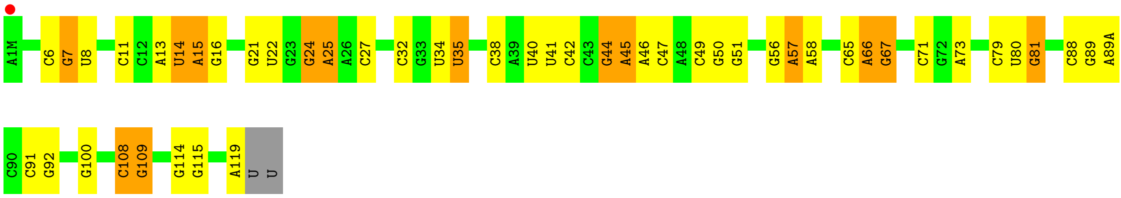
- Molecule 26: 5S rRNA

Chain RB:



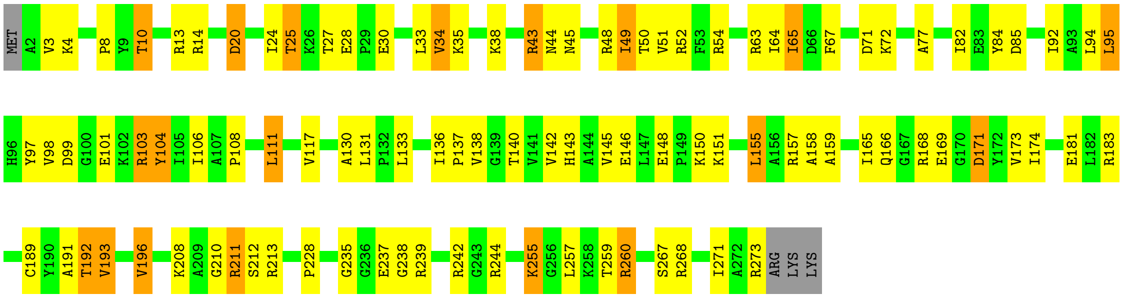
- Molecule 26: 5S rRNA

Chain YB:



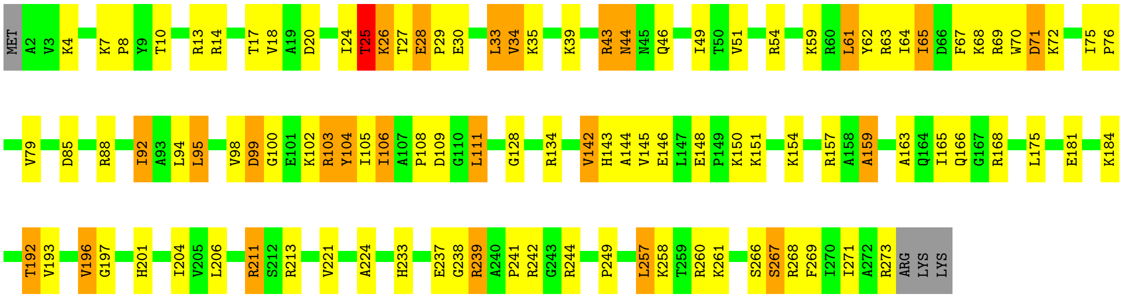
- Molecule 27: 50S ribosomal protein L2

Chain RD:



- Molecule 27: 50S ribosomal protein L2

Chain YD: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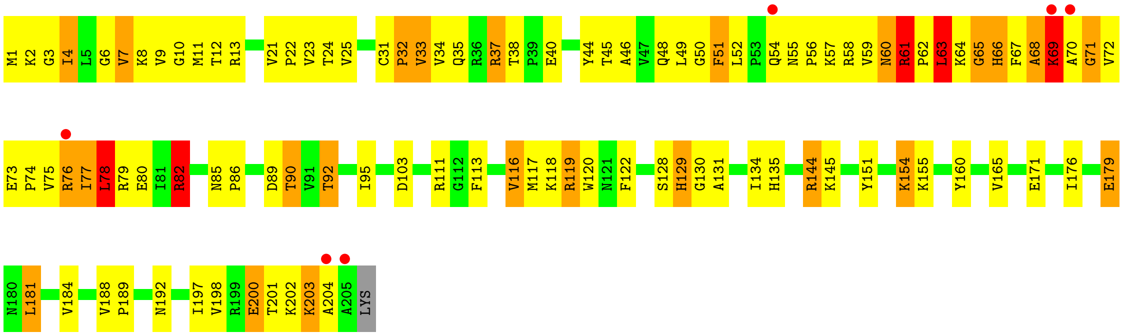
V79 D85 R88 I92 A93 L94 L95 V98 D99 G100 E101 K102 R103 Y104 I105 I106 A107 P108 D109 G110 L111 G128 R134 V142 H143 A144 V145 E146 L147 E148 P149 K150 K151 K154 R157 A158 A159 A163 Q164 I165 Q166 G167 R168 L175 E181 K184
T192 V193 V196 G197 H201 I204 V205 L206 R211 S212 R213 V221 A224 H233 E237 G238 R239 A240 P241 R242 G243 R244 P249 L257 K258 T259 R260 K261 S266 S267 R268 F269 I270 I271 A272 R273 ARG LYS LYS

- Molecule 28: 50S ribosomal protein L3

Chain RE:


M1 K2 G3 I4 L5 G6 V7 K8 V9 G10 M11 T12 R13 V21 P22 V23 T24 V25 C31 P32 V33 V34 Q35 R36 R37 T38 P39 E40 Y44 T45 A46 V47 Q48 L49 G50 F51 L52 P53 Q54 N55 P56 K57 R58 V59 N60 R61 P62 L63 K64 G65 H66 F67 A68 K69 A70 G71 V72
E73 P74 V75 R76 I77 L78 R79 E80 I81 R82 N85 P86 D89 T90 V91 T92 I95 D103 R111 G112 F113 V116 M117 K118 R119 W120 N121 F122 S128 H129 G130 A131 I134 H135 R144 K145 Y151 K154 K155 Y160 V165 E171 I176 E179
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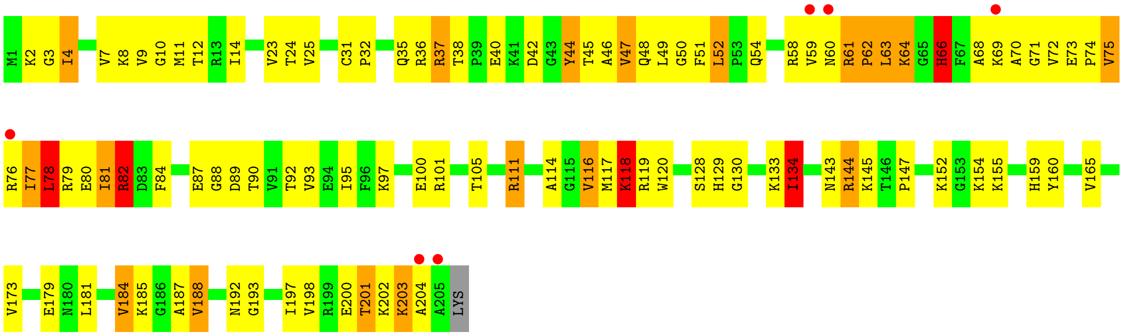
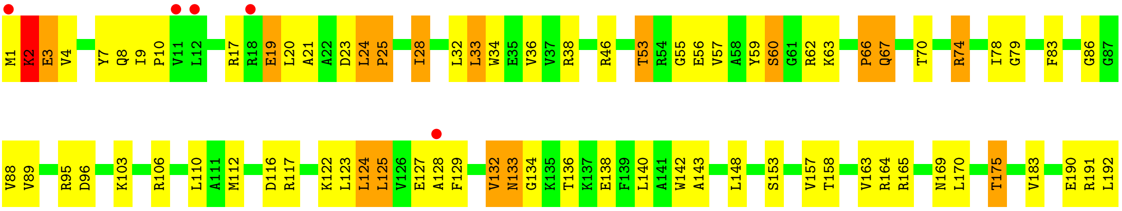
- Molecule 28: 50S ribosomal protein L3

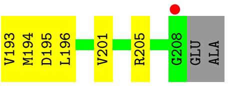
Chain YE:


M1 K2 G3 I4 V7 K8 V9 G10 M11 T12 R13 I14 V23 T24 V25 C31 P32 Q35 R36 R37 T38 P39 E40 K41 D42 G43 Y44 T45 A46 V47 Q48 L49 G50 F51 L52 P53 Q54 R58 V59 N60 R61 P62 L63 K64 G65 H66 F67 A68 K69 A70 G71 V72 E73 P74 V75
R76 I77 L78 R79 E80 I81 R82 D83 F84 E87 G88 D89 T90 V91 T92 V93 E94 I95 F96 K97 E100 R101 T105 R111 A114 G115 V116 M117 K118 R119 W120 S128 H129 G130 K133 I134 N143 R144 K145 T146 P147 K152 G153 K154 K155 H159 Y160 V165
V173 E179 N180 L181 V184 K185 G186 A187 V188 N192 G193 I197 V198 R199 E200 T201 K202 K203 A204 A205 LYS

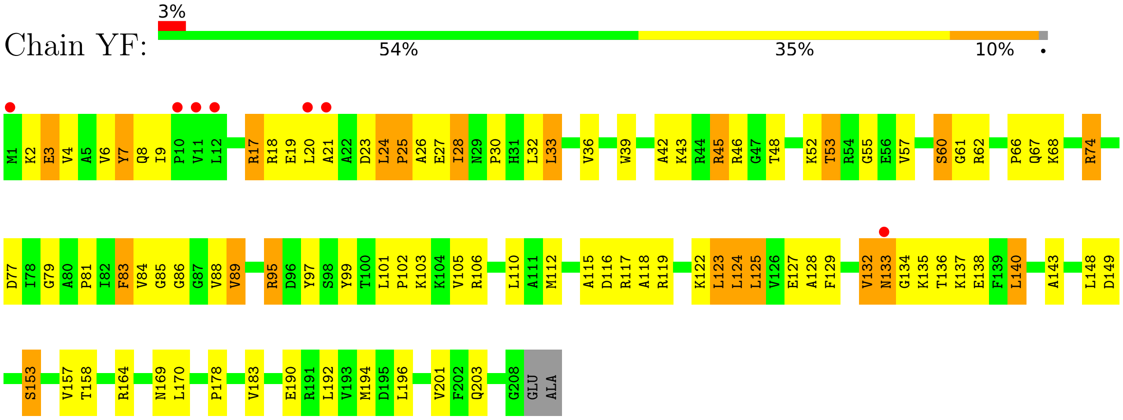
- Molecule 29: 50S ribosomal protein L4

Chain RF:

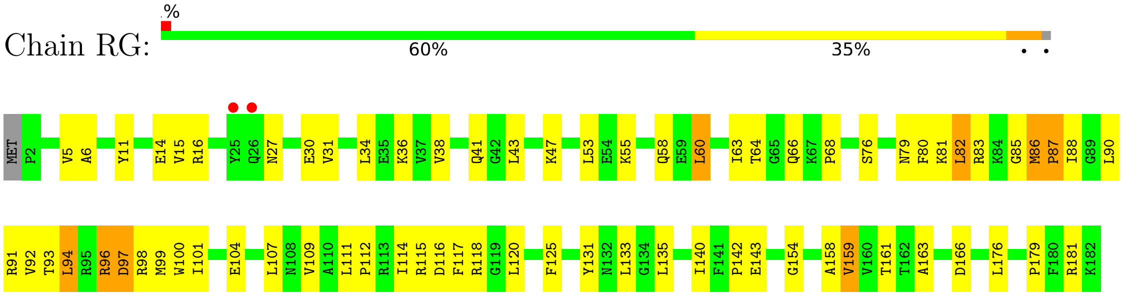

M1 K2 E3 V4 Y7 Q8 I9 P10 V11 L12 R17 R18 E19 L20 A21 A22 D23 L24 P25 I28 L32 L33 W34 E35 V36 V37 R38 R46 T53 R54 G55 E56 V57 A58 Y59 S60 G61 R62 K63 P66 Q67 T70 R74 I78 G79 F83 G86 G87
V88 V89 R95 D96 K103 R106 L110 A111 M112 D116 R117 K122 L123 L124 L125 V126 E127 A128 F129 V132 N133 G134 K135 T136 K137 E138 F139 L140 A141 W142 A143 L148 S153 V157 T158 V163 R164 R165 N169 L170 T175 V183 E190 R191 L192



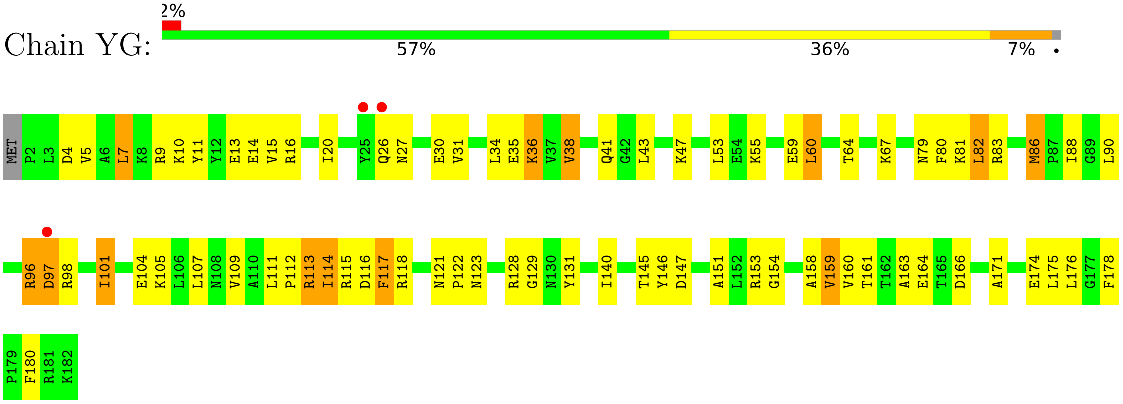
- Molecule 29: 50S ribosomal protein L4



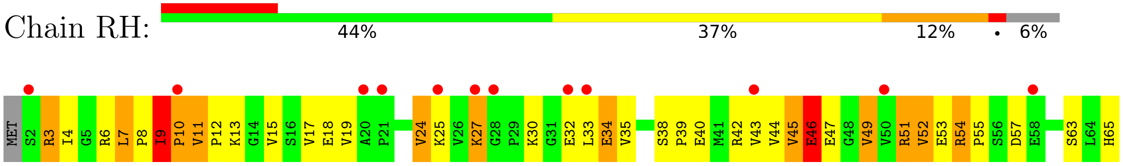
- Molecule 30: 50S ribosomal protein L5

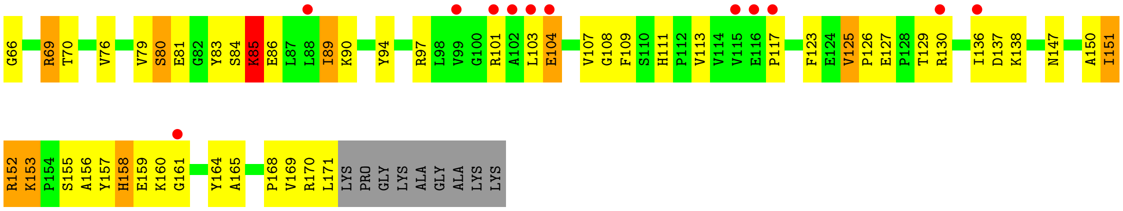


- Molecule 30: 50S ribosomal protein L5



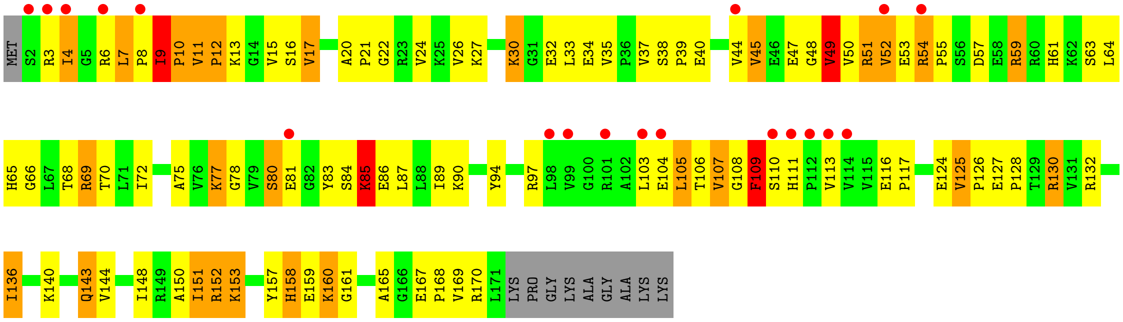
- Molecule 31: 50S ribosomal protein L6





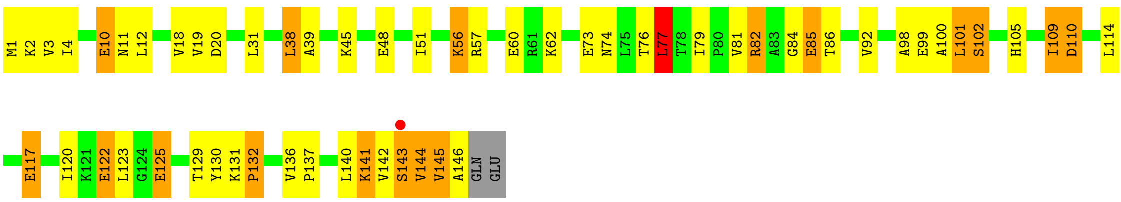
- Molecule 31: 50S ribosomal protein L6

Chain YH:



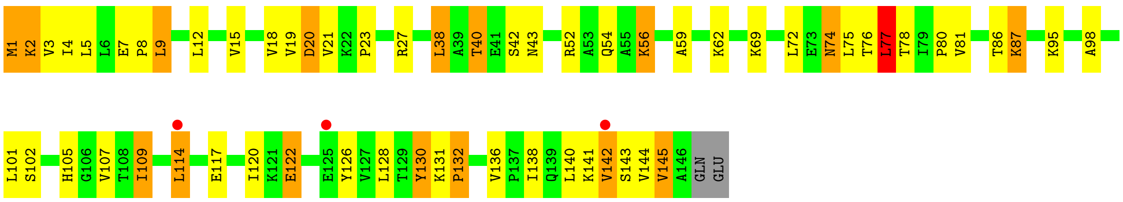
- Molecule 32: 50S ribosomal protein L9

Chain RI:



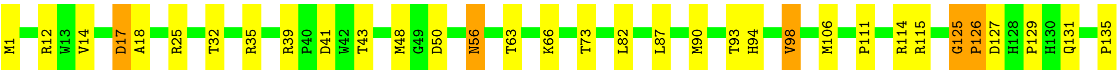
- Molecule 32: 50S ribosomal protein L9

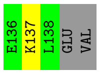
Chain YI:



- Molecule 33: 50S ribosomal protein L13

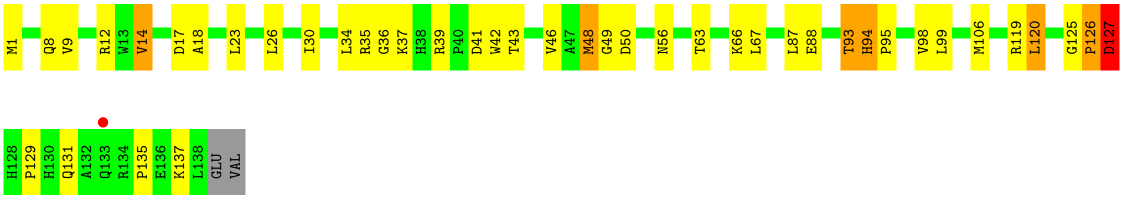
Chain RN:





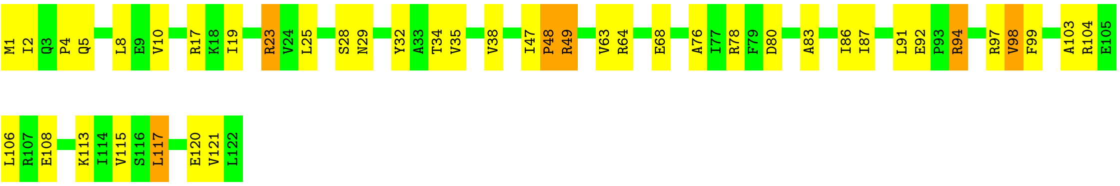
- Molecule 33: 50S ribosomal protein L13

Chain YN:



- Molecule 34: 50S ribosomal protein L14

Chain RO:

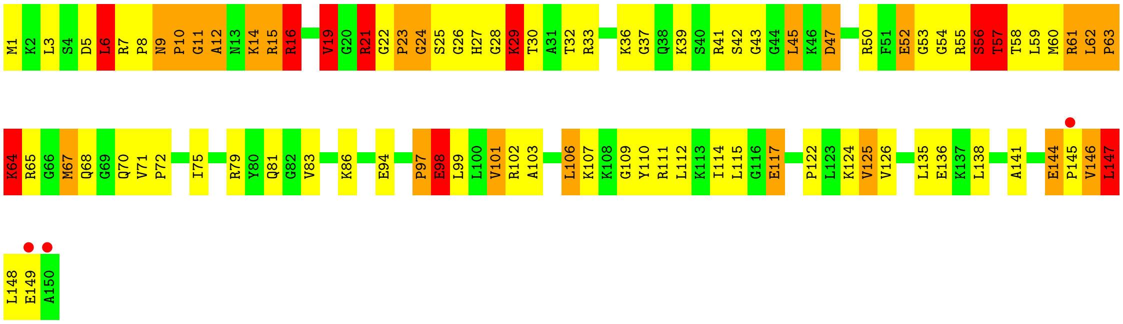


- Molecule 34: 50S ribosomal protein L14

Chain YO:

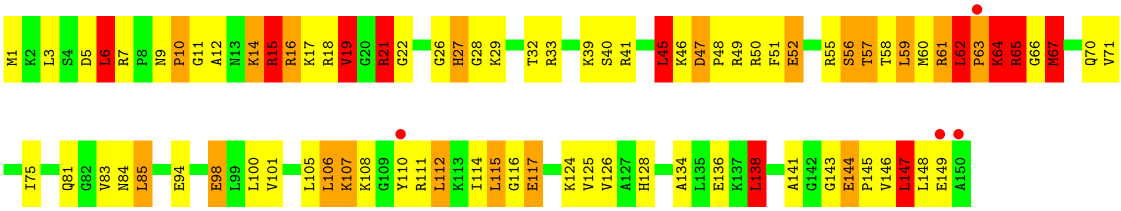
- Molecule 35: 50S ribosomal protein L15

Chain RP:

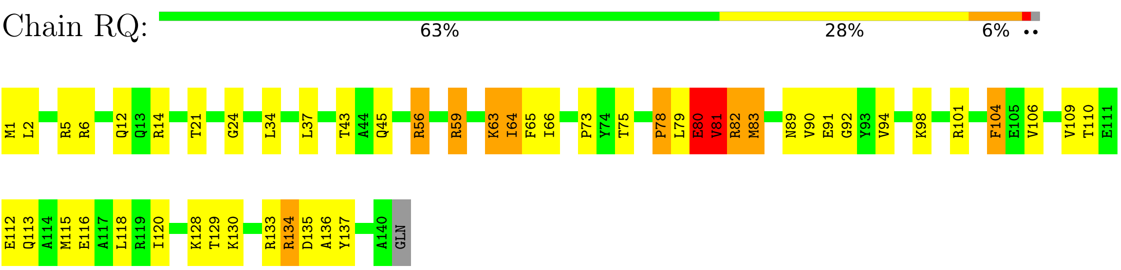


- Molecule 35: 50S ribosomal protein L15

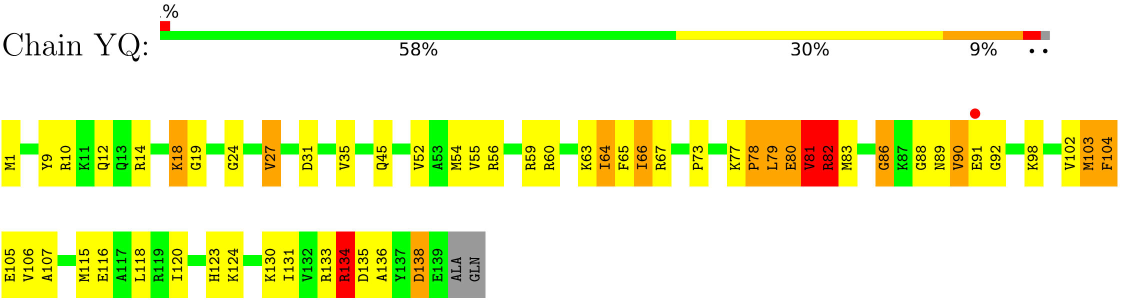
Chain YP:



