



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 09:23 pm BST

PDB ID : 4W4G
Title : Postcleavage state of 70S bound to HigB toxin and AAA (lysine) codon
Authors : Schureck, M.A.; Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2014-08-14
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

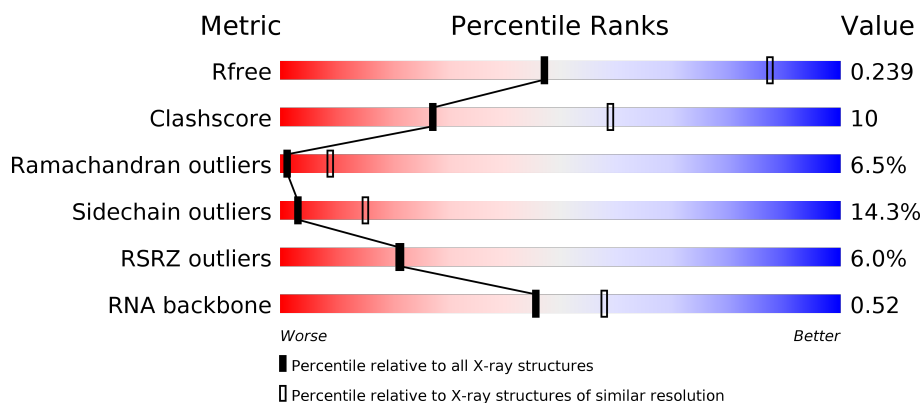
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div>3%</div> <div>56%</div> <div>32%</div> <div>10%</div> <div>.</div> </div>
1	XA	1522	<div> <div>4%</div> <div>57%</div> <div>34%</div> <div>7%</div> <div>.</div> </div>
2	QB	256	<div> <div>10%</div> <div>52%</div> <div>31%</div> <div>8%</div> <div>8%</div> </div>
2	XB	256	<div> <div>6%</div> <div>50%</div> <div>34%</div> <div>8%</div> <div>8%</div> </div>

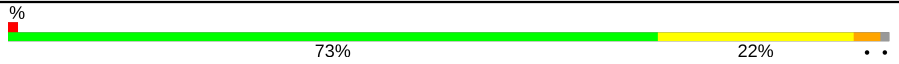



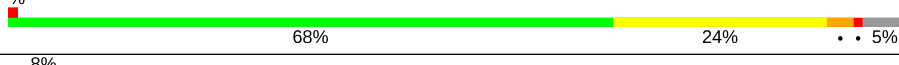
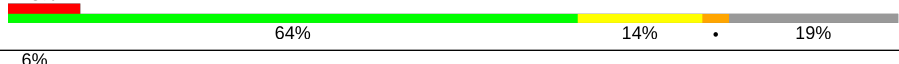
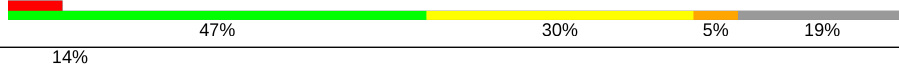
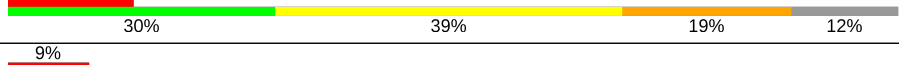
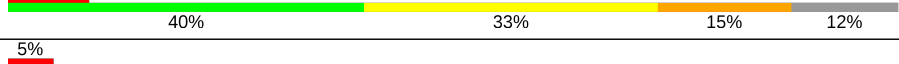


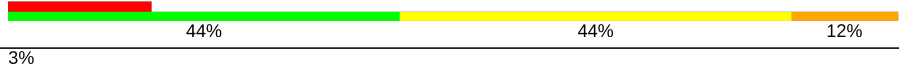

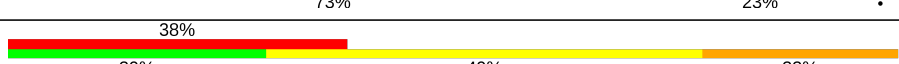
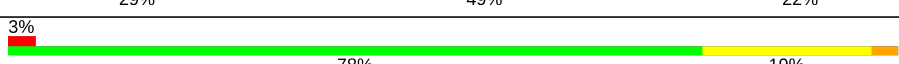
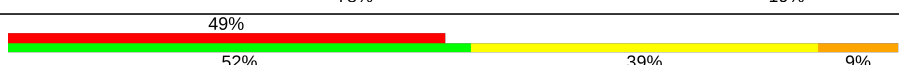
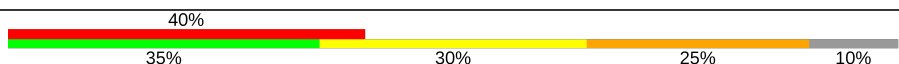
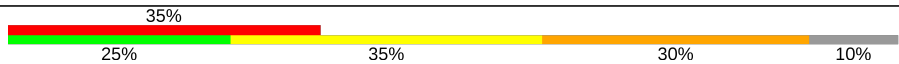



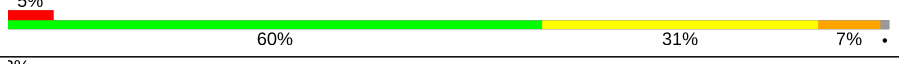
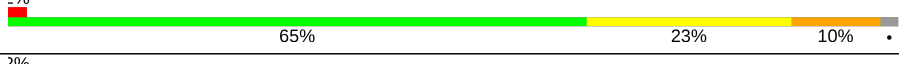


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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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

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Mol	Chain	Length	Quality of chain
27	RD	276	
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	

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Mol	Chain	Length	Quality of chain
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	

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Mol	Chain	Length	Quality of chain
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	

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
23	A3P	XX	20	-	-	-	X
56	MG	QA	1626	-	-	-	X
56	MG	QA	1645	-	-	-	X
56	MG	QA	1690	-	-	-	X
56	MG	QA	1704	-	-	-	X
56	MG	QA	1706	-	-	-	X
56	MG	QA	1709	-	-	-	X
56	MG	QA	1715	-	-	-	X
56	MG	QA	1732	-	-	-	X
56	MG	QA	1735	-	-	-	X
56	MG	QV	103	-	-	-	X
56	MG	R2	101	-	-	-	X
56	MG	RA	3001	-	-	-	X
56	MG	RA	3007	-	-	-	X
56	MG	RA	3050	-	-	-	X
56	MG	RA	3074	-	-	-	X
56	MG	RA	3132	-	-	-	X
56	MG	RA	3135	-	-	-	X
56	MG	RA	3161	-	-	-	X
56	MG	RA	3175	-	-	-	X
56	MG	RA	3216	-	-	-	X
56	MG	RA	3233	-	-	-	X
56	MG	RA	3239	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3245	-	-	-	X
56	MG	RA	3251	-	-	-	X
56	MG	RA	3267	-	-	-	X
56	MG	RA	3272	-	-	-	X
56	MG	RA	3274	-	-	-	X
56	MG	RA	3295	-	-	-	X
56	MG	RA	3309	-	-	-	X
56	MG	RA	3314	-	-	-	X
56	MG	RA	3315	-	-	-	X
56	MG	RA	3319	-	-	-	X
56	MG	RA	3326	-	-	-	X
56	MG	RA	3327	-	-	-	X
56	MG	RA	3341	-	-	-	X
56	MG	RA	3350	-	-	-	X
56	MG	RA	3351	-	-	-	X
56	MG	RA	3388	-	-	-	X
56	MG	RA	3402	-	-	-	X
56	MG	RA	3405	-	-	-	X
56	MG	RQ	201	-	-	-	X
56	MG	RU	201	-	-	-	X
56	MG	XA	1637	-	-	-	X
56	MG	XA	1647	-	-	-	X
56	MG	XA	1660	-	-	-	X
56	MG	XA	1689	-	-	-	X
56	MG	XA	1702	-	-	-	X
56	MG	XA	1706	-	-	-	X
56	MG	XA	1728	-	-	-	X
56	MG	XA	1731	-	-	-	X
56	MG	XA	1754	-	-	-	X
56	MG	YA	3001	-	-	-	X
56	MG	YA	3151	-	-	-	X
56	MG	YA	3181	-	-	-	X
56	MG	YA	3266	-	-	-	X
56	MG	YA	3276	-	-	-	X
56	MG	YA	3285	-	-	-	X
56	MG	YA	3291	-	-	-	X
56	MG	YA	3298	-	-	-	X
56	MG	YA	3312	-	-	-	X
56	MG	YA	3336	-	-	-	X
56	MG	YA	3347	-	-	-	X
56	MG	YA	3349	-	-	-	X
56	MG	YA	3351	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3369	-	-	-	X
56	MG	YA	3375	-	-	-	X
56	MG	YA	3379	-	-	-	X
56	MG	YA	3389	-	-	-	X
56	MG	YA	3418	-	-	-	X
56	MG	YA	3434	-	-	-	X
56	MG	YA	3446	-	-	-	X
56	MG	YQ	202	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 297400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			399	177	82	121	19			
23	XX	18	Total	C	N	O	P	0	0	0
			399	177	82	121	19			

- Molecule 24 is a protein called Host inhibition of growth B.

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

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QY	0	MET	-	insertion	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	-	insertion	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	C	N	O	P	0	0	0
			62269	27713	11649	20016	2891			
25	YA	2875	Total	C	N	O	P	0	0	0
			61924	27560	11583	19906	2875			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
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
46	R0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			
46	Y0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	Y9	36	Total	C	N	O	S	0	0	0
			298	183	67	45	3			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	140	Total 140	Mg 140	0	0
56	YV	1	Total 1	Mg 1	0	0
56	RP	2	Total 2	Mg 2	0	0
56	YA	464	Total 464	Mg 464	0	0
56	Y5	2	Total 2	Mg 2	0	0
56	YH	1	Total 1	Mg 1	0	0
56	YR	1	Total 1	Mg 1	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	YD	1	Total 1	Mg 1	0	0
56	QV	5	Total 5	Mg 5	0	0
56	YO	1	Total 1	Mg 1	0	0
56	XA	160	Total 160	Mg 160	0	0
56	YY	1	Total 1	Mg 1	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	XN	1	Total 1	Mg 1	0	0
56	QL	1	Total 1	Mg 1	0	0
56	YU	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	Y0	3	Total 3	Mg 3	0	0
56	YG	1	Total 1	Mg 1	0	0
56	YQ	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RY	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	XF	1	Total 1	Mg 1	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RD	2	Total 2	Mg 2	0	0
56	XL	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	R5	3	Total 3	Mg 3	0	0
56	RA	413	Total 413	Mg 413	0	0
56	YP	2	Total 2	Mg 2	0	0
56	RE	1	Total 1	Mg 1	0	0
56	R2	1	Total 1	Mg 1	0	0
56	YB	5	Total 5	Mg 5	0	0
56	R0	2	Total 2	Mg 2	0	0
56	XV	4	Total 4	Mg 4	0	0
56	RB	4	Total 4	Mg 4	0	0
56	QE	1	Total 1	Mg 1	0	0
56	XD	1	Total 1	Mg 1	0	0
56	RF	1	Total 1	Mg 1	0	0
56	YE	2	Total 2	Mg 2	0	0

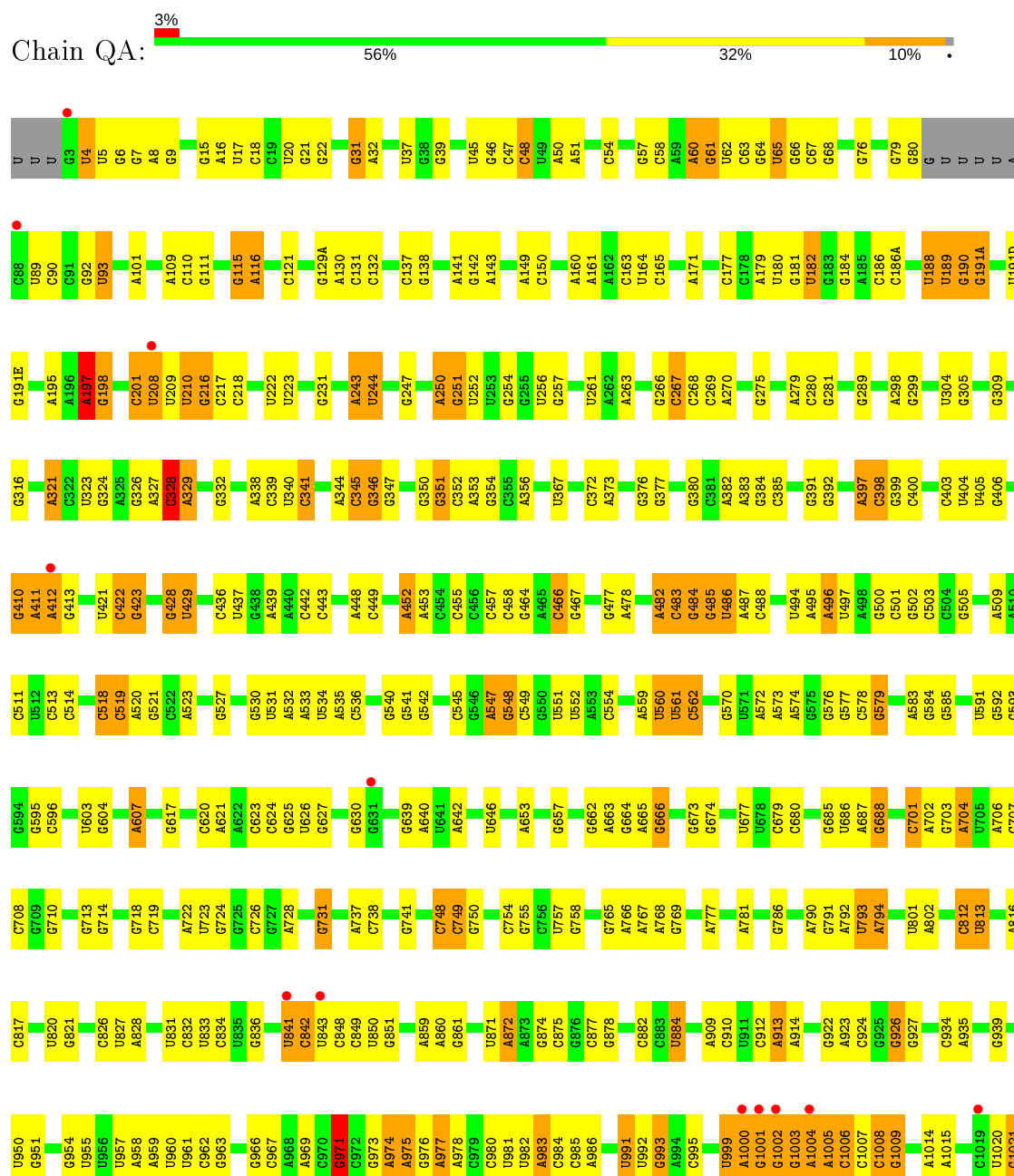
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

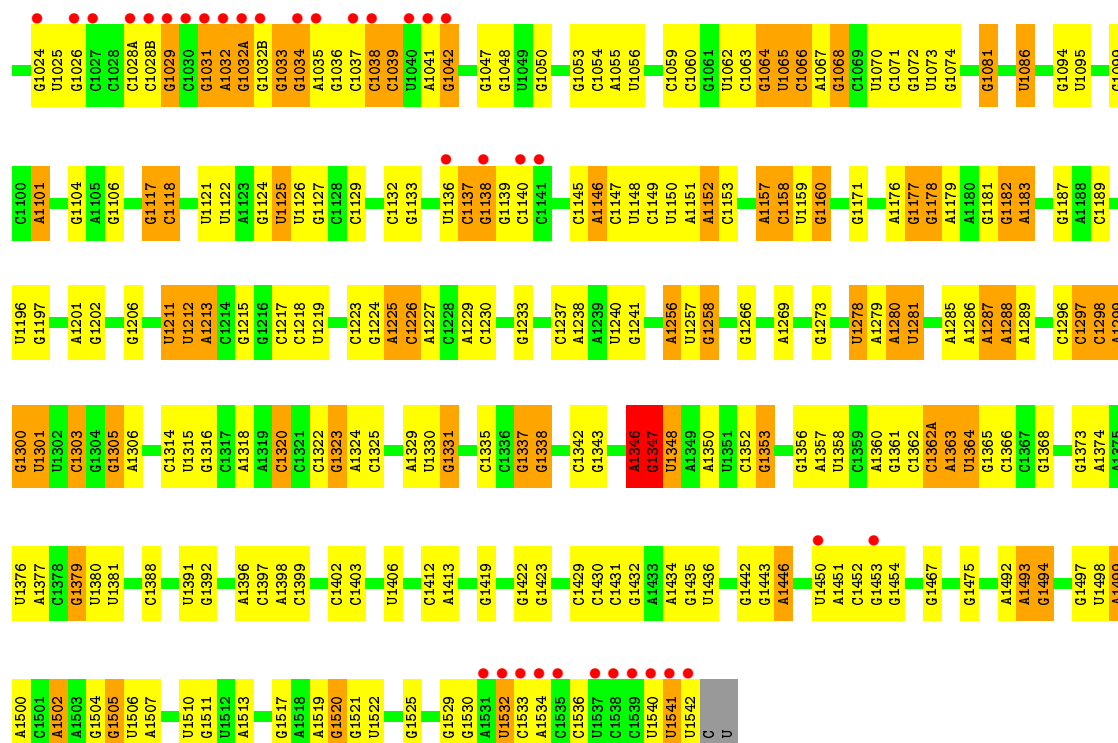
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XD	1	Total 1	Zn 1	0	0
57	QD	1	Total 1	Zn 1	0	0
57	QN	1	Total 1	Zn 1	0	0
57	XN	1	Total 1	Zn 1	0	0

3 Residue-property plots

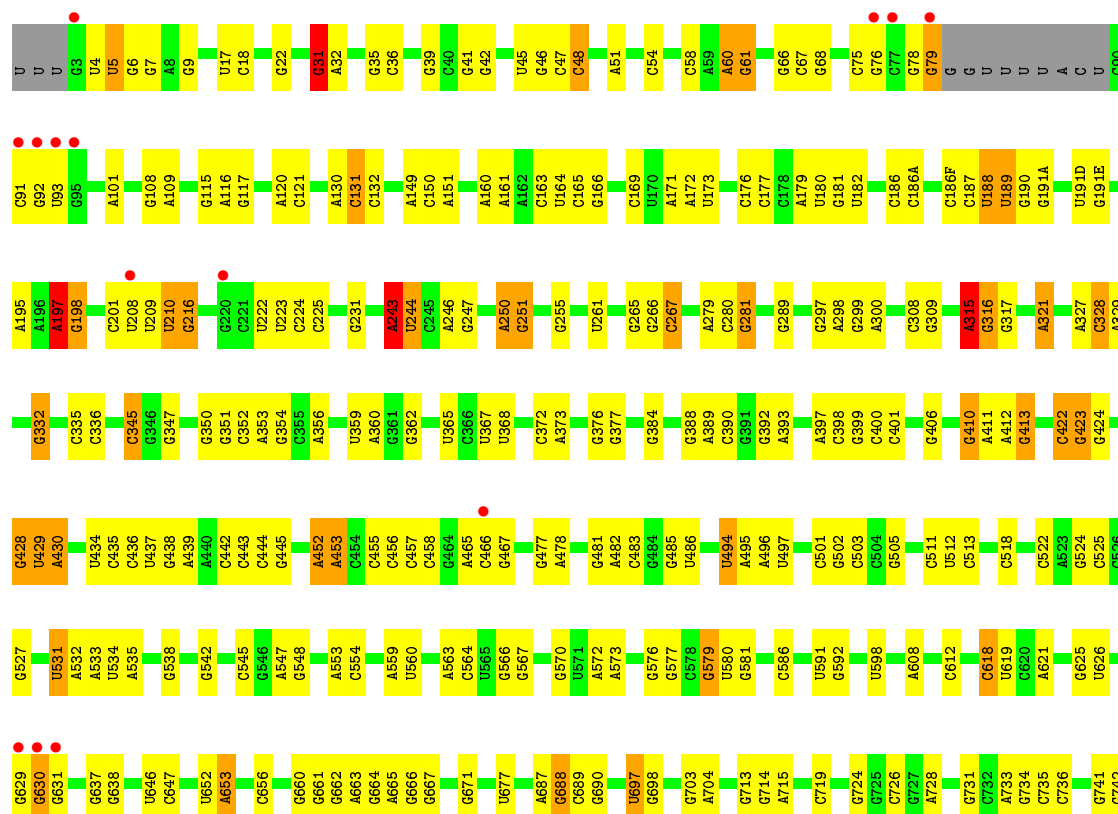
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

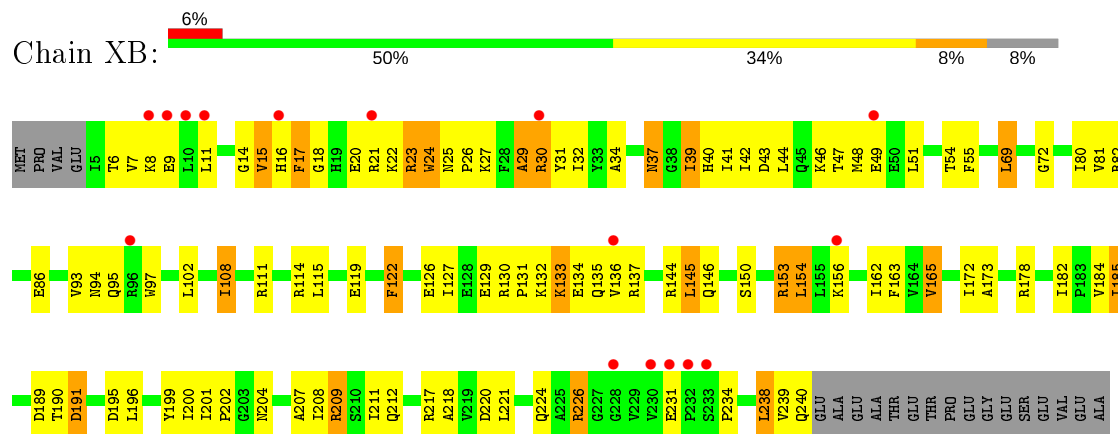




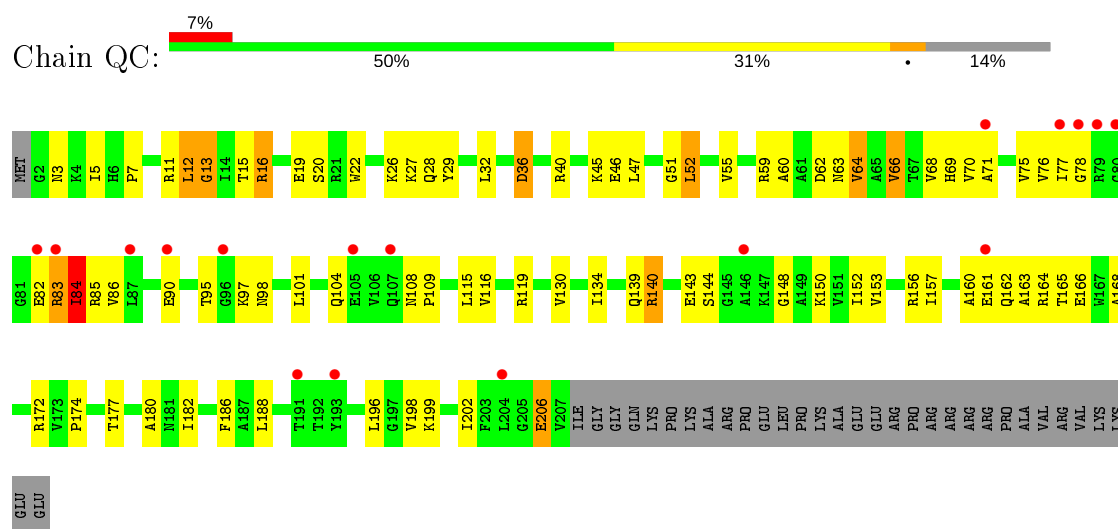
• Molecule 1: 16S rRNA



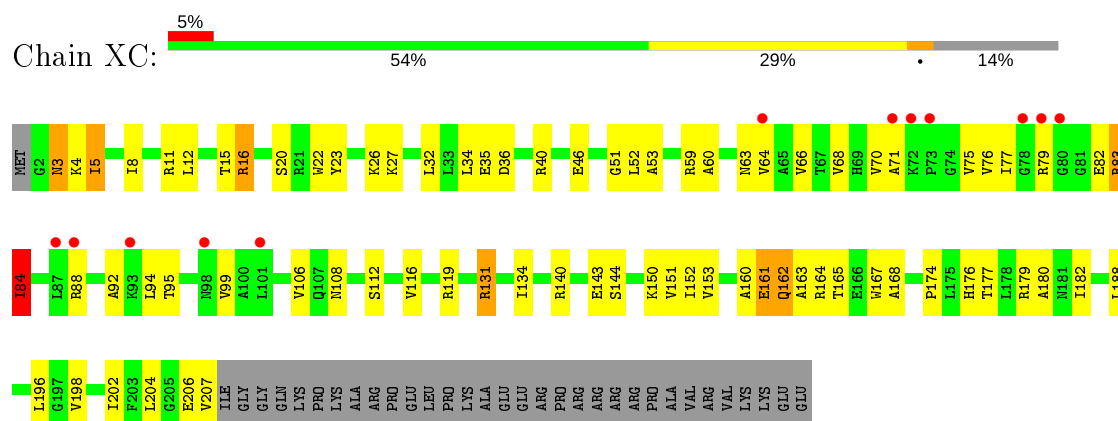
- Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

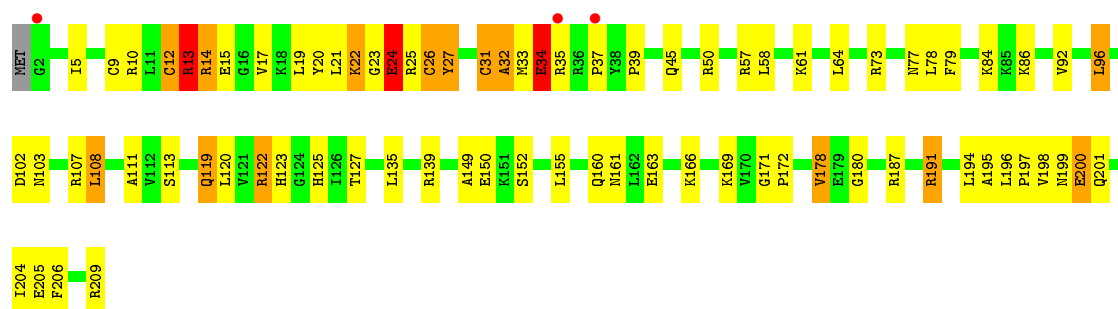


- Molecule 3: 30S ribosomal protein S3

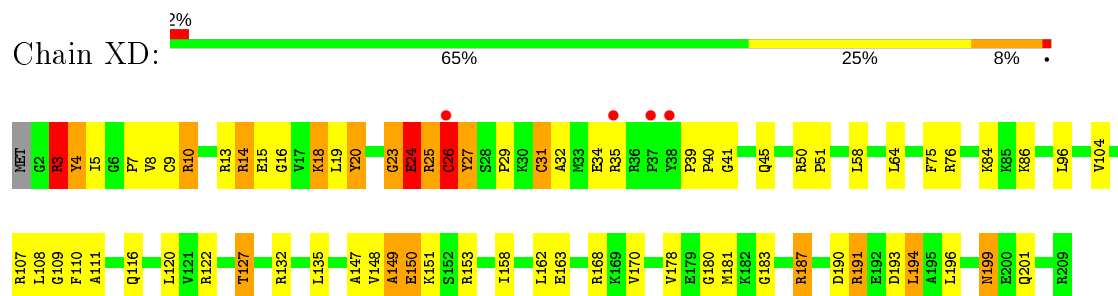


- Molecule 4: 30S ribosomal protein S4

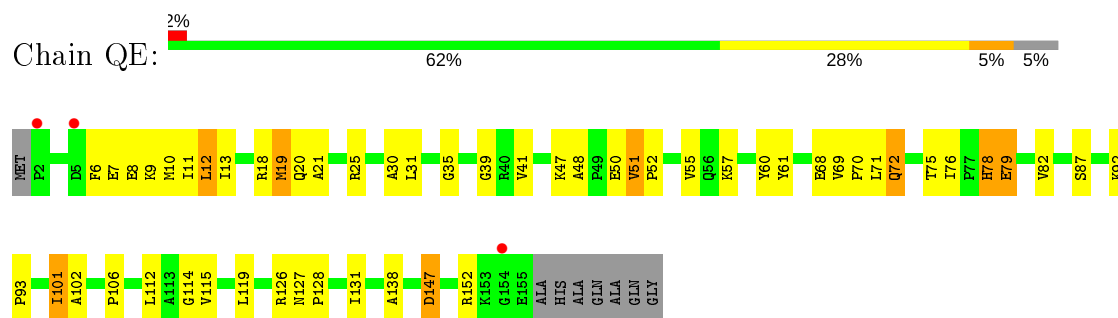




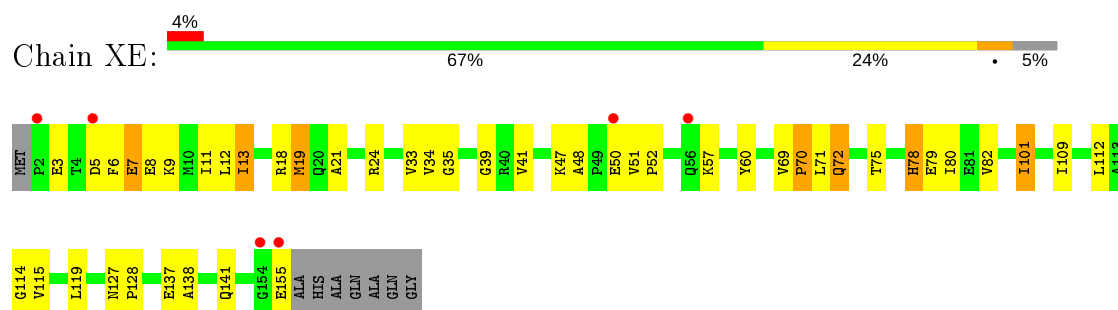
- Molecule 4: 30S ribosomal protein S4



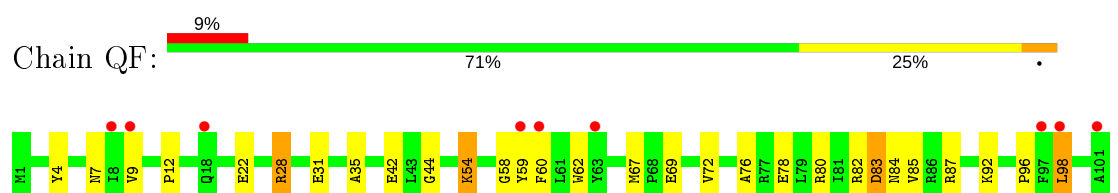
- Molecule 5: 30S ribosomal protein S5



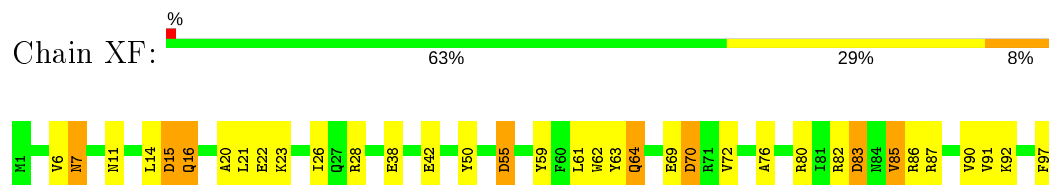
- Molecule 5: 30S ribosomal protein S5



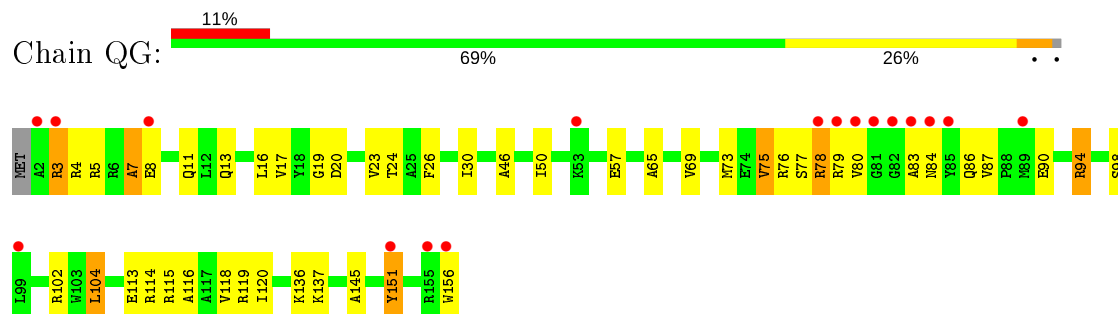
- Molecule 6: 30S ribosomal protein S6



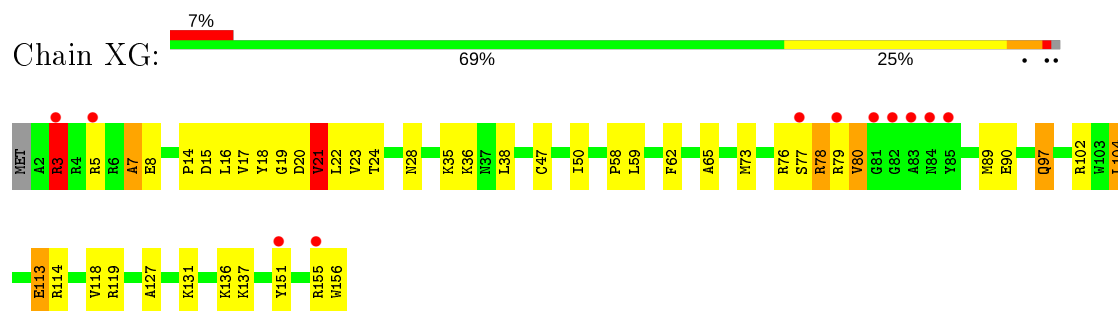
- Molecule 6: 30S ribosomal protein S6



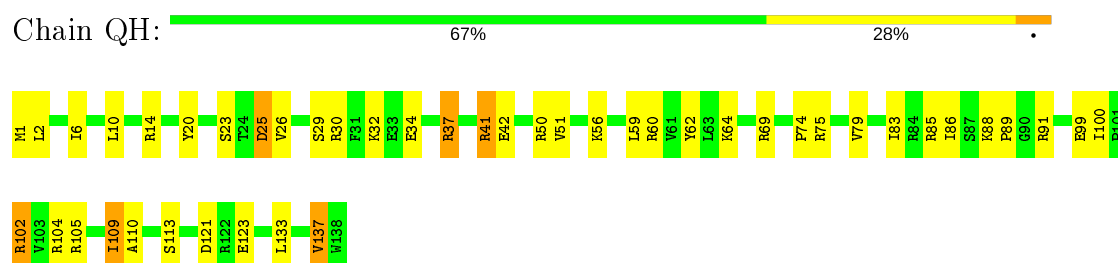
- Molecule 7: 30S ribosomal protein S7



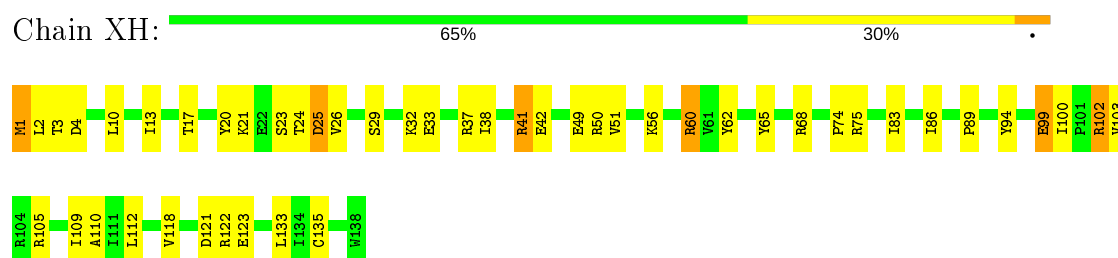
- Molecule 7: 30S ribosomal protein S7



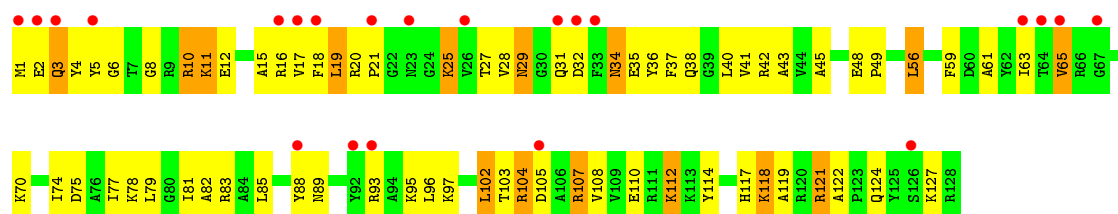
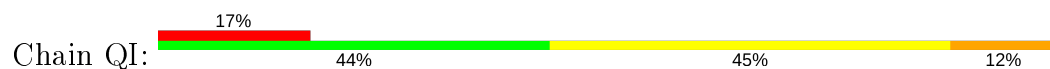
- Molecule 8: 30S ribosomal protein S8



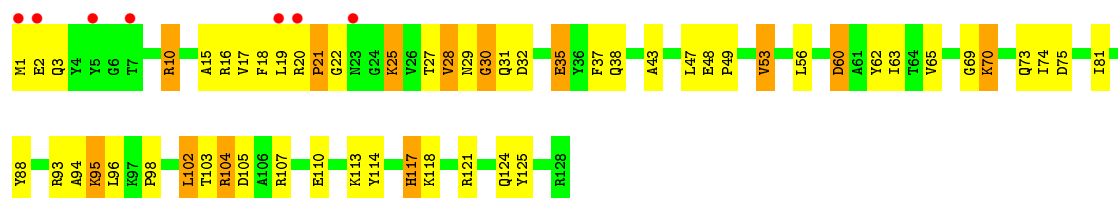
- Molecule 8: 30S ribosomal protein S8



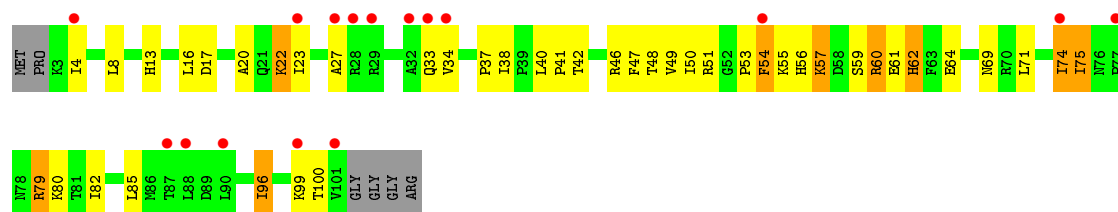
- Molecule 9: 30S ribosomal protein S9



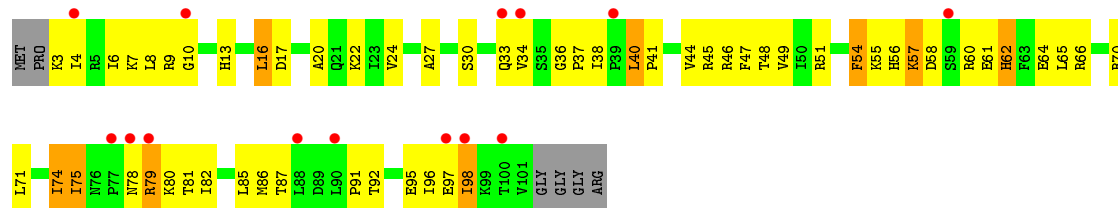
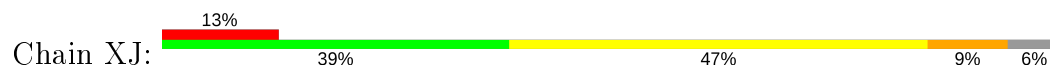
- Molecule 9: 30S ribosomal protein S9



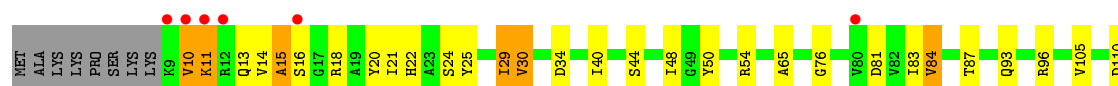
- Molecule 10: 30S ribosomal protein S10

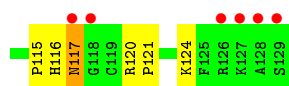


- Molecule 10: 30S ribosomal protein S10

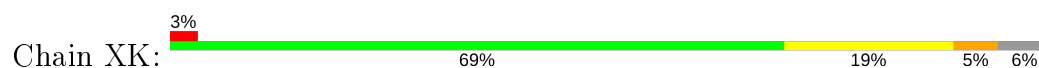


- Molecule 11: 30S ribosomal protein S11





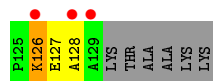
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