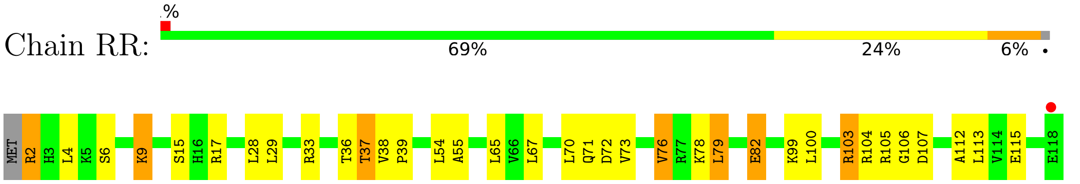
- Molecule 36: 50S ribosomal protein L16



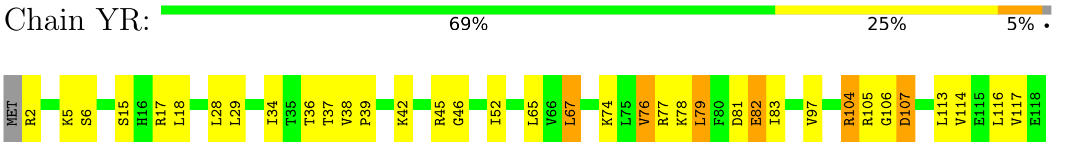
- Molecule 36: 50S ribosomal protein L16



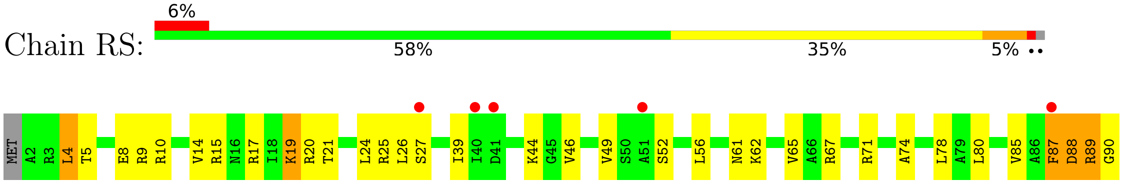
- Molecule 37: 50S ribosomal protein L17

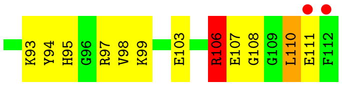


- Molecule 37: 50S ribosomal protein L17



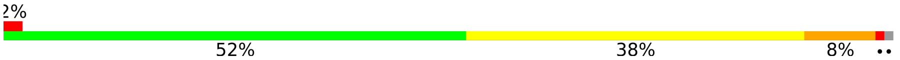
- Molecule 38: 50S ribosomal protein L18

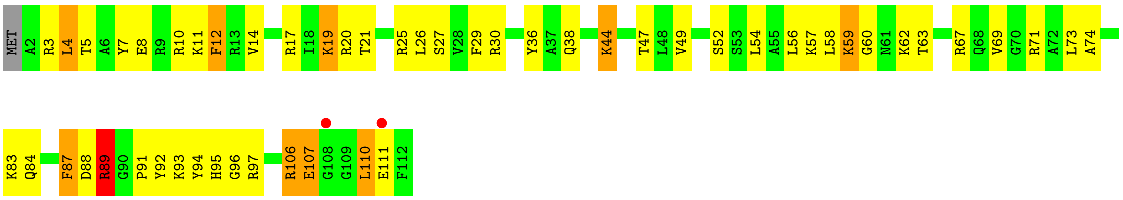




- Molecule 38: 50S ribosomal protein L18

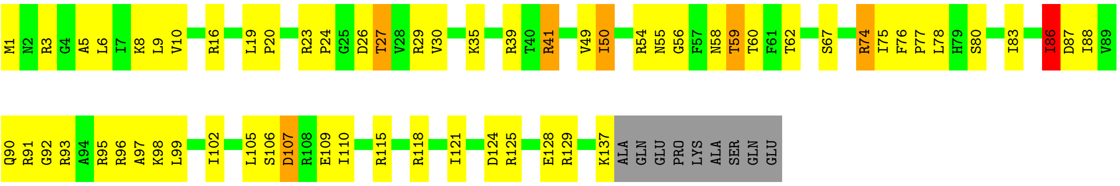
Chain YS:





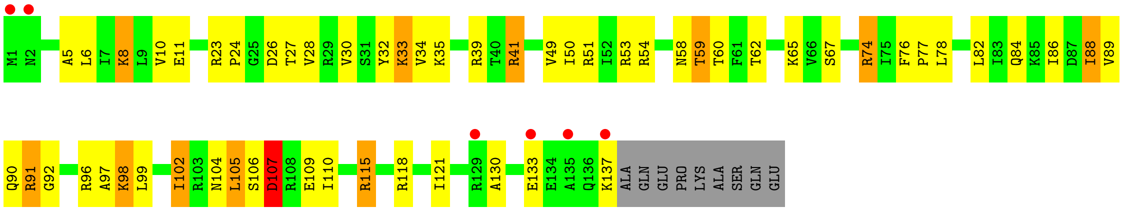
- Molecule 39: 50S ribosomal protein L19

Chain RT:



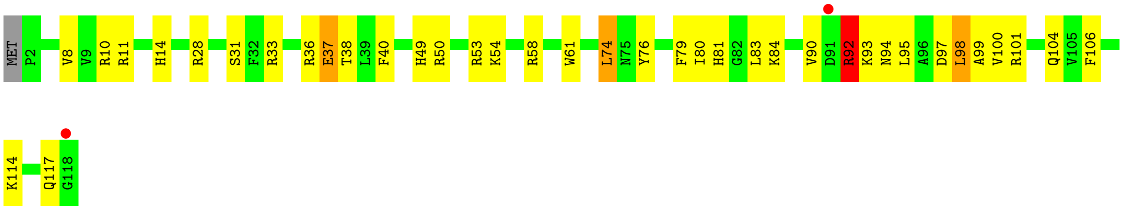
- Molecule 39: 50S ribosomal protein L19

Chain YT:



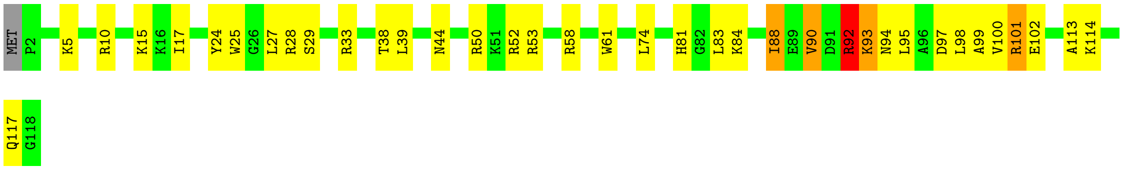
- Molecule 40: 50S ribosomal protein L20

Chain RU:



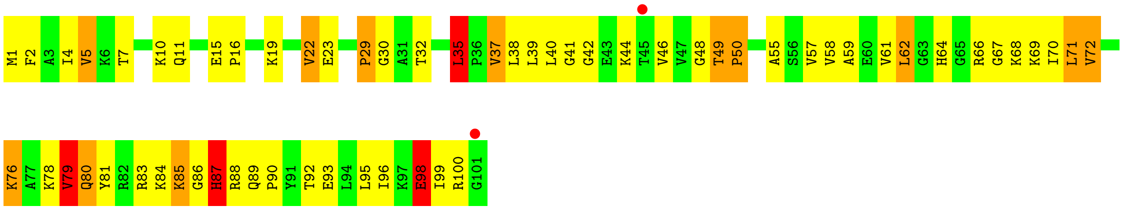
- Molecule 40: 50S ribosomal protein L20

Chain YU:



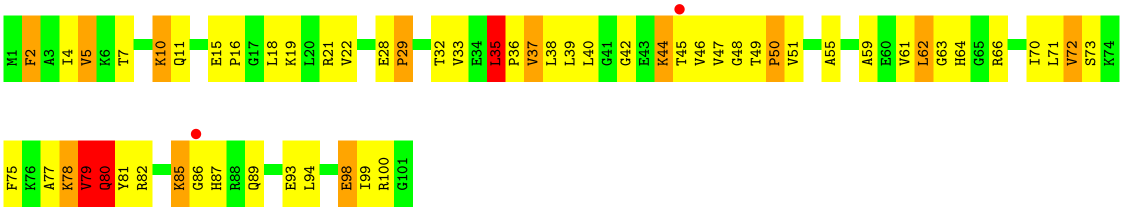
- Molecule 41: 50S ribosomal protein L21

Chain RV:



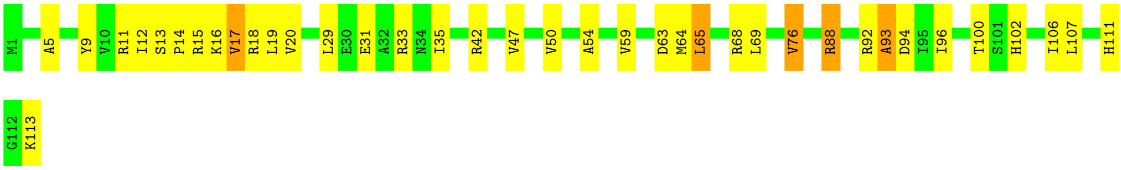
- Molecule 41: 50S ribosomal protein L21

Chain YV:



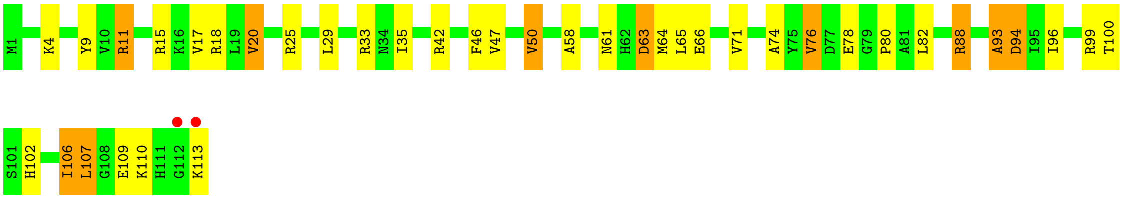
- Molecule 42: 50S ribosomal protein L22

Chain RW:

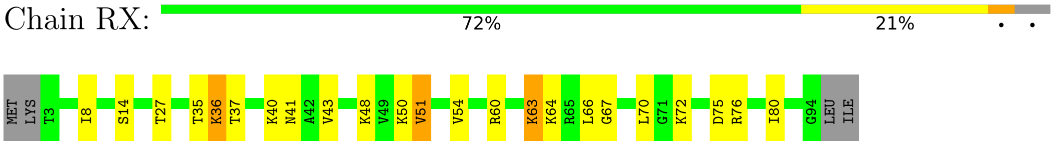


- Molecule 42: 50S ribosomal protein L22

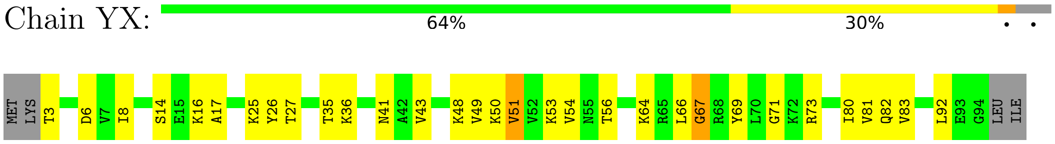
Chain YW:



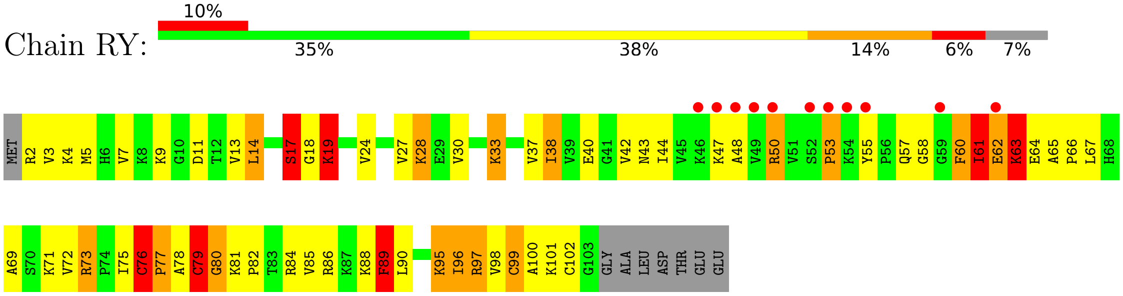
- Molecule 43: 50S ribosomal protein L23



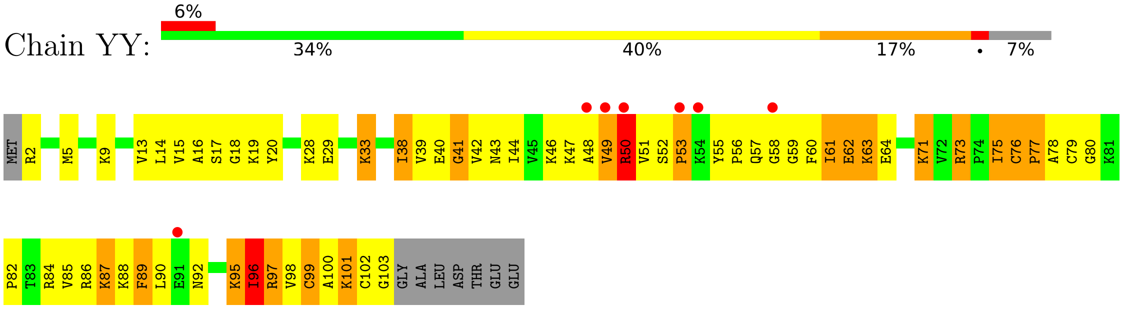
- Molecule 43: 50S ribosomal protein L23



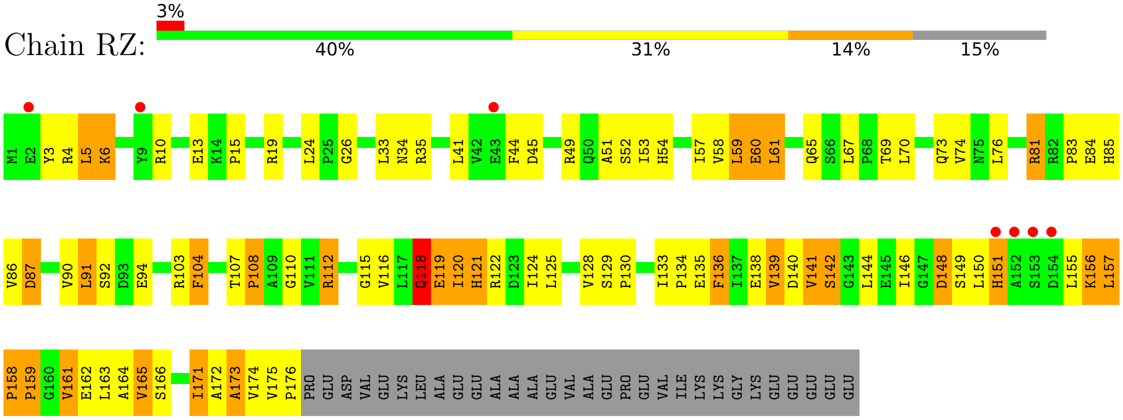
- Molecule 44: 50S ribosomal protein L24



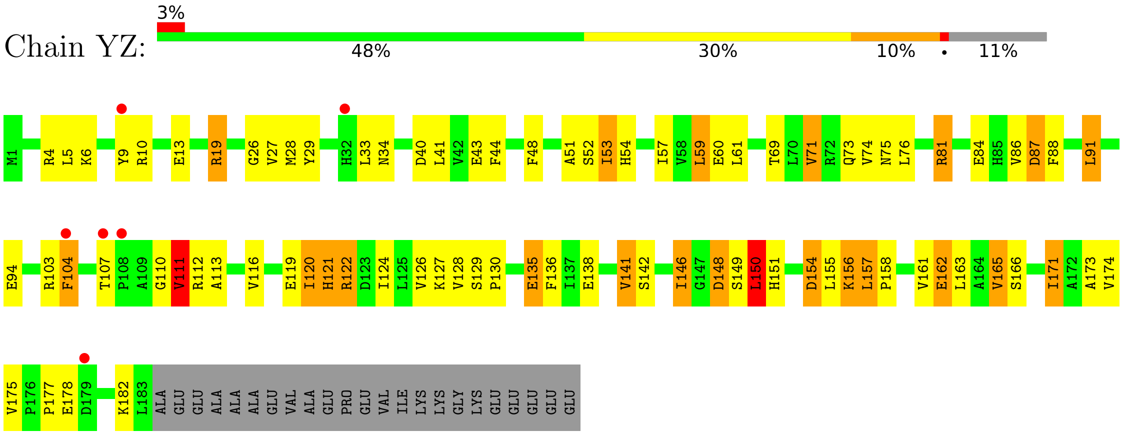
- Molecule 44: 50S ribosomal protein L24



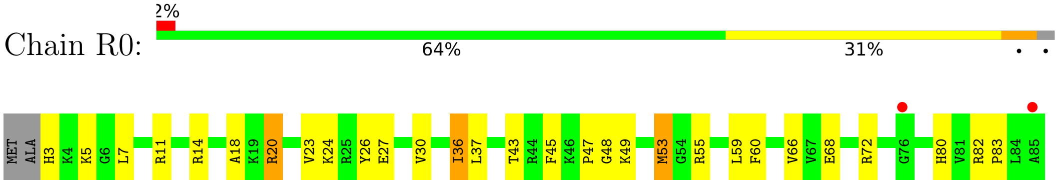
- Molecule 45: 50S ribosomal protein L25



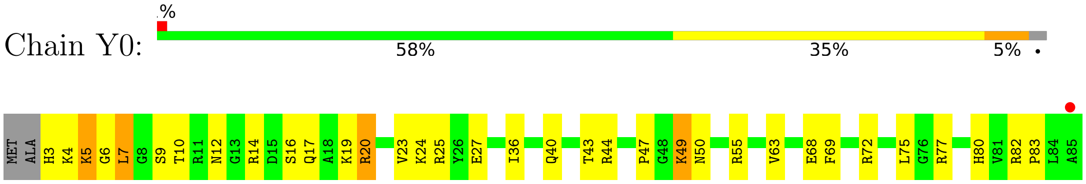
- Molecule 45: 50S ribosomal protein L25



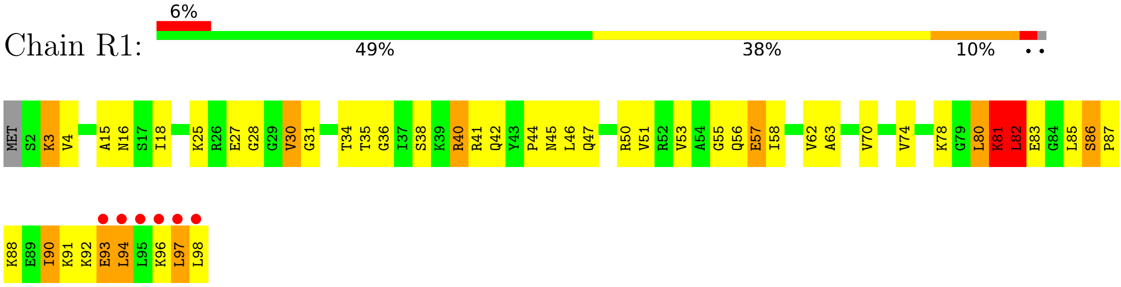
- Molecule 46: 50S ribosomal protein L27



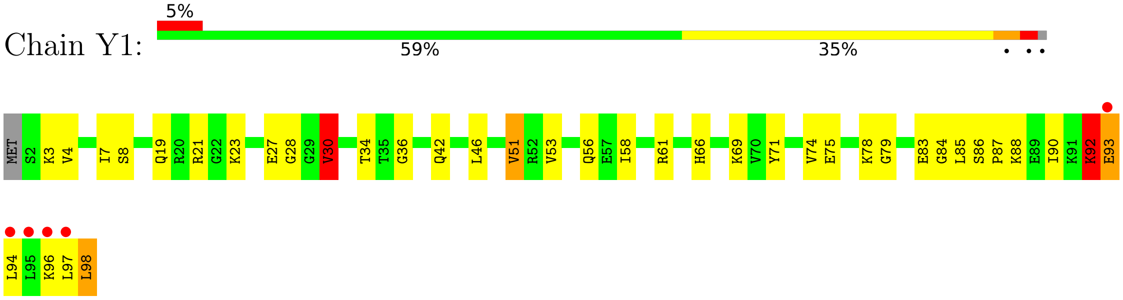
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28

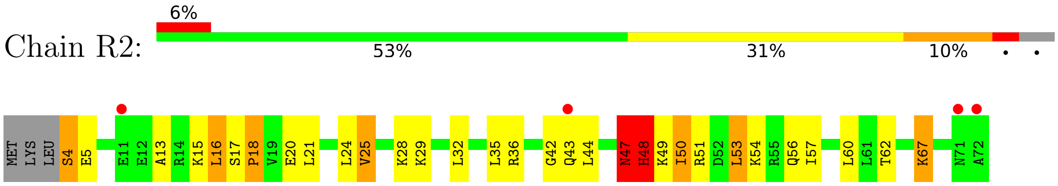


- Molecule 47: 50S ribosomal protein L28



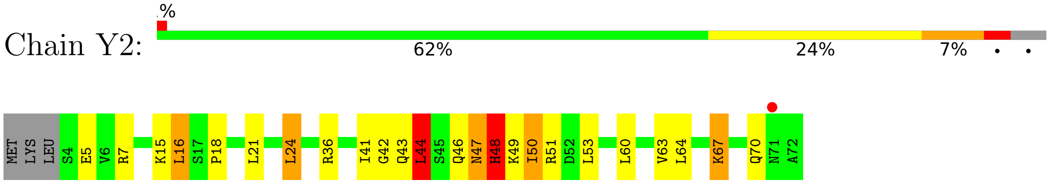
- Molecule 48: 50S ribosomal protein L29

Chain R2:



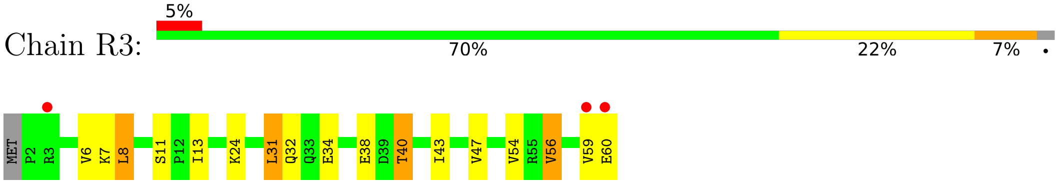
- Molecule 48: 50S ribosomal protein L29

Chain Y2:



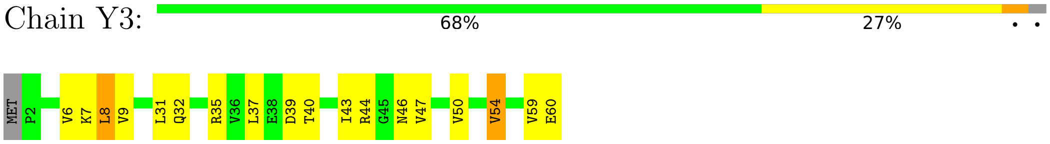
- Molecule 49: 50S ribosomal protein L30

Chain R3:



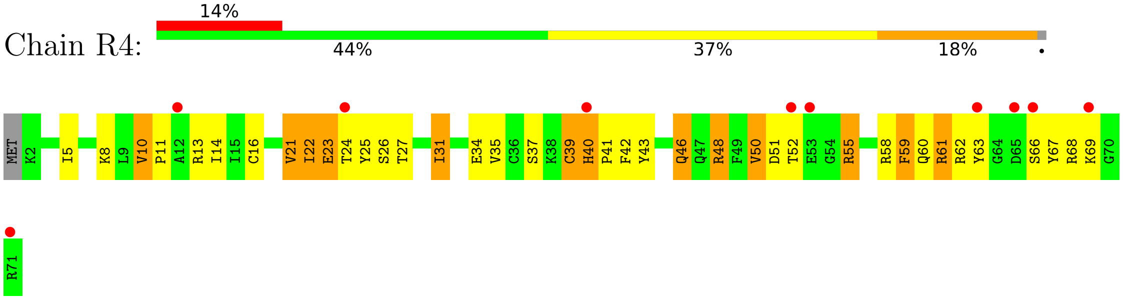
- Molecule 49: 50S ribosomal protein L30

Chain Y3:



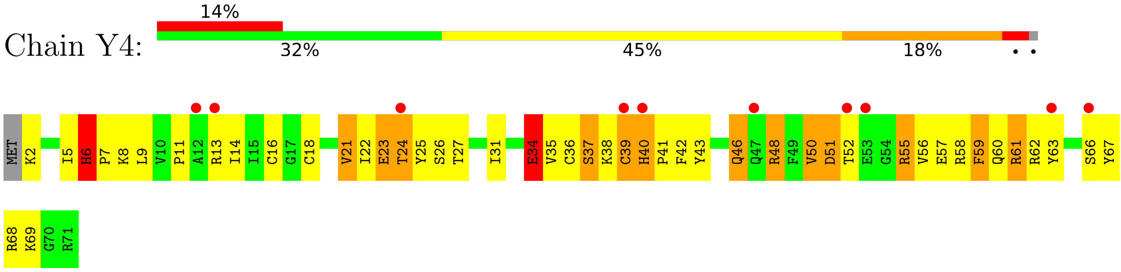
- Molecule 50: 50S ribosomal protein L31