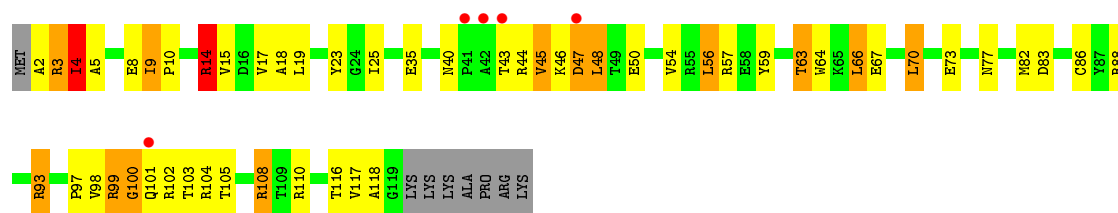


- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13





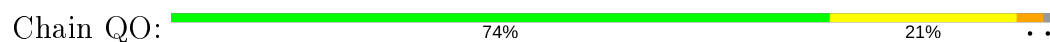
- Molecule 14: 30S ribosomal protein S14



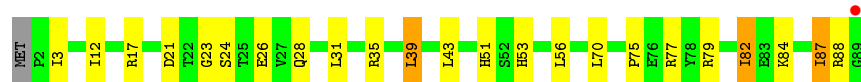
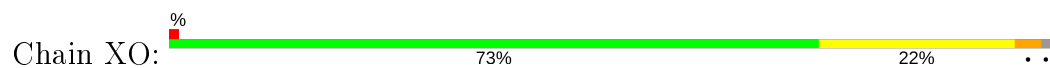
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



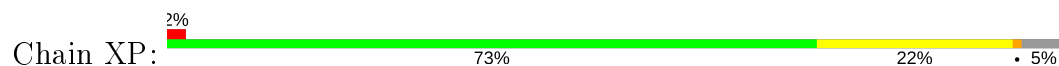
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

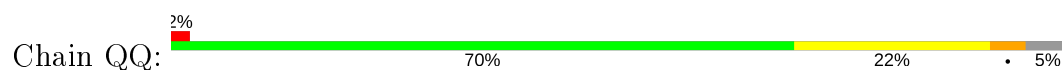


- Molecule 16: 30S ribosomal protein S16





- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



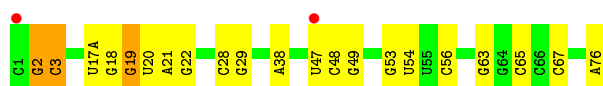
- Molecule 18: 30S ribosomal protein S18



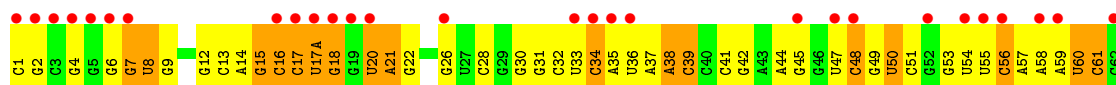
- Molecule 19: 30S ribosomal protein S19



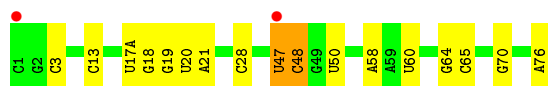
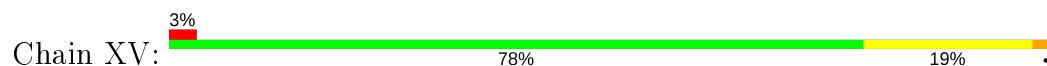
- Molecule 19: 30S ribosomal protein S19



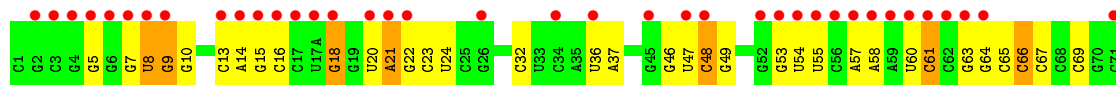
- Molecule 22: tRNA fMet



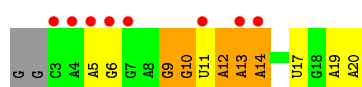
- Molecule 22: tRNA fMet



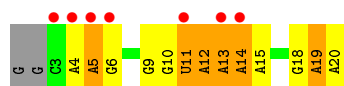
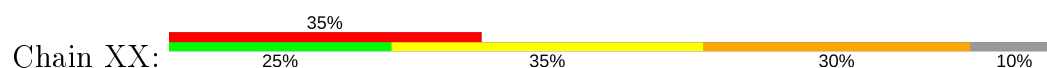
- Molecule 22: tRNA fMet



- Molecule 23: messenger RNA



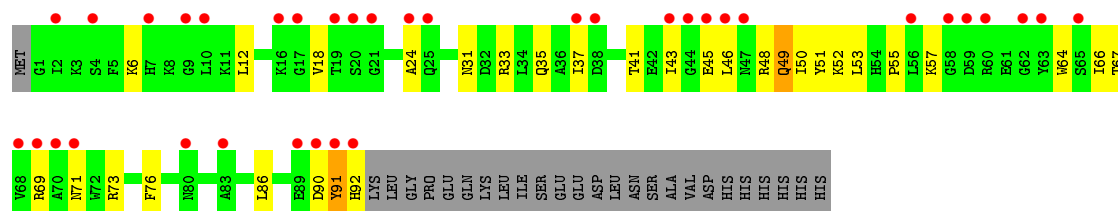
- Molecule 23: messenger RNA



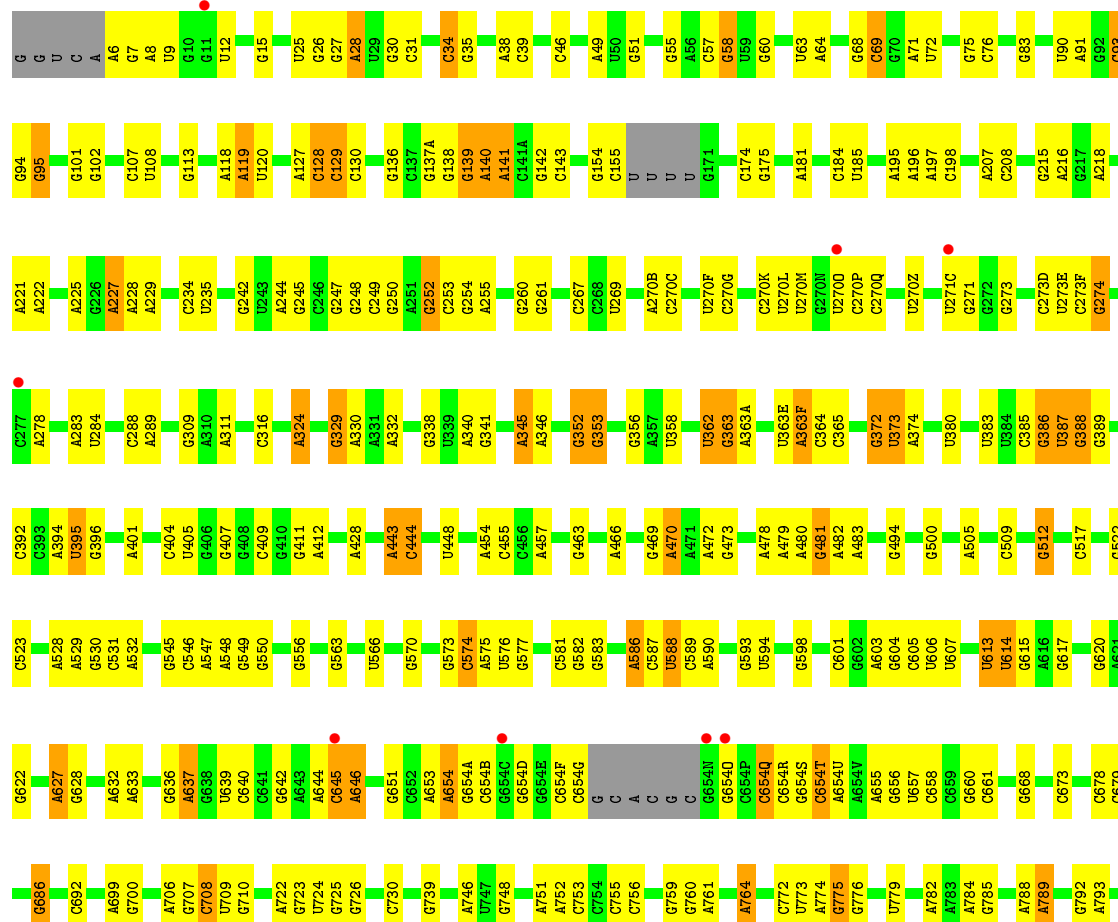
- Molecule 24: Host inhibition of growth B

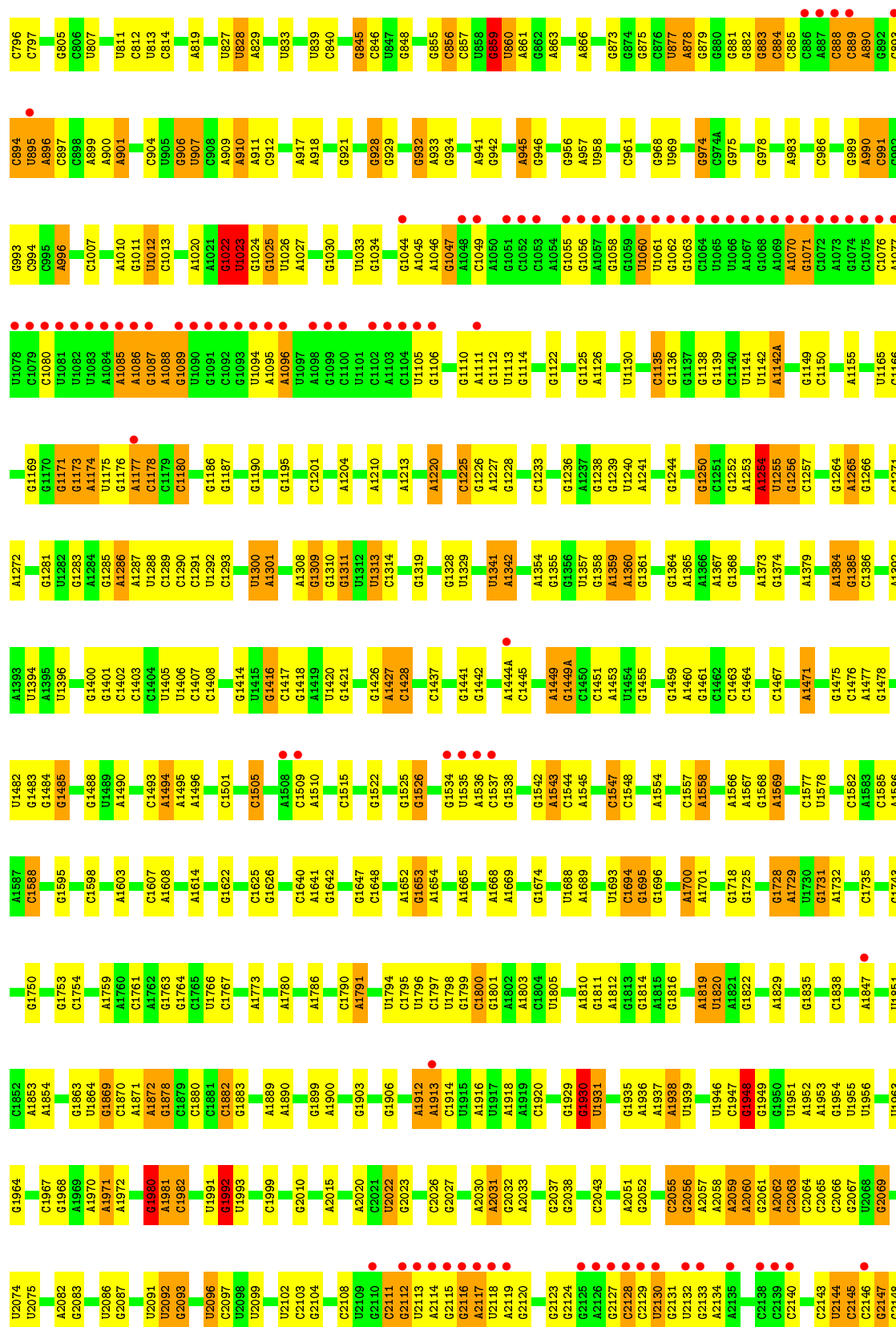


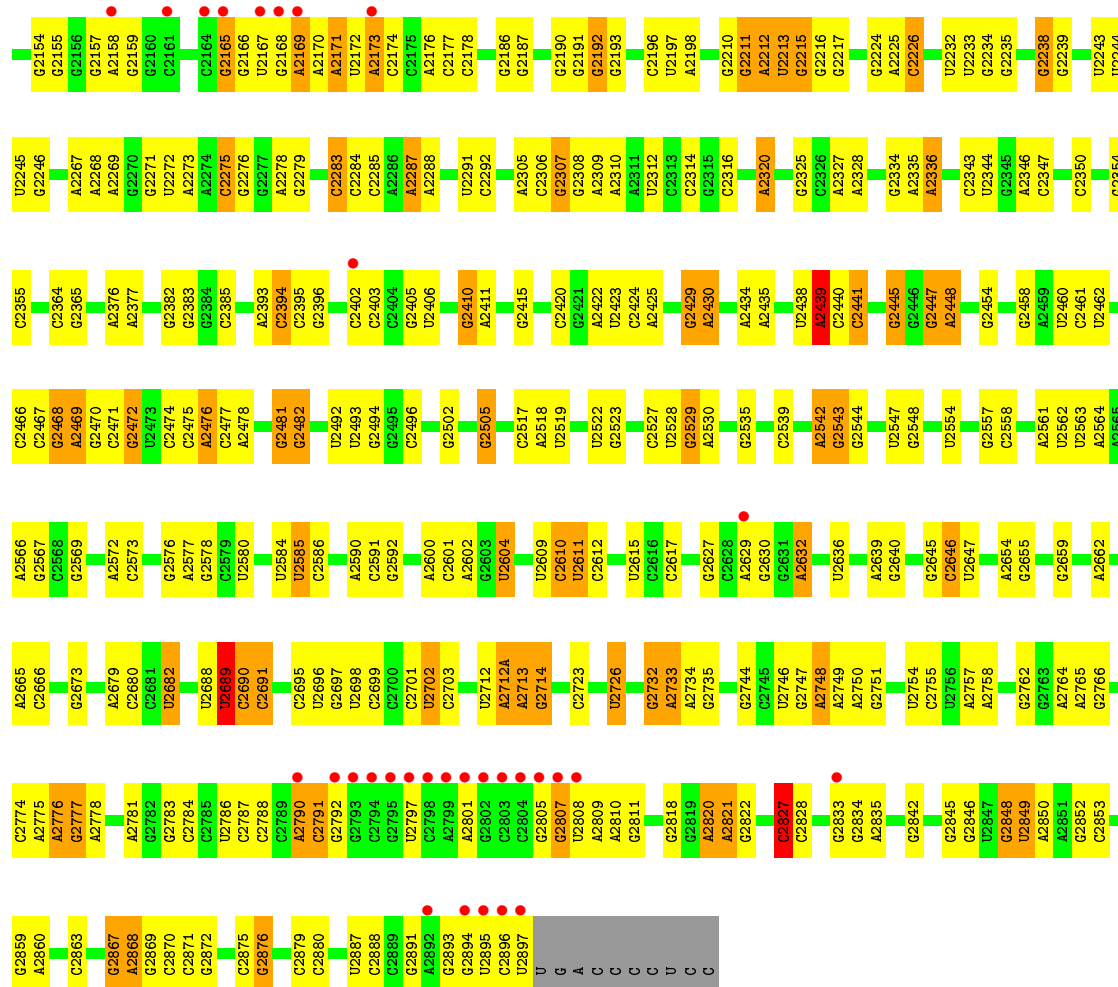
- Molecule 24: Host inhibition of growth B



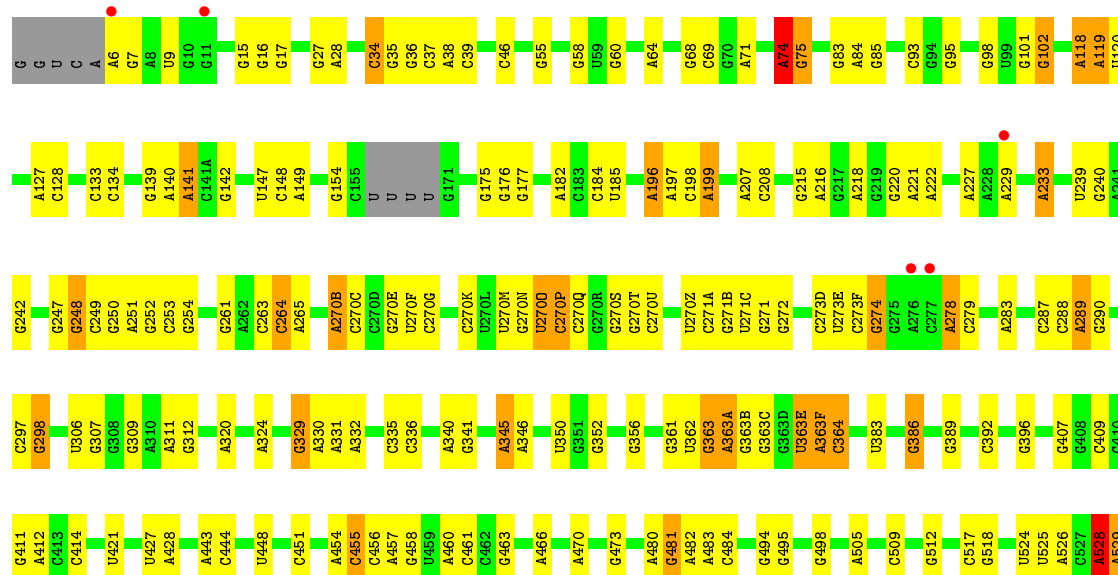
- Molecule 25: 23S rRNA

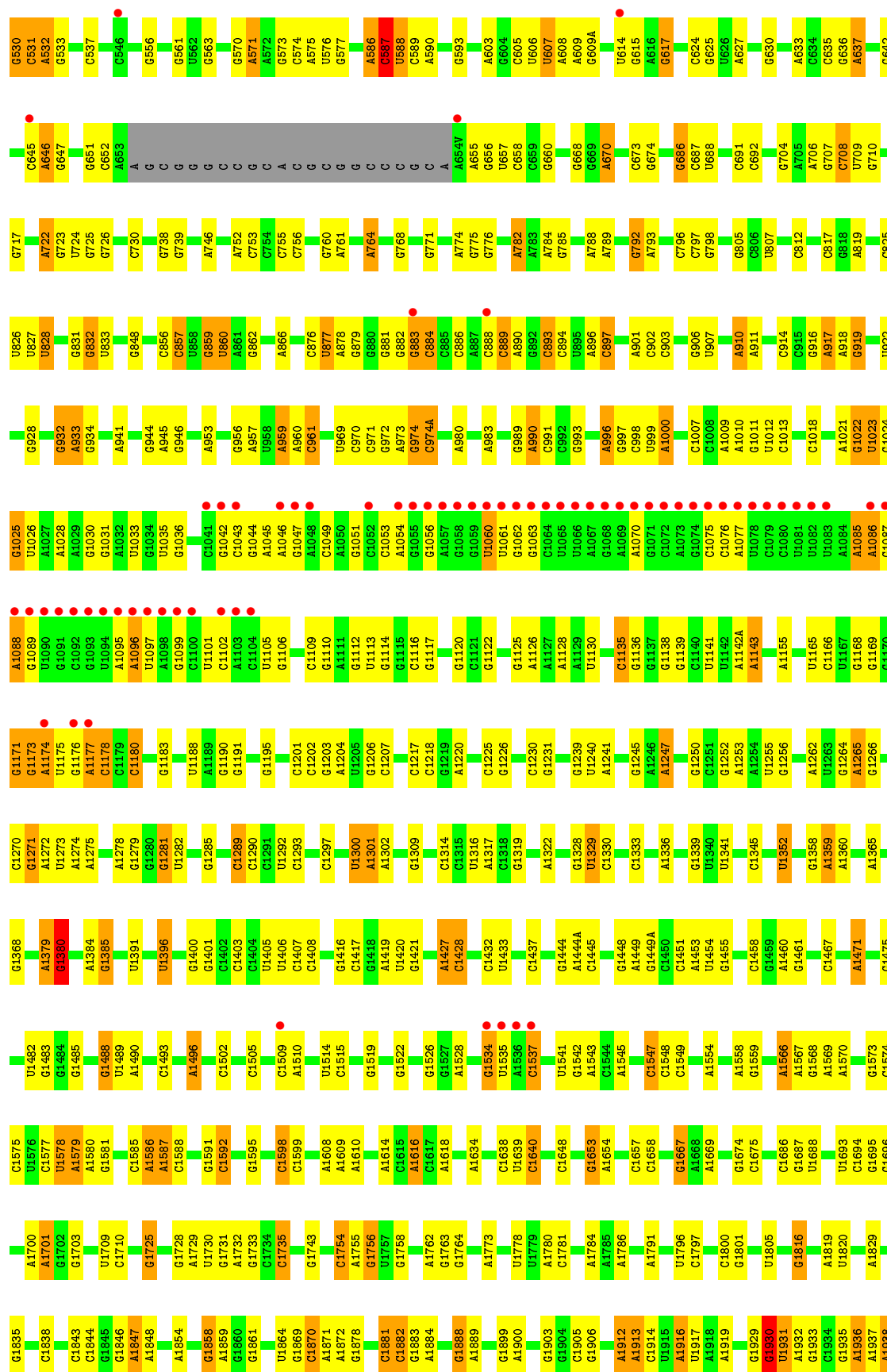


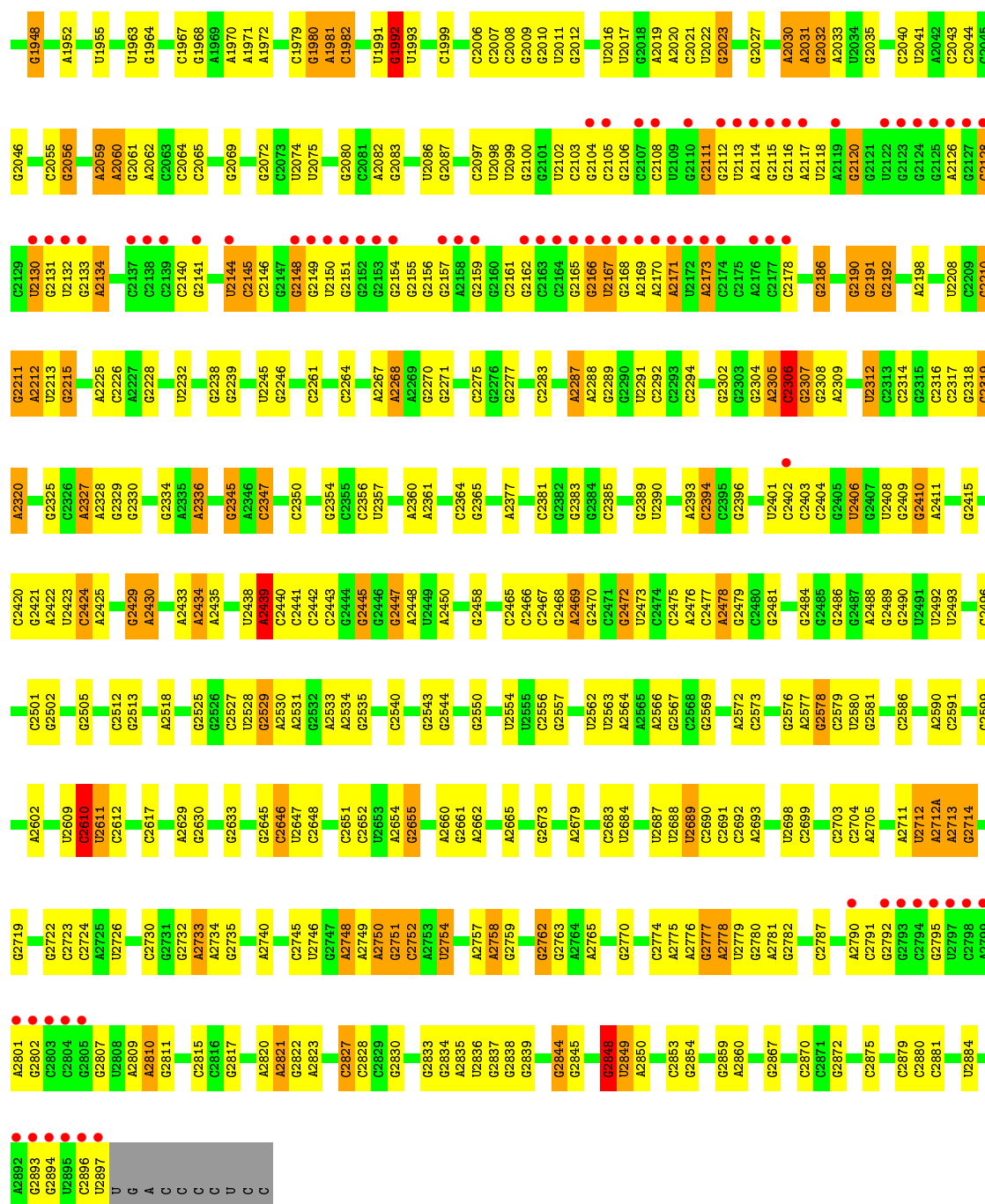




● Molecule 25: 23S rRNA

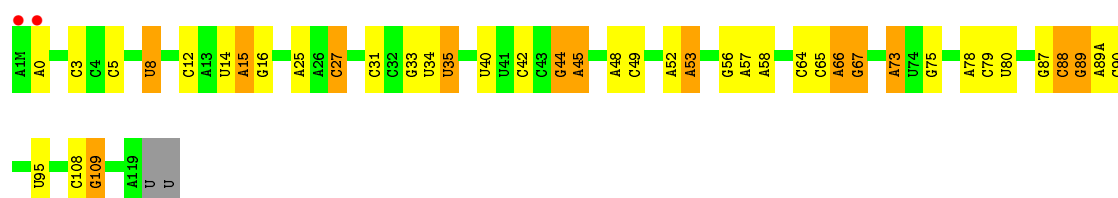




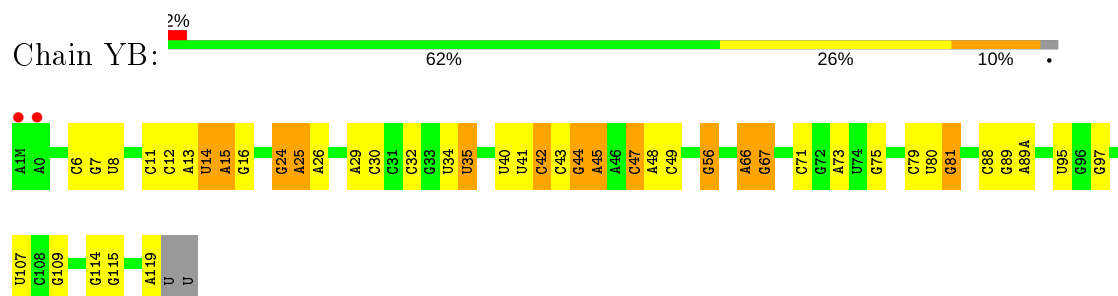


• Molecule 26: 5S rRNA

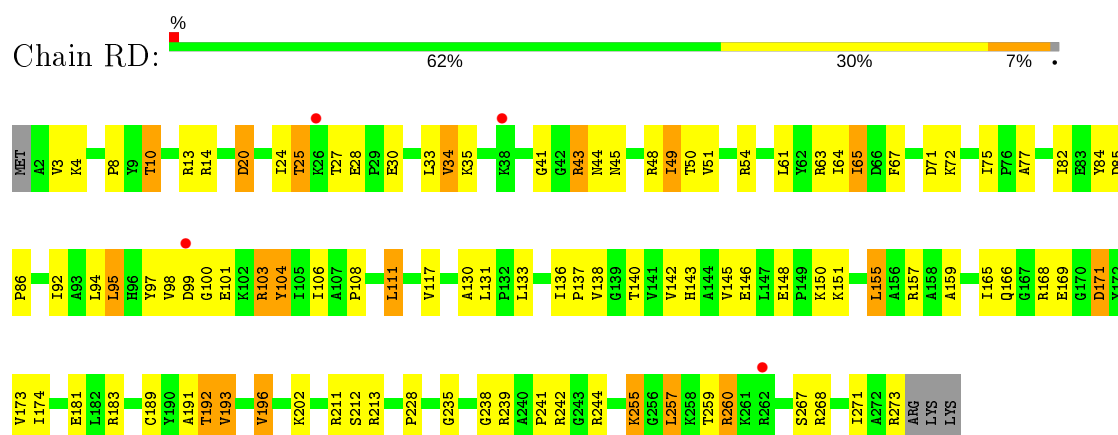
Chain RB: 2% 65% 23% 10%



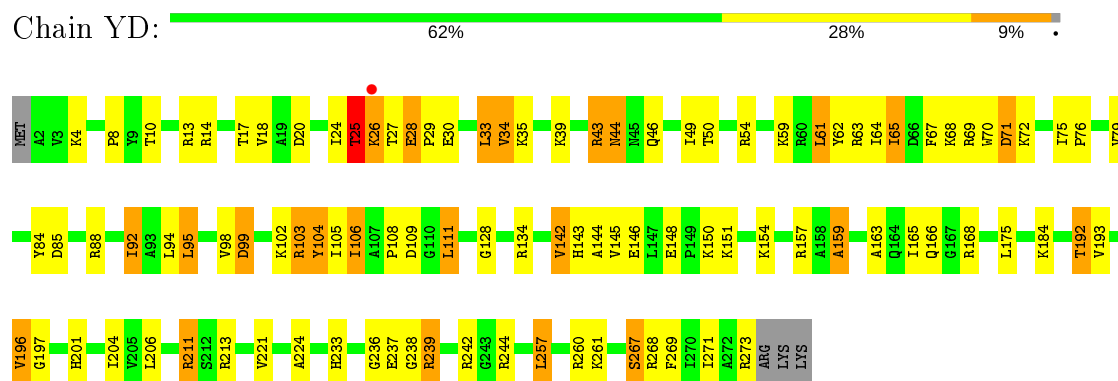
- Molecule 26: 5S rRNA



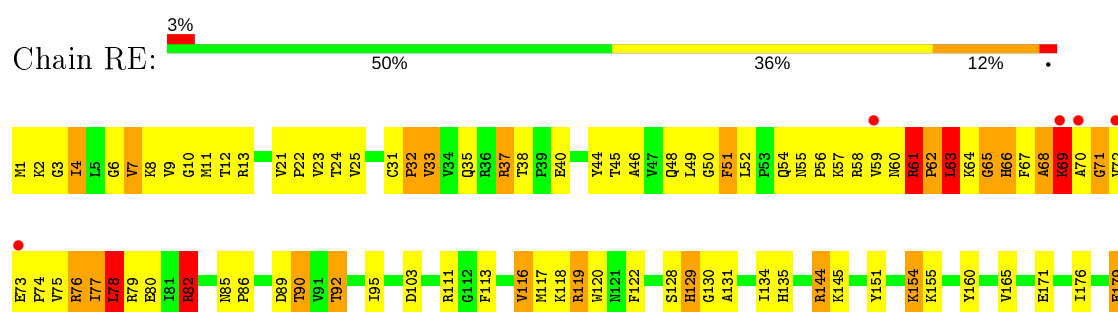
- Molecule 27: 50S ribosomal protein L2



- Molecule 27: 50S ribosomal protein L2

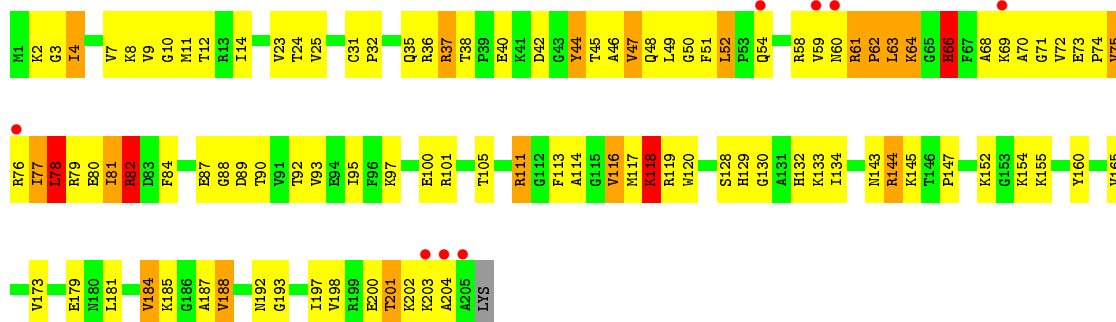


- Molecule 28: 50S ribosomal protein L3

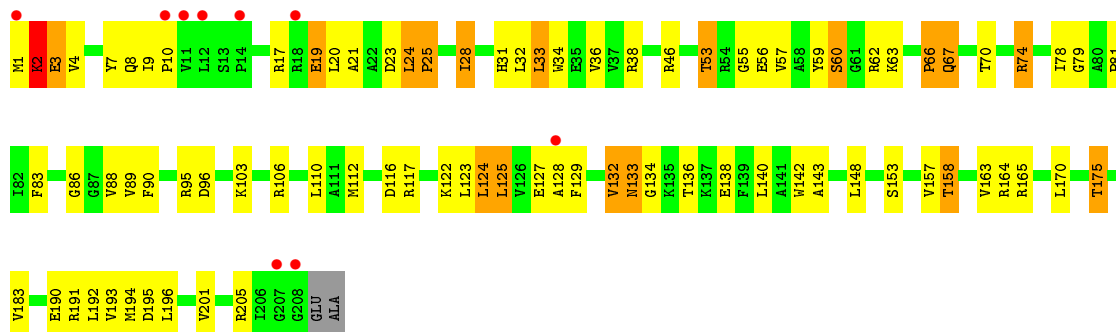




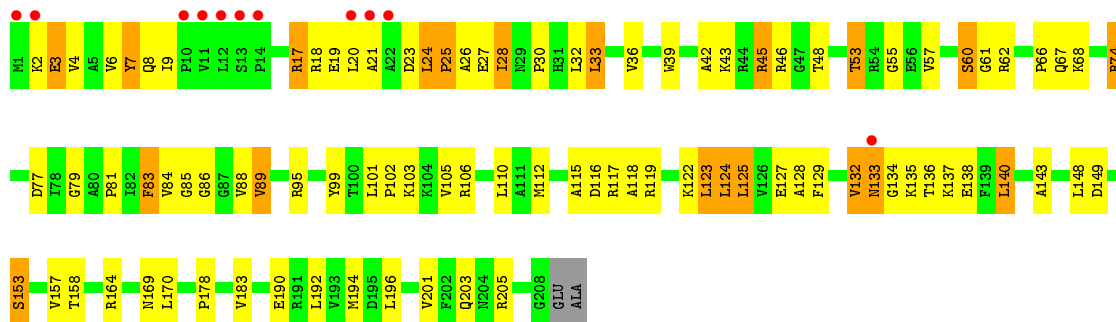
- Molecule 28: 50S ribosomal protein L3



- Molecule 29: 50S ribosomal protein L4

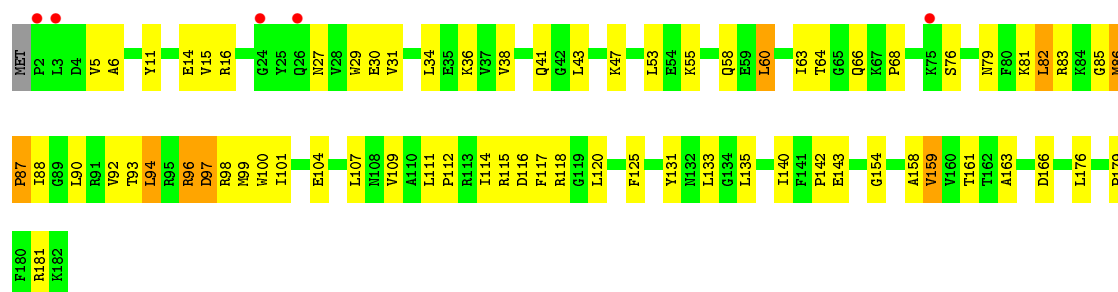


- Molecule 29: 50S ribosomal protein L4

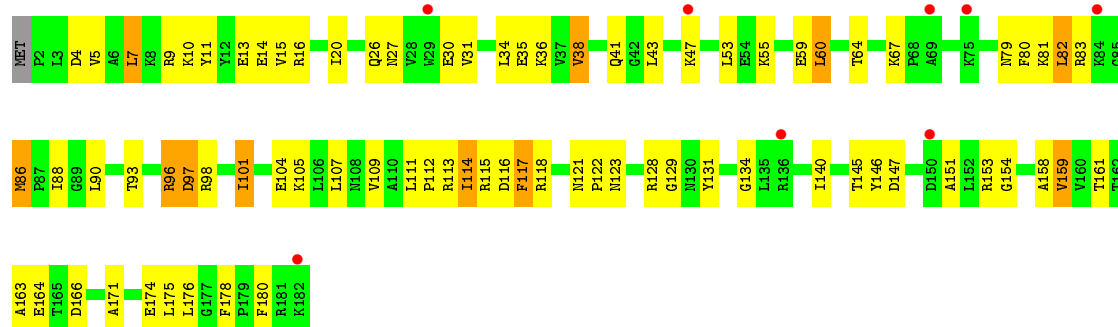


- Molecule 30: 50S ribosomal protein L5

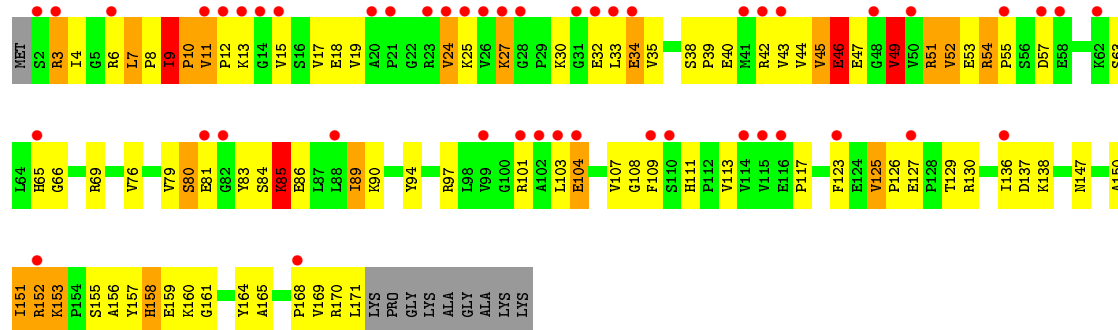




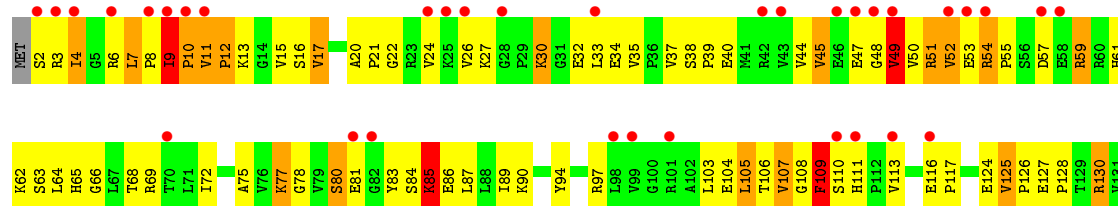
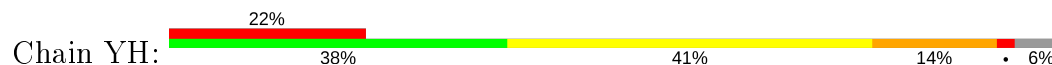
• Molecule 30: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L6

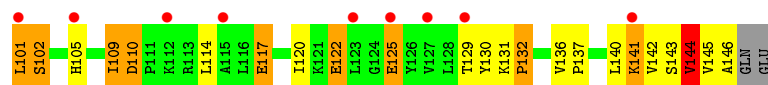


• Molecule 31: 50S ribosomal protein L6

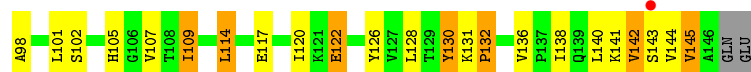




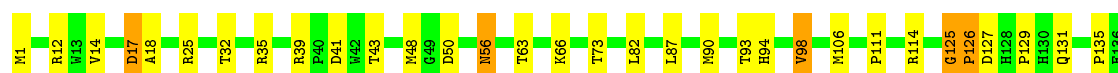
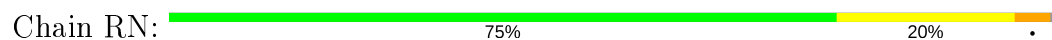
- Molecule 32: 50S ribosomal protein L9



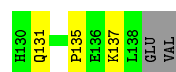
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13

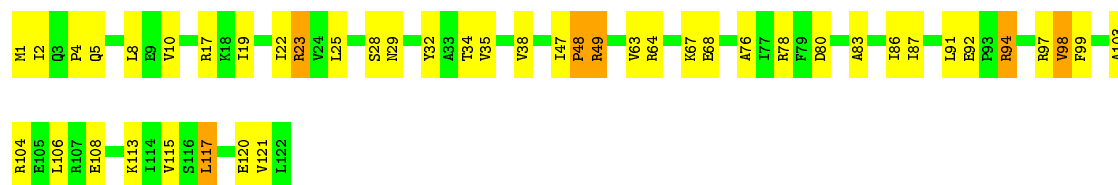


- Molecule 33: 50S ribosomal protein L13



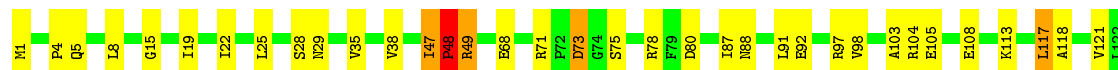
- Molecule 34: 50S ribosomal protein L14





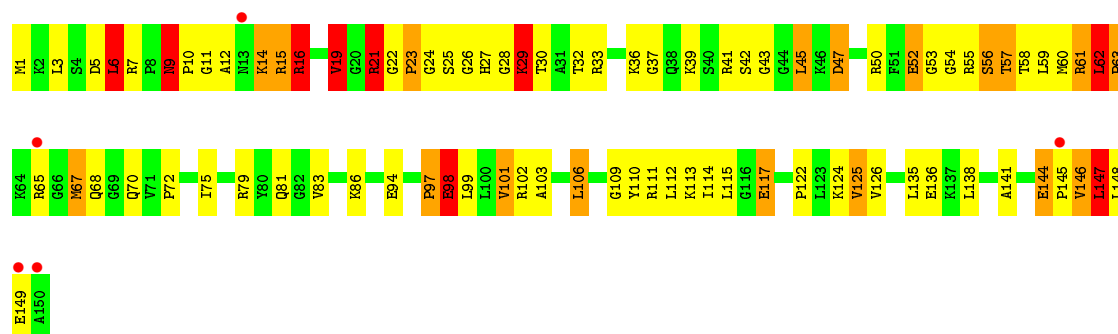
- Molecule 34: 50S ribosomal protein L14

Chain YO: 71% 25% ..