Chain R4:



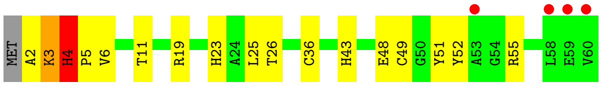
- Molecule 50: 50S ribosomal protein L31

Chain Y4:



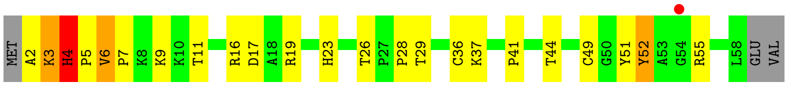
- Molecule 51: 50S ribosomal protein L32

Chain R5:



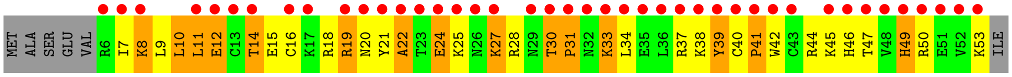
- Molecule 51: 50S ribosomal protein L32

Chain Y5:



- Molecule 52: 50S ribosomal protein L33

Chain R6:

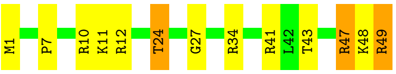


- Molecule 52: 50S ribosomal protein L33

Chain Y6:

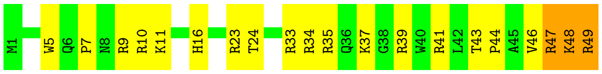
- Molecule 53: 50S ribosomal protein L34

Chain R7:



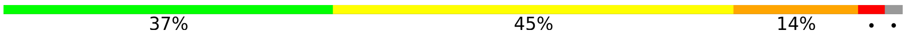
- Molecule 53: 50S ribosomal protein L34

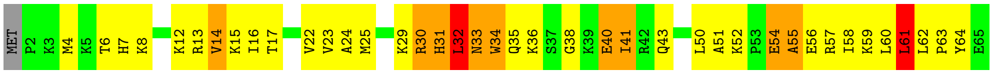
Chain Y7:



- Molecule 54: 50S ribosomal protein L35

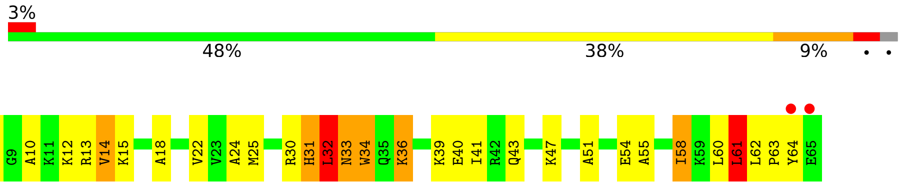
Chain R8:





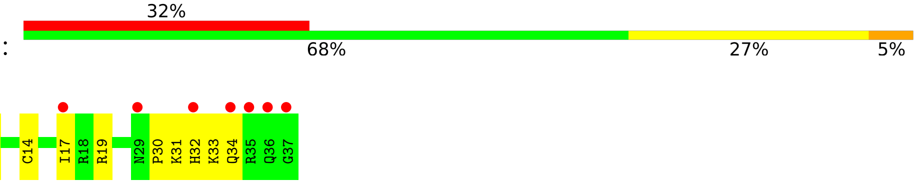
- Molecule 54: 50S ribosomal protein L35

Chain Y8:



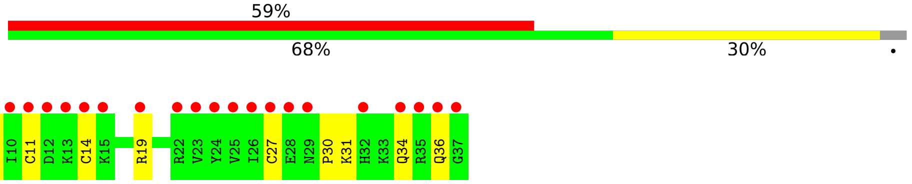
- Molecule 55: 50S ribosomal protein L36

Chain R9:



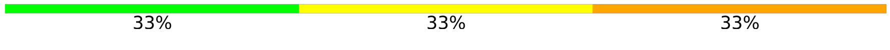
- Molecule 55: 50S ribosomal protein L36

Chain Y9:



- Molecule 56: CC-puromycin

Chain Z6:



- Molecule 56: CC-puromycin

Chain Z7:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	213.45Å 452.92Å 608.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.60 49.92 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.92-3.60) 98.7 (49.92-3.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.234 0.201 , 0.236	Depositor DCC
R_{free} test set	30161 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å^2)	86.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 93.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	294410	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PPU, ZN, A2M

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	0.33	1/36346 (0.0%)	0.82	16/56724 (0.0%)
1	XA	0.35	0/36276	0.83	15/56615 (0.0%)
2	QB	0.25	0/1950	0.49	0/2630
2	XB	0.26	0/1950	0.49	1/2630 (0.0%)
3	QC	0.24	0/1636	0.47	0/2205
3	XC	0.27	0/1636	0.48	0/2205
4	QD	0.28	0/1733	0.50	0/2318
4	XD	0.28	0/1733	0.50	0/2318
5	QE	0.28	0/1195	0.48	0/1609
5	XE	0.29	0/1195	0.48	0/1609
6	QF	0.25	0/856	0.44	0/1154
6	XF	0.28	0/856	0.45	0/1154
7	QG	0.24	0/1276	0.45	0/1709
7	XG	0.27	0/1276	0.46	0/1709
8	QH	0.25	0/1136	0.47	0/1527
8	XH	0.27	0/1136	0.45	0/1527
9	QI	0.24	0/1037	0.48	0/1389
9	XI	0.26	0/1037	0.48	0/1389
10	QJ	0.24	0/814	0.45	0/1095
10	XJ	0.24	0/814	0.46	0/1095
11	QK	0.24	0/916	0.44	0/1234
11	XK	0.28	0/916	0.48	0/1234
12	QL	0.31	0/991	0.52	1/1327 (0.1%)
12	XL	0.36	0/991	0.56	1/1327 (0.1%)
13	QM	0.26	0/947	0.53	1/1270 (0.1%)
13	XM	0.25	0/947	0.53	0/1270
14	QN	0.25	0/501	0.47	0/664
14	XN	0.29	0/501	0.49	0/664
15	QO	0.24	0/745	0.39	0/992
15	XO	0.27	0/745	0.43	0/992
16	QP	0.26	0/721	0.46	0/970
16	XP	0.25	0/721	0.45	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.26	0/847	0.46	0/1131
17	XQ	0.30	0/847	0.47	0/1131
18	QR	0.25	0/590	0.48	0/782
18	XR	0.26	0/590	0.52	0/782
19	QS	0.27	0/670	0.53	0/901
19	XS	0.29	0/670	0.52	0/901
20	QT	0.25	0/765	0.49	1/1007 (0.1%)
20	XT	0.25	0/765	0.48	0/1007
21	QU	0.23	0/221	0.47	0/288
21	XU	0.24	0/221	0.45	0/288
22	QV	0.34	0/1832	0.83	0/2855
22	XV	0.35	0/1832	0.81	0/2855
23	QX	0.70	0/417	1.26	3/649 (0.5%)
23	XX	0.62	0/417	1.24	0/649
24	QY	0.26	0/773	0.40	0/1043
24	XY	0.26	0/773	0.41	0/1043
25	RA	0.41	0/69742	0.89	17/108874 (0.0%)
25	YA	0.44	1/69356 (0.0%)	0.91	31/108271 (0.0%)
26	RB	0.31	0/2928	0.82	0/4568
26	YB	0.34	0/2928	0.85	0/4568
27	RD	0.34	0/2165	0.56	0/2919
27	YD	0.37	0/2165	0.60	0/2919
28	RE	0.30	0/1601	0.55	0/2160
28	YE	0.34	0/1601	0.58	0/2160
29	RF	0.35	0/1662	0.58	0/2249
29	YF	0.31	0/1662	0.57	0/2249
30	RG	0.25	0/1499	0.47	0/2016
30	YG	0.26	0/1499	0.46	0/2016
31	RH	0.25	0/1332	0.60	1/1802 (0.1%)
31	YH	0.27	0/1332	0.61	1/1802 (0.1%)
32	RI	0.24	0/1151	0.54	0/1558
32	YI	0.28	0/1151	0.58	0/1558
33	RN	0.28	0/1131	0.50	0/1525
33	YN	0.29	0/1131	0.50	0/1525
34	RO	0.32	0/943	0.51	0/1269
34	YO	0.33	0/943	0.53	0/1269
35	RP	0.34	0/1162	0.66	0/1544
35	YP	0.35	0/1162	0.68	2/1544 (0.1%)
36	RQ	0.36	0/1133	0.58	0/1515
36	YQ	0.35	0/1128	0.58	1/1508 (0.1%)
37	RR	0.27	0/974	0.51	0/1302
37	YR	0.30	0/974	0.53	0/1302
38	RS	0.25	0/892	0.49	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YS	0.29	0/892	0.54	0/1187
39	RT	0.27	0/1155	0.46	0/1542
39	YT	0.30	0/1155	0.47	0/1542
40	RU	0.32	0/982	0.53	0/1306
40	YU	0.33	0/982	0.52	0/1306
41	RV	0.38	0/790	0.69	1/1057 (0.1%)
41	YV	0.35	0/790	0.67	1/1057 (0.1%)
42	RW	0.30	0/911	0.51	0/1220
42	YW	0.30	0/911	0.52	0/1220
43	RX	0.32	0/739	0.51	0/993
43	YX	0.35	0/739	0.52	0/993
44	RY	0.33	0/798	0.59	0/1064
44	YY	0.32	0/798	0.59	0/1064
45	RZ	0.29	0/1435	0.57	0/1947
45	YZ	0.30	0/1493	0.60	0/2026
46	R0	0.32	0/666	0.52	0/885
46	Y0	0.32	0/666	0.58	0/885
47	R1	0.31	0/770	0.57	0/1022
47	Y1	0.36	0/770	0.59	0/1022
48	R2	0.28	0/583	0.57	0/771
48	Y2	0.33	0/583	0.59	1/771 (0.1%)
49	R3	0.29	0/474	0.44	0/635
49	Y3	0.28	0/474	0.47	0/635
50	R4	0.24	0/586	0.46	0/785
50	Y4	0.30	0/586	0.51	0/785
51	R5	0.30	0/473	0.58	1/639 (0.2%)
51	Y5	0.50	1/456 (0.2%)	0.71	2/617 (0.3%)
52	R6	0.29	0/424	0.67	0/565
52	Y6	0.44	0/424	0.82	0/565
53	R7	0.33	0/438	0.49	0/575
53	Y7	0.34	0/438	0.53	0/575
54	R8	0.42	0/525	0.75	0/691
54	Y8	0.38	0/525	0.66	0/691
55	R9	0.26	0/310	0.42	0/407
55	Y9	0.24	0/302	0.42	0/397
56	Z6	0.54	0/40	0.56	0/60
56	Z7	0.31	0/40	0.59	0/60
All	All	0.37	3/318230 (0.0%)	0.79	98/475578 (0.0%)

All (3) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	QA	1336	C	C3'-C2'	5.34	1.58	1.52
25	YA	1762	A	O3'-P	-5.30	1.54	1.61
51	Y5	7	PRO	N-CD	5.29	1.55	1.47

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	XL	24	VAL	C-N-CD	6.00	140.99	128.40
51	Y5	4	HIS	C-N-CD	6.00	140.99	128.40
25	YA	2655	G	O4'-C1'-N9	5.98	112.98	108.20
25	YA	1313	U	C2-N1-C1'	5.98	124.87	117.70
1	QA	328	C	P-O3'-C3'	5.94	126.83	119.70

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	32472	0	16393	434	0
1	XA	32409	0	16361	385	0
2	QB	1915	0	1969	55	0
2	XB	1915	0	1969	60	0
3	QC	1612	0	1677	51	0
3	XC	1612	0	1677	40	0
4	QD	1703	0	1765	43	0
4	XD	1703	0	1765	36	0
5	QE	1178	0	1233	31	0
5	XE	1178	0	1234	22	0
6	QF	843	0	857	19	0
6	XF	843	0	857	21	0
7	QG	1257	0	1296	22	0
7	XG	1257	0	1296	31	0
8	QH	1116	0	1177	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	XH	1116	0	1177	26	0
9	QI	1018	0	1049	55	0
9	XI	1018	0	1049	41	0
10	QJ	801	0	849	36	0
10	XJ	801	0	849	44	0
11	QK	901	0	926	26	0
11	XK	901	0	926	20	0
12	QL	975	0	1062	28	0
12	XL	975	0	1062	21	0
13	QM	937	0	994	37	0
13	XM	937	0	994	56	0
14	QN	492	0	530	17	0
14	XN	492	0	528	12	0
15	QO	734	0	771	14	0
15	XO	734	0	771	14	0
16	QP	705	0	725	15	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	13	0
17	XQ	834	0	904	18	0
18	QR	585	0	657	10	0
18	XR	585	0	657	19	0
19	QS	656	0	678	44	0
19	XS	656	0	678	36	0
20	QT	763	0	861	21	0
20	XT	763	0	861	27	0
21	QU	217	0	234	11	0
21	XU	217	0	234	15	0
22	QV	1640	0	837	8	0
22	XV	1640	0	837	6	0
23	QX	440	9	224	25	0
23	XX	440	9	224	18	0
24	QY	756	0	749	46	0
24	XY	756	0	749	39	0
25	RA	62269	0	31392	699	0
25	YA	61924	0	31215	651	0
26	RB	2617	0	1328	27	0
26	YB	2617	0	1328	34	0
27	RD	2115	0	2195	65	0
27	YD	2115	0	2195	78	0
28	RE	1568	0	1634	101	0
28	YE	1568	0	1634	77	0
29	RF	1627	0	1680	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	YF	1627	0	1680	65	0
30	RG	1474	0	1535	44	0
30	YG	1474	0	1535	47	0
31	RH	1307	0	1382	91	0
31	YH	1307	0	1381	83	0
32	RI	1136	0	1223	53	0
32	YI	1136	0	1223	71	0
33	RN	1104	0	1180	14	0
33	YN	1104	0	1180	22	0
34	RO	933	0	996	29	0
34	YO	933	0	996	24	0
35	RP	1145	0	1228	127	0
35	YP	1145	0	1228	125	0
36	RQ	1112	0	1170	35	0
36	YQ	1107	0	1166	37	0
37	RR	960	0	1021	15	0
37	YR	960	0	1021	21	0
38	RS	882	0	943	29	0
38	YS	882	0	943	35	0
39	RT	1141	0	1202	43	0
39	YT	1141	0	1202	38	0
40	RU	964	0	1022	38	0
40	YU	964	0	1022	34	0
41	RV	779	0	852	60	0
41	YV	779	0	852	54	0
42	RW	900	0	964	22	0
42	YW	900	0	964	23	0
43	RX	725	0	778	16	0
43	YX	725	0	778	19	0
44	RY	785	0	877	67	0
44	YY	785	0	878	47	0
45	RZ	1404	0	1437	92	0
45	YZ	1461	0	1493	47	0
46	R0	657	0	683	23	0
46	Y0	657	0	683	25	0
47	R1	763	0	848	32	0
47	Y1	763	0	848	22	0
48	R2	581	0	629	17	0
48	Y2	581	0	629	15	0
49	R3	469	0	518	9	0
49	Y3	469	0	518	8	0
50	R4	573	0	565	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	Y4	573	0	565	40	0
51	R5	459	0	480	9	0
51	Y5	442	0	465	16	0
52	R6	417	0	441	25	0
52	Y6	417	0	441	51	0
53	R7	430	0	480	7	0
53	Y7	430	0	480	12	0
54	R8	517	0	582	50	0
54	Y8	517	0	582	68	0
55	R9	307	0	338	10	0
55	Y9	299	0	326	7	0
56	Z6	74	0	51	6	0
56	Z7	74	0	51	23	0
57	QA	147	0	0	0	0
57	QD	1	0	0	0	0
57	QE	1	0	0	0	0
57	QL	1	0	0	0	0
57	QV	5	0	0	0	0
57	R0	3	0	0	0	0
57	R2	1	0	0	0	0
57	R5	3	0	0	0	0
57	RA	431	0	0	0	0
57	RB	5	0	0	0	0
57	RD	2	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	2	0	0	0	0
57	RR	1	0	0	0	0
57	RY	2	0	0	0	0
57	XA	161	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XN	1	0	0	0	0
57	XV	4	0	0	0	0
57	Y0	3	0	0	0	0
57	Y1	1	0	0	0	0
57	Y5	3	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	473	0	0	0	0
57	YB	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YD	1	0	0	0	0
57	YE	1	0	0	0	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YH	2	0	0	0	0
57	YN	1	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	2	0	0	0	0
57	YR	1	0	0	0	0
57	YU	1	0	0	0	0
57	YV	1	0	0	0	0
57	YY	1	0	0	0	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
All	All	294392	18	199957	5185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5185 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)
41:YV:49:THR:CG2	41:YV:50:PRO:HD3	1.35	1.52
31:RH:9:ILE:CG2	31:RH:10:PRO:HA	1.36	1.51
31:YH:9:ILE:CG2	31:YH:10:PRO:HA	1.39	1.47
50:Y4:6:HIS:HB2	50:Y4:7:PRO:CD	1.43	1.47
41:RV:49:THR:CG2	41:RV:50:PRO:HD3	1.48	1.42

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	234/256 (91%)	186 (80%)	29 (12%)	19 (8%)	1	11
2	XB	234/256 (91%)	189 (81%)	27 (12%)	18 (8%)	1	12
3	QC	204/239 (85%)	161 (79%)	27 (13%)	16 (8%)	1	11
3	XC	204/239 (85%)	160 (78%)	32 (16%)	12 (6%)	1	18
4	QD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	2	19
4	XD	206/209 (99%)	168 (82%)	22 (11%)	16 (8%)	1	11
5	QE	152/162 (94%)	135 (89%)	12 (8%)	5 (3%)	4	31
5	XE	152/162 (94%)	137 (90%)	9 (6%)	6 (4%)	3	27
6	QF	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
6	XF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	QG	153/156 (98%)	136 (89%)	13 (8%)	4 (3%)	5	35
7	XG	153/156 (98%)	134 (88%)	15 (10%)	4 (3%)	5	35
8	QH	136/138 (99%)	126 (93%)	7 (5%)	3 (2%)	6	39
8	XH	136/138 (99%)	123 (90%)	10 (7%)	3 (2%)	6	39
9	QI	126/128 (98%)	94 (75%)	24 (19%)	8 (6%)	1	17
9	XI	126/128 (98%)	96 (76%)	23 (18%)	7 (6%)	2	19
10	QJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	3	26
10	XJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	2	20
11	QK	119/129 (92%)	102 (86%)	13 (11%)	4 (3%)	3	31
11	XK	119/129 (92%)	105 (88%)	10 (8%)	4 (3%)	3	31
12	QL	123/132 (93%)	99 (80%)	16 (13%)	8 (6%)	1	16
12	XL	123/132 (93%)	97 (79%)	18 (15%)	8 (6%)	1	16
13	QM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	8
13	XM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	8
14	QN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	20
14	XN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	20
15	QO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	XO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	QP	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
16	XP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	QQ	98/105 (93%)	90 (92%)	7 (7%)	1 (1%)	15	55
17	XQ	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	7	41
18	QR	69/88 (78%)	61 (88%)	8 (12%)	0	100	100
18	XR	69/88 (78%)	62 (90%)	6 (9%)	1 (1%)	11	48
19	QS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	5
19	XS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	5
20	QT	97/106 (92%)	79 (81%)	15 (16%)	3 (3%)	4	32
20	XT	97/106 (92%)	80 (82%)	14 (14%)	3 (3%)	4	32
21	QU	23/25 (92%)	16 (70%)	6 (26%)	1 (4%)	2	24
21	XU	23/25 (92%)	18 (78%)	3 (13%)	2 (9%)	1	9
24	QY	90/118 (76%)	84 (93%)	5 (6%)	1 (1%)	14	53
24	XY	90/118 (76%)	80 (89%)	8 (9%)	2 (2%)	6	39
27	RD	270/276 (98%)	224 (83%)	38 (14%)	8 (3%)	4	33
27	YD	270/276 (98%)	228 (84%)	32 (12%)	10 (4%)	3	28
28	RE	203/206 (98%)	137 (68%)	38 (19%)	28 (14%)	0	4
28	YE	203/206 (98%)	133 (66%)	40 (20%)	30 (15%)	0	3
29	RF	206/210 (98%)	167 (81%)	26 (13%)	13 (6%)	1	17
29	YF	206/210 (98%)	168 (82%)	22 (11%)	16 (8%)	1	11
30	RG	179/182 (98%)	141 (79%)	26 (14%)	12 (7%)	1	15
30	YG	179/182 (98%)	146 (82%)	22 (12%)	11 (6%)	1	17
31	RH	168/180 (93%)	104 (62%)	37 (22%)	27 (16%)	0	3
31	YH	168/180 (93%)	98 (58%)	42 (25%)	28 (17%)	0	3
32	RI	144/148 (97%)	109 (76%)	28 (19%)	7 (5%)	2	21
32	YI	144/148 (97%)	116 (81%)	24 (17%)	4 (3%)	5	34
33	RN	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	2	20
33	YN	136/140 (97%)	110 (81%)	19 (14%)	7 (5%)	2	20
34	RO	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	59
34	YO	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	19	59
35	RP	148/150 (99%)	97 (66%)	23 (16%)	28 (19%)	0	2
35	YP	148/150 (99%)	102 (69%)	22 (15%)	24 (16%)	0	3
36	RQ	138/141 (98%)	110 (80%)	17 (12%)	11 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	YQ	137/141 (97%)	111 (81%)	15 (11%)	11 (8%)	1	11
37	RR	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	30
37	YR	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	5	35
38	RS	109/112 (97%)	84 (77%)	17 (16%)	8 (7%)	1	13
38	YS	109/112 (97%)	85 (78%)	13 (12%)	11 (10%)	0	7
39	RT	135/146 (92%)	109 (81%)	24 (18%)	2 (2%)	10	47
39	YT	135/146 (92%)	113 (84%)	17 (13%)	5 (4%)	3	28
40	RU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	9	45
40	YU	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	5	35
41	RV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	3
41	YV	99/101 (98%)	71 (72%)	15 (15%)	13 (13%)	0	4
42	RW	111/113 (98%)	107 (96%)	1 (1%)	3 (3%)	5	35
42	YW	111/113 (98%)	104 (94%)	3 (3%)	4 (4%)	3	29
43	RX	90/96 (94%)	76 (84%)	12 (13%)	2 (2%)	6	39
43	YX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	39
44	RY	100/110 (91%)	56 (56%)	28 (28%)	16 (16%)	0	3
44	YY	100/110 (91%)	57 (57%)	27 (27%)	16 (16%)	0	3
45	RZ	174/206 (84%)	116 (67%)	33 (19%)	25 (14%)	0	4
45	YZ	181/206 (88%)	122 (67%)	42 (23%)	17 (9%)	0	8
46	R0	81/85 (95%)	73 (90%)	5 (6%)	3 (4%)	3	28
46	Y0	81/85 (95%)	67 (83%)	11 (14%)	3 (4%)	3	28
47	R1	95/98 (97%)	71 (75%)	12 (13%)	12 (13%)	0	5
47	Y1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	17
48	R2	67/72 (93%)	54 (81%)	8 (12%)	5 (8%)	1	12
48	Y2	67/72 (93%)	56 (84%)	5 (8%)	6 (9%)	1	9
49	R3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
49	Y3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
50	R4	68/71 (96%)	43 (63%)	12 (18%)	13 (19%)	0	2
50	Y4	68/71 (96%)	38 (56%)	15 (22%)	15 (22%)	0	1
51	R5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	30
51	Y5	55/60 (92%)	48 (87%)	4 (7%)	3 (6%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	R6	46/54 (85%)	22 (48%)	15 (33%)	9 (20%)	0	2
52	Y6	46/54 (85%)	16 (35%)	16 (35%)	14 (30%)	0	0
53	R7	47/49 (96%)	47 (100%)	0	0	100	100
53	Y7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
54	R8	62/65 (95%)	48 (77%)	7 (11%)	7 (11%)	0	6
54	Y8	62/65 (95%)	49 (79%)	6 (10%)	7 (11%)	0	6
55	R9	35/37 (95%)	34 (97%)	0	1 (3%)	4	33
55	Y9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11649/12360 (94%)	9390 (81%)	1489 (13%)	770 (7%)	1	16