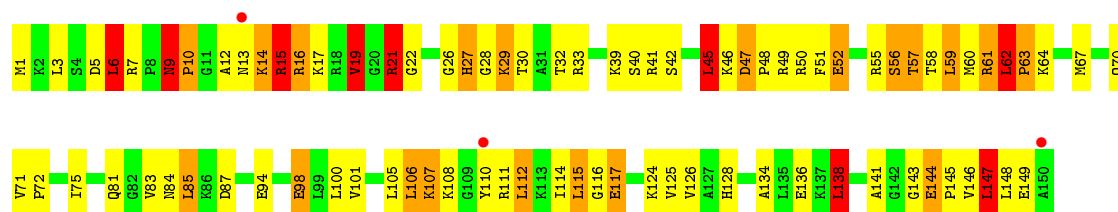
- Molecule 35: 50S ribosomal protein L15

Chain RP: 3% 43% 39% 12% 6%



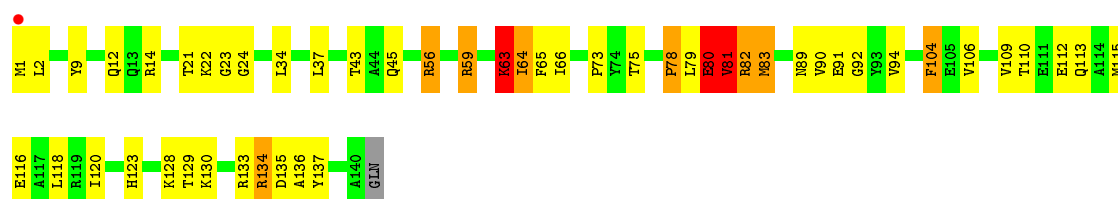
- Molecule 35: 50S ribosomal protein L15

Chain YP: 2% 43% 37% 13% 6%

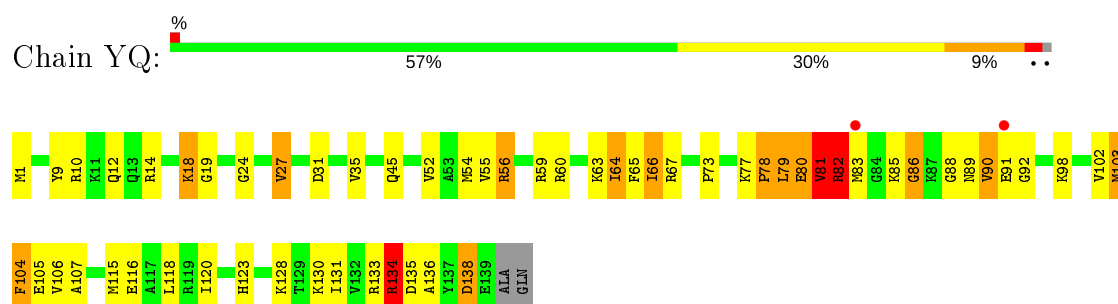


- Molecule 36: 50S ribosomal protein L16

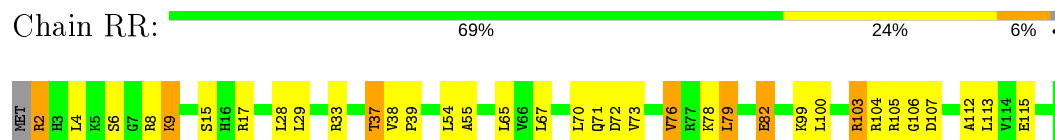
Chain RQ: % 63% 28% 6% ..



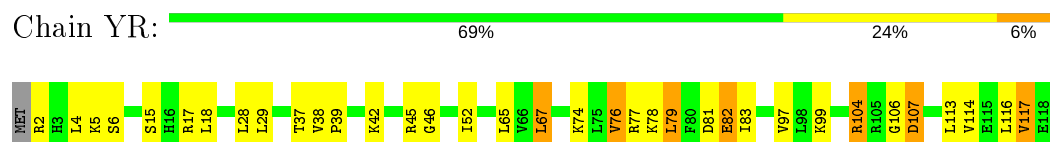
- Molecule 36: 50S ribosomal protein L16



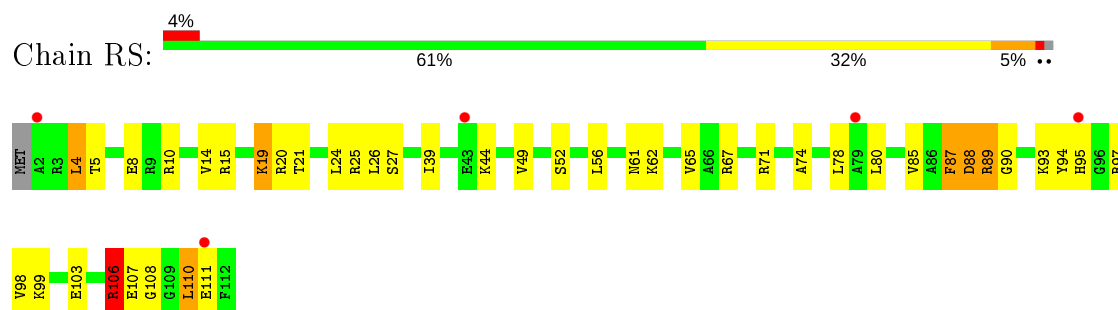
- Molecule 37: 50S ribosomal protein L17



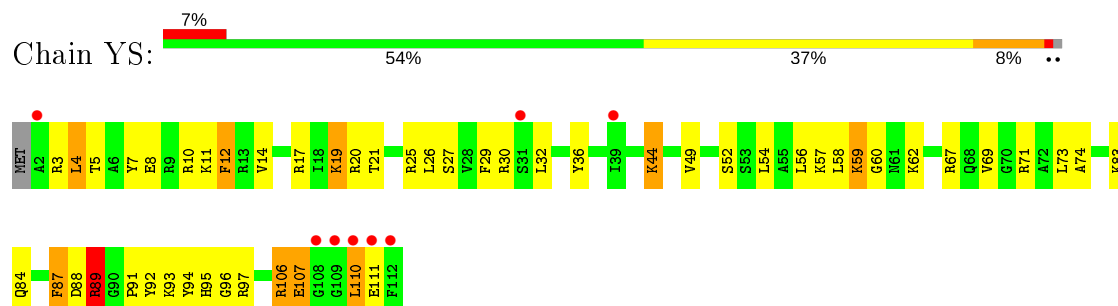
- Molecule 37: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L18

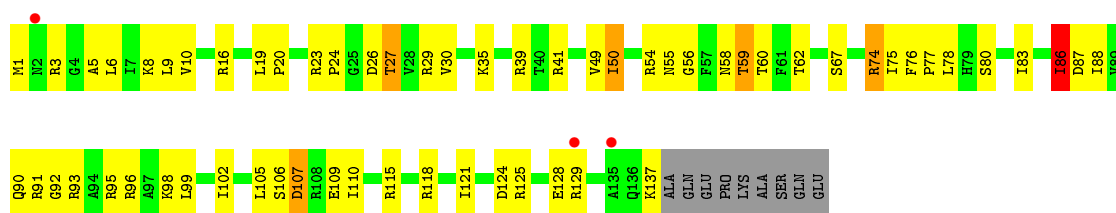


- Molecule 38: 50S ribosomal protein L18

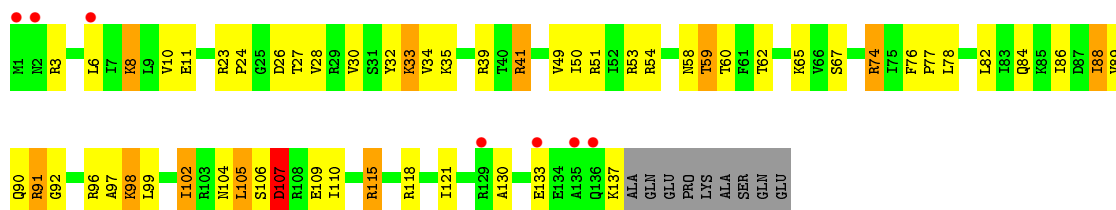


- Molecule 39: 50S ribosomal protein L19

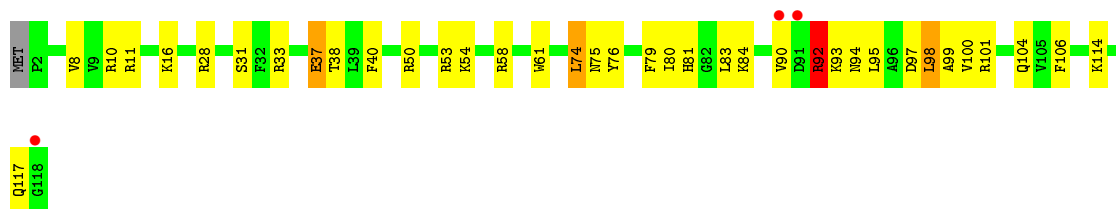




• Molecule 39: 50S ribosomal protein L19



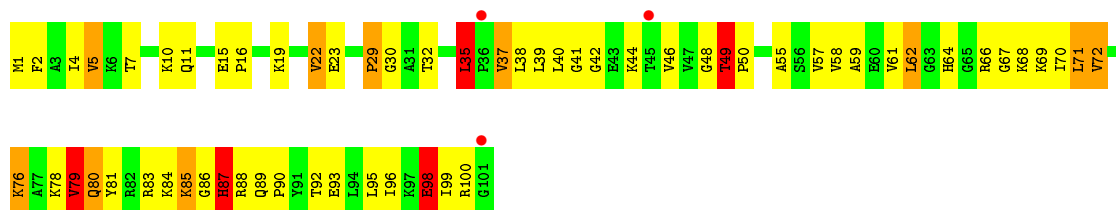
• Molecule 40: 50S ribosomal protein L20



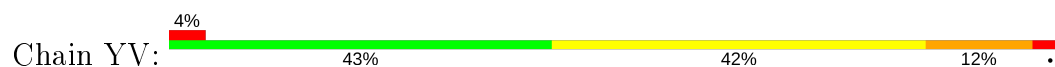
• Molecule 40: 50S ribosomal protein L20

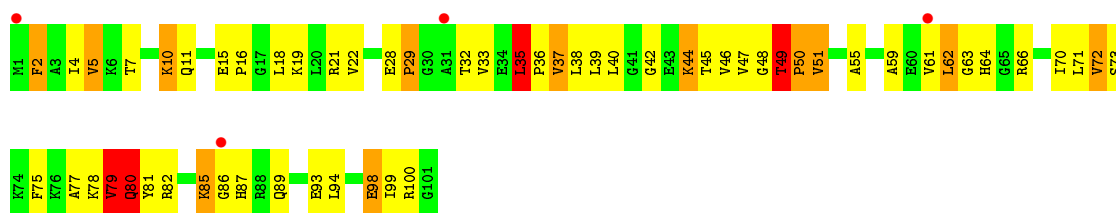


• Molecule 41: 50S ribosomal protein L21

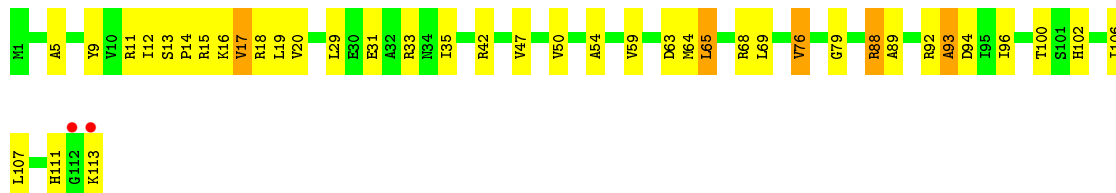


• Molecule 41: 50S ribosomal protein L21

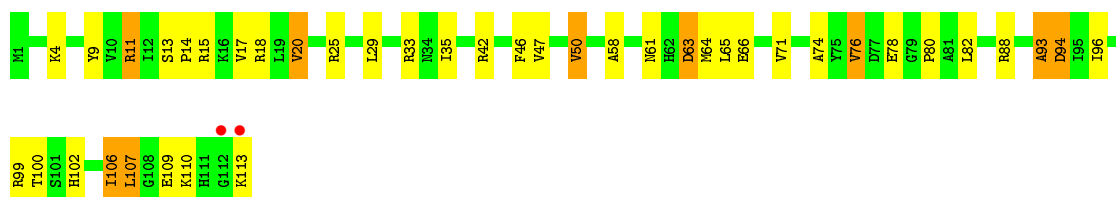




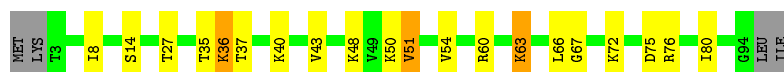
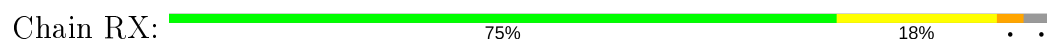
• Molecule 42: 50S ribosomal protein L22



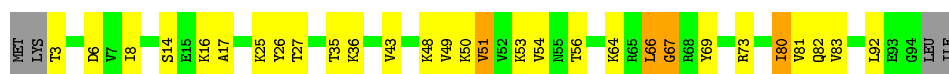
• Molecule 42: 50S ribosomal protein L22



• Molecule 43: 50S ribosomal protein L23



• Molecule 43: 50S ribosomal protein L23

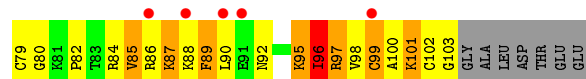
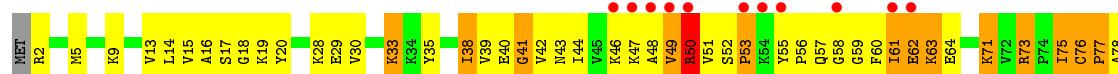


• Molecule 44: 50S ribosomal protein L24

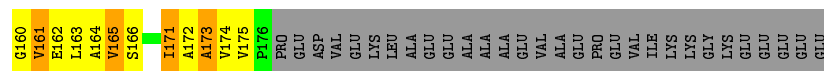
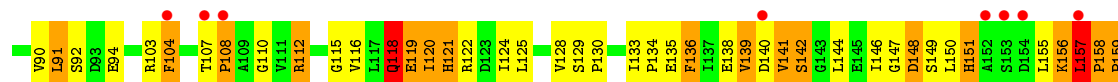
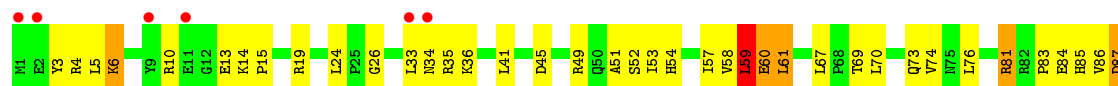




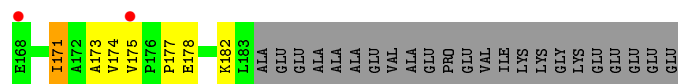
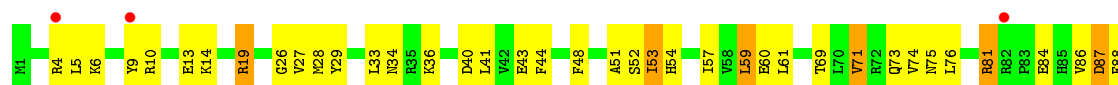
• Molecule 44: 50S ribosomal protein L24



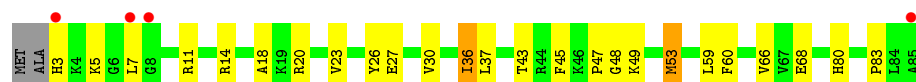
• Molecule 45: 50S ribosomal protein L25



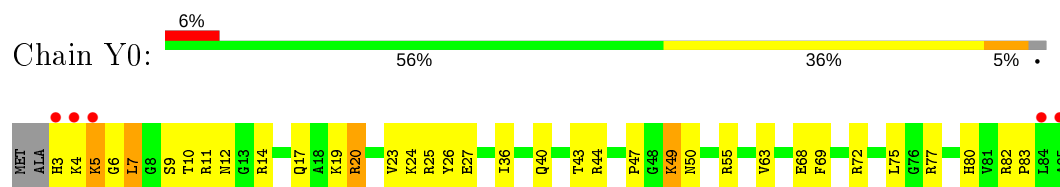
• Molecule 45: 50S ribosomal protein L25



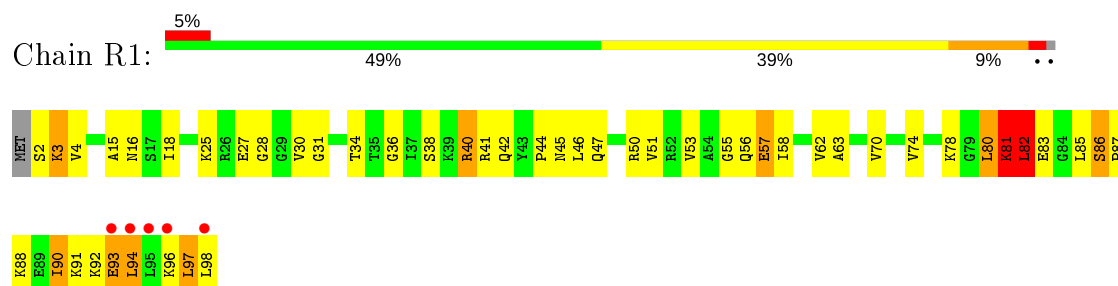
• Molecule 46: 50S ribosomal protein L27



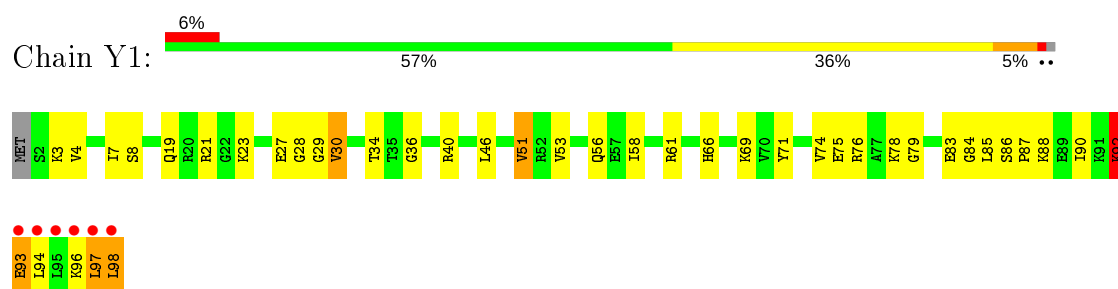
- Molecule 46: 50S ribosomal protein L27



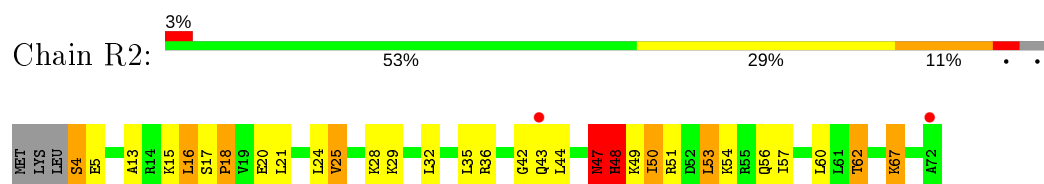
- Molecule 47: 50S ribosomal protein L28



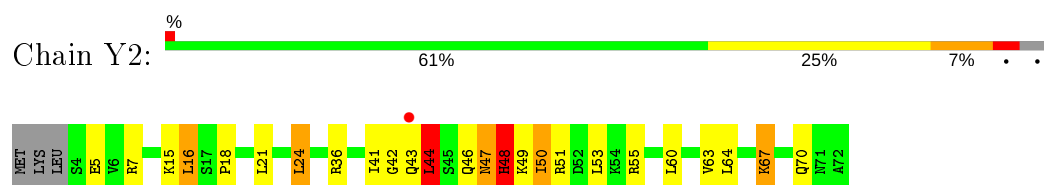
- Molecule 47: 50S ribosomal protein L28



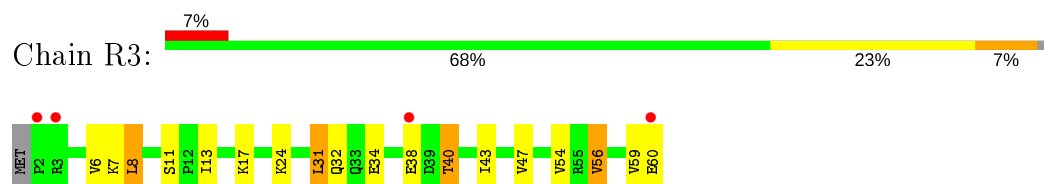
- Molecule 48: 50S ribosomal protein L29



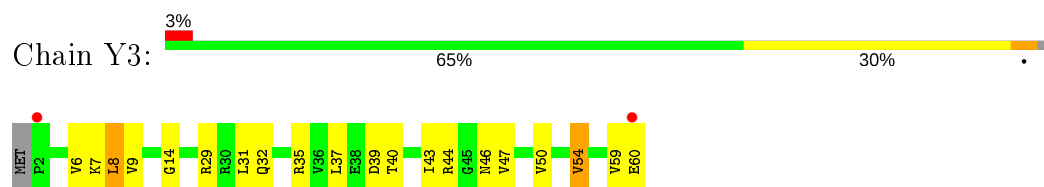
- Molecule 48: 50S ribosomal protein L29



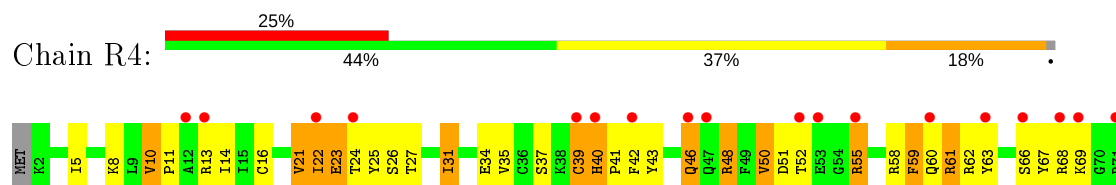
- Molecule 49: 50S ribosomal protein L30



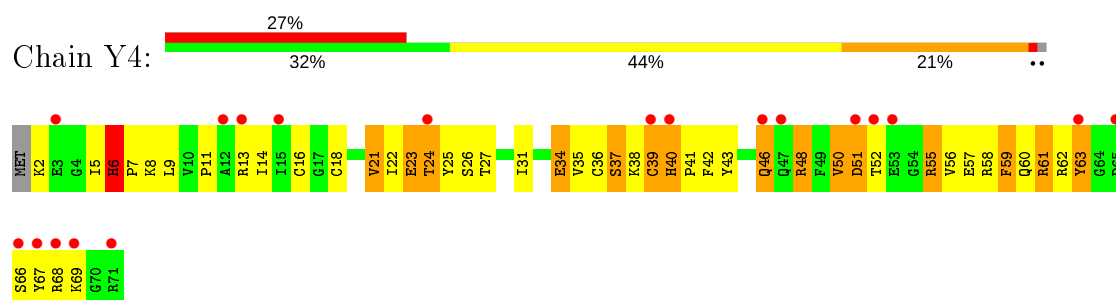
- Molecule 49: 50S ribosomal protein L30



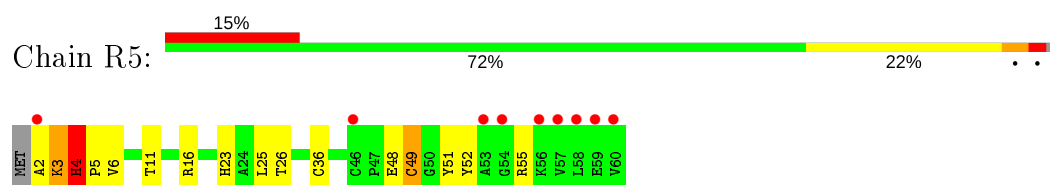
- Molecule 50: 50S ribosomal protein L31



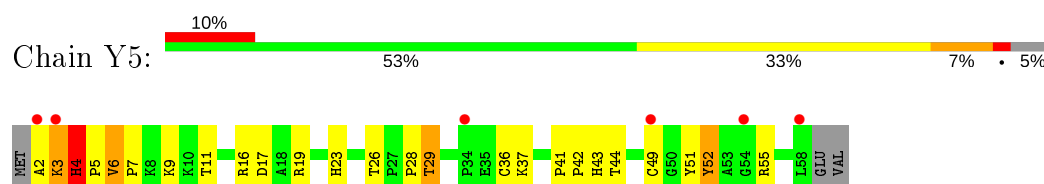
- Molecule 50: 50S ribosomal protein L31



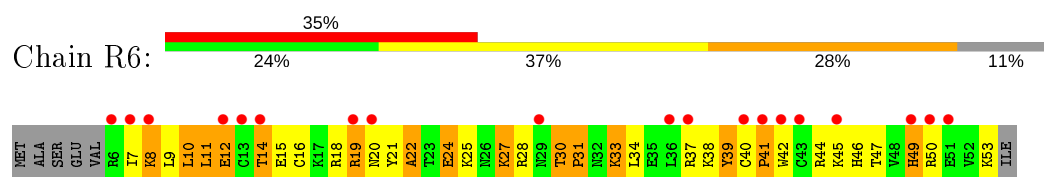
- Molecule 51: 50S ribosomal protein L32



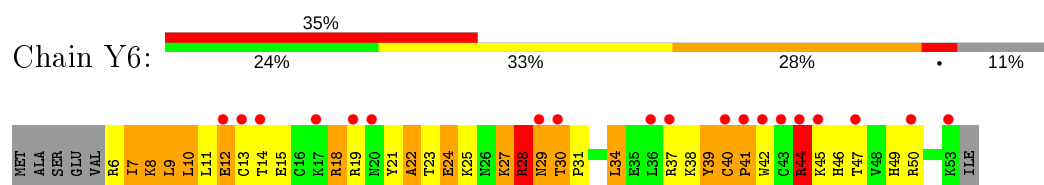
- Molecule 51: 50S ribosomal protein L32



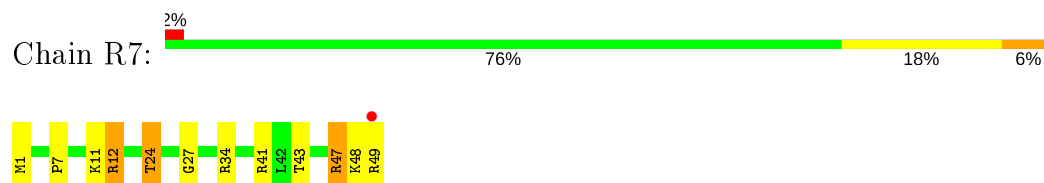
- Molecule 52: 50S ribosomal protein L33



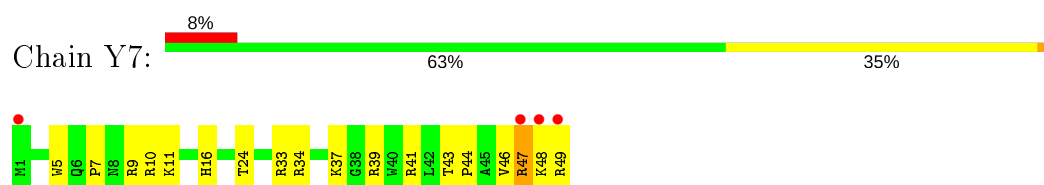
- Molecule 52: 50S ribosomal protein L33



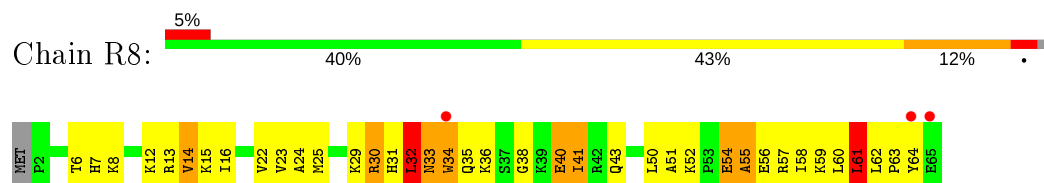
- Molecule 53: 50S ribosomal protein L34



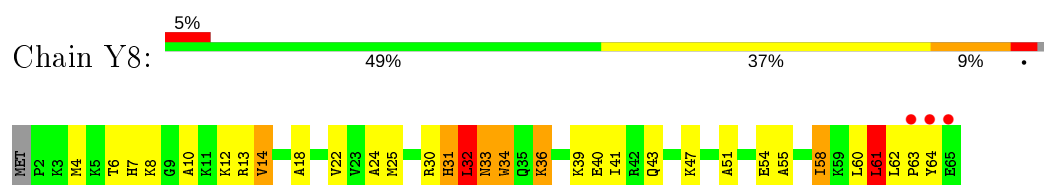
- Molecule 53: 50S ribosomal protein L34



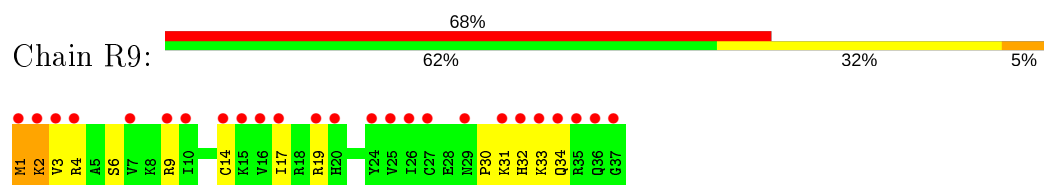
- Molecule 54: 50S ribosomal protein L35



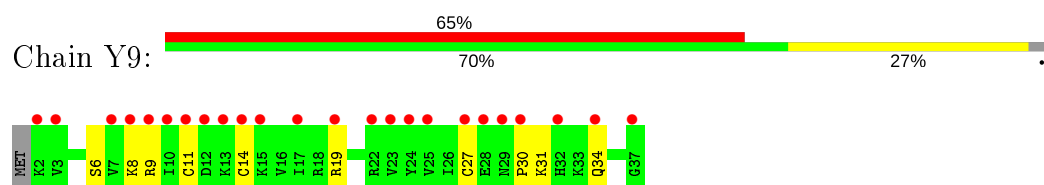
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	214.11Å 453.88Å 607.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 3.30 34.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (34.96-3.30) 94.3 (34.96-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.209 , 0.238 0.211 , 0.239	Depositor DCC
R_{free} test set	38567 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	297400	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A3P, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	QA	0.31	0/36346	0.80	11/56724 (0.0%)
1	XA	0.32	0/36276	0.81	17/56615 (0.0%)
2	QB	0.25	0/1950	0.50	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	0.29	0/1733	0.50	0/2318
4	XD	0.28	0/1733	0.50	0/2318
5	QE	0.28	0/1195	0.47	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	0.25	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	0.28	0/916	0.45	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	1/991 (0.1%)	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	0.26	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	0.27	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	0.25	0/221	0.45	0/288
22	QV	0.29	0/1832	0.78	0/2855
22	QW	0.21	0/1832	0.75	0/2855
22	XV	0.31	0/1832	0.79	0/2855
22	XW	0.19	0/1832	0.77	0/2855
23	QX	0.47	0/420	0.99	0/654
23	XX	0.48	0/420	1.03	0/654
24	QY	0.36	0/773	0.46	0/1043
24	XY	0.33	0/773	0.46	0/1043
25	RA	0.38	1/69742 (0.0%)	0.84	27/108874 (0.0%)
25	YA	0.39	0/69356	0.85	27/108271 (0.0%)
26	RB	0.28	0/2928	0.79	0/4568
26	YB	0.29	0/2928	0.78	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	0.59	0/2160
29	RF	0.35	0/1662	0.58	0/2249
29	YF	0.31	0/1662	0.58	0/2249
30	RG	0.25	0/1499	0.47	0/2016
30	YG	0.25	0/1499	0.46	0/2016
31	RH	0.27	0/1332	0.65	1/1802 (0.1%)
31	YH	0.29	0/1332	0.67	1/1802 (0.1%)
32	RI	0.24	0/1151	0.53	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	0.65	0/1544
35	YP	0.35	0/1162	0.73	3/1544 (0.2%)
36	RQ	0.34	0/1133	0.57	0/1515
36	YQ	0.35	0/1128	0.58	1/1508 (0.1%)
37	RR	0.27	0/974	0.51	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.30	0/974	0.53	0/1302
38	RS	0.25	0/892	0.48	0/1187
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	0.43	0/790	0.73	2/1057 (0.2%)
41	YV	0.40	0/790	0.71	2/1057 (0.2%)
42	RW	0.30	0/911	0.51	0/1220
42	YW	0.31	0/911	0.52	0/1220
43	RX	0.31	0/739	0.51	0/993
43	YX	0.35	0/739	0.53	0/993
44	RY	0.33	0/798	0.59	0/1064
44	YY	0.32	0/798	0.59	0/1064
45	RZ	0.37	2/1435 (0.1%)	0.59	2/1947 (0.1%)
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	0.58	0/771
48	Y2	0.34	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	0.27	0/586	0.53	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	0.47	0/424	0.86	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	0.43	0/407
55	Y9	0.24	0/301	0.41	0/397
All	All	0.34	5/321819 (0.0%)	0.76	103/481178 (0.0%)

All (5) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	RZ	158	PRO	N-CD	5.37	1.55	1.47
51	Y5	7	PRO	N-CD	5.31	1.55	1.47
45	RZ	159	PRO	N-CD	5.29	1.55	1.47
12	XL	25	PRO	N-CD	5.03	1.54	1.47
25	RA	1980	G	O3'-P	-5.03	1.55	1.61

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	YH	9	ILE	C-N-CD	-11.91	94.41	120.60
31	RH	9	ILE	C-N-CD	-10.87	96.68	120.60
1	XA	315	A	P-O3'-C3'	9.29	130.84	119.70
25	RA	1022	G	O3'-P-O5'	8.26	119.69	104.00
1	XA	960	U	P-O3'-C3'	8.23	129.57	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	16392	426	0
1	XA	32409	0	16360	366	0
2	QB	1915	0	1969	56	0
2	XB	1915	0	1969	60	0
3	QC	1612	0	1677	48	0
3	XC	1612	0	1677	39	0
4	QD	1703	0	1766	55	0
4	XD	1703	0	1766	35	0
5	QE	1178	0	1234	40	0
5	XE	1178	0	1234	23	0
6	QF	843	0	857	18	0
6	XF	843	0	857	29	0
7	QG	1257	0	1296	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	33	0
8	QH	1116	0	1177	30	0
8	XH	1116	0	1177	25	0
9	QI	1018	0	1049	49	0
9	XI	1018	0	1049	44	0
10	QJ	801	0	849	38	0
10	XJ	801	0	849	42	0
11	QK	901	0	926	26	0
11	XK	901	0	926	20	0
12	QL	975	0	1062	29	0
12	XL	975	0	1062	24	0
13	QM	937	0	995	27	0
13	XM	937	0	995	56	0
14	QN	492	0	530	20	0
14	XN	492	0	529	12	0
15	QO	734	0	771	14	0
15	XO	734	0	771	15	0
16	QP	705	0	725	15	0
16	XP	705	0	725	10	0
17	QQ	834	0	904	15	0
17	XQ	834	0	904	17	0
18	QR	585	0	657	10	0
18	XR	585	0	657	19	0
19	QS	656	0	678	46	0
19	XS	656	0	678	41	0
20	QT	763	0	861	25	0
20	XT	763	0	861	28	0
21	QU	217	0	234	9	0
21	XU	217	0	234	14	0
22	QV	1640	0	837	9	0
22	QW	1640	0	837	56	0
22	XV	1640	0	837	6	0
22	XW	1640	0	837	25	0
23	QX	399	0	196	11	0
23	XX	399	0	196	16	0
24	QY	756	0	749	19	0
24	XY	756	0	749	19	0
25	RA	62269	0	31391	631	0
25	YA	61924	0	31215	613	0
26	RB	2617	0	1328	25	0
26	YB	2617	0	1328	30	0
27	RD	2115	0	2195	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	YD	2115	0	2195	75	0
28	RE	1568	0	1634	93	0
28	YE	1568	0	1634	71	0
29	RF	1627	0	1680	57	0
29	YF	1627	0	1680	57	0
30	RG	1474	0	1535	48	0
30	YG	1474	0	1535	44	0
31	RH	1307	0	1382	76	0
31	YH	1307	0	1382	68	0
32	RI	1136	0	1223	39	0
32	YI	1136	0	1223	67	0
33	RN	1104	0	1180	14	0
33	YN	1104	0	1180	22	0
34	RO	933	0	996	35	0
34	YO	933	0	996	24	0
35	RP	1145	0	1228	86	0
35	YP	1145	0	1228	83	0
36	RQ	1112	0	1170	32	0
36	YQ	1107	0	1165	38	0
37	RR	960	0	1021	15	0
37	YR	960	0	1021	24	0
38	RS	882	0	943	27	0
38	YS	882	0	943	32	0
39	RT	1141	0	1202	45	0
39	YT	1141	0	1202	36	0
40	RU	964	0	1022	36	0
40	YU	964	0	1022	29	0
41	RV	779	0	852	53	0
41	YV	779	0	852	57	0
42	RW	900	0	964	26	0
42	YW	900	0	964	23	0
43	RX	725	0	778	13	0
43	YX	725	0	778	20	0
44	RY	785	0	878	66	0
44	YY	785	0	878	51	0
45	RZ	1404	0	1437	93	0
45	YZ	1461	0	1493	47	0
46	R0	657	0	683	19	0
46	Y0	657	0	683	25	0
47	R1	763	0	848	29	0
47	Y1	763	0	848	25	0
48	R2	581	0	629	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Y2	581	0	629	16	0
49	R3	469	0	518	10	0
49	Y3	469	0	518	10	0
50	R4	573	0	565	21	0
50	Y4	573	0	565	37	0
51	R5	459	0	480	9	0
51	Y5	442	0	465	21	0
52	R6	417	0	441	26	0
52	Y6	417	0	441	40	0
53	R7	430	0	480	6	0
53	Y7	430	0	480	10	0
54	R8	517	0	582	37	0
54	Y8	517	0	582	32	0
55	R9	307	0	338	13	0
55	Y9	298	0	326	8	0
56	QA	140	0	0	0	0
56	QE	1	0	0	0	0
56	QL	1	0	0	0	0
56	QV	5	0	0	0	0
56	R0	2	0	0	0	0
56	R2	1	0	0	0	0
56	R5	3	0	0	0	0
56	RA	413	0	0	0	0
56	RB	4	0	0	0	0
56	RD	2	0	0	0	0
56	RE	1	0	0	0	0
56	RF	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0
56	RR	1	0	0	0	0
56	RU	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	160	0	0	0	0
56	XD	1	0	0	0	0
56	XF	1	0	0	0	0
56	XL	1	0	0	0	0
56	XN	1	0	0	0	0
56	XV	4	0	0	0	0
56	Y0	3	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	2	0	0	0	0
56	Y7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YA	464	0	0	0	0
56	YB	5	0	0	0	0
56	YD	1	0	0	0	0
56	YE	2	0	0	0	0
56	YG	1	0	0	0	0
56	YH	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	2	0	0	0	0
56	YQ	2	0	0	0	0
56	YR	1	0	0	0	0
56	YU	1	0	0	0	0
56	YV	1	0	0	0	0
56	YY	1	0	0	0	0
57	QD	1	0	0	0	0
57	QN	1	0	0	0	0
57	XD	1	0	0	0	0
57	XN	1	0	0	0	0
All	All	297400	0	201477	4861	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 10.