5 of 770 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	29	ALA
2	QB	165	VAL
2	QB	195	ASP
2	QB	238	LEU
3	QC	64	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	204/220 (93%)	173 (85%)	31 (15%)	3	19
2	XB	204/220 (93%)	176 (86%)	28 (14%)	3	22
3	QC	160/188 (85%)	142 (89%)	18 (11%)	6	30
3	XC	160/188 (85%)	141 (88%)	19 (12%)	5	27
4	QD	180/181 (99%)	157 (87%)	23 (13%)	4	24
4	XD	180/181 (99%)	156 (87%)	24 (13%)	4	23
5	QE	119/123 (97%)	101 (85%)	18 (15%)	3	19
5	XE	119/123 (97%)	106 (89%)	13 (11%)	6	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	QF	90/90 (100%)	85 (94%)	5 (6%)	21	56
6	XF	90/90 (100%)	77 (86%)	13 (14%)	3	20
7	QG	126/127 (99%)	112 (89%)	14 (11%)	6	31
7	XG	126/127 (99%)	109 (86%)	17 (14%)	4	23
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11	42
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	32
9	QI	99/99 (100%)	79 (80%)	20 (20%)	1	8
9	XI	99/99 (100%)	80 (81%)	19 (19%)	1	9
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	23
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	2	17
11	QK	92/99 (93%)	82 (89%)	10 (11%)	6	32
11	XK	92/99 (93%)	83 (90%)	9 (10%)	8	36
12	QL	104/109 (95%)	89 (86%)	15 (14%)	3	20
12	XL	104/109 (95%)	87 (84%)	17 (16%)	2	15
13	QM	94/101 (93%)	80 (85%)	14 (15%)	3	19
13	XM	94/101 (93%)	82 (87%)	12 (13%)	4	24
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	79
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	34
15	QO	79/80 (99%)	74 (94%)	5 (6%)	18	53
15	XO	79/80 (99%)	74 (94%)	5 (6%)	18	53
16	QP	72/74 (97%)	64 (89%)	8 (11%)	6	31
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6	31
17	QQ	95/97 (98%)	90 (95%)	5 (5%)	22	58
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	46
18	QR	62/77 (80%)	56 (90%)	6 (10%)	8	36
18	XR	62/77 (80%)	54 (87%)	8 (13%)	4	24
19	QS	71/80 (89%)	54 (76%)	17 (24%)	0	4
19	XS	71/80 (89%)	58 (82%)	13 (18%)	1	10
20	QT	76/82 (93%)	62 (82%)	14 (18%)	1	10
20	XT	76/82 (93%)	66 (87%)	10 (13%)	4	23
21	QU	20/20 (100%)	18 (90%)	2 (10%)	7	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	XU	20/20 (100%)	18 (90%)	2 (10%)	7	35
24	QY	79/103 (77%)	73 (92%)	6 (8%)	13	45
24	XY	79/103 (77%)	74 (94%)	5 (6%)	18	53
27	RD	214/218 (98%)	178 (83%)	36 (17%)	2	14
27	YD	214/218 (98%)	179 (84%)	35 (16%)	2	15
28	RE	165/166 (99%)	137 (83%)	28 (17%)	2	14
28	YE	165/166 (99%)	138 (84%)	27 (16%)	2	15
29	RF	165/166 (99%)	139 (84%)	26 (16%)	2	17
29	YF	165/166 (99%)	141 (86%)	24 (14%)	3	20
30	RG	155/156 (99%)	147 (95%)	8 (5%)	23	58
30	YG	155/156 (99%)	138 (89%)	17 (11%)	6	31
31	RH	142/148 (96%)	123 (87%)	19 (13%)	4	23
31	YH	142/148 (96%)	115 (81%)	27 (19%)	1	9
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1	8
32	YI	122/124 (98%)	99 (81%)	23 (19%)	1	9
33	RN	117/119 (98%)	107 (92%)	10 (8%)	10	41
33	YN	117/119 (98%)	104 (89%)	13 (11%)	6	31
34	RO	100/100 (100%)	91 (91%)	9 (9%)	9	39
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	35
35	RP	116/116 (100%)	80 (69%)	36 (31%)	0	2
35	YP	116/116 (100%)	84 (72%)	32 (28%)	0	3
36	RQ	110/111 (99%)	93 (84%)	17 (16%)	2	18
36	YQ	110/111 (99%)	93 (84%)	17 (16%)	2	18
37	RR	100/101 (99%)	82 (82%)	18 (18%)	1	11
37	YR	100/101 (99%)	87 (87%)	13 (13%)	4	24
38	RS	87/88 (99%)	80 (92%)	7 (8%)	12	43
38	YS	87/88 (99%)	73 (84%)	14 (16%)	2	16
39	RT	120/127 (94%)	100 (83%)	20 (17%)	2	14
39	YT	120/127 (94%)	98 (82%)	22 (18%)	1	10
40	RU	93/94 (99%)	85 (91%)	8 (9%)	10	41
40	YU	93/94 (99%)	85 (91%)	8 (9%)	10	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	9
41	YV	82/82 (100%)	63 (77%)	19 (23%)	1	5
42	RW	92/92 (100%)	82 (89%)	10 (11%)	6	32
42	YW	92/92 (100%)	79 (86%)	13 (14%)	3	21
43	RX	74/78 (95%)	65 (88%)	9 (12%)	5	26
43	YX	74/78 (95%)	68 (92%)	6 (8%)	11	43
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	4
44	YY	85/91 (93%)	61 (72%)	24 (28%)	0	3
45	RZ	155/179 (87%)	129 (83%)	26 (17%)	2	14
45	YZ	162/179 (90%)	134 (83%)	28 (17%)	2	12
46	R0	66/67 (98%)	62 (94%)	4 (6%)	18	53
46	Y0	66/67 (98%)	58 (88%)	8 (12%)	5	26
47	R1	82/83 (99%)	68 (83%)	14 (17%)	2	13
47	Y1	82/83 (99%)	72 (88%)	10 (12%)	5	26
48	R2	64/67 (96%)	52 (81%)	12 (19%)	1	9
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	32
49	R3	51/52 (98%)	44 (86%)	7 (14%)	3	22
49	Y3	51/52 (98%)	47 (92%)	4 (8%)	12	44
50	R4	62/63 (98%)	47 (76%)	15 (24%)	0	4
50	Y4	62/63 (98%)	44 (71%)	18 (29%)	0	2
51	R5	51/52 (98%)	41 (80%)	10 (20%)	1	8
51	Y5	49/52 (94%)	42 (86%)	7 (14%)	3	21
52	R6	47/52 (90%)	32 (68%)	15 (32%)	0	2
52	Y6	47/52 (90%)	30 (64%)	17 (36%)	0	1
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2	14
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	14
54	R8	54/55 (98%)	43 (80%)	11 (20%)	1	8
54	Y8	54/55 (98%)	44 (82%)	10 (18%)	1	10
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	55
55	Y9	33/34 (97%)	33 (100%)	0	100	100
All	All	9856/10268 (96%)	8435 (86%)	1421 (14%)	3	20

5 of 1421 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	XR	37	VAL
35	YP	56	SER
20	XT	93	GLU
18	XR	31	LEU
29	YF	136	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
37	YR	3	HIS
40	YU	81	HIS
40	YU	117	GLN
40	RU	81	HIS
45	RZ	118	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1522 (99%)	286 (18%)	44 (2%)
1	XA	1506/1522 (98%)	290 (19%)	35 (2%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	13 (17%)	1 (1%)
23	QX	19/25 (76%)	13 (68%)	2 (10%)
23	XX	19/25 (76%)	8 (42%)	2 (10%)
25	RA	2888/2916 (99%)	575 (19%)	45 (1%)
25	YA	2872/2916 (98%)	560 (19%)	39 (1%)
26	RB	121/124 (97%)	21 (17%)	1 (0%)
26	YB	121/124 (97%)	20 (16%)	2 (1%)
56	Z6	1/3 (33%)	0	0
56	Z7	1/3 (33%)	0	0
All	All	9209/9334 (98%)	1801 (19%)	171 (1%)

5 of 1801 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G

5 of 171 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	818	G
25	YA	1085	A
1	XA	1004	A
25	YA	74	A
25	YA	1762	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	A2M	XX	20	23	18,25,26	0.99	1 (5%)	18,36,39	1.49	3 (16%)
23	A2M	QX	21	1,23	18,25,26	1.16	1 (5%)	18,36,39	1.39	4 (22%)
23	A2M	XX	21	23	18,25,26	1.08	2 (11%)	18,36,39	1.41	2 (11%)
23	A2M	QX	19	23	18,25,26	1.03	1 (5%)	18,36,39	1.41	3 (16%)
56	PPU	Z6	76	56,25	32,40,41	0.90	1 (3%)	33,57,60	1.73	7 (21%)
56	PPU	Z7	76	56,25	32,40,41	0.90	1 (3%)	33,57,60	1.36	6 (18%)
23	A2M	XX	19	23	18,25,26	0.98	1 (5%)	18,36,39	1.85	5 (27%)
23	A2M	QX	20	23	18,25,26	1.20	2 (11%)	18,36,39	1.40	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	A2M	XX	20	23	-	0/5/27/28	0/3/3/3
23	A2M	QX	21	1,23	-	5/5/27/28	0/3/3/3
23	A2M	XX	21	23	-	4/5/27/28	0/3/3/3
23	A2M	QX	19	23	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z6	76	56,25	-	1/21/43/44	0/4/4/4
56	PPU	Z7	76	56,25	-	7/21/43/44	0/4/4/4
23	A2M	XX	19	23	-	2/5/27/28	0/3/3/3
23	A2M	QX	20	23	-	0/5/27/28	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A2M	C5-C4	3.07	1.49	1.40
23	QX	21	A2M	C5-C4	2.75	1.48	1.40
23	QX	19	A2M	C5-C4	2.52	1.47	1.40
23	XX	21	A2M	O4’-C1’	2.47	1.44	1.41
23	XX	19	A2M	C5-C4	2.39	1.47	1.40

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z6	76	PPU	N1-C6-N6	6.36	123.75	117.06
23	XX	19	A2M	N3-C2-N1	-3.97	122.47	128.68
23	QX	19	A2M	N3-C2-N1	-3.70	122.89	128.68
56	Z6	76	PPU	C9-N6-C6	-3.57	108.69	119.51
23	XX	19	A2M	C1’-N9-C4	-3.47	120.54	126.64

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	QX	21	A2M	C1’-C2’-O2’-CM’
23	XX	21	A2M	O4’-C4’-C5’-O5’
23	XX	21	A2M	C3’-C4’-C5’-O5’
23	XX	21	A2M	C1’-C2’-O2’-CM’
56	Z7	76	PPU	C-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	XX	20	A2M	1	0
23	QX	21	A2M	3	0
23	XX	21	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	QX	19	A2M	1	0
56	Z6	76	PPU	5	0
56	Z7	76	PPU	12	0
23	XX	19	A2M	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1285 ligands modelled in this entry, 1285 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	QA	1511/1522 (99%)	0.09	32 (2%)	63	48	52, 94, 194, 353	0
1	XA	1508/1522 (99%)	0.03	36 (2%)	59	42	41, 84, 179, 401	0
2	QB	236/256 (92%)	0.22	11 (4%)	31	19	76, 141, 220, 278	0
2	XB	236/256 (92%)	-0.03	1 (0%)	92	86	56, 119, 205, 243	0
3	QC	206/239 (86%)	0.30	5 (2%)	59	42	81, 126, 222, 383	0
3	XC	206/239 (86%)	0.08	1 (0%)	91	83	58, 106, 171, 346	0
4	QD	208/209 (99%)	-0.25	0	100	100	53, 85, 131, 188	0
4	XD	208/209 (99%)	-0.18	0	100	100	56, 87, 139, 181	0
5	QE	154/162 (95%)	-0.05	0	100	100	45, 86, 147, 236	0
5	XE	154/162 (95%)	-0.09	0	100	100	41, 77, 151, 303	0
6	QF	101/101 (100%)	0.15	4 (3%)	38	25	75, 119, 160, 179	0
6	XF	101/101 (100%)	-0.35	1 (0%)	82	70	49, 83, 120, 199	0
7	QG	155/156 (99%)	0.40	13 (8%)	11	7	83, 138, 199, 270	0
7	XG	155/156 (99%)	0.20	9 (5%)	23	13	70, 111, 186, 242	0
8	QH	138/138 (100%)	-0.10	0	100	100	52, 93, 131, 193	0
8	XH	138/138 (100%)	-0.06	0	100	100	55, 83, 120, 154	0
9	QI	128/128 (100%)	0.85	18 (14%)	2	2	87, 160, 242, 319	0
9	XI	128/128 (100%)	0.09	2 (1%)	72	57	66, 119, 199, 272	0
10	QJ	99/105 (94%)	0.67	8 (8%)	12	7	94, 155, 255, 330	0
10	XJ	99/105 (94%)	0.57	8 (8%)	12	7	73, 136, 199, 337	0
11	QK	121/129 (93%)	0.36	7 (5%)	23	13	65, 110, 191, 294	0
11	XK	121/129 (93%)	-0.05	4 (3%)	46	31	50, 85, 156, 284	0
12	QL	125/132 (94%)	0.01	2 (1%)	72	57	52, 78, 121, 306	0
12	XL	125/132 (94%)	-0.08	2 (1%)	72	57	46, 73, 119, 225	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	QM	118/126 (93%)	0.31	6 (5%)	28	17	92, 139, 223, 308	0
13	XM	118/126 (93%)	0.18	2 (1%)	70	55	61, 120, 172, 350	0
14	QN	60/61 (98%)	0.08	2 (3%)	46	31	82, 124, 170, 221	0
14	XN	60/61 (98%)	-0.17	0	100	100	72, 100, 128, 193	0
15	QO	88/89 (98%)	0.01	0	100	100	58, 94, 138, 168	0
15	XO	88/89 (98%)	-0.20	1 (1%)	80	68	45, 78, 134, 146	0
16	QP	84/88 (95%)	0.14	0	100	100	56, 81, 121, 206	0
16	XP	84/88 (95%)	0.35	1 (1%)	79	66	58, 90, 134, 294	0
17	QQ	100/105 (95%)	-0.07	1 (1%)	82	70	51, 91, 126, 136	0
17	XQ	100/105 (95%)	-0.05	0	100	100	51, 83, 119, 217	0
18	QR	71/88 (80%)	0.29	2 (2%)	53	37	77, 119, 180, 288	0
18	XR	71/88 (80%)	-0.11	0	100	100	50, 81, 183, 271	0
19	QS	82/93 (88%)	0.71	9 (10%)	5	3	96, 150, 245, 348	0
19	XS	82/93 (88%)	0.46	3 (3%)	41	27	72, 128, 212, 281	0
20	QT	99/106 (93%)	0.23	6 (6%)	21	12	55, 97, 153, 209	0
20	XT	99/106 (93%)	0.35	4 (4%)	38	25	63, 106, 171, 235	0
21	QU	25/25 (100%)	1.22	4 (16%)	1	1	104, 142, 192, 230	0
21	XU	25/25 (100%)	1.02	5 (20%)	1	0	91, 117, 148, 176	0
22	QV	77/77 (100%)	0.18	3 (3%)	39	25	45, 95, 141, 191	0
22	XV	77/77 (100%)	0.03	1 (1%)	77	63	41, 86, 120, 188	0
23	QX	17/25 (68%)	3.24	12 (70%)	0	0	73, 229, 280, 291	0
23	XX	17/25 (68%)	3.47	11 (64%)	0	0	58, 223, 329, 349	0
24	QY	92/118 (77%)	0.88	3 (3%)	46	31	58, 116, 149, 189	0
24	XY	92/118 (77%)	0.81	5 (5%)	25	16	72, 113, 143, 177	0
25	RA	2891/2916 (99%)	0.26	163 (5%)	24	14	36, 68, 244, 472	0
25	YA	2875/2916 (98%)	0.29	162 (5%)	24	14	32, 61, 254, 518	0
26	RB	122/124 (98%)	-0.06	2 (1%)	72	57	72, 115, 150, 204	0
26	YB	122/124 (98%)	-0.05	1 (0%)	86	75	72, 95, 141, 236	0
27	RD	272/276 (98%)	-0.21	0	100	100	29, 66, 111, 221	0
27	YD	272/276 (98%)	-0.27	0	100	100	19, 51, 94, 175	0
28	RE	205/206 (99%)	0.09	6 (2%)	51	35	42, 84, 156, 368	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	YE	205/206 (99%)	0.13	6 (2%)	51	35	31, 73, 154, 409	0
29	RF	208/210 (99%)	-0.26	6 (2%)	51	35	27, 58, 160, 285	0
29	YF	208/210 (99%)	-0.12	7 (3%)	45	30	32, 69, 206, 333	0
30	RG	181/182 (99%)	0.07	2 (1%)	80	68	68, 120, 176, 225	0
30	YG	181/182 (99%)	-0.01	3 (1%)	70	55	65, 105, 154, 215	0
31	RH	170/180 (94%)	0.94	24 (14%)	2	2	82, 161, 292, 396	0
31	YH	170/180 (94%)	0.69	19 (11%)	5	3	66, 132, 250, 421	0
32	RI	146/148 (98%)	0.33	1 (0%)	87	78	64, 112, 168, 286	0
32	YI	146/148 (98%)	0.11	3 (2%)	63	48	47, 99, 175, 333	0
33	RN	138/140 (98%)	-0.07	0	100	100	54, 87, 135, 192	0
33	YN	138/140 (98%)	-0.07	1 (0%)	87	78	47, 79, 134, 185	0
34	RO	122/122 (100%)	-0.34	0	100	100	37, 72, 107, 153	0
34	YO	122/122 (100%)	-0.28	0	100	100	31, 64, 98, 132	0
35	RP	150/150 (100%)	0.11	3 (2%)	65	49	29, 79, 147, 252	0
35	YP	150/150 (100%)	0.11	4 (2%)	54	38	37, 73, 131, 253	0
36	RQ	140/141 (99%)	-0.11	0	100	100	41, 85, 142, 208	0
36	YQ	139/141 (98%)	-0.14	1 (0%)	87	78	39, 74, 127, 231	0
37	RR	117/118 (99%)	-0.05	1 (0%)	84	73	41, 75, 114, 165	0
37	YR	117/118 (99%)	-0.20	0	100	100	39, 65, 100, 157	0
38	RS	111/112 (99%)	0.44	7 (6%)	20	11	65, 117, 178, 256	0
38	YS	111/112 (99%)	0.03	2 (1%)	68	53	58, 94, 154, 253	0
39	RT	137/146 (93%)	-0.04	0	100	100	52, 88, 171, 361	0
39	YT	137/146 (93%)	-0.03	6 (4%)	34	21	45, 74, 201, 347	0
40	RU	117/118 (99%)	-0.23	2 (1%)	70	55	30, 66, 135, 205	0
40	YU	117/118 (99%)	-0.30	0	100	100	38, 69, 133, 179	0
41	RV	101/101 (100%)	0.02	2 (1%)	65	49	37, 84, 144, 284	0
41	YV	101/101 (100%)	-0.08	2 (1%)	65	49	43, 92, 135, 361	0
42	RW	113/113 (100%)	-0.19	0	100	100	40, 64, 130, 201	0
42	YW	113/113 (100%)	0.00	2 (1%)	68	53	33, 62, 110, 192	0
43	RX	92/96 (95%)	-0.00	0	100	100	48, 80, 118, 155	0
43	YX	92/96 (95%)	-0.27	0	100	100	32, 65, 113, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	RY	102/110 (92%)	0.75	11 (10%)	5	3	50, 84, 222, 392	0
44	YY	102/110 (92%)	0.56	7 (6%)	16	10	52, 94, 210, 487	0
45	RZ	176/206 (85%)	0.33	7 (3%)	38	25	63, 117, 216, 401	0
45	YZ	183/206 (88%)	0.19	6 (3%)	46	31	64, 113, 192, 282	0
46	R0	83/85 (97%)	0.06	2 (2%)	59	42	50, 75, 111, 253	0
46	Y0	83/85 (97%)	0.11	1 (1%)	79	66	39, 69, 98, 204	0
47	R1	97/98 (98%)	0.30	6 (6%)	20	12	41, 76, 203, 321	0
47	Y1	97/98 (98%)	0.18	5 (5%)	27	17	30, 61, 190, 315	0
48	R2	69/72 (95%)	0.01	4 (5%)	23	13	49, 99, 191, 258	0
48	Y2	69/72 (95%)	-0.22	1 (1%)	75	61	41, 78, 123, 222	0
49	R3	59/60 (98%)	0.64	3 (5%)	28	17	42, 72, 131, 159	0
49	Y3	59/60 (98%)	0.18	0	100	100	47, 81, 131, 164	0
50	R4	70/71 (98%)	0.79	10 (14%)	2	2	99, 196, 456, 558	0
50	Y4	70/71 (98%)	0.71	10 (14%)	2	2	94, 171, 356, 481	0
51	R5	59/60 (98%)	0.06	4 (6%)	17	10	40, 75, 185, 238	0
51	Y5	57/60 (95%)	-0.13	1 (1%)	68	53	24, 70, 159, 234	0
52	R6	48/54 (88%)	3.90	42 (87%)	0	0	126, 181, 242, 300	0
52	Y6	48/54 (88%)	3.85	40 (83%)	0	0	119, 172, 254, 281	0
53	R7	49/49 (100%)	-0.10	0	100	100	33, 54, 146, 188	0
53	Y7	49/49 (100%)	-0.08	0	100	100	20, 45, 117, 224	0
54	R8	64/65 (98%)	0.00	0	100	100	34, 66, 138, 223	0
54	Y8	64/65 (98%)	-0.02	2 (3%)	49	33	31, 62, 118, 203	0
55	R9	37/37 (100%)	1.50	12 (32%)	0	0	76, 134, 192, 230	0
55	Y9	36/37 (97%)	2.53	22 (61%)	0	0	102, 141, 190, 242	0
56	Z6	2/3 (66%)	-0.01	0	100	100	42, 42, 42, 55	0
56	Z7	2/3 (66%)	0.68	0	100	100	62, 62, 62, 63	0
All	All	21070/21694 (97%)	0.17	879 (4%)	36	23	19, 85, 199, 558	0

The worst 5 of 879 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	2114	A	20.8
25	YA	2110	G	16.2