The worst 5 of 4861 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)
28:RE:51:PHE:O	28:RE:74:PRO:HB3	1.29	1.31
13:XM:8:GLU:O	13:XM:9:ILE:HG22	1.09	1.26
5:QE:11:ILE:O	5:QE:12:LEU:HG	1.07	1.21
32:YI:78:THR:H	32:YI:142:VAL:CG2	1.54	1.19
45:RZ:163:LEU:HD11	45:RZ:165:VAL:CG1	1.72	1.19

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	234/256 (91%)	186 (80%)	29 (12%)	19 (8%)	1	6
2	XB	234/256 (91%)	189 (81%)	27 (12%)	18 (8%)	1	6
3	QC	204/239 (85%)	162 (79%)	26 (13%)	16 (8%)	1	6
3	XC	204/239 (85%)	160 (78%)	31 (15%)	13 (6%)	1	9
4	QD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	2	12
4	XD	206/209 (99%)	168 (82%)	22 (11%)	16 (8%)	1	6
5	QE	152/162 (94%)	136 (90%)	11 (7%)	5 (3%)	4	22
5	XE	152/162 (94%)	137 (90%)	9 (6%)	6 (4%)	3	18
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	27
7	XG	153/156 (98%)	133 (87%)	15 (10%)	5 (3%)	4	22
8	QH	136/138 (99%)	126 (93%)	7 (5%)	3 (2%)	6	30
8	XH	136/138 (99%)	123 (90%)	10 (7%)	3 (2%)	6	30
9	QI	126/128 (98%)	94 (75%)	24 (19%)	8 (6%)	1	9
9	XI	126/128 (98%)	96 (76%)	23 (18%)	7 (6%)	2	11
10	QJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	3	17
10	XJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	2	13
11	QK	119/129 (92%)	101 (85%)	13 (11%)	5 (4%)	3	17
11	XK	119/129 (92%)	105 (88%)	10 (8%)	4 (3%)	3	22
12	QL	123/132 (93%)	99 (80%)	16 (13%)	8 (6%)	1	9
12	XL	123/132 (93%)	97 (79%)	18 (15%)	8 (6%)	1	9
13	QM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	4
13	XM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	4
14	QN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	13
14	XN	58/61 (95%)	50 (86%)	5 (9%)	3 (5%)	2	13
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	46
17	XQ	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	7	32
18	QR	69/88 (78%)	61 (88%)	8 (12%)	0	100	100
18	XR	69/88 (78%)	62 (90%)	6 (9%)	1 (1%)	11	38
19	QS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	1
19	XS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	1
20	QT	97/106 (92%)	79 (81%)	15 (16%)	3 (3%)	4	23
20	XT	97/106 (92%)	80 (82%)	14 (14%)	3 (3%)	4	23
21	QU	23/25 (92%)	16 (70%)	6 (26%)	1 (4%)	2	16
21	XU	23/25 (92%)	18 (78%)	3 (13%)	2 (9%)	1	5
24	QY	90/118 (76%)	82 (91%)	8 (9%)	0	100	100
24	XY	90/118 (76%)	81 (90%)	9 (10%)	0	100	100
27	RD	270/276 (98%)	224 (83%)	38 (14%)	8 (3%)	4	24
27	YD	270/276 (98%)	228 (84%)	32 (12%)	10 (4%)	3	20
28	RE	203/206 (98%)	137 (68%)	37 (18%)	29 (14%)	0	1
28	YE	203/206 (98%)	134 (66%)	40 (20%)	29 (14%)	0	1
29	RF	206/210 (98%)	167 (81%)	26 (13%)	13 (6%)	1	9
29	YF	206/210 (98%)	168 (82%)	22 (11%)	16 (8%)	1	6
30	RG	179/182 (98%)	141 (79%)	26 (14%)	12 (7%)	1	8
30	YG	179/182 (98%)	147 (82%)	21 (12%)	11 (6%)	1	10
31	RH	168/180 (93%)	104 (62%)	37 (22%)	27 (16%)	0	1
31	YH	168/180 (93%)	98 (58%)	42 (25%)	28 (17%)	0	1
32	RI	144/148 (97%)	109 (76%)	29 (20%)	6 (4%)	3	17
32	YI	144/148 (97%)	116 (81%)	24 (17%)	4 (3%)	5	25
33	RN	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	2	13
33	YN	136/140 (97%)	110 (81%)	19 (14%)	7 (5%)	2	13
34	RO	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	51
34	YO	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	19	51
35	RP	148/150 (99%)	99 (67%)	24 (16%)	25 (17%)	0	1
35	YP	148/150 (99%)	102 (69%)	25 (17%)	21 (14%)	0	1
36	RQ	138/141 (98%)	110 (80%)	17 (12%)	11 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	YQ	137/141 (97%)	111 (81%)	15 (11%)	11 (8%)	1	6
37	RR	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	21
37	YR	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	5	27
38	RS	109/112 (97%)	84 (77%)	17 (16%)	8 (7%)	1	7
38	YS	109/112 (97%)	85 (78%)	13 (12%)	11 (10%)	0	3
39	RT	135/146 (92%)	109 (81%)	24 (18%)	2 (2%)	10	38
39	YT	135/146 (92%)	113 (84%)	17 (13%)	5 (4%)	3	20
40	RU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	9	35
40	YU	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	5	27
41	RV	99/101 (98%)	73 (74%)	12 (12%)	14 (14%)	0	1
41	YV	99/101 (98%)	71 (72%)	14 (14%)	14 (14%)	0	1
42	RW	111/113 (98%)	107 (96%)	1 (1%)	3 (3%)	5	26
42	YW	111/113 (98%)	104 (94%)	3 (3%)	4 (4%)	3	20
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	30
43	YX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	30
44	RY	100/110 (91%)	56 (56%)	27 (27%)	17 (17%)	0	1
44	YY	100/110 (91%)	57 (57%)	27 (27%)	16 (16%)	0	1
45	RZ	174/206 (84%)	116 (67%)	36 (21%)	22 (13%)	0	1
45	YZ	181/206 (88%)	122 (67%)	42 (23%)	17 (9%)	0	4
46	R0	81/85 (95%)	73 (90%)	5 (6%)	3 (4%)	3	20
46	Y0	81/85 (95%)	67 (83%)	11 (14%)	3 (4%)	3	20
47	R1	95/98 (97%)	71 (75%)	12 (13%)	12 (13%)	0	1
47	Y1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	9
48	R2	67/72 (93%)	54 (81%)	8 (12%)	5 (8%)	1	7
48	Y2	67/72 (93%)	56 (84%)	5 (8%)	6 (9%)	1	4
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	1
50	Y4	68/71 (96%)	38 (56%)	15 (22%)	15 (22%)	0	0
51	R5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	21
51	Y5	55/60 (92%)	48 (87%)	4 (7%)	3 (6%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	R6	46/54 (85%)	22 (48%)	15 (33%)	9 (20%)	0	0
52	Y6	46/54 (85%)	16 (35%)	18 (39%)	12 (26%)	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	2
54	Y8	62/65 (95%)	49 (79%)	6 (10%)	7 (11%)	0	2
55	R9	35/37 (95%)	34 (97%)	0	1 (3%)	4	24
55	Y9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11649/12360 (94%)	9394 (81%)	1496 (13%)	759 (6%)	1	9

5 of 759 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%)	174 (85%)	30 (15%)	3	14
2	XB	204/220 (93%)	176 (86%)	28 (14%)	3	16
3	QC	160/188 (85%)	142 (89%)	18 (11%)	6	22
3	XC	160/188 (85%)	142 (89%)	18 (11%)	6	22
4	QD	180/181 (99%)	157 (87%)	23 (13%)	4	18
4	XD	180/181 (99%)	155 (86%)	25 (14%)	3	16
5	QE	119/123 (97%)	103 (87%)	16 (13%)	4	16
5	XE	119/123 (97%)	106 (89%)	13 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	QF	90/90 (100%)	85 (94%)	5 (6%)	21	52
6	XF	90/90 (100%)	77 (86%)	13 (14%)	3	15
7	QG	126/127 (99%)	112 (89%)	14 (11%)	6	23
7	XG	126/127 (99%)	110 (87%)	16 (13%)	4	19
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11	35
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	24
9	QI	99/99 (100%)	78 (79%)	21 (21%)	1	4
9	XI	99/99 (100%)	80 (81%)	19 (19%)	1	6
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	16
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	2	12
11	QK	92/99 (93%)	81 (88%)	11 (12%)	5	20
11	XK	92/99 (93%)	83 (90%)	9 (10%)	8	29
12	QL	104/109 (95%)	89 (86%)	15 (14%)	3	15
12	XL	104/109 (95%)	87 (84%)	17 (16%)	2	10
13	QM	94/101 (93%)	80 (85%)	14 (15%)	3	13
13	XM	94/101 (93%)	82 (87%)	12 (13%)	4	18
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	76
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	27
15	QO	79/80 (99%)	74 (94%)	5 (6%)	18	47
15	XO	79/80 (99%)	74 (94%)	5 (6%)	18	47
16	QP	72/74 (97%)	64 (89%)	8 (11%)	6	23
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6	23
17	QQ	95/97 (98%)	90 (95%)	5 (5%)	22	53
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	40
18	QR	62/77 (80%)	56 (90%)	6 (10%)	8	29
18	XR	62/77 (80%)	54 (87%)	8 (13%)	4	18
19	QS	71/80 (89%)	54 (76%)	17 (24%)	0	2
19	XS	71/80 (89%)	58 (82%)	13 (18%)	1	7
20	QT	76/82 (93%)	62 (82%)	14 (18%)	1	7
20	XT	76/82 (93%)	66 (87%)	10 (13%)	4	17
21	QU	20/20 (100%)	18 (90%)	2 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	XU	20/20 (100%)	18 (90%)	2 (10%)	7	27
24	QY	79/103 (77%)	73 (92%)	6 (8%)	13	39
24	XY	79/103 (77%)	74 (94%)	5 (6%)	18	47
27	RD	214/218 (98%)	178 (83%)	36 (17%)	2	9
27	YD	214/218 (98%)	179 (84%)	35 (16%)	2	10
28	RE	165/166 (99%)	138 (84%)	27 (16%)	2	10
28	YE	165/166 (99%)	138 (84%)	27 (16%)	2	10
29	RF	165/166 (99%)	139 (84%)	26 (16%)	2	11
29	YF	165/166 (99%)	142 (86%)	23 (14%)	3	16
30	RG	155/156 (99%)	147 (95%)	8 (5%)	23	54
30	YG	155/156 (99%)	138 (89%)	17 (11%)	6	24
31	RH	142/148 (96%)	124 (87%)	18 (13%)	4	19
31	YH	142/148 (96%)	116 (82%)	26 (18%)	1	7
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1	5
32	YI	122/124 (98%)	99 (81%)	23 (19%)	1	6
33	RN	117/119 (98%)	107 (92%)	10 (8%)	10	35
33	YN	117/119 (98%)	104 (89%)	13 (11%)	6	23
34	RO	100/100 (100%)	91 (91%)	9 (9%)	9	32
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	27
35	RP	116/116 (100%)	82 (71%)	34 (29%)	0	1
35	YP	116/116 (100%)	85 (73%)	31 (27%)	0	1
36	RQ	110/111 (99%)	93 (84%)	17 (16%)	2	12
36	YQ	110/111 (99%)	93 (84%)	17 (16%)	2	12
37	RR	100/101 (99%)	82 (82%)	18 (18%)	1	7
37	YR	100/101 (99%)	87 (87%)	13 (13%)	4	17
38	RS	87/88 (99%)	80 (92%)	7 (8%)	12	37
38	YS	87/88 (99%)	73 (84%)	14 (16%)	2	10
39	RT	120/127 (94%)	100 (83%)	20 (17%)	2	10
39	YT	120/127 (94%)	98 (82%)	22 (18%)	1	7
40	RU	93/94 (99%)	85 (91%)	8 (9%)	10	35
40	YU	93/94 (99%)	85 (91%)	8 (9%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	5
41	YV	82/82 (100%)	63 (77%)	19 (23%)	1	3
42	RW	92/92 (100%)	82 (89%)	10 (11%)	6	24
42	YW	92/92 (100%)	79 (86%)	13 (14%)	3	16
43	RX	74/78 (95%)	65 (88%)	9 (12%)	5	20
43	YX	74/78 (95%)	68 (92%)	6 (8%)	11	36
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	2
44	YY	85/91 (93%)	61 (72%)	24 (28%)	0	1
45	RZ	155/179 (87%)	127 (82%)	28 (18%)	1	7
45	YZ	162/179 (90%)	134 (83%)	28 (17%)	2	8
46	R0	66/67 (98%)	62 (94%)	4 (6%)	18	48
46	Y0	66/67 (98%)	58 (88%)	8 (12%)	5	20
47	R1	82/83 (99%)	68 (83%)	14 (17%)	2	9
47	Y1	82/83 (99%)	72 (88%)	10 (12%)	5	20
48	R2	64/67 (96%)	52 (81%)	12 (19%)	1	6
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	24
49	R3	51/52 (98%)	44 (86%)	7 (14%)	3	16
49	Y3	51/52 (98%)	47 (92%)	4 (8%)	12	38
50	R4	62/63 (98%)	47 (76%)	15 (24%)	0	2
50	Y4	62/63 (98%)	44 (71%)	18 (29%)	0	1
51	R5	51/52 (98%)	40 (78%)	11 (22%)	1	4
51	Y5	49/52 (94%)	42 (86%)	7 (14%)	3	15
52	R6	47/52 (90%)	32 (68%)	15 (32%)	0	1
52	Y6	47/52 (90%)	30 (64%)	17 (36%)	0	0
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2	10
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	10
54	R8	54/55 (98%)	44 (82%)	10 (18%)	1	7
54	Y8	54/55 (98%)	44 (82%)	10 (18%)	1	7
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	49
55	Y9	33/34 (97%)	33 (100%)	0	100	100
All	All	9856/10268 (96%)	8442 (86%)	1414 (14%)	3	15

5 of 1414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	R4	16	CYS
6	XF	83	ASP
45	YZ	71	VAL
51	R5	36	CYS
2	XB	185	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
45	RZ	118	GLN
50	Y4	6	HIS
7	XG	97	GLN
7	QG	86	GLN
3	XC	108	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1522 (99%)	303 (20%)	42 (2%)
1	XA	1506/1522 (98%)	291 (19%)	37 (2%)
22	QV	76/77 (98%)	15 (19%)	0
22	QW	76/77 (98%)	21 (27%)	2 (2%)
22	XV	76/77 (98%)	10 (13%)	1 (1%)
22	XW	76/77 (98%)	18 (23%)	0
23	QX	16/20 (80%)	6 (37%)	2 (12%)
23	XX	16/20 (80%)	6 (37%)	0
25	RA	2888/2916 (99%)	575 (19%)	52 (1%)
25	YA	2872/2916 (98%)	560 (19%)	39 (1%)
26	RB	121/124 (97%)	23 (19%)	1 (0%)
26	YB	121/124 (97%)	20 (16%)	2 (1%)
All	All	9353/9472 (98%)	1848 (19%)	178 (1%)

5 of 1848 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	9	G
1	QA	22	G
1	QA	32	A

5 of 178 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2092	U
1	XA	5	U
25	YA	2191	G
25	RA	2166	G
25	RA	2518	A

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

2 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	A3P	QX	20	23	23,28,29	1.08	1 (4%)	23,42,45	1.37	4 (17%)
23	A3P	XX	20	23	23,28,29	1.00	1 (4%)	23,42,45	1.40	3 (13%)

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	A3P	QX	20	23	-	5/8/30/31	0/3/3/3
23	A3P	XX	20	23	-	1/8/30/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	C5-C4	2.58	1.47	1.40
23	XX	20	A3P	C5-C4	2.49	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	XX	20	A3P	N3-C2-N1	-3.47	123.25	128.68
23	QX	20	A3P	C4-C5-N7	-3.32	105.94	109.40
23	QX	20	A3P	N3-C2-N1	-3.28	123.55	128.68
23	XX	20	A3P	C3'-C2'-C1'	2.97	106.47	99.89
23	XX	20	A3P	C4-C5-N7	-2.74	106.55	109.40