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Mol	Chain	Res	Type	RSRZ
25	RA	2139	C	15.4
25	YA	2138	C	14.7
25	YA	2165	G	14.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	A2M	XX	21	23/24	0.76	0.37	111,165,165,165	0
23	A2M	QX	21	23/24	0.79	0.40	111,168,168,168	0
23	A2M	QX	20	23/24	0.90	0.28	111,117,117,117	0
23	A2M	XX	19	23/24	0.91	0.27	96,96,111,111	0
23	A2M	XX	20	23/24	0.91	0.31	105,105,111,111	0
23	A2M	QX	19	23/24	0.93	0.26	111,115,115,115	0
56	PPU	Z7	76	37/38	0.93	0.31	61,61,61,61	0
56	PPU	Z6	76	37/38	0.96	0.24	41,47,54,58	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3286	1/1	0.07	0.46	47,47,47,47	0
57	MG	QD	302	1/1	0.37	1.32	78,78,78,78	0
57	MG	YA	3222	1/1	0.38	0.49	78,78,78,78	0
57	MG	YG	201	1/1	0.40	0.23	85,85,85,85	0
57	MG	YA	3226	1/1	0.41	0.48	55,55,55,55	0
57	MG	RA	3292	1/1	0.43	0.54	52,52,52,52	0
57	MG	RA	3400	1/1	0.44	0.50	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XV	103	1/1	0.44	0.41	62,62,62,62	0
57	MG	RA	3300	1/1	0.44	0.73	44,44,44,44	0
57	MG	QA	1658	1/1	0.46	0.58	34,34,34,34	0
57	MG	QA	1747	1/1	0.48	0.41	111,111,111,111	0
57	MG	YA	3410	1/1	0.48	0.34	43,43,43,43	0
57	MG	YA	3169	1/1	0.48	0.80	61,61,61,61	0
57	MG	YA	3399	1/1	0.49	0.66	73,73,73,73	0
57	MG	RA	3221	1/1	0.50	1.18	46,46,46,46	0
57	MG	QA	1711	1/1	0.50	0.63	70,70,70,70	0
57	MG	YA	3468	1/1	0.51	0.36	44,44,44,44	0
57	MG	QA	1693	1/1	0.51	0.16	47,47,47,47	0
57	MG	QA	1647	1/1	0.52	0.23	72,72,72,72	0
57	MG	YA	3181	1/1	0.53	0.30	58,58,58,58	0
57	MG	QA	1731	1/1	0.53	0.35	54,54,54,54	0
57	MG	QA	1671	1/1	0.54	0.62	38,38,38,38	0
57	MG	QA	1668	1/1	0.54	0.39	50,50,50,50	0
57	MG	XA	1742	1/1	0.54	0.85	62,62,62,62	0
57	MG	YA	3352	1/1	0.54	0.50	65,65,65,65	0
57	MG	RA	3278	1/1	0.55	0.43	68,68,68,68	0
57	MG	YA	3446	1/1	0.55	0.34	49,49,49,49	0
57	MG	YA	3353	1/1	0.56	0.48	34,34,34,34	0
57	MG	RA	3110	1/1	0.56	0.31	38,38,38,38	0
57	MG	YA	3377	1/1	0.57	0.52	85,85,85,85	0
57	MG	RA	3298	1/1	0.57	0.75	79,79,79,79	0
57	MG	XA	1760	1/1	0.57	0.24	71,71,71,71	0
57	MG	YA	3301	1/1	0.58	0.85	65,65,65,65	0
57	MG	YA	3333	1/1	0.59	0.81	47,47,47,47	0
57	MG	RA	3318	1/1	0.59	0.36	38,38,38,38	0
57	MG	RA	3335	1/1	0.59	1.11	44,44,44,44	0
57	MG	QA	1719	1/1	0.60	0.82	68,68,68,68	0
57	MG	RA	3342	1/1	0.60	0.49	109,109,109,109	0
57	MG	YA	3423	1/1	0.60	0.51	50,50,50,50	0
57	MG	YA	3355	1/1	0.60	0.32	39,39,39,39	0
57	MG	YA	3265	1/1	0.60	0.69	56,56,56,56	0
57	MG	YA	3392	1/1	0.60	0.31	52,52,52,52	0
57	MG	XA	1749	1/1	0.61	0.40	81,81,81,81	0
57	MG	RA	3206	1/1	0.61	0.23	30,30,30,30	0
57	MG	XA	1714	1/1	0.62	0.83	54,54,54,54	0
57	MG	RD	301	1/1	0.62	0.54	35,35,35,35	0
57	MG	XA	1688	1/1	0.62	0.51	37,37,37,37	0
57	MG	XA	1689	1/1	0.62	1.16	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YQ	202	1/1	0.62	0.60	39,39,39,39	0
57	MG	Y5	103	1/1	0.62	0.62	50,50,50,50	0
57	MG	YA	3182	1/1	0.63	0.40	51,51,51,51	0
57	MG	RA	3365	1/1	0.63	0.27	58,58,58,58	0
57	MG	RA	3048	1/1	0.63	0.62	27,27,27,27	0
57	MG	QA	1703	1/1	0.63	0.30	57,57,57,57	0
57	MG	RA	3134	1/1	0.63	0.38	39,39,39,39	0
57	MG	RA	3394	1/1	0.64	0.53	39,39,39,39	0
57	MG	YA	3368	1/1	0.64	0.51	36,36,36,36	0
57	MG	XA	1722	1/1	0.64	1.08	74,74,74,74	0
57	MG	YA	3471	1/1	0.64	0.56	85,85,85,85	0
57	MG	XA	1752	1/1	0.64	0.37	62,62,62,62	0
57	MG	YA	3242	1/1	0.64	0.37	54,54,54,54	0
57	MG	XA	1755	1/1	0.64	0.45	61,61,61,61	0
57	MG	YA	3459	1/1	0.65	0.54	42,42,42,42	0
57	MG	QA	1663	1/1	0.65	1.31	64,64,64,64	0
57	MG	YA	3146	1/1	0.65	0.48	63,63,63,63	0
57	MG	RA	3173	1/1	0.65	0.48	50,50,50,50	0
57	MG	RA	3370	1/1	0.65	0.71	101,101,101,101	0
57	MG	YA	3348	1/1	0.65	0.25	45,45,45,45	0
57	MG	RA	3326	1/1	0.66	0.55	65,65,65,65	0
57	MG	YA	3325	1/1	0.66	0.94	53,53,53,53	0
57	MG	RA	3330	1/1	0.66	0.20	64,64,64,64	0
57	MG	RA	3275	1/1	0.66	0.64	79,79,79,79	0
57	MG	RA	3248	1/1	0.66	0.30	23,23,23,23	0
57	MG	YA	3376	1/1	0.67	0.37	82,82,82,82	0
57	MG	QA	1696	1/1	0.67	1.04	64,64,64,64	0
57	MG	RA	3327	1/1	0.67	0.41	71,71,71,71	0
57	MG	QA	1695	1/1	0.67	0.34	48,48,48,48	0
57	MG	YB	206	1/1	0.67	0.23	50,50,50,50	0
57	MG	YA	3405	1/1	0.67	0.43	33,33,33,33	0
57	MG	XA	1700	1/1	0.67	0.59	36,36,36,36	0
57	MG	XA	1709	1/1	0.67	1.07	63,63,63,63	0
57	MG	RA	3040	1/1	0.68	0.18	19,19,19,19	0
57	MG	YA	3349	1/1	0.68	0.42	63,63,63,63	0
57	MG	RA	3167	1/1	0.68	0.36	25,25,25,25	0
57	MG	YA	3443	1/1	0.68	0.29	65,65,65,65	0
57	MG	QA	1724	1/1	0.68	0.27	60,60,60,60	0
57	MG	XA	1656	1/1	0.68	0.09	50,50,50,50	0
57	MG	XA	1676	1/1	0.68	0.48	44,44,44,44	0
57	MG	YA	3372	1/1	0.68	0.49	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3182	1/1	0.68	0.41	56,56,56,56	0
57	MG	YF	301	1/1	0.68	0.33	38,38,38,38	0
57	MG	QA	1710	1/1	0.68	0.51	59,59,59,59	0
57	MG	YA	3184	1/1	0.68	0.42	49,49,49,49	0
57	MG	YA	3338	1/1	0.68	0.58	57,57,57,57	0
57	MG	YA	3172	1/1	0.69	0.36	43,43,43,43	0
57	MG	RA	3334	1/1	0.69	0.67	40,40,40,40	0
57	MG	YA	3394	1/1	0.69	0.26	61,61,61,61	0
57	MG	RA	3203	1/1	0.69	0.22	29,29,29,29	0
57	MG	RA	3339	1/1	0.69	0.17	69,69,69,69	0
57	MG	XA	1736	1/1	0.69	0.16	45,45,45,45	0
57	MG	R0	102	1/1	0.69	0.46	47,47,47,47	0
57	MG	YA	3426	1/1	0.69	0.19	45,45,45,45	0
57	MG	XA	1630	1/1	0.69	0.53	46,46,46,46	0
57	MG	RA	3102	1/1	0.70	0.52	56,56,56,56	0
57	MG	YA	3356	1/1	0.70	0.20	55,55,55,55	0
57	MG	YA	3303	1/1	0.70	0.44	47,47,47,47	0
57	MG	YA	3096	1/1	0.70	0.29	36,36,36,36	0
57	MG	YA	3109	1/1	0.70	0.34	31,31,31,31	0
57	MG	RA	3340	1/1	0.70	0.47	56,56,56,56	0
57	MG	YA	3388	1/1	0.70	0.39	55,55,55,55	0
57	MG	YA	3150	1/1	0.70	0.37	44,44,44,44	0
57	MG	QA	1742	1/1	0.70	0.57	57,57,57,57	0
57	MG	YA	3351	1/1	0.70	0.45	48,48,48,48	0
57	MG	QE	201	1/1	0.70	0.26	62,62,62,62	0
57	MG	YA	3179	1/1	0.70	0.46	64,64,64,64	0
57	MG	YA	3318	1/1	0.71	0.81	48,48,48,48	0
57	MG	YA	3390	1/1	0.71	0.26	54,54,54,54	0
57	MG	RA	3416	1/1	0.71	0.29	61,61,61,61	0
57	MG	QA	1744	1/1	0.71	0.72	44,44,44,44	0
57	MG	XA	1720	1/1	0.71	0.83	62,62,62,62	0
57	MG	QA	1672	1/1	0.71	0.73	71,71,71,71	0
57	MG	YA	3461	1/1	0.71	0.43	57,57,57,57	0
57	MG	YA	3425	1/1	0.72	0.45	61,61,61,61	0
57	MG	RA	3187	1/1	0.72	0.40	42,42,42,42	0
57	MG	YA	3431	1/1	0.72	0.36	65,65,65,65	0
57	MG	YA	3217	1/1	0.72	0.25	46,46,46,46	0
57	MG	RA	3431	1/1	0.72	0.52	34,34,34,34	0
57	MG	QA	1718	1/1	0.72	0.49	66,66,66,66	0
57	MG	RA	3372	1/1	0.72	0.43	44,44,44,44	0
57	MG	RA	3333	1/1	0.72	0.47	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3268	1/1	0.72	0.38	51,51,51,51	0
57	MG	QA	1743	1/1	0.72	0.34	71,71,71,71	0
57	MG	RA	3403	1/1	0.72	0.33	59,59,59,59	0
57	MG	XA	1729	1/1	0.72	1.08	48,48,48,48	0
57	MG	YA	3306	1/1	0.72	0.67	54,54,54,54	0
57	MG	YA	3367	1/1	0.72	0.30	57,57,57,57	0
57	MG	RA	3324	1/1	0.73	0.27	62,62,62,62	0
57	MG	XA	1702	1/1	0.73	0.35	38,38,38,38	0
57	MG	XA	1730	1/1	0.73	0.29	55,55,55,55	0
57	MG	RA	3001	1/1	0.73	0.71	60,60,60,60	0
57	MG	R2	101	1/1	0.73	0.38	80,80,80,80	0
57	MG	YA	3419	1/1	0.73	0.17	54,54,54,54	0
57	MG	QA	1637	1/1	0.73	0.48	61,61,61,61	0
57	MG	RA	3262	1/1	0.74	0.46	62,62,62,62	0
57	MG	XA	1739	1/1	0.74	0.24	49,49,49,49	0
57	MG	YA	3183	1/1	0.74	0.32	28,28,28,28	0
57	MG	RA	3269	1/1	0.74	0.49	50,50,50,50	0
57	MG	YA	3113	1/1	0.74	0.42	37,37,37,37	0
57	MG	YA	3141	1/1	0.74	0.27	31,31,31,31	0
57	MG	RA	3219	1/1	0.74	0.31	31,31,31,31	0
57	MG	YA	3342	1/1	0.74	0.79	43,43,43,43	0
57	MG	RA	3390	1/1	0.74	0.20	53,53,53,53	0
57	MG	YA	3260	1/1	0.74	0.40	48,48,48,48	0
57	MG	YA	3264	1/1	0.74	0.52	60,60,60,60	0
57	MG	RA	3417	1/1	0.74	0.20	45,45,45,45	0
57	MG	YA	3409	1/1	0.74	0.69	54,54,54,54	0
57	MG	XA	1756	1/1	0.74	0.54	59,59,59,59	0
57	MG	XA	1631	1/1	0.74	0.29	74,74,74,74	0
57	MG	QA	1734	1/1	0.75	0.34	53,53,53,53	0
57	MG	RA	3421	1/1	0.75	0.43	43,43,43,43	0
57	MG	YA	3167	1/1	0.75	0.96	49,49,49,49	0
57	MG	YA	3438	1/1	0.75	0.19	54,54,54,54	0
57	MG	YA	3237	1/1	0.75	0.43	26,26,26,26	0
57	MG	YA	3168	1/1	0.75	0.48	34,34,34,34	0
57	MG	XL	201	1/1	0.75	0.17	43,43,43,43	0
57	MG	RA	3430	1/1	0.75	0.27	38,38,38,38	0
57	MG	RA	3294	1/1	0.75	0.24	48,48,48,48	0
57	MG	QA	1707	1/1	0.75	0.61	64,64,64,64	0
57	MG	RP	202	1/1	0.75	0.36	34,34,34,34	0
57	MG	RA	3362	1/1	0.75	0.33	45,45,45,45	0
57	MG	YA	3145	1/1	0.75	0.23	32,32,32,32	0
57	MG	YA	3357	1/1	0.75	0.50	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	YA	3191	1/1	0.75	0.59	28,28,28,28	0
57	MG	RA	3255	1/1	0.76	0.09	40,40,40,40	0
57	MG	YA	3228	1/1	0.76	1.27	51,51,51,51	0
57	MG	RY	202	1/1	0.76	0.56	66,66,66,66	0
57	MG	RA	3204	1/1	0.76	0.68	34,34,34,34	0
57	MG	YA	3152	1/1	0.76	0.27	34,34,34,34	0
57	MG	RA	3265	1/1	0.76	0.18	33,33,33,33	0
57	MG	XA	1710	1/1	0.76	0.50	57,57,57,57	0
57	MG	XA	1757	1/1	0.76	0.39	66,66,66,66	0
57	MG	XA	1759	1/1	0.76	0.12	36,36,36,36	0
57	MG	RA	3176	1/1	0.76	0.42	51,51,51,51	0
57	MG	YA	3451	1/1	0.76	0.46	63,63,63,63	0
57	MG	XD	302	1/1	0.76	0.10	77,77,77,77	0
57	MG	RA	3428	1/1	0.76	0.46	41,41,41,41	0
57	MG	YA	3309	1/1	0.76	0.85	56,56,56,56	0
57	MG	YA	3315	1/1	0.76	0.22	55,55,55,55	0
57	MG	XA	1635	1/1	0.76	0.21	44,44,44,44	0
57	MG	XA	1652	1/1	0.76	0.92	41,41,41,41	0
57	MG	RA	3142	1/1	0.76	0.40	48,48,48,48	0
57	MG	RA	3089	1/1	0.76	0.50	33,33,33,33	0
57	MG	QA	1733	1/1	0.76	0.35	57,57,57,57	0
57	MG	XA	1697	1/1	0.77	0.33	52,52,52,52	0
57	MG	RA	3380	1/1	0.77	0.33	45,45,45,45	0
57	MG	RA	3266	1/1	0.77	0.74	48,48,48,48	0
57	MG	RA	3251	1/1	0.77	0.39	58,58,58,58	0
57	MG	YA	3202	1/1	0.77	0.54	22,22,22,22	0
57	MG	YA	3210	1/1	0.77	0.16	29,29,29,29	0
57	MG	RA	3198	1/1	0.77	0.29	49,49,49,49	0
57	MG	RA	3311	1/1	0.77	0.79	61,61,61,61	0
57	MG	QA	1740	1/1	0.77	0.59	69,69,69,69	0
57	MG	RA	3210	1/1	0.77	0.37	29,29,29,29	0
57	MG	YD	301	1/1	0.77	0.53	21,21,21,21	0
57	MG	YA	3316	1/1	0.77	0.65	53,53,53,53	0
57	MG	YA	3127	1/1	0.77	0.13	48,48,48,48	0
57	MG	YA	3322	1/1	0.77	0.68	42,42,42,42	0
57	MG	RA	3338	1/1	0.77	0.43	52,52,52,52	0
57	MG	YA	3354	1/1	0.78	0.43	67,67,67,67	0
57	MG	RA	3100	1/1	0.78	0.18	14,14,14,14	0
57	MG	YA	3195	1/1	0.78	0.29	30,30,30,30	0
57	MG	XA	1751	1/1	0.78	0.34	59,59,59,59	0
57	MG	QA	1678	1/1	0.78	0.24	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	YA	3439	1/1	0.78	0.34	53,53,53,53	0
57	MG	YA	3440	1/1	0.78	0.29	75,75,75,75	0
57	MG	XA	1753	1/1	0.78	0.32	67,67,67,67	0
57	MG	RA	3284	1/1	0.78	0.67	41,41,41,41	0
57	MG	YA	3447	1/1	0.78	0.25	38,38,38,38	0
57	MG	QA	1629	1/1	0.78	0.45	46,46,46,46	0
57	MG	RA	3425	1/1	0.78	0.49	46,46,46,46	0
57	MG	QA	1613	1/1	0.78	0.43	50,50,50,50	0
57	MG	YA	3466	1/1	0.78	0.35	58,58,58,58	0
57	MG	RA	3212	1/1	0.78	0.31	19,19,19,19	0
57	MG	XA	1725	1/1	0.78	0.45	64,64,64,64	0
57	MG	YA	3343	1/1	0.78	0.45	25,25,25,25	0
57	MG	RA	3140	1/1	0.78	0.17	59,59,59,59	0
57	MG	XA	1686	1/1	0.78	0.47	47,47,47,47	0
57	MG	RA	3302	1/1	0.78	0.55	36,36,36,36	0
57	MG	QL	201	1/1	0.78	0.23	49,49,49,49	0
57	MG	RA	3316	1/1	0.78	0.58	52,52,52,52	0
57	MG	XA	1718	1/1	0.79	0.71	51,51,51,51	0
57	MG	YA	3313	1/1	0.79	0.18	65,65,65,65	0
57	MG	QA	1677	1/1	0.79	0.19	86,86,86,86	0
57	MG	XA	1721	1/1	0.79	0.23	57,57,57,57	0
57	MG	RB	203	1/1	0.79	0.36	31,31,31,31	0
57	MG	YA	3373	1/1	0.79	0.60	42,42,42,42	0
57	MG	YA	3156	1/1	0.79	0.22	40,40,40,40	0
57	MG	RA	3218	1/1	0.79	0.18	39,39,39,39	0
57	MG	XA	1726	1/1	0.79	0.39	56,56,56,56	0
57	MG	RA	3325	1/1	0.79	0.52	67,67,67,67	0
57	MG	QA	1716	1/1	0.79	0.97	35,35,35,35	0
57	MG	YA	3261	1/1	0.79	0.39	54,54,54,54	0
57	MG	RA	3353	1/1	0.79	0.39	43,43,43,43	0
57	MG	YA	3400	1/1	0.79	0.42	80,80,80,80	0
57	MG	YA	3094	1/1	0.79	0.37	75,75,75,75	0
57	MG	RA	3177	1/1	0.79	0.49	45,45,45,45	0
57	MG	RA	3234	1/1	0.79	0.50	36,36,36,36	0
57	MG	RA	3270	1/1	0.79	0.56	35,35,35,35	0
57	MG	RA	3151	1/1	0.79	0.34	35,35,35,35	0
57	MG	YU	201	1/1	0.79	0.43	60,60,60,60	0
57	MG	QA	1640	1/1	0.79	0.36	58,58,58,58	0
57	MG	YA	3347	1/1	0.80	0.39	44,44,44,44	0
57	MG	YA	3300	1/1	0.80	0.61	35,35,35,35	0
57	MG	RA	3186	1/1	0.80	0.54	40,40,40,40	0
57	MG	RA	3090	1/1	0.80	0.33	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RB	205	1/1	0.80	0.39	58,58,58,58	0
57	MG	YA	3452	1/1	0.80	0.56	58,58,58,58	0
57	MG	XA	1646	1/1	0.80	0.21	57,57,57,57	0
57	MG	YA	3135	1/1	0.80	0.76	39,39,39,39	0
57	MG	QA	1683	1/1	0.80	0.87	42,42,42,42	0
57	MG	XA	1735	1/1	0.80	0.43	18,18,18,18	0
57	MG	YA	3412	1/1	0.80	0.34	49,49,49,49	0
57	MG	RA	3343	1/1	0.80	0.14	48,48,48,48	0
57	MG	XA	1666	1/1	0.80	0.48	46,46,46,46	0
57	MG	RA	3347	1/1	0.80	0.96	65,65,65,65	0
57	MG	RA	3163	1/1	0.80	0.52	61,61,61,61	0
57	MG	YA	3278	1/1	0.80	0.99	33,33,33,33	0
57	MG	QA	1746	1/1	0.80	0.09	44,44,44,44	0
57	MG	YA	3293	1/1	0.80	0.15	33,33,33,33	0
57	MG	YA	3381	1/1	0.81	0.27	35,35,35,35	0
57	MG	YA	3384	1/1	0.81	0.99	53,53,53,53	0
57	MG	QA	1690	1/1	0.81	0.49	27,27,27,27	0
57	MG	QA	1745	1/1	0.81	0.19	72,72,72,72	0
57	MG	RA	3091	1/1	0.81	0.22	29,29,29,29	0
57	MG	XA	1723	1/1	0.81	0.36	35,35,35,35	0
57	MG	YA	3101	1/1	0.81	0.35	22,22,22,22	0
57	MG	YA	3230	1/1	0.81	0.61	53,53,53,53	0
57	MG	YA	3404	1/1	0.81	0.83	54,54,54,54	0
57	MG	YA	3232	1/1	0.81	0.13	27,27,27,27	0
57	MG	RA	3223	1/1	0.81	0.74	36,36,36,36	0
57	MG	QA	1630	1/1	0.81	0.24	55,55,55,55	0
57	MG	QA	1705	1/1	0.81	0.46	47,47,47,47	0
57	MG	YA	3130	1/1	0.81	0.20	28,28,28,28	0
57	MG	R5	102	1/1	0.81	0.44	33,33,33,33	0
57	MG	XA	1758	1/1	0.81	0.68	58,58,58,58	0
57	MG	XA	1681	1/1	0.81	1.09	49,49,49,49	0
57	MG	XA	1717	1/1	0.81	0.28	31,31,31,31	0
57	MG	Y0	101	1/1	0.81	0.29	12,12,12,12	0
57	MG	QA	1621	1/1	0.81	0.19	49,49,49,49	0
57	MG	RA	3345	1/1	0.82	0.39	36,36,36,36	0
57	MG	QV	105	1/1	0.82	0.22	34,34,34,34	0
57	MG	RA	3309	1/1	0.82	0.22	49,49,49,49	0
57	MG	RA	3249	1/1	0.82	0.68	41,41,41,41	0
57	MG	YA	3310	1/1	0.82	0.74	50,50,50,50	0
57	MG	YA	3457	1/1	0.82	0.18	63,63,63,63	0
57	MG	YA	3250	1/1	0.82	0.54	67,67,67,67	0
57	MG	RA	3059	1/1	0.82	0.18	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3423	1/1	0.82	0.44	48,48,48,48	0
57	MG	QA	1728	1/1	0.82	0.17	36,36,36,36	0
57	MG	YA	3469	1/1	0.82	0.35	70,70,70,70	0
57	MG	XA	1612	1/1	0.82	0.32	49,49,49,49	0
57	MG	RA	3147	1/1	0.82	0.19	65,65,65,65	0
57	MG	QA	1698	1/1	0.82	0.34	69,69,69,69	0
57	MG	YA	3374	1/1	0.82	0.23	38,38,38,38	0
57	MG	YA	3279	1/1	0.82	0.17	71,71,71,71	0
57	MG	YA	3284	1/1	0.82	0.35	57,57,57,57	0
57	MG	YA	3225	1/1	0.82	0.30	43,43,43,43	0
57	MG	YY	201	1/1	0.82	0.30	33,33,33,33	0
57	MG	RA	3119	1/1	0.82	0.45	67,67,67,67	0
57	MG	RA	3237	1/1	0.82	0.39	54,54,54,54	0
57	MG	QA	1737	1/1	0.83	0.25	47,47,47,47	0
57	MG	YA	3164	1/1	0.83	0.75	48,48,48,48	0
57	MG	YA	3383	1/1	0.83	0.23	47,47,47,47	0
57	MG	YA	3088	1/1	0.83	0.56	21,21,21,21	0
57	MG	RA	3412	1/1	0.83	0.42	57,57,57,57	0
57	MG	YA	3450	1/1	0.83	0.39	49,49,49,49	0
57	MG	RE	302	1/1	0.83	0.31	53,53,53,53	0
57	MG	QA	1612	1/1	0.83	0.80	37,37,37,37	0
57	MG	RR	201	1/1	0.83	0.44	21,21,21,21	0
57	MG	RA	3366	1/1	0.83	0.18	58,58,58,58	0
57	MG	QA	1709	1/1	0.83	0.59	45,45,45,45	0
57	MG	YA	3465	1/1	0.83	0.43	47,47,47,47	0
57	MG	QA	1628	1/1	0.83	0.16	61,61,61,61	0
57	MG	RA	3154	1/1	0.83	0.41	48,48,48,48	0
57	MG	XA	1692	1/1	0.83	0.18	71,71,71,71	0
57	MG	YA	3360	1/1	0.83	0.43	41,41,41,41	0
57	MG	YA	3365	1/1	0.83	0.65	24,24,24,24	0
57	MG	RA	3263	1/1	0.83	0.29	50,50,50,50	0
57	MG	YA	3267	1/1	0.83	0.86	49,49,49,49	0
57	MG	RA	3392	1/1	0.83	0.27	43,43,43,43	0
57	MG	YA	3328	1/1	0.83	0.42	55,55,55,55	0
57	MG	YA	3430	1/1	0.83	0.16	43,43,43,43	0
57	MG	RA	3285	1/1	0.83	0.47	35,35,35,35	0
57	MG	YA	3436	1/1	0.83	0.26	22,22,22,22	0
57	MG	RA	3242	1/1	0.83	0.41	28,28,28,28	0
57	MG	Y7	101	1/1	0.83	0.41	43,43,43,43	0
57	MG	QA	1625	1/1	0.84	0.22	59,59,59,59	0
57	MG	YA	3236	1/1	0.84	0.13	23,23,23,23	0
57	MG	XA	1672	1/1	0.84	0.28	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3013	1/1	0.84	0.47	32,32,32,32	0
57	MG	RA	3427	1/1	0.84	0.28	56,56,56,56	0
57	MG	YA	3255	1/1	0.84	0.41	41,41,41,41	0
57	MG	YA	3382	1/1	0.84	0.26	37,37,37,37	0
57	MG	RA	3408	1/1	0.84	0.12	62,62,62,62	0
57	MG	RA	3022	1/1	0.84	0.35	52,52,52,52	0
57	MG	RA	3414	1/1	0.84	0.44	45,45,45,45	0
57	MG	XA	1625	1/1	0.84	0.20	75,75,75,75	0
57	MG	RA	3415	1/1	0.84	0.30	50,50,50,50	0
57	MG	RB	204	1/1	0.84	0.12	41,41,41,41	0
57	MG	YA	3398	1/1	0.84	0.20	36,36,36,36	0
57	MG	XA	1633	1/1	0.84	0.25	49,49,49,49	0
57	MG	XA	1703	1/1	0.84	0.38	48,48,48,48	0
57	MG	YA	3283	1/1	0.84	0.60	66,66,66,66	0
57	MG	XA	1743	1/1	0.84	0.34	50,50,50,50	0
57	MG	XA	1704	1/1	0.84	0.28	55,55,55,55	0
57	MG	YA	3292	1/1	0.84	0.50	33,33,33,33	0
57	MG	YA	3134	1/1	0.84	0.37	37,37,37,37	0
57	MG	XA	1706	1/1	0.84	0.36	41,41,41,41	0
57	MG	YH	202	1/1	0.84	0.21	59,59,59,59	0
57	MG	YQ	201	1/1	0.84	0.18	52,52,52,52	0
57	MG	YA	3422	1/1	0.84	0.52	27,27,27,27	0
57	MG	RA	3341	1/1	0.84	0.28	46,46,46,46	0
57	MG	RA	3092	1/1	0.84	0.57	36,36,36,36	0
57	MG	RA	3419	1/1	0.84	0.27	47,47,47,47	0
57	MG	XA	1654	1/1	0.84	0.57	26,26,26,26	0
57	MG	RA	3313	1/1	0.84	0.36	50,50,50,50	0
57	MG	YA	3294	1/1	0.85	0.53	37,37,37,37	0
57	MG	YA	3432	1/1	0.85	0.44	31,31,31,31	0
57	MG	YA	3295	1/1	0.85	0.38	46,46,46,46	0
57	MG	RA	3407	1/1	0.85	0.39	56,56,56,56	0
57	MG	RA	3360	1/1	0.85	0.33	64,64,64,64	0
57	MG	XA	1639	1/1	0.85	0.39	58,58,58,58	0
57	MG	QA	1659	1/1	0.85	0.39	31,31,31,31	0
57	MG	YA	3307	1/1	0.85	0.23	43,43,43,43	0
57	MG	XA	1754	1/1	0.85	0.16	84,84,84,84	0
57	MG	XA	1647	1/1	0.85	0.23	83,83,83,83	0
57	MG	QA	1706	1/1	0.85	0.27	48,48,48,48	0
57	MG	RD	302	1/1	0.85	0.50	29,29,29,29	0
57	MG	YA	3240	1/1	0.85	0.22	43,43,43,43	0
57	MG	RA	3276	1/1	0.85	1.05	65,65,65,65	0
57	MG	YA	3460	1/1	0.85	0.37	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	XA	1663	1/1	0.85	0.42	30,30,30,30	0
57	MG	RA	3254	1/1	0.85	0.41	50,50,50,50	0
57	MG	RA	3233	1/1	0.85	0.36	37,37,37,37	0
57	MG	YA	3467	1/1	0.85	0.39	48,48,48,48	0
57	MG	RA	3256	1/1	0.85	0.36	47,47,47,47	0
57	MG	XA	1677	1/1	0.85	0.15	39,39,39,39	0
57	MG	QA	1735	1/1	0.85	0.14	40,40,40,40	0
57	MG	YA	3091	1/1	0.85	0.68	26,26,26,26	0
57	MG	YA	3346	1/1	0.85	0.66	45,45,45,45	0
57	MG	QA	1682	1/1	0.85	0.95	39,39,39,39	0
57	MG	YA	3276	1/1	0.85	0.38	53,53,53,53	0
57	MG	RA	3241	1/1	0.85	0.34	38,38,38,38	0
57	MG	RA	3397	1/1	0.85	0.39	34,34,34,34	0
57	MG	YA	3280	1/1	0.85	0.35	70,70,70,70	0
57	MG	QV	104	1/1	0.85	0.34	52,52,52,52	0
57	MG	XA	1629	1/1	0.85	0.15	53,53,53,53	0
57	MG	RA	3402	1/1	0.85	0.17	32,32,32,32	0
57	MG	QA	1609	1/1	0.85	0.32	57,57,57,57	0
57	MG	YA	3220	1/1	0.85	0.57	39,39,39,39	0
57	MG	XA	1695	1/1	0.86	0.18	71,71,71,71	0
57	MG	RA	3413	1/1	0.86	0.35	35,35,35,35	0
57	MG	RA	3348	1/1	0.86	0.36	68,68,68,68	0
57	MG	YA	3401	1/1	0.86	0.25	56,56,56,56	0
57	MG	QA	1639	1/1	0.86	0.20	49,49,49,49	0
57	MG	RA	3358	1/1	0.86	1.04	57,57,57,57	0
57	MG	YA	3312	1/1	0.86	0.86	40,40,40,40	0
57	MG	RA	3181	1/1	0.86	0.52	62,62,62,62	0
57	MG	YA	3411	1/1	0.86	0.43	35,35,35,35	0
57	MG	RA	3146	1/1	0.86	0.20	25,25,25,25	0
57	MG	RA	3279	1/1	0.86	0.40	40,40,40,40	0
57	MG	RA	3422	1/1	0.86	0.48	45,45,45,45	0
57	MG	RA	3283	1/1	0.86	0.33	37,37,37,37	0
57	MG	XA	1636	1/1	0.86	0.63	43,43,43,43	0
57	MG	YA	3231	1/1	0.86	0.27	44,44,44,44	0
57	MG	YA	3332	1/1	0.86	0.66	36,36,36,36	0
57	MG	QA	1608	1/1	0.86	0.30	25,25,25,25	0
57	MG	XA	1719	1/1	0.86	0.61	71,71,71,71	0
57	MG	RA	3222	1/1	0.86	0.46	30,30,30,30	0
57	MG	YA	3238	1/1	0.86	0.44	48,48,48,48	0
57	MG	YA	3239	1/1	0.86	0.31	29,29,29,29	0
57	MG	QA	1662	1/1	0.86	0.21	56,56,56,56	0
57	MG	XA	1651	1/1	0.86	0.42	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3246	1/1	0.86	0.39	43,43,43,43	0
57	MG	RA	3388	1/1	0.86	0.52	18,18,18,18	0
57	MG	YA	3251	1/1	0.86	0.59	48,48,48,48	0
57	MG	YA	3253	1/1	0.86	0.59	25,25,25,25	0
57	MG	XA	1724	1/1	0.86	0.35	48,48,48,48	0
57	MG	YA	3455	1/1	0.86	0.27	36,36,36,36	0
57	MG	YA	3258	1/1	0.86	0.29	48,48,48,48	0
57	MG	RA	3260	1/1	0.86	0.59	65,65,65,65	0
57	MG	RB	201	1/1	0.86	0.37	30,30,30,30	0
57	MG	RA	3337	1/1	0.86	0.23	58,58,58,58	0
57	MG	QA	1620	1/1	0.86	0.57	30,30,30,30	0
57	MG	XA	1670	1/1	0.86	0.20	30,30,30,30	0
57	MG	YA	3155	1/1	0.86	0.18	27,27,27,27	0
57	MG	RA	3064	1/1	0.86	0.58	15,15,15,15	0
57	MG	RA	3068	1/1	0.86	0.32	14,14,14,14	0
57	MG	QA	1729	1/1	0.86	0.16	54,54,54,54	0
57	MG	RA	3268	1/1	0.86	0.44	35,35,35,35	0
57	MG	XA	1683	1/1	0.86	0.51	45,45,45,45	0
57	MG	YA	3170	1/1	0.86	0.54	7,7,7,7	0
57	MG	XA	1684	1/1	0.86	0.32	41,41,41,41	0
57	MG	RA	3406	1/1	0.86	0.34	49,49,49,49	0
57	MG	QA	1666	1/1	0.86	0.45	51,51,51,51	0
57	MG	RA	3314	1/1	0.86	1.19	47,47,47,47	0
57	MG	RA	3244	1/1	0.86	0.20	45,45,45,45	0
57	MG	XA	1693	1/1	0.86	0.15	25,25,25,25	0
57	MG	YA	3393	1/1	0.86	0.14	39,39,39,39	0
57	MG	YA	3187	1/1	0.86	0.48	35,35,35,35	0
57	MG	YA	3396	1/1	0.86	0.35	59,59,59,59	0
57	MG	YA	3142	1/1	0.87	0.51	50,50,50,50	0
57	MG	YA	3249	1/1	0.87	0.33	46,46,46,46	0
57	MG	YA	3350	1/1	0.87	0.25	28,28,28,28	0
57	MG	QA	1638	1/1	0.87	0.23	67,67,67,67	0
57	MG	XA	1712	1/1	0.87	0.18	53,53,53,53	0
57	MG	RA	3132	1/1	0.87	0.54	35,35,35,35	0
57	MG	RA	3228	1/1	0.87	0.25	47,47,47,47	0
57	MG	YA	3215	1/1	0.87	0.26	15,15,15,15	0
57	MG	RA	3230	1/1	0.87	0.21	73,73,73,73	0
57	MG	XA	1745	1/1	0.87	0.12	47,47,47,47	0
57	MG	YA	3358	1/1	0.87	0.67	25,25,25,25	0
57	MG	YA	3158	1/1	0.87	0.26	43,43,43,43	0
57	MG	YA	3160	1/1	0.87	0.37	42,42,42,42	0
57	MG	YA	3366	1/1	0.87	0.47	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1668	1/1	0.87	0.36	29,29,29,29	0
57	MG	RA	3049	1/1	0.87	0.29	1,1,1,1	0
57	MG	YA	3369	1/1	0.87	0.26	58,58,58,58	0
57	MG	RA	3050	1/1	0.87	0.51	23,23,23,23	0
57	MG	YA	3105	1/1	0.87	0.57	45,45,45,45	0
57	MG	QA	1717	1/1	0.87	0.43	55,55,55,55	0
57	MG	YA	3235	1/1	0.87	0.46	19,19,19,19	0
57	MG	RA	3095	1/1	0.87	0.77	47,47,47,47	0
57	MG	XA	1678	1/1	0.87	0.70	65,65,65,65	0
57	MG	QA	1627	1/1	0.87	0.40	52,52,52,52	0
57	MG	XA	1705	1/1	0.87	0.62	30,30,30,30	0
57	MG	QA	1648	1/1	0.87	0.12	74,74,74,74	0
57	MG	YA	3387	1/1	0.87	0.21	49,49,49,49	0
57	MG	RA	3081	1/1	0.87	0.12	20,20,20,20	0
57	MG	XA	1741	1/1	0.88	0.16	44,44,44,44	0
57	MG	YA	3327	1/1	0.88	0.40	30,30,30,30	0
57	MG	YA	3407	1/1	0.88	0.49	7,7,7,7	0
57	MG	RA	3211	1/1	0.88	0.10	26,26,26,26	0
57	MG	XA	1694	1/1	0.88	0.19	43,43,43,43	0
57	MG	QA	1721	1/1	0.88	1.37	46,46,46,46	0
57	MG	YA	3151	1/1	0.88	0.54	15,15,15,15	0
57	MG	YA	3418	1/1	0.88	0.17	19,19,19,19	0
57	MG	XA	1748	1/1	0.88	1.16	55,55,55,55	0
57	MG	RA	3367	1/1	0.88	0.44	43,43,43,43	0
57	MG	RA	3215	1/1	0.88	0.32	29,29,29,29	0
57	MG	RA	3328	1/1	0.88	0.45	37,37,37,37	0
57	MG	YA	3252	1/1	0.88	0.46	47,47,47,47	0
57	MG	QA	1738	1/1	0.88	0.11	42,42,42,42	0
57	MG	RA	3179	1/1	0.88	0.32	43,43,43,43	0
57	MG	RA	3180	1/1	0.88	0.47	18,18,18,18	0
57	MG	RA	3286	1/1	0.88	0.38	34,34,34,34	0
57	MG	QA	1674	1/1	0.88	0.42	57,57,57,57	0
57	MG	RA	3259	1/1	0.88	0.34	39,39,39,39	0
57	MG	XA	1661	1/1	0.88	0.44	28,28,28,28	0
57	MG	YA	3266	1/1	0.88	0.89	43,43,43,43	0
57	MG	YA	3175	1/1	0.88	0.18	34,34,34,34	0
57	MG	QA	1697	1/1	0.88	0.43	34,34,34,34	0
57	MG	RA	3401	1/1	0.88	0.63	60,60,60,60	0
57	MG	QA	1689	1/1	0.88	0.37	30,30,30,30	0
57	MG	RA	3152	1/1	0.88	0.84	33,33,33,33	0
57	MG	YA	3060	1/1	0.88	0.35	11,11,11,11	0
57	MG	YA	3282	1/1	0.88	0.21	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	YA	3067	1/1	0.88	0.22	6,6,6,6	0
57	MG	YA	3073	1/1	0.88	0.57	24,24,24,24	0
57	MG	RA	3308	1/1	0.88	0.62	63,63,63,63	0
57	MG	YA	3291	1/1	0.88	0.88	34,34,34,34	0
57	MG	YA	3200	1/1	0.88	0.39	32,32,32,32	0
57	MG	YA	3089	1/1	0.88	0.26	44,44,44,44	0
57	MG	RQ	202	1/1	0.88	0.25	74,74,74,74	0
57	MG	YA	3211	1/1	0.88	0.10	67,67,67,67	0
57	MG	RA	3264	1/1	0.88	0.72	39,39,39,39	0
57	MG	RA	3231	1/1	0.88	0.61	30,30,30,30	0
57	MG	YA	3099	1/1	0.88	0.17	10,10,10,10	0
57	MG	RA	3153	1/1	0.88	0.17	13,13,13,13	0
57	MG	YA	3224	1/1	0.88	0.25	15,15,15,15	0
57	MG	XA	1682	1/1	0.88	0.18	51,51,51,51	0
57	MG	YP	202	1/1	0.88	0.39	38,38,38,38	0
57	MG	QA	1618	1/1	0.88	0.44	32,32,32,32	0
57	MG	QA	1692	1/1	0.88	0.46	47,47,47,47	0
57	MG	QA	1636	1/1	0.88	0.67	47,47,47,47	0
57	MG	RA	3323	1/1	0.88	0.12	37,37,37,37	0
57	MG	QA	1661	1/1	0.88	0.26	57,57,57,57	0
57	MG	XA	1737	1/1	0.88	0.20	40,40,40,40	0
57	MG	RA	3363	1/1	0.88	0.45	46,46,46,46	0
57	MG	YA	3417	1/1	0.89	0.27	78,78,78,78	0
57	MG	YA	3198	1/1	0.89	0.37	25,25,25,25	0
57	MG	XA	1626	1/1	0.89	0.42	28,28,28,28	0
57	MG	RA	3158	1/1	0.89	0.32	59,59,59,59	0
57	MG	YA	3209	1/1	0.89	0.51	19,19,19,19	0
57	MG	RA	3160	1/1	0.89	0.36	58,58,58,58	0
57	MG	RA	3288	1/1	0.89	0.45	56,56,56,56	0
57	MG	YA	3427	1/1	0.89	0.22	27,27,27,27	0
57	MG	RA	3196	1/1	0.89	0.66	39,39,39,39	0
57	MG	YA	3216	1/1	0.89	0.27	24,24,24,24	0
57	MG	RA	3331	1/1	0.89	0.33	59,59,59,59	0
57	MG	QA	1741	1/1	0.89	0.52	45,45,45,45	0
57	MG	YA	3221	1/1	0.89	0.25	28,28,28,28	0
57	MG	YA	3139	1/1	0.89	0.12	38,38,38,38	0
57	MG	RA	3296	1/1	0.89	0.36	46,46,46,46	0
57	MG	RA	3166	1/1	0.89	0.59	30,30,30,30	0
57	MG	RA	3389	1/1	0.89	0.40	9,9,9,9	0
57	MG	YA	3371	1/1	0.89	0.45	57,57,57,57	0
57	MG	XA	1648	1/1	0.89	0.20	39,39,39,39	0
57	MG	QV	102	1/1	0.89	0.22	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3302	1/1	0.89	0.42	57,57,57,57	0
57	MG	XA	1707	1/1	0.89	0.40	35,35,35,35	0
57	MG	RA	3205	1/1	0.89	0.19	34,34,34,34	0
57	MG	RA	3306	1/1	0.89	0.55	43,43,43,43	0
57	MG	RA	3172	1/1	0.89	0.44	50,50,50,50	0
57	MG	RA	3399	1/1	0.89	0.23	46,46,46,46	0
57	MG	RA	3240	1/1	0.89	0.44	56,56,56,56	0
57	MG	RA	3106	1/1	0.89	0.31	32,32,32,32	0
57	MG	QV	103	1/1	0.89	0.43	8,8,8,8	0
57	MG	RP	201	1/1	0.89	0.21	35,35,35,35	0
57	MG	YA	3244	1/1	0.89	0.74	34,34,34,34	0
57	MG	YA	3001	1/1	0.89	0.80	28,28,28,28	0
57	MG	YA	3472	1/1	0.89	0.36	45,45,45,45	0
57	MG	YB	203	1/1	0.89	0.35	16,16,16,16	0
57	MG	YA	3022	1/1	0.89	0.52	54,54,54,54	0
57	MG	RA	3061	1/1	0.89	0.42	28,28,28,28	0
57	MG	RQ	201	1/1	0.89	0.43	37,37,37,37	0
57	MG	RA	3213	1/1	0.89	0.32	30,30,30,30	0
57	MG	YA	3180	1/1	0.89	0.33	38,38,38,38	0
57	MG	QA	1633	1/1	0.89	0.32	39,39,39,39	0
57	MG	RA	3320	1/1	0.89	0.46	58,58,58,58	0
57	MG	RA	3354	1/1	0.89	0.55	82,82,82,82	0
57	MG	YR	201	1/1	0.89	0.39	12,12,12,12	0
57	MG	YA	3344	1/1	0.89	0.23	71,71,71,71	0
57	MG	RA	3355	1/1	0.89	0.10	51,51,51,51	0
57	MG	RA	3133	1/1	0.89	0.59	39,39,39,39	0
57	MG	Y0	103	1/1	0.89	0.28	18,18,18,18	0
57	MG	Y5	102	1/1	0.89	0.41	16,16,16,16	0
57	MG	QA	1646	1/1	0.89	0.52	70,70,70,70	0
57	MG	RA	3157	1/1	0.89	0.20	79,79,79,79	0
57	MG	RA	3282	1/1	0.90	0.13	47,47,47,47	0
57	MG	XA	1632	1/1	0.90	0.48	20,20,20,20	0
57	MG	YA	3117	1/1	0.90	0.40	34,34,34,34	0
57	MG	YA	3375	1/1	0.90	0.28	30,30,30,30	0
57	MG	QA	1665	1/1	0.90	0.50	52,52,52,52	0
57	MG	RA	3135	1/1	0.90	0.98	49,49,49,49	0
57	MG	QA	1704	1/1	0.90	0.54	35,35,35,35	0
57	MG	QA	1601	1/1	0.90	0.40	11,11,11,11	0
57	MG	YA	3204	1/1	0.90	0.29	34,34,34,34	0
57	MG	YA	3263	1/1	0.90	0.47	50,50,50,50	0
57	MG	YA	3386	1/1	0.90	0.31	58,58,58,58	0
57	MG	YA	3454	1/1	0.90	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1642	1/1	0.90	0.13	43,43,43,43	0
57	MG	RA	3321	1/1	0.90	0.39	37,37,37,37	0
57	MG	QA	1723	1/1	0.90	0.19	50,50,50,50	0
57	MG	RA	3042	1/1	0.90	0.32	9,9,9,9	0
57	MG	RA	3087	1/1	0.90	0.20	36,36,36,36	0
57	MG	QA	1712	1/1	0.90	0.33	38,38,38,38	0
57	MG	RA	3127	1/1	0.90	0.17	33,33,33,33	0
57	MG	XA	1655	1/1	0.90	0.47	41,41,41,41	0
57	MG	XA	1698	1/1	0.90	0.48	112,112,112,112	0
57	MG	YA	3005	1/1	0.90	0.22	9,9,9,9	0
57	MG	XA	1699	1/1	0.90	0.25	31,31,31,31	0
57	MG	YA	3057	1/1	0.90	0.22	59,59,59,59	0
57	MG	QA	1614	1/1	0.90	0.30	44,44,44,44	0
57	MG	RA	3253	1/1	0.90	0.32	21,21,21,21	0
57	MG	XA	1738	1/1	0.90	0.45	35,35,35,35	0
57	MG	YA	3083	1/1	0.90	0.12	21,21,21,21	0
57	MG	R5	103	1/1	0.90	0.07	34,34,34,34	0
57	MG	RA	3208	1/1	0.90	0.48	52,52,52,52	0
57	MG	YN	201	1/1	0.90	0.25	44,44,44,44	0
57	MG	RA	3307	1/1	0.90	0.43	43,43,43,43	0
57	MG	YA	3177	1/1	0.90	0.32	26,26,26,26	0
57	MG	YA	3362	1/1	0.90	0.85	31,31,31,31	0
57	MG	YA	3178	1/1	0.90	0.18	47,47,47,47	0
57	MG	QA	1675	1/1	0.90	0.18	36,36,36,36	0
57	MG	XA	1744	1/1	0.90	0.28	36,36,36,36	0
57	MG	RA	3232	1/1	0.90	0.31	39,39,39,39	0
57	MG	XA	1746	1/1	0.90	0.21	63,63,63,63	0
57	MG	YA	3428	1/1	0.90	0.27	39,39,39,39	0
57	MG	YA	3370	1/1	0.90	0.49	39,39,39,39	0
57	MG	RA	3281	1/1	0.90	0.15	40,40,40,40	0
58	ZN	XN	101	1/1	0.90	0.15	78,78,78,78	0
57	MG	YA	3336	1/1	0.91	0.27	32,32,32,32	0
57	MG	YA	3248	1/1	0.91	0.35	15,15,15,15	0
57	MG	YA	3035	1/1	0.91	0.26	26,26,26,26	0
57	MG	QA	1650	1/1	0.91	0.38	31,31,31,31	0
57	MG	RA	3374	1/1	0.91	0.35	18,18,18,18	0
57	MG	XA	1621	1/1	0.91	0.44	39,39,39,39	0
57	MG	YA	3069	1/1	0.91	0.41	18,18,18,18	0
57	MG	QA	1631	1/1	0.91	0.51	41,41,41,41	0
57	MG	YA	3257	1/1	0.91	0.32	51,51,51,51	0
57	MG	XA	1732	1/1	0.91	0.09	52,52,52,52	0
57	MG	RA	3384	1/1	0.91	0.27	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	RA	3387	1/1	0.91	0.41	24,24,24,24	0
57	MG	RA	3424	1/1	0.91	0.21	45,45,45,45	0
57	MG	RA	3200	1/1	0.91	0.36	20,20,20,20	0
57	MG	YA	3434	1/1	0.91	0.27	21,21,21,21	0
57	MG	YA	3095	1/1	0.91	0.77	16,16,16,16	0
57	MG	YA	3185	1/1	0.91	0.58	9,9,9,9	0
57	MG	RA	3426	1/1	0.91	0.25	24,24,24,24	0
57	MG	YA	3097	1/1	0.91	0.33	22,22,22,22	0
57	MG	YA	3359	1/1	0.91	0.39	52,52,52,52	0
57	MG	YA	3269	1/1	0.91	0.18	35,35,35,35	0
57	MG	YA	3194	1/1	0.91	0.17	56,56,56,56	0
57	MG	YA	3098	1/1	0.91	0.45	69,69,69,69	0
57	MG	RA	3165	1/1	0.91	0.18	71,71,71,71	0
57	MG	QA	1702	1/1	0.91	0.14	99,99,99,99	0
57	MG	YA	3453	1/1	0.91	0.21	33,33,33,33	0
57	MG	RA	3344	1/1	0.91	0.23	39,39,39,39	0
57	MG	YA	3108	1/1	0.91	0.40	22,22,22,22	0
57	MG	QA	1670	1/1	0.91	0.43	53,53,53,53	0
57	MG	YA	3458	1/1	0.91	0.14	49,49,49,49	0
57	MG	YA	3285	1/1	0.91	0.30	42,42,42,42	0
57	MG	RA	3395	1/1	0.91	0.54	46,46,46,46	0
57	MG	YA	3290	1/1	0.91	0.31	22,22,22,22	0
57	MG	YA	3114	1/1	0.91	0.42	36,36,36,36	0
57	MG	RA	3396	1/1	0.91	0.15	43,43,43,43	0
57	MG	YA	3120	1/1	0.91	0.16	37,37,37,37	0
57	MG	RA	3168	1/1	0.91	0.31	43,43,43,43	0
57	MG	YA	3379	1/1	0.91	0.20	44,44,44,44	0
57	MG	RA	3293	1/1	0.91	0.60	21,21,21,21	0
57	MG	YA	3299	1/1	0.91	0.28	70,70,70,70	0
57	MG	QA	1606	1/1	0.91	0.24	12,12,12,12	0
57	MG	RA	3105	1/1	0.91	0.16	38,38,38,38	0
57	MG	RA	3028	1/1	0.91	0.34	34,34,34,34	0
57	MG	RA	3035	1/1	0.91	0.29	59,59,59,59	0
57	MG	RA	3301	1/1	0.91	0.32	34,34,34,34	0
57	MG	RA	3113	1/1	0.91	0.25	33,33,33,33	0
57	MG	QA	1679	1/1	0.91	0.22	39,39,39,39	0
57	MG	YA	3147	1/1	0.91	0.44	20,20,20,20	0
57	MG	RA	3364	1/1	0.91	0.20	67,67,67,67	0
57	MG	YA	3233	1/1	0.91	0.44	35,35,35,35	0
57	MG	XA	1667	1/1	0.91	0.81	27,27,27,27	0
57	MG	RY	201	1/1	0.91	0.20	24,24,24,24	0
57	MG	QA	1680	1/1	0.91	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3155	1/1	0.91	0.20	27,27,27,27	0
57	MG	XA	1675	1/1	0.91	0.77	29,29,29,29	0
57	MG	RA	3129	1/1	0.91	0.34	19,19,19,19	0
57	MG	R5	101	1/1	0.91	0.20	25,25,25,25	0
57	MG	YA	3007	1/1	0.91	0.50	13,13,13,13	0
58	ZN	QN	100	1/1	0.91	0.14	90,90,90,90	0
57	MG	QA	1660	1/1	0.91	0.41	20,20,20,20	0
57	MG	YA	3048	1/1	0.92	0.21	32,32,32,32	0
57	MG	YA	3243	1/1	0.92	0.19	56,56,56,56	0
57	MG	QA	1643	1/1	0.92	0.30	59,59,59,59	0
57	MG	RA	3322	1/1	0.92	0.28	30,30,30,30	0
57	MG	YA	3065	1/1	0.92	0.23	16,16,16,16	0
57	MG	YA	3340	1/1	0.92	0.52	52,52,52,52	0
57	MG	YA	3341	1/1	0.92	0.23	56,56,56,56	0
57	MG	YA	3171	1/1	0.92	0.11	35,35,35,35	0
57	MG	YA	3424	1/1	0.92	0.18	28,28,28,28	0
57	MG	RA	3084	1/1	0.92	0.31	28,28,28,28	0
57	MG	RA	3359	1/1	0.92	0.36	42,42,42,42	0
57	MG	RA	3044	1/1	0.92	0.42	2,2,2,2	0
57	MG	RA	3111	1/1	0.92	0.20	38,38,38,38	0
57	MG	YA	3254	1/1	0.92	0.18	41,41,41,41	0
57	MG	YA	3084	1/1	0.92	0.39	29,29,29,29	0
57	MG	R0	101	1/1	0.92	0.29	14,14,14,14	0
57	MG	QA	1685	1/1	0.92	0.09	25,25,25,25	0
57	MG	YA	3090	1/1	0.92	0.32	34,34,34,34	0
57	MG	YA	3437	1/1	0.92	0.26	74,74,74,74	0
57	MG	RA	3226	1/1	0.92	0.31	49,49,49,49	0
57	MG	RA	3201	1/1	0.92	0.46	27,27,27,27	0
57	MG	RA	3171	1/1	0.92	0.80	38,38,38,38	0
57	MG	YA	3442	1/1	0.92	0.20	49,49,49,49	0
57	MG	YA	3186	1/1	0.92	0.41	27,27,27,27	0
57	MG	QA	1617	1/1	0.92	0.38	37,37,37,37	0
57	MG	XA	1608	1/1	0.92	0.26	27,27,27,27	0
57	MG	YA	3193	1/1	0.92	0.73	27,27,27,27	0
57	MG	XA	1611	1/1	0.92	0.69	36,36,36,36	0
57	MG	YA	3274	1/1	0.92	0.34	33,33,33,33	0
57	MG	YA	3363	1/1	0.92	0.58	29,29,29,29	0
57	MG	RA	3418	1/1	0.92	0.24	39,39,39,39	0
57	MG	YA	3197	1/1	0.92	0.27	23,23,23,23	0
57	MG	QA	1736	1/1	0.92	0.56	49,49,49,49	0
57	MG	QA	1603	1/1	0.92	0.19	53,53,53,53	0
57	MG	YA	3281	1/1	0.92	0.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	YA	3201	1/1	0.92	0.32	30,30,30,30	0
57	MG	RA	3093	1/1	0.92	0.28	21,21,21,21	0
57	MG	XA	1628	1/1	0.92	0.37	33,33,33,33	0
57	MG	RA	3378	1/1	0.92	0.14	112,112,112,112	0
57	MG	RA	3336	1/1	0.92	0.11	32,32,32,32	0
57	MG	RA	3305	1/1	0.92	0.17	24,24,24,24	0
57	MG	RA	3209	1/1	0.92	0.50	34,34,34,34	0
57	MG	YA	3122	1/1	0.92	0.35	44,44,44,44	0
57	MG	RA	3156	1/1	0.92	0.10	36,36,36,36	0
57	MG	YA	3218	1/1	0.92	0.35	23,23,23,23	0
57	MG	YB	204	1/1	0.92	0.14	54,54,54,54	0
57	MG	YA	3219	1/1	0.92	0.40	27,27,27,27	0
57	MG	XA	1634	1/1	0.92	0.30	17,17,17,17	0
57	MG	RA	3271	1/1	0.92	0.53	14,14,14,14	0
57	MG	QA	1623	1/1	0.92	0.61	37,37,37,37	0
57	MG	RA	3310	1/1	0.92	0.44	69,69,69,69	0
57	MG	RA	3039	1/1	0.92	0.49	7,7,7,7	0
57	MG	QA	1739	1/1	0.92	0.15	57,57,57,57	0
57	MG	RA	3246	1/1	0.92	0.23	22,22,22,22	0
57	MG	RA	3214	1/1	0.92	0.39	63,63,63,63	0
57	MG	RA	3398	1/1	0.92	0.10	38,38,38,38	0
57	MG	RA	3185	1/1	0.92	0.11	31,31,31,31	0
57	MG	RE	301	1/1	0.92	0.29	8,8,8,8	0
57	MG	XA	1716	1/1	0.92	0.64	39,39,39,39	0
57	MG	RA	3350	1/1	0.92	0.22	53,53,53,53	0
57	MG	Y1	101	1/1	0.92	0.30	17,17,17,17	0
57	MG	YA	3317	1/1	0.92	0.19	35,35,35,35	0
57	MG	RF	301	1/1	0.92	0.10	27,27,27,27	0
57	MG	YA	3019	1/1	0.92	0.36	14,14,14,14	0
57	MG	RA	3217	1/1	0.92	0.18	16,16,16,16	0
57	MG	XA	1662	1/1	0.92	0.35	13,13,13,13	0
57	MG	QA	1708	1/1	0.93	0.43	19,19,19,19	0
57	MG	QA	1722	1/1	0.93	0.27	49,49,49,49	0
57	MG	YA	3262	1/1	0.93	0.39	14,14,14,14	0
57	MG	RA	3287	1/1	0.93	0.16	33,33,33,33	0
57	MG	RA	3037	1/1	0.93	0.19	1,1,1,1	0
57	MG	XA	1620	1/1	0.93	0.21	30,30,30,30	0
57	MG	RA	3083	1/1	0.93	0.09	19,19,19,19	0
57	MG	YA	3100	1/1	0.93	0.39	23,23,23,23	0
57	MG	RA	3329	1/1	0.93	0.25	47,47,47,47	0
57	MG	RA	3369	1/1	0.93	0.70	46,46,46,46	0
57	MG	YA	3273	1/1	0.93	0.30	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	QA	1699	1/1	0.93	0.26	72,72,72,72	0
57	MG	QA	1700	1/1	0.93	0.83	35,35,35,35	0
57	MG	RA	3120	1/1	0.93	0.29	67,67,67,67	0
57	MG	RA	3123	1/1	0.93	0.40	33,33,33,33	0
57	MG	RA	3299	1/1	0.93	0.20	76,76,76,76	0
57	MG	RA	3381	1/1	0.93	0.70	11,11,11,11	0
57	MG	YA	3214	1/1	0.93	0.23	34,34,34,34	0
57	MG	RA	3224	1/1	0.93	0.48	37,37,37,37	0
57	MG	YA	3449	1/1	0.93	0.35	39,39,39,39	0
57	MG	RA	3385	1/1	0.93	0.38	3,3,3,3	0
57	MG	RA	3126	1/1	0.93	0.56	67,67,67,67	0
57	MG	RA	3199	1/1	0.93	0.32	5,5,5,5	0
57	MG	RA	3162	1/1	0.93	0.16	23,23,23,23	0
57	MG	QA	1602	1/1	0.93	0.61	20,20,20,20	0
57	MG	QA	1694	1/1	0.93	0.18	31,31,31,31	0
57	MG	XA	1761	1/1	0.93	0.10	68,68,68,68	0
57	MG	RA	3393	1/1	0.93	0.15	29,29,29,29	0
57	MG	XA	1650	1/1	0.93	0.51	20,20,20,20	0
57	MG	QA	1669	1/1	0.93	0.10	48,48,48,48	0
57	MG	YA	3148	1/1	0.93	0.78	9,9,9,9	0
57	MG	XV	104	1/1	0.93	0.15	16,16,16,16	0
57	MG	XA	1711	1/1	0.93	0.59	24,24,24,24	0
57	MG	QA	1732	1/1	0.93	0.42	60,60,60,60	0
57	MG	XA	1653	1/1	0.93	0.18	29,29,29,29	0
57	MG	QA	1615	1/1	0.93	0.20	59,59,59,59	0
57	MG	YA	3020	1/1	0.93	0.28	19,19,19,19	0
57	MG	RA	3238	1/1	0.93	0.25	9,9,9,9	0
57	MG	RA	3169	1/1	0.93	0.85	39,39,39,39	0
57	MG	YA	3042	1/1	0.93	0.29	4,4,4,4	0
57	MG	XA	1658	1/1	0.93	0.21	25,25,25,25	0
57	MG	XA	1660	1/1	0.93	0.20	27,27,27,27	0
57	MG	YA	3058	1/1	0.93	0.20	39,39,39,39	0
57	MG	RA	3277	1/1	0.93	0.36	51,51,51,51	0
57	MG	YA	3245	1/1	0.93	0.38	33,33,33,33	0
57	MG	RA	3058	1/1	0.93	0.21	31,31,31,31	0
57	MG	RA	3352	1/1	0.93	0.83	39,39,39,39	0
57	MG	RA	3317	1/1	0.93	0.52	36,36,36,36	0
57	MG	YA	3329	1/1	0.93	0.24	34,34,34,34	0
57	MG	RA	3099	1/1	0.93	0.43	32,32,32,32	0
57	MG	YA	3076	1/1	0.93	0.42	24,24,24,24	0
57	MG	YV	201	1/1	0.93	0.33	11,11,11,11	0
57	MG	QA	1681	1/1	0.93	0.23	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3357	1/1	0.93	0.33	45,45,45,45	0
57	MG	YA	3339	1/1	0.93	0.37	31,31,31,31	0
57	MG	RA	3245	1/1	0.93	0.50	30,30,30,30	0
57	MG	YA	3413	1/1	0.93	0.19	36,36,36,36	0
57	MG	RA	3409	1/1	0.93	0.35	0,0,0,0	0
57	MG	QA	1634	1/1	0.93	0.32	65,65,65,65	0
57	MG	RA	3104	1/1	0.93	0.17	34,34,34,34	0
57	MG	YA	3259	1/1	0.93	0.22	43,43,43,43	0
57	MG	XV	102	1/1	0.94	0.29	0,0,0,0	0
57	MG	RA	3202	1/1	0.94	0.10	40,40,40,40	0
57	MG	YA	3402	1/1	0.94	0.48	14,14,14,14	0
57	MG	QA	1673	1/1	0.94	0.26	72,72,72,72	0
57	MG	RA	3086	1/1	0.94	0.20	20,20,20,20	0
57	MG	RA	3303	1/1	0.94	0.15	44,44,44,44	0
57	MG	YA	3314	1/1	0.94	0.28	43,43,43,43	0
57	MG	XA	1665	1/1	0.94	0.21	19,19,19,19	0
57	MG	RA	3052	1/1	0.94	0.21	38,38,38,38	0
57	MG	XA	1607	1/1	0.94	0.31	32,32,32,32	0
57	MG	RA	3053	1/1	0.94	0.55	26,26,26,26	0
57	MG	YA	3321	1/1	0.94	0.22	36,36,36,36	0
57	MG	XA	1610	1/1	0.94	0.38	22,22,22,22	0
57	MG	YA	3040	1/1	0.94	0.19	5,5,5,5	0
57	MG	RA	3149	1/1	0.94	0.63	1,1,1,1	0
57	MG	YA	3043	1/1	0.94	0.44	7,7,7,7	0
57	MG	RA	3056	1/1	0.94	0.84	32,32,32,32	0
57	MG	YA	3330	1/1	0.94	0.47	24,24,24,24	0
57	MG	YA	3159	1/1	0.94	0.39	26,26,26,26	0
57	MG	XA	1614	1/1	0.94	0.16	40,40,40,40	0
57	MG	YA	3163	1/1	0.94	0.23	21,21,21,21	0
57	MG	YA	3429	1/1	0.94	0.19	81,81,81,81	0
57	MG	YA	3337	1/1	0.94	0.41	4,4,4,4	0
57	MG	XA	1728	1/1	0.94	0.39	46,46,46,46	0
57	MG	YA	3247	1/1	0.94	0.46	30,30,30,30	0
57	MG	QA	1720	1/1	0.94	0.19	35,35,35,35	0
57	MG	YA	3061	1/1	0.94	0.22	10,10,10,10	0
57	MG	QA	1713	1/1	0.94	0.36	32,32,32,32	0
57	MG	XA	1622	1/1	0.94	0.78	35,35,35,35	0
57	MG	XA	1734	1/1	0.94	0.19	15,15,15,15	0
57	MG	YA	3345	1/1	0.94	0.27	29,29,29,29	0
57	MG	RA	3386	1/1	0.94	0.19	36,36,36,36	0
57	MG	YA	3173	1/1	0.94	0.22	43,43,43,43	0
57	MG	YA	3444	1/1	0.94	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1684	1/1	0.94	0.26	42,42,42,42	0
57	MG	YA	3081	1/1	0.94	0.20	26,26,26,26	0
57	MG	YA	3082	1/1	0.94	0.29	20,20,20,20	0
57	MG	RA	3124	1/1	0.94	0.21	45,45,45,45	0
57	MG	RA	3094	1/1	0.94	0.21	47,47,47,47	0
57	MG	YA	3087	1/1	0.94	0.24	18,18,18,18	0
57	MG	RA	3346	1/1	0.94	0.68	53,53,53,53	0
57	MG	RA	3019	1/1	0.94	0.30	16,16,16,16	0
57	MG	RA	3216	1/1	0.94	0.28	20,20,20,20	0
57	MG	RB	202	1/1	0.94	0.39	27,27,27,27	0
57	MG	YA	3093	1/1	0.94	0.11	41,41,41,41	0
57	MG	RA	3247	1/1	0.94	0.30	35,35,35,35	0
57	MG	RA	3351	1/1	0.94	0.22	70,70,70,70	0
57	MG	RA	3319	1/1	0.94	0.14	95,95,95,95	0
57	MG	YA	3270	1/1	0.94	0.85	37,37,37,37	0
57	MG	RA	3096	1/1	0.94	0.73	29,29,29,29	0
57	MG	QA	1657	1/1	0.94	0.36	21,21,21,21	0
57	MG	RA	3192	1/1	0.94	0.26	22,22,22,22	0
57	MG	YA	3277	1/1	0.94	0.14	83,83,83,83	0
57	MG	RA	3356	1/1	0.94	0.13	56,56,56,56	0
57	MG	YA	3199	1/1	0.94	0.25	11,11,11,11	0
57	MG	YB	202	1/1	0.94	0.56	31,31,31,31	0
57	MG	RA	3220	1/1	0.94	0.23	34,34,34,34	0
57	MG	YA	3103	1/1	0.94	0.13	42,42,42,42	0
57	MG	RA	3078	1/1	0.94	0.29	12,12,12,12	0
57	MG	YA	3106	1/1	0.94	0.49	12,12,12,12	0
57	MG	YA	3205	1/1	0.94	0.24	32,32,32,32	0
57	MG	YA	3206	1/1	0.94	0.22	27,27,27,27	0
57	MG	RA	3023	1/1	0.94	0.54	3,3,3,3	0
57	MG	QA	1654	1/1	0.94	0.49	34,34,34,34	0
57	MG	YA	3111	1/1	0.94	0.25	21,21,21,21	0
57	MG	RA	3257	1/1	0.94	0.54	48,48,48,48	0
57	MG	XA	1708	1/1	0.94	0.26	54,54,54,54	0
57	MG	RA	3136	1/1	0.94	0.35	61,61,61,61	0
57	MG	YA	3385	1/1	0.94	0.27	40,40,40,40	0
57	MG	YA	3119	1/1	0.94	0.55	40,40,40,40	0
57	MG	YA	3298	1/1	0.94	0.68	41,41,41,41	0
57	MG	RA	3138	1/1	0.94	0.30	49,49,49,49	0
57	MG	Y0	102	1/1	0.94	0.10	24,24,24,24	0
57	MG	RA	3261	1/1	0.94	0.52	30,30,30,30	0
57	MG	YA	3124	1/1	0.94	0.18	16,16,16,16	0
57	MG	RA	3227	1/1	0.94	0.51	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1713	1/1	0.94	0.20	31,31,31,31	0
57	MG	YA	3304	1/1	0.94	0.46	27,27,27,27	0
57	MG	YA	3305	1/1	0.94	0.47	38,38,38,38	0
57	MG	XN	102	1/1	0.94	0.22	54,54,54,54	0
57	MG	RA	3030	1/1	0.95	0.30	16,16,16,16	0
57	MG	YA	3414	1/1	0.95	0.11	127,127,127,127	0
57	MG	RA	3183	1/1	0.95	0.50	67,67,67,67	0
57	MG	XA	1604	1/1	0.95	0.34	19,19,19,19	0
57	MG	YA	3256	1/1	0.95	0.17	15,15,15,15	0
57	MG	YA	3421	1/1	0.95	0.25	33,33,33,33	0
57	MG	RA	3383	1/1	0.95	0.34	26,26,26,26	0
57	MG	RA	3128	1/1	0.95	0.13	37,37,37,37	0
57	MG	QA	1619	1/1	0.95	0.48	10,10,10,10	0
57	MG	QA	1655	1/1	0.95	0.29	29,29,29,29	0
57	MG	RA	3038	1/1	0.95	0.44	39,39,39,39	0
57	MG	RA	3195	1/1	0.95	0.21	20,20,20,20	0
57	MG	YA	3189	1/1	0.95	0.35	25,25,25,25	0
57	MG	RA	3349	1/1	0.95	0.48	49,49,49,49	0
57	MG	YA	3104	1/1	0.95	0.14	50,50,50,50	0
57	MG	RA	3252	1/1	0.95	0.12	62,62,62,62	0
57	MG	RA	3391	1/1	0.95	0.23	32,32,32,32	0
57	MG	QA	1725	1/1	0.95	0.29	41,41,41,41	0
57	MG	RA	3071	1/1	0.95	0.35	41,41,41,41	0
57	MG	QA	1604	1/1	0.95	0.14	31,31,31,31	0
57	MG	YA	3112	1/1	0.95	0.26	29,29,29,29	0
57	MG	RA	3137	1/1	0.95	0.32	22,22,22,22	0
57	MG	YA	3015	1/1	0.95	0.28	17,17,17,17	0
57	MG	YA	3016	1/1	0.95	0.12	17,17,17,17	0
57	MG	YA	3018	1/1	0.95	0.38	11,11,11,11	0
57	MG	XA	1680	1/1	0.95	0.23	25,25,25,25	0
57	MG	YA	3445	1/1	0.95	0.25	25,25,25,25	0
57	MG	RA	3002	1/1	0.95	0.32	24,24,24,24	0
57	MG	YA	3361	1/1	0.95	0.34	37,37,37,37	0
57	MG	RA	3043	1/1	0.95	0.48	7,7,7,7	0
57	MG	YA	3126	1/1	0.95	0.25	41,41,41,41	0
57	MG	YA	3212	1/1	0.95	0.66	25,25,25,25	0
57	MG	YA	3213	1/1	0.95	0.63	30,30,30,30	0
57	MG	YA	3031	1/1	0.95	0.33	26,26,26,26	0
57	MG	RA	3295	1/1	0.95	0.21	41,41,41,41	0
57	MG	YA	3131	1/1	0.95	0.17	27,27,27,27	0
57	MG	YA	3456	1/1	0.95	0.33	125,125,125,125	0
57	MG	YA	3133	1/1	0.95	0.60	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3037	1/1	0.95	0.18	11,11,11,11	0
57	MG	YA	3039	1/1	0.95	0.48	9,9,9,9	0
57	MG	RA	3141	1/1	0.95	0.18	41,41,41,41	0
57	MG	XA	1685	1/1	0.95	0.15	17,17,17,17	0
57	MG	YA	3463	1/1	0.95	0.22	48,48,48,48	0
57	MG	QA	1688	1/1	0.95	0.29	32,32,32,32	0
57	MG	YA	3045	1/1	0.95	0.41	8,8,8,8	0
57	MG	YA	3046	1/1	0.95	0.16	23,23,23,23	0
57	MG	RA	3045	1/1	0.95	0.32	11,11,11,11	0
57	MG	YA	3380	1/1	0.95	0.58	38,38,38,38	0
57	MG	YA	3227	1/1	0.95	0.16	44,44,44,44	0
57	MG	YA	3050	1/1	0.95	0.30	7,7,7,7	0
57	MG	YA	3149	1/1	0.95	0.38	37,37,37,37	0
57	MG	YA	3051	1/1	0.95	0.44	4,4,4,4	0
57	MG	RA	3014	1/1	0.95	0.23	1,1,1,1	0
57	MG	XA	1690	1/1	0.95	0.39	29,29,29,29	0
57	MG	YA	3308	1/1	0.95	0.30	26,26,26,26	0
57	MG	YA	3234	1/1	0.95	0.51	31,31,31,31	0
57	MG	XA	1691	1/1	0.95	0.19	27,27,27,27	0
57	MG	YA	3391	1/1	0.95	0.71	44,44,44,44	0
57	MG	RA	3332	1/1	0.95	0.35	40,40,40,40	0
57	MG	YP	201	1/1	0.95	0.18	8,8,8,8	0
57	MG	YA	3062	1/1	0.95	0.45	32,32,32,32	0
57	MG	RA	3207	1/1	0.95	0.49	20,20,20,20	0
57	MG	YA	3395	1/1	0.95	0.56	55,55,55,55	0
57	MG	XA	1740	1/1	0.95	0.44	69,69,69,69	0
57	MG	XA	1645	1/1	0.95	0.53	41,41,41,41	0
57	MG	RA	3175	1/1	0.95	0.10	45,45,45,45	0
57	MG	RA	3236	1/1	0.95	0.35	23,23,23,23	0
57	MG	RA	3017	1/1	0.95	0.42	5,5,5,5	0
57	MG	XA	1649	1/1	0.95	0.22	13,13,13,13	0
57	MG	QA	1730	1/1	0.95	0.17	40,40,40,40	0
57	MG	XA	1701	1/1	0.95	0.37	30,30,30,30	0
57	MG	QA	1626	1/1	0.95	0.12	40,40,40,40	0
57	MG	QA	1607	1/1	0.95	0.51	26,26,26,26	0
57	MG	QA	1691	1/1	0.95	0.37	26,26,26,26	0
57	MG	RA	3376	1/1	0.95	0.33	25,25,25,25	0
57	MG	RA	3243	1/1	0.95	0.11	37,37,37,37	0
57	MG	RA	3097	1/1	0.96	0.22	17,17,17,17	0
57	MG	RA	3150	1/1	0.96	0.42	42,42,42,42	0
57	MG	YA	3378	1/1	0.96	0.70	40,40,40,40	0
57	MG	RA	3382	1/1	0.96	0.25	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1611	1/1	0.96	0.33	33,33,33,33	0
57	MG	QA	1632	1/1	0.96	0.28	46,46,46,46	0
57	MG	XA	1687	1/1	0.96	0.98	53,53,53,53	0
57	MG	QA	1624	1/1	0.96	0.12	41,41,41,41	0
57	MG	YA	3006	1/1	0.96	0.36	18,18,18,18	0
57	MG	YA	3153	1/1	0.96	0.49	36,36,36,36	0
57	MG	RA	3103	1/1	0.96	0.34	36,36,36,36	0
57	MG	YA	3013	1/1	0.96	0.36	2,2,2,2	0
57	MG	YA	3157	1/1	0.96	0.32	19,19,19,19	0
57	MG	QA	1649	1/1	0.96	0.30	22,22,22,22	0
57	MG	QA	1701	1/1	0.96	0.13	48,48,48,48	0
57	MG	RA	3024	1/1	0.96	0.38	42,42,42,42	0
57	MG	XA	1602	1/1	0.96	0.50	6,6,6,6	0
57	MG	YA	3275	1/1	0.96	0.29	40,40,40,40	0
57	MG	RA	3108	1/1	0.96	0.29	25,25,25,25	0
57	MG	YA	3165	1/1	0.96	0.27	37,37,37,37	0
57	MG	YA	3166	1/1	0.96	0.48	10,10,10,10	0
57	MG	XA	1605	1/1	0.96	0.37	23,23,23,23	0
57	MG	YA	3023	1/1	0.96	0.40	2,2,2,2	0
57	MG	YA	3025	1/1	0.96	0.55	25,25,25,25	0
57	MG	YA	3027	1/1	0.96	0.44	15,15,15,15	0
57	MG	YA	3403	1/1	0.96	0.26	27,27,27,27	0
57	MG	XA	1696	1/1	0.96	0.33	20,20,20,20	0
57	MG	YA	3034	1/1	0.96	0.24	24,24,24,24	0
57	MG	XA	1606	1/1	0.96	0.42	10,10,10,10	0
57	MG	YA	3174	1/1	0.96	0.31	24,24,24,24	0
57	MG	YA	3287	1/1	0.96	0.17	34,34,34,34	0
57	MG	YA	3288	1/1	0.96	0.25	50,50,50,50	0
57	MG	RA	3109	1/1	0.96	0.43	11,11,11,11	0
57	MG	RA	3267	1/1	0.96	0.35	51,51,51,51	0
57	MG	QA	1667	1/1	0.96	0.17	39,39,39,39	0
57	MG	YA	3415	1/1	0.96	0.51	24,24,24,24	0
57	MG	YA	3416	1/1	0.96	0.21	46,46,46,46	0
57	MG	RA	3066	1/1	0.96	0.30	17,17,17,17	0
57	MG	RA	3164	1/1	0.96	0.25	34,34,34,34	0
57	MG	XA	1613	1/1	0.96	0.12	18,18,18,18	0
57	MG	QA	1605	1/1	0.96	0.28	35,35,35,35	0
57	MG	XA	1619	1/1	0.96	0.34	13,13,13,13	0
57	MG	RA	3273	1/1	0.96	0.09	53,53,53,53	0
57	MG	RA	3274	1/1	0.96	0.28	41,41,41,41	0
57	MG	YA	3053	1/1	0.96	0.68	5,5,5,5	0
57	MG	RA	3114	1/1	0.96	0.25	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1623	1/1	0.96	0.09	33,33,33,33	0
57	MG	YA	3190	1/1	0.96	0.50	19,19,19,19	0
57	MG	XA	1624	1/1	0.96	0.09	51,51,51,51	0
57	MG	YA	3192	1/1	0.96	0.07	32,32,32,32	0
57	MG	RA	3117	1/1	0.96	0.56	28,28,28,28	0
57	MG	RA	3069	1/1	0.96	0.36	23,23,23,23	0
57	MG	RA	3031	1/1	0.96	0.26	16,16,16,16	0
57	MG	RA	3170	1/1	0.96	0.49	64,64,64,64	0
57	MG	RA	3405	1/1	0.96	0.50	52,52,52,52	0
57	MG	YA	3070	1/1	0.96	0.23	47,47,47,47	0
57	MG	YA	3071	1/1	0.96	0.30	11,11,11,11	0
57	MG	RA	3122	1/1	0.96	0.24	21,21,21,21	0
57	MG	RA	3073	1/1	0.96	0.33	32,32,32,32	0
57	MG	RA	3225	1/1	0.96	0.18	23,23,23,23	0
57	MG	YA	3319	1/1	0.96	0.29	41,41,41,41	0
57	MG	RA	3074	1/1	0.96	0.34	16,16,16,16	0
57	MG	RA	3410	1/1	0.96	0.15	49,49,49,49	0
57	MG	RA	3174	1/1	0.96	0.54	1,1,1,1	0
57	MG	YA	3448	1/1	0.96	0.20	20,20,20,20	0
57	MG	XA	1637	1/1	0.96	0.23	49,49,49,49	0
57	MG	RA	3076	1/1	0.96	0.29	13,13,13,13	0
57	MG	XA	1641	1/1	0.96	0.11	38,38,38,38	0
57	MG	RA	3034	1/1	0.96	0.24	41,41,41,41	0
57	MG	YA	3331	1/1	0.96	0.48	19,19,19,19	0
57	MG	XA	1727	1/1	0.96	0.18	31,31,31,31	0
57	MG	YA	3092	1/1	0.96	0.25	12,12,12,12	0
57	MG	QA	1726	1/1	0.96	0.15	48,48,48,48	0
57	MG	RA	3290	1/1	0.96	0.13	49,49,49,49	0
57	MG	RA	3291	1/1	0.96	0.32	39,39,39,39	0
57	MG	XA	1731	1/1	0.96	0.26	27,27,27,27	0
57	MG	RA	3178	1/1	0.96	0.27	45,45,45,45	0
57	MG	QA	1727	1/1	0.96	0.25	77,77,77,77	0
57	MG	RA	3420	1/1	0.96	0.27	74,74,74,74	0
57	MG	RA	3130	1/1	0.96	0.11	34,34,34,34	0
57	MG	QA	1715	1/1	0.96	0.14	46,46,46,46	0
57	MG	QA	1676	1/1	0.96	0.32	40,40,40,40	0
57	MG	QA	1622	1/1	0.96	0.19	20,20,20,20	0
57	MG	RA	3184	1/1	0.96	0.36	28,28,28,28	0
57	MG	RA	3088	1/1	0.96	0.45	15,15,15,15	0
57	MG	XA	1657	1/1	0.96	0.50	34,34,34,34	0
57	MG	YB	201	1/1	0.96	0.43	28,28,28,28	0
57	MG	RA	3005	1/1	0.96	0.14	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1659	1/1	0.96	0.69	22,22,22,22	0
57	MG	RA	3007	1/1	0.96	0.43	13,13,13,13	0
57	MG	RA	3188	1/1	0.96	0.46	38,38,38,38	0
57	MG	XA	1747	1/1	0.96	0.27	55,55,55,55	0
57	MG	YE	301	1/1	0.96	0.29	4,4,4,4	0
57	MG	YA	3116	1/1	0.96	0.55	17,17,17,17	0
57	MG	RA	3361	1/1	0.96	0.26	35,35,35,35	0
57	MG	YH	201	1/1	0.96	0.20	80,80,80,80	0
57	MG	YA	3118	1/1	0.96	0.28	23,23,23,23	0
57	MG	RA	3304	1/1	0.96	0.28	36,36,36,36	0
57	MG	YA	3241	1/1	0.96	0.27	19,19,19,19	0
57	MG	RA	3009	1/1	0.96	0.60	16,16,16,16	0
57	MG	RA	3010	1/1	0.96	0.20	16,16,16,16	0
57	MG	RA	3047	1/1	0.96	0.55	5,5,5,5	0
57	MG	RA	3197	1/1	0.96	0.32	17,17,17,17	0
57	MG	YA	3364	1/1	0.96	0.50	52,52,52,52	0
57	MG	RA	3011	1/1	0.96	0.54	8,8,8,8	0
57	MG	RA	3250	1/1	0.96	0.31	31,31,31,31	0
57	MG	RA	3143	1/1	0.96	0.29	4,4,4,4	0
57	MG	RA	3012	1/1	0.96	0.24	4,4,4,4	0
57	MG	RA	3373	1/1	0.96	0.14	52,52,52,52	0
57	MG	QA	1687	1/1	0.96	0.29	50,50,50,50	0
57	MG	Y5	101	1/1	0.96	0.13	7,7,7,7	0
57	MG	YA	3138	1/1	0.96	0.24	17,17,17,17	0
57	MG	RA	3315	1/1	0.96	0.44	25,25,25,25	0
57	MG	YA	3140	1/1	0.96	0.19	30,30,30,30	0
57	MG	RA	3148	1/1	0.96	0.32	10,10,10,10	0
58	ZN	XD	301	1/1	0.96	0.34	66,66,66,66	0
57	MG	XF	201	1/1	0.96	0.38	41,41,41,41	0
57	MG	QA	1652	1/1	0.97	0.19	20,20,20,20	0
57	MG	XA	1627	1/1	0.97	0.11	73,73,73,73	0
57	MG	RA	3297	1/1	0.97	0.31	49,49,49,49	0
57	MG	RA	3125	1/1	0.97	0.22	29,29,29,29	0
57	MG	RA	3098	1/1	0.97	0.38	11,11,11,11	0
57	MG	YA	3003	1/1	0.97	0.35	10,10,10,10	0
57	MG	RA	3075	1/1	0.97	0.22	14,14,14,14	0
57	MG	YA	3335	1/1	0.97	0.36	31,31,31,31	0
57	MG	QA	1653	1/1	0.97	0.34	25,25,25,25	0
57	MG	RA	3032	1/1	0.97	0.40	26,26,26,26	0
57	MG	YA	3009	1/1	0.97	0.46	10,10,10,10	0
57	MG	YA	3010	1/1	0.97	0.20	1,1,1,1	0
57	MG	YA	3012	1/1	0.97	0.24	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	QA	1635	1/1	0.97	0.23	30,30,30,30	0
57	MG	YA	3014	1/1	0.97	0.29	18,18,18,18	0
57	MG	RA	3368	1/1	0.97	0.29	59,59,59,59	0
57	MG	RA	3272	1/1	0.97	0.12	35,35,35,35	0
57	MG	YA	3017	1/1	0.97	0.38	2,2,2,2	0
57	MG	YA	3433	1/1	0.97	0.22	33,33,33,33	0
57	MG	RA	3082	1/1	0.97	0.43	22,22,22,22	0
57	MG	YA	3435	1/1	0.97	0.16	35,35,35,35	0
57	MG	RA	3371	1/1	0.97	0.21	33,33,33,33	0
57	MG	QA	1686	1/1	0.97	0.11	31,31,31,31	0
57	MG	RA	3159	1/1	0.97	0.34	19,19,19,19	0
57	MG	XA	1644	1/1	0.97	0.28	24,24,24,24	0
57	MG	YA	3188	1/1	0.97	0.28	43,43,43,43	0
57	MG	RA	3036	1/1	0.97	0.37	4,4,4,4	0
57	MG	RA	3375	1/1	0.97	0.28	10,10,10,10	0
57	MG	YA	3028	1/1	0.97	0.20	14,14,14,14	0
57	MG	YA	3110	1/1	0.97	0.30	27,27,27,27	0
57	MG	YA	3029	1/1	0.97	0.23	18,18,18,18	0
57	MG	YA	3271	1/1	0.97	0.30	25,25,25,25	0
57	MG	YA	3272	1/1	0.97	0.36	49,49,49,49	0
57	MG	RA	3161	1/1	0.97	0.18	44,44,44,44	0
57	MG	QA	1714	1/1	0.97	0.32	66,66,66,66	0
57	MG	RA	3379	1/1	0.97	0.18	44,44,44,44	0
57	MG	RA	3016	1/1	0.97	0.08	7,7,7,7	0
57	MG	YA	3038	1/1	0.97	0.32	38,38,38,38	0
57	MG	RA	3312	1/1	0.97	0.30	1,1,1,1	0
57	MG	RA	3280	1/1	0.97	0.16	20,20,20,20	0
57	MG	RA	3190	1/1	0.97	0.46	10,10,10,10	0
57	MG	YA	3203	1/1	0.97	0.11	18,18,18,18	0
57	MG	RA	3191	1/1	0.97	0.17	10,10,10,10	0
57	MG	YA	3044	1/1	0.97	0.44	2,2,2,2	0
57	MG	RA	3060	1/1	0.97	0.25	18,18,18,18	0
57	MG	YA	3208	1/1	0.97	0.31	7,7,7,7	0
57	MG	YA	3462	1/1	0.97	0.54	39,39,39,39	0
57	MG	XA	1609	1/1	0.97	0.08	53,53,53,53	0
57	MG	YA	3464	1/1	0.97	0.14	46,46,46,46	0
57	MG	YA	3129	1/1	0.97	0.39	20,20,20,20	0
57	MG	YA	3047	1/1	0.97	0.59	32,32,32,32	0
57	MG	YA	3289	1/1	0.97	0.30	31,31,31,31	0
57	MG	RA	3193	1/1	0.97	0.69	17,17,17,17	0
57	MG	YA	3132	1/1	0.97	0.38	59,59,59,59	0
57	MG	YA	3470	1/1	0.97	0.20	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1750	1/1	0.97	0.21	46,46,46,46	0
57	MG	QA	1610	1/1	0.97	0.09	48,48,48,48	0
57	MG	YA	3052	1/1	0.97	0.61	26,26,26,26	0
57	MG	YA	3136	1/1	0.97	0.34	28,28,28,28	0
57	MG	YA	3296	1/1	0.97	0.50	34,34,34,34	0
57	MG	YA	3297	1/1	0.97	0.45	31,31,31,31	0
57	MG	YB	205	1/1	0.97	0.11	58,58,58,58	0
57	MG	QA	1656	1/1	0.97	0.28	16,16,16,16	0
57	MG	YA	3054	1/1	0.97	0.21	0,0,0,0	0
57	MG	YA	3056	1/1	0.97	0.22	4,4,4,4	0
57	MG	RA	3021	1/1	0.97	0.47	25,25,25,25	0
57	MG	RA	3115	1/1	0.97	0.37	13,13,13,13	0
57	MG	XA	1617	1/1	0.97	0.56	36,36,36,36	0
57	MG	XA	1618	1/1	0.97	0.62	23,23,23,23	0
57	MG	RA	3429	1/1	0.97	0.15	19,19,19,19	0
57	MG	YA	3063	1/1	0.97	0.51	4,4,4,4	0
57	MG	QA	1664	1/1	0.97	0.23	23,23,23,23	0
57	MG	YA	3229	1/1	0.97	0.29	54,54,54,54	0
57	MG	YA	3066	1/1	0.97	0.33	29,29,29,29	0
57	MG	RA	3145	1/1	0.97	0.25	20,20,20,20	0
57	MG	YA	3068	1/1	0.97	0.28	35,35,35,35	0
57	MG	XA	1715	1/1	0.97	0.36	27,27,27,27	0
57	MG	RA	3006	1/1	0.97	0.29	3,3,3,3	0
57	MG	QA	1642	1/1	0.97	0.20	51,51,51,51	0
57	MG	YA	3072	1/1	0.97	0.32	12,12,12,12	0
57	MG	RA	3072	1/1	0.97	0.35	4,4,4,4	0
57	MG	YA	3074	1/1	0.97	0.43	13,13,13,13	0
57	MG	YA	3406	1/1	0.97	0.35	8,8,8,8	0
57	MG	QA	1651	1/1	0.97	0.25	31,31,31,31	0
57	MG	YA	3320	1/1	0.97	0.21	56,56,56,56	0
57	MG	YA	3162	1/1	0.97	0.18	38,38,38,38	0
57	MG	YA	3077	1/1	0.97	0.49	8,8,8,8	0
57	MG	YA	3080	1/1	0.97	0.51	2,2,2,2	0
57	MG	YA	3326	1/1	0.97	0.19	64,64,64,64	0
57	MG	YA	3107	1/1	0.98	0.14	2,2,2,2	0
57	MG	RA	3144	1/1	0.98	0.37	11,11,11,11	0
57	MG	RA	3229	1/1	0.98	0.30	16,16,16,16	0
57	MG	XA	1615	1/1	0.98	0.55	46,46,46,46	0
57	MG	RA	3046	1/1	0.98	0.16	17,17,17,17	0
57	MG	RA	3118	1/1	0.98	0.20	5,5,5,5	0
57	MG	RA	3027	1/1	0.98	0.31	8,8,8,8	0
57	MG	RA	3077	1/1	0.98	0.49	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3115	1/1	0.98	0.16	3,3,3,3	0
57	MG	YA	3049	1/1	0.98	0.43	4,4,4,4	0
57	MG	RA	3018	1/1	0.98	0.34	17,17,17,17	0
57	MG	XA	1664	1/1	0.98	0.31	14,14,14,14	0
57	MG	RA	3235	1/1	0.98	0.10	20,20,20,20	0
57	MG	YA	3196	1/1	0.98	0.40	22,22,22,22	0
57	MG	RA	3079	1/1	0.98	0.34	5,5,5,5	0
57	MG	YA	3121	1/1	0.98	0.36	11,11,11,11	0
57	MG	RA	3080	1/1	0.98	0.44	4,4,4,4	0
57	MG	YA	3123	1/1	0.98	0.32	5,5,5,5	0
57	MG	YA	3055	1/1	0.98	0.46	5,5,5,5	0
57	MG	RA	3063	1/1	0.98	0.29	23,23,23,23	0
57	MG	YA	3441	1/1	0.98	0.40	9,9,9,9	0
57	MG	XA	1669	1/1	0.98	0.27	25,25,25,25	0
57	MG	RA	3404	1/1	0.98	0.19	51,51,51,51	0
57	MG	YA	3059	1/1	0.98	0.22	7,7,7,7	0
57	MG	XA	1671	1/1	0.98	0.11	6,6,6,6	0
57	MG	YA	3207	1/1	0.98	0.61	13,13,13,13	0
57	MG	RA	3239	1/1	0.98	0.21	20,20,20,20	0
57	MG	XA	1673	1/1	0.98	0.21	45,45,45,45	0
57	MG	XA	1674	1/1	0.98	0.09	18,18,18,18	0
57	MG	YA	3002	1/1	0.98	0.20	5,5,5,5	0
57	MG	RA	3101	1/1	0.98	0.28	37,37,37,37	0
57	MG	YA	3137	1/1	0.98	0.26	5,5,5,5	0
57	MG	YA	3004	1/1	0.98	0.30	4,4,4,4	0
57	MG	RA	3003	1/1	0.98	0.38	16,16,16,16	0
57	MG	RA	3065	1/1	0.98	0.18	32,32,32,32	0
57	MG	QA	1644	1/1	0.98	0.25	19,19,19,19	0
57	MG	YA	3008	1/1	0.98	0.15	20,20,20,20	0
57	MG	YA	3143	1/1	0.98	0.39	28,28,28,28	0
57	MG	YA	3144	1/1	0.98	0.46	41,41,41,41	0
57	MG	XA	1679	1/1	0.98	0.30	41,41,41,41	0
57	MG	RA	3085	1/1	0.98	0.17	26,26,26,26	0
57	MG	RA	3411	1/1	0.98	0.40	44,44,44,44	0
57	MG	YA	3075	1/1	0.98	0.20	19,19,19,19	0
57	MG	RA	3131	1/1	0.98	0.13	20,20,20,20	0
57	MG	RA	3377	1/1	0.98	0.42	10,10,10,10	0
57	MG	YA	3078	1/1	0.98	0.29	28,28,28,28	0
57	MG	YA	3079	1/1	0.98	0.44	7,7,7,7	0
57	MG	RA	3067	1/1	0.98	0.48	20,20,20,20	0
57	MG	YA	3154	1/1	0.98	0.21	17,17,17,17	0
57	MG	RA	3107	1/1	0.98	0.36	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1638	1/1	0.98	0.34	57,57,57,57	0
57	MG	RA	3015	1/1	0.98	0.36	10,10,10,10	0
57	MG	YA	3473	1/1	0.98	0.40	8,8,8,8	0
57	MG	YA	3389	1/1	0.98	0.14	55,55,55,55	0
57	MG	XA	1640	1/1	0.98	0.46	23,23,23,23	0
57	MG	YA	3311	1/1	0.98	0.14	60,60,60,60	0
57	MG	YA	3085	1/1	0.98	0.17	7,7,7,7	0
57	MG	YA	3086	1/1	0.98	0.23	38,38,38,38	0
57	MG	RA	3189	1/1	0.98	0.51	21,21,21,21	0
57	MG	YA	3021	1/1	0.98	0.44	11,11,11,11	0
57	MG	QA	1616	1/1	0.98	0.20	52,52,52,52	0
57	MG	YA	3397	1/1	0.98	0.06	41,41,41,41	0
57	MG	XA	1601	1/1	0.98	0.36	7,7,7,7	0
57	MG	YA	3024	1/1	0.98	0.44	12,12,12,12	0
57	MG	RA	3070	1/1	0.98	0.41	18,18,18,18	0
57	MG	YA	3026	1/1	0.98	0.23	8,8,8,8	0
57	MG	XA	1603	1/1	0.98	0.15	19,19,19,19	0
57	MG	RA	3054	1/1	0.98	0.39	0,0,0,0	0
57	MG	YA	3323	1/1	0.98	0.29	1,1,1,1	0
57	MG	YA	3324	1/1	0.98	0.57	4,4,4,4	0
57	MG	RA	3112	1/1	0.98	0.16	36,36,36,36	0
57	MG	YA	3030	1/1	0.98	0.48	6,6,6,6	0
57	MG	YA	3408	1/1	0.98	0.07	46,46,46,46	0
57	MG	RA	3139	1/1	0.98	0.19	15,15,15,15	0
57	MG	YA	3033	1/1	0.98	0.23	10,10,10,10	0
57	MG	QV	101	1/1	0.98	0.23	19,19,19,19	0
57	MG	YA	3176	1/1	0.98	0.35	3,3,3,3	0
57	MG	RA	3057	1/1	0.98	0.28	5,5,5,5	0
57	MG	YA	3102	1/1	0.98	0.31	18,18,18,18	0
57	MG	RA	3289	1/1	0.98	0.12	14,14,14,14	0
57	MG	YA	3334	1/1	0.98	0.60	24,24,24,24	0
57	MG	RA	3026	1/1	0.98	0.25	5,5,5,5	0
57	MG	RA	3258	1/1	0.98	0.26	32,32,32,32	0
57	MG	RA	3116	1/1	0.98	0.46	30,30,30,30	0
57	MG	YA	3420	1/1	0.98	0.19	33,33,33,33	0
57	MG	XA	1616	1/1	0.99	0.29	11,11,11,11	0
57	MG	RA	3051	1/1	0.99	0.36	11,11,11,11	0
57	MG	RA	3033	1/1	0.99	0.28	12,12,12,12	0
57	MG	RA	3020	1/1	0.99	0.37	9,9,9,9	0
57	MG	RA	3008	1/1	0.99	0.14	35,35,35,35	0
57	MG	RA	3055	1/1	0.99	0.24	17,17,17,17	0
57	MG	RA	3194	1/1	0.99	0.38	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	YA	3125	1/1	0.99	0.28	13,13,13,13	0
57	MG	QA	1645	1/1	0.99	0.17	52,52,52,52	0
57	MG	YA	3011	1/1	0.99	0.62	3,3,3,3	0
57	MG	YA	3128	1/1	0.99	0.08	27,27,27,27	0
57	MG	YA	3032	1/1	0.99	0.27	7,7,7,7	0
57	MG	RA	3029	1/1	0.99	0.19	14,14,14,14	0
57	MG	QA	1641	1/1	0.99	0.32	28,28,28,28	0
57	MG	RA	3004	1/1	0.99	0.56	3,3,3,3	0
57	MG	YA	3036	1/1	0.99	0.44	7,7,7,7	0
57	MG	XA	1643	1/1	0.99	0.29	29,29,29,29	0
57	MG	YA	3161	1/1	0.99	0.22	10,10,10,10	0
57	MG	R0	103	1/1	0.99	0.29	22,22,22,22	0
57	MG	XV	101	1/1	0.99	0.19	7,7,7,7	0
57	MG	RA	3025	1/1	0.99	0.28	10,10,10,10	0
57	MG	YA	3064	1/1	0.99	0.15	11,11,11,11	0
57	MG	YA	3041	1/1	0.99	0.31	23,23,23,23	0
57	MG	RA	3121	1/1	0.99	0.21	5,5,5,5	0
57	MG	RA	3041	1/1	0.99	0.33	7,7,7,7	0
58	ZN	QD	301	1/1	0.99	0.32	44,44,44,44	0
57	MG	YA	3223	1/1	0.99	0.29	25,25,25,25	0
57	MG	XA	1733	1/1	0.99	0.38	8,8,8,8	0
57	MG	RA	3062	1/1	0.99	0.35	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.