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	QX	20	A3P	C3'-O3'-P1-O1P
23	QX	20	A3P	C2'-C3'-O3'-P1
23	QX	20	A3P	C4'-C3'-O3'-P1
23	QX	20	A3P	C3'-C4'-C5'-O5'
23	QX	20	A3P	C3'-O3'-P1-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	QX	20	A3P	1	0
23	XX	20	A3P	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1244 ligands modelled in this entry, 1244 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1511/1522 (99%)	0.12	47 (3%) 49 48	47, 90, 193, 346	0
1	XA	1508/1522 (99%)	0.11	58 (3%) 40 37	42, 85, 179, 385	0
2	QB	236/256 (92%)	0.41	25 (10%) 6 6	95, 145, 216, 283	0
2	XB	236/256 (92%)	0.34	16 (6%) 17 17	80, 127, 194, 248	0
3	QC	206/239 (86%)	0.56	17 (8%) 11 11	86, 129, 209, 279	0
3	XC	206/239 (86%)	0.31	12 (5%) 23 22	73, 111, 176, 256	0
4	QD	208/209 (99%)	-0.01	3 (1%) 75 75	58, 81, 132, 231	0
4	XD	208/209 (99%)	0.00	4 (1%) 66 65	63, 92, 153, 186	0
5	QE	154/162 (95%)	-0.04	3 (1%) 66 65	57, 83, 141, 207	0
5	XE	154/162 (95%)	0.13	6 (3%) 39 37	56, 83, 145, 244	0
6	QF	101/101 (100%)	0.66	9 (8%) 9 10	92, 138, 183, 203	0
6	XF	101/101 (100%)	0.03	1 (0%) 82 82	60, 90, 119, 171	0
7	QG	155/156 (99%)	0.68	17 (10%) 5 5	96, 144, 192, 282	0
7	XG	155/156 (99%)	0.38	11 (7%) 16 16	87, 115, 173, 226	0
8	QH	138/138 (100%)	-0.16	0 100 100	59, 91, 128, 188	0
8	XH	138/138 (100%)	-0.04	0 100 100	64, 88, 121, 174	0
9	QI	128/128 (100%)	1.03	22 (17%) 1 1	88, 168, 229, 293	0
9	XI	128/128 (100%)	0.64	7 (5%) 25 23	83, 136, 203, 246	0
10	QJ	99/105 (94%)	0.95	16 (16%) 1 2	92, 168, 228, 284	0
10	XJ	99/105 (94%)	0.92	14 (14%) 2 2	78, 141, 219, 279	0
11	QK	121/129 (93%)	0.75	12 (9%) 7 7	66, 117, 191, 242	0
11	XK	121/129 (93%)	0.19	4 (3%) 46 44	52, 84, 161, 197	0
12	QL	125/132 (94%)	0.02	1 (0%) 86 86	53, 71, 115, 232	0
12	XL	125/132 (94%)	0.01	3 (2%) 59 56	52, 71, 105, 204	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	118/126 (93%)	0.56	8 (6%) 17 17	93, 148, 218, 278	0
13	XM	118/126 (93%)	0.38	5 (4%) 36 34	82, 126, 181, 267	0
14	QN	60/61 (98%)	0.63	7 (11%) 4 4	98, 127, 180, 208	0
14	XN	60/61 (98%)	0.41	3 (5%) 28 27	81, 102, 132, 248	0
15	QO	88/89 (98%)	0.14	0 100 100	63, 89, 143, 153	0
15	XO	88/89 (98%)	-0.02	1 (1%) 80 81	54, 80, 125, 147	0
16	QP	84/88 (95%)	0.01	2 (2%) 59 56	61, 77, 115, 213	0
16	XP	84/88 (95%)	0.03	2 (2%) 59 56	75, 98, 139, 217	0
17	QQ	100/105 (95%)	0.13	2 (2%) 65 64	60, 85, 113, 137	0
17	XQ	100/105 (95%)	0.02	1 (1%) 82 82	58, 85, 117, 209	0
18	QR	71/88 (80%)	0.45	7 (9%) 7 7	92, 124, 204, 224	0
18	XR	71/88 (80%)	0.21	5 (7%) 16 16	63, 86, 179, 224	0
19	QS	82/93 (88%)	0.82	13 (15%) 1 2	96, 159, 239, 270	0
19	XS	82/93 (88%)	0.54	8 (9%) 7 7	91, 129, 221, 278	0
20	QT	99/106 (93%)	0.38	5 (5%) 28 26	65, 99, 158, 210	0
20	XT	99/106 (93%)	0.24	2 (2%) 65 64	79, 113, 174, 201	0
21	QU	25/25 (100%)	1.84	8 (32%) 0 0	109, 136, 171, 253	0
21	XU	25/25 (100%)	1.28	4 (16%) 1 2	95, 118, 171, 181	0
22	QV	77/77 (100%)	0.35	2 (2%) 56 53	47, 91, 145, 216	0
22	QW	77/77 (100%)	1.92	29 (37%) 0 0	60, 203, 273, 298	0
22	XV	77/77 (100%)	0.18	2 (2%) 56 53	47, 90, 138, 204	0
22	XW	77/77 (100%)	2.04	38 (49%) 0 0	71, 225, 299, 354	0
23	QX	17/20 (85%)	2.07	8 (47%) 0 0	59, 207, 269, 270	0
23	XX	17/20 (85%)	2.03	7 (41%) 0 0	52, 200, 283, 301	0
24	QY	92/118 (77%)	0.74	8 (8%) 10 10	66, 123, 158, 177	0
24	XY	92/118 (77%)	1.88	36 (39%) 0 0	79, 160, 201, 212	0
25	RA	2891/2916 (99%)	0.13	133 (4%) 32 30	35, 64, 209, 371	0
25	YA	2875/2916 (98%)	0.12	148 (5%) 28 26	33, 60, 231, 360	0
26	RB	122/124 (98%)	0.12	2 (1%) 72 70	67, 110, 153, 202	0
26	YB	122/124 (98%)	0.15	2 (1%) 72 70	74, 102, 152, 201	0
27	RD	272/276 (98%)	-0.07	4 (1%) 73 72	37, 65, 112, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
27	YD	272/276 (98%)	-0.17	1 (0%)	92	93	32, 48, 92, 192	0
28	RE	205/206 (99%)	0.14	7 (3%)	45	43	41, 79, 169, 273	0
28	YE	205/206 (99%)	0.23	8 (3%)	39	37	40, 78, 163, 260	0
29	RF	208/210 (99%)	0.04	9 (4%)	35	34	35, 60, 170, 262	0
29	YF	208/210 (99%)	0.08	11 (5%)	26	24	35, 73, 173, 250	0
30	RG	181/182 (99%)	0.35	5 (2%)	53	51	85, 125, 168, 187	0
30	YG	181/182 (99%)	0.48	8 (4%)	34	33	85, 122, 183, 239	0
31	RH	170/180 (94%)	1.51	48 (28%)	0	0	99, 169, 244, 283	0
31	YH	170/180 (94%)	1.14	39 (22%)	0	1	75, 147, 231, 277	0
32	RI	146/148 (98%)	0.77	21 (14%)	2	2	70, 125, 186, 284	0
32	YI	146/148 (98%)	0.28	5 (3%)	45	43	47, 100, 178, 253	0
33	RN	138/140 (98%)	-0.11	0	100	100	49, 78, 131, 230	0
33	YN	138/140 (98%)	-0.04	0	100	100	53, 85, 143, 177	0
34	RO	122/122 (100%)	-0.16	0	100	100	48, 68, 105, 143	0
34	YO	122/122 (100%)	-0.29	0	100	100	46, 64, 92, 136	0
35	RP	150/150 (100%)	0.10	5 (3%)	46	44	37, 78, 157, 260	0
35	YP	150/150 (100%)	0.19	3 (2%)	65	64	40, 75, 139, 253	0
36	RQ	140/141 (99%)	-0.03	1 (0%)	87	88	47, 77, 136, 200	0
36	YQ	139/141 (98%)	0.03	2 (1%)	75	75	50, 79, 131, 251	0
37	RR	117/118 (99%)	-0.19	0	100	100	50, 73, 111, 146	0
37	YR	117/118 (99%)	-0.15	0	100	100	48, 68, 101, 145	0
38	RS	111/112 (99%)	0.26	5 (4%)	33	32	82, 114, 162, 217	0
38	YS	111/112 (99%)	0.37	8 (7%)	15	15	78, 102, 155, 196	0
39	RT	137/146 (93%)	0.11	3 (2%)	62	60	58, 83, 174, 271	0
39	YT	137/146 (93%)	0.18	7 (5%)	28	26	55, 79, 183, 256	0
40	RU	117/118 (99%)	-0.22	3 (2%)	56	53	40, 63, 130, 251	0
40	YU	117/118 (99%)	-0.02	2 (1%)	70	68	47, 76, 150, 184	0
41	RV	101/101 (100%)	0.05	3 (2%)	50	49	40, 83, 148, 267	0
41	YV	101/101 (100%)	0.36	4 (3%)	38	36	46, 103, 153, 191	0
42	RW	113/113 (100%)	-0.05	2 (1%)	68	67	40, 61, 127, 192	0
42	YW	113/113 (100%)	0.02	2 (1%)	68	67	42, 64, 112, 207	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
43	RX	92/96 (95%)	-0.11	0	100	100	57, 77, 114, 151	0
43	YX	92/96 (95%)	-0.14	0	100	100	43, 62, 99, 124	0
44	RY	102/110 (92%)	0.86	18 (17%)	1	1	57, 88, 196, 277	0
44	YY	102/110 (92%)	0.78	16 (15%)	2	2	63, 102, 218, 267	0
45	RZ	176/206 (85%)	0.48	14 (7%)	12	11	76, 116, 207, 274	0
45	YZ	183/206 (88%)	0.42	14 (7%)	13	12	75, 120, 186, 245	0
46	R0	83/85 (97%)	0.16	4 (4%)	30	28	46, 72, 159, 246	0
46	Y0	83/85 (97%)	0.21	5 (6%)	21	21	46, 76, 141, 197	0
47	R1	97/98 (98%)	0.43	5 (5%)	27	25	44, 73, 173, 231	0
47	Y1	97/98 (98%)	0.34	6 (6%)	20	20	36, 57, 166, 259	0
48	R2	69/72 (95%)	0.10	2 (2%)	51	50	66, 99, 165, 209	0
48	Y2	69/72 (95%)	0.05	1 (1%)	75	75	52, 76, 141, 198	0
49	R3	59/60 (98%)	0.06	4 (6%)	17	17	54, 68, 118, 154	0
49	Y3	59/60 (98%)	0.06	2 (3%)	45	43	59, 86, 131, 188	0
50	R4	70/71 (98%)	1.24	18 (25%)	0	0	100, 181, 261, 319	0
50	Y4	70/71 (98%)	1.23	19 (27%)	0	0	108, 173, 248, 312	0
51	R5	59/60 (98%)	0.55	9 (15%)	2	2	32, 68, 183, 221	0
51	Y5	57/60 (95%)	0.44	6 (10%)	6	6	31, 77, 168, 220	0
52	R6	48/54 (88%)	2.05	19 (39%)	0	0	80, 144, 220, 264	0
52	Y6	48/54 (88%)	1.88	19 (39%)	0	0	84, 123, 179, 225	0
53	R7	49/49 (100%)	-0.22	1 (2%)	65	64	29, 46, 128, 207	0
53	Y7	49/49 (100%)	-0.07	4 (8%)	11	11	20, 42, 117, 204	0
54	R8	64/65 (98%)	0.15	3 (4%)	31	29	36, 60, 143, 194	0
54	Y8	64/65 (98%)	0.18	3 (4%)	31	29	29, 59, 98, 237	0
55	R9	37/37 (100%)	2.73	25 (67%)	0	0	97, 141, 178, 209	0
55	Y9	36/37 (97%)	2.83	24 (66%)	0	0	84, 133, 171, 215	0
All	All	21220/21832 (97%)	0.25	1263 (5%)	21	21	20, 85, 198, 385	0

The worst 5 of 1263 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	1075	C	14.9
1	XA	1026	G	12.6

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Mol	Chain	Res	Type	RSRZ
25	RA	1057	A	12.6
28	YE	204	ALA	12.2
44	RY	48	ALA	11.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	A3P	XX	20	26/27	0.77	0.44	222,222,222,222	0
23	A3P	QX	20	26/27	0.85	0.23	175,175,175,175	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	XA	1706	1/1	0.30	0.86	81,81,81,81	0
56	MG	RA	3295	1/1	0.35	0.67	58,58,58,58	0
56	MG	XA	1702	1/1	0.38	0.72	101,101,101,101	0
56	MG	YA	3427	1/1	0.42	0.28	99,99,99,99	0
56	MG	RA	3132	1/1	0.46	1.34	58,58,58,58	0
56	MG	YA	3232	1/1	0.48	0.26	57,57,57,57	0
56	MG	RA	3243	1/1	0.49	0.32	54,54,54,54	0
56	MG	RA	3334	1/1	0.51	0.31	55,55,55,55	0
56	MG	XA	1678	1/1	0.52	0.22	70,70,70,70	0
56	MG	RA	3297	1/1	0.53	0.29	68,68,68,68	0
56	MG	YA	3279	1/1	0.54	0.30	66,66,66,66	0
56	MG	QA	1733	1/1	0.54	0.27	65,65,65,65	0
56	MG	RA	3216	1/1	0.54	0.41	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1625	1/1	0.54	0.31	87,87,87,87	0
56	MG	XA	1657	1/1	0.55	0.22	59,59,59,59	0
56	MG	RA	3319	1/1	0.55	0.55	96,96,96,96	0
56	MG	XA	1637	1/1	0.56	0.40	48,48,48,48	0
56	MG	QA	1709	1/1	0.57	0.44	59,59,59,59	0
56	MG	RA	3001	1/1	0.57	0.64	73,73,73,73	0
56	MG	RA	3074	1/1	0.59	0.44	33,33,33,33	0
56	MG	YQ	202	1/1	0.60	0.52	66,66,66,66	0
56	MG	RA	3324	1/1	0.60	0.18	62,62,62,62	0
56	MG	RA	3267	1/1	0.60	0.91	63,63,63,63	0
56	MG	XA	1754	1/1	0.61	0.69	119,119,119,119	0
56	MG	QA	1726	1/1	0.61	0.32	56,56,56,56	0
56	MG	YA	3407	1/1	0.62	0.15	44,44,44,44	0
56	MG	XA	1745	1/1	0.62	0.37	99,99,99,99	0
56	MG	YA	3338	1/1	0.63	0.16	63,63,63,63	0
56	MG	RA	3274	1/1	0.63	0.50	64,64,64,64	0
56	MG	RA	3405	1/1	0.63	0.63	74,74,74,74	0
56	MG	RA	3135	1/1	0.64	0.47	86,86,86,86	0
56	MG	RA	3161	1/1	0.64	0.58	71,71,71,71	0
56	MG	YA	3397	1/1	0.65	0.25	58,58,58,58	0
56	MG	YA	3001	1/1	0.65	0.78	70,70,70,70	0
56	MG	RA	3326	1/1	0.65	0.51	52,52,52,52	0
56	MG	RA	3175	1/1	0.66	0.43	57,57,57,57	0
56	MG	QA	1699	1/1	0.66	0.23	60,60,60,60	0
56	MG	YA	3460	1/1	0.66	0.23	82,82,82,82	0
56	MG	XA	1725	1/1	0.66	0.27	51,51,51,51	0
56	MG	RA	3331	1/1	0.66	0.20	74,74,74,74	0
56	MG	YA	3369	1/1	0.66	0.43	83,83,83,83	0
56	MG	QA	1706	1/1	0.66	0.78	50,50,50,50	0
56	MG	RU	201	1/1	0.67	0.53	63,63,63,63	0
56	MG	XA	1714	1/1	0.67	0.16	81,81,81,81	0
56	MG	YA	3181	1/1	0.67	0.55	64,64,64,64	0
56	MG	YA	3401	1/1	0.68	0.24	166,166,166,166	0
56	MG	RA	3155	1/1	0.68	0.27	55,55,55,55	0
56	MG	YA	3375	1/1	0.68	0.44	68,68,68,68	0
56	MG	RA	3233	1/1	0.68	0.46	50,50,50,50	0
56	MG	YA	3422	1/1	0.68	0.24	63,63,63,63	0
56	MG	YA	3174	1/1	0.68	0.35	66,66,66,66	0
56	MG	RA	3251	1/1	0.68	0.56	59,59,59,59	0
56	MG	YA	3300	1/1	0.68	0.36	74,74,74,74	0
56	MG	YA	3224	1/1	0.68	0.33	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3150	1/1	0.69	0.40	69,69,69,69	0
56	MG	RA	3007	1/1	0.69	0.99	40,40,40,40	0
56	MG	YA	3351	1/1	0.69	0.58	74,74,74,74	0
56	MG	QA	1645	1/1	0.69	0.59	75,75,75,75	0
56	MG	YA	3446	1/1	0.69	0.70	68,68,68,68	0
56	MG	QA	1694	1/1	0.70	0.21	86,86,86,86	0
56	MG	XA	1647	1/1	0.70	0.48	67,67,67,67	0
56	MG	YH	201	1/1	0.70	0.15	105,105,105,105	0
56	MG	XA	1739	1/1	0.70	0.15	57,57,57,57	0
56	MG	R2	101	1/1	0.71	0.51	74,74,74,74	0
56	MG	RA	3144	1/1	0.71	0.33	51,51,51,51	0
56	MG	YA	3336	1/1	0.71	0.67	75,75,75,75	0
56	MG	RA	3351	1/1	0.72	0.50	54,54,54,54	0
56	MG	RA	3402	1/1	0.72	0.41	61,61,61,61	0
56	MG	QA	1698	1/1	0.72	0.34	101,101,101,101	0
56	MG	YA	3418	1/1	0.72	0.52	52,52,52,52	0
56	MG	RA	3090	1/1	0.72	0.24	61,61,61,61	0
57	ZN	QN	100	1/1	0.72	0.15	100,100,100,100	0
56	MG	YA	3386	1/1	0.72	0.34	48,48,48,48	0
56	MG	YA	3291	1/1	0.72	0.60	63,63,63,63	0
56	MG	RA	3327	1/1	0.72	0.54	69,69,69,69	0
56	MG	YA	3298	1/1	0.72	0.49	82,82,82,82	0
56	MG	RA	3309	1/1	0.73	0.70	69,69,69,69	0
56	MG	YA	3331	1/1	0.73	0.32	56,56,56,56	0
56	MG	RA	3388	1/1	0.73	0.41	84,84,84,84	0
56	MG	RA	3174	1/1	0.73	0.25	64,64,64,64	0
56	MG	XA	1728	1/1	0.73	0.90	73,73,73,73	0
56	MG	QV	103	1/1	0.74	0.45	55,55,55,55	0
56	MG	YA	3379	1/1	0.74	0.49	87,87,87,87	0
56	MG	YA	3434	1/1	0.74	0.50	67,67,67,67	0
56	MG	RA	3262	1/1	0.74	0.19	38,38,38,38	0
56	MG	RA	3245	1/1	0.74	0.49	41,41,41,41	0
56	MG	XA	1716	1/1	0.74	0.34	58,58,58,58	0
56	MG	YA	3444	1/1	0.75	0.27	56,56,56,56	0
56	MG	XA	1746	1/1	0.75	0.35	67,67,67,67	0
56	MG	YA	3373	1/1	0.75	0.25	41,41,41,41	0
56	MG	YA	3089	1/1	0.75	0.34	42,42,42,42	0
56	MG	XA	1617	1/1	0.75	0.27	50,50,50,50	0
56	MG	YA	3285	1/1	0.75	0.52	68,68,68,68	0
56	MG	XA	1758	1/1	0.75	0.38	60,60,60,60	0
56	MG	RA	3333	1/1	0.75	0.24	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3334	1/1	0.76	0.37	65,65,65,65	0
56	MG	XA	1689	1/1	0.76	0.70	55,55,55,55	0
56	MG	YA	3151	1/1	0.76	0.45	26,26,26,26	0
56	MG	YA	3131	1/1	0.76	0.35	48,48,48,48	0
56	MG	RA	3396	1/1	0.76	0.25	49,49,49,49	0
56	MG	XA	1659	1/1	0.76	0.20	76,76,76,76	0
56	MG	RA	3131	1/1	0.76	0.39	65,65,65,65	0
56	MG	RA	3272	1/1	0.76	0.90	49,49,49,49	0
56	MG	QA	1690	1/1	0.76	0.41	80,80,80,80	0
56	MG	QA	1732	1/1	0.76	0.52	63,63,63,63	0
56	MG	RA	3325	1/1	0.76	0.25	56,56,56,56	0
56	MG	YA	3425	1/1	0.77	0.24	43,43,43,43	0
56	MG	XA	1740	1/1	0.77	0.34	50,50,50,50	0
56	MG	XA	1731	1/1	0.77	0.63	59,59,59,59	0
56	MG	XA	1743	1/1	0.77	0.15	39,39,39,39	0
56	MG	RA	3082	1/1	0.77	0.24	15,15,15,15	0
56	MG	YB	205	1/1	0.77	0.28	62,62,62,62	0
56	MG	XL	201	1/1	0.77	0.19	60,60,60,60	0
56	MG	RA	3259	1/1	0.77	0.38	57,57,57,57	0
56	MG	QA	1715	1/1	0.77	0.54	74,74,74,74	0
56	MG	RA	3400	1/1	0.77	0.37	59,59,59,59	0
56	MG	YA	3380	1/1	0.77	0.21	65,65,65,65	0
56	MG	YA	3390	1/1	0.77	0.29	92,92,92,92	0
56	MG	RA	3048	1/1	0.77	0.40	21,21,21,21	0
56	MG	RA	3182	1/1	0.78	0.30	38,38,38,38	0
56	MG	YA	3165	1/1	0.78	0.21	50,50,50,50	0
56	MG	YA	3276	1/1	0.78	0.47	61,61,61,61	0
56	MG	QA	1672	1/1	0.78	0.19	49,49,49,49	0
56	MG	QA	1704	1/1	0.78	0.42	60,60,60,60	0
56	MG	YA	3347	1/1	0.78	0.77	74,74,74,74	0
56	MG	YA	3312	1/1	0.78	0.90	52,52,52,52	0
56	MG	YA	3349	1/1	0.78	0.54	58,58,58,58	0
56	MG	YA	3442	1/1	0.78	0.31	77,77,77,77	0
56	MG	YA	3307	1/1	0.78	0.31	101,101,101,101	0
56	MG	RA	3314	1/1	0.78	0.74	60,60,60,60	0
56	MG	QA	1626	1/1	0.78	0.53	59,59,59,59	0
56	MG	RA	3095	1/1	0.78	0.15	62,62,62,62	0
56	MG	XA	1696	1/1	0.78	0.30	56,56,56,56	0
56	MG	RA	3350	1/1	0.78	0.98	61,61,61,61	0
56	MG	RA	3239	1/1	0.78	0.47	52,52,52,52	0
56	MG	RA	3210	1/1	0.78	0.29	41,41,41,41	0
56	MG	RA	3315	1/1	0.78	0.40	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1619	1/1	0.79	0.22	27,27,27,27	0
56	MG	QA	1641	1/1	0.79	0.20	50,50,50,50	0
56	MG	YA	3337	1/1	0.79	0.30	46,46,46,46	0
56	MG	RA	3283	1/1	0.79	0.38	40,40,40,40	0
56	MG	RQ	201	1/1	0.79	0.45	52,52,52,52	0
56	MG	XA	1630	1/1	0.79	0.36	35,35,35,35	0
56	MG	XA	1635	1/1	0.79	0.19	45,45,45,45	0
56	MG	RA	3223	1/1	0.79	0.38	67,67,67,67	0
56	MG	XA	1660	1/1	0.79	0.63	60,60,60,60	0
56	MG	YA	3454	1/1	0.79	0.23	59,59,59,59	0
56	MG	YA	3368	1/1	0.79	0.29	53,53,53,53	0
56	MG	QA	1735	1/1	0.79	0.49	75,75,75,75	0
56	MG	YA	3081	1/1	0.79	0.23	35,35,35,35	0
56	MG	YA	3173	1/1	0.79	0.14	41,41,41,41	0
56	MG	RA	3341	1/1	0.79	0.46	41,41,41,41	0
56	MG	RA	3329	1/1	0.79	0.24	60,60,60,60	0
56	MG	YA	3219	1/1	0.79	0.11	38,38,38,38	0
56	MG	YA	3266	1/1	0.79	0.83	71,71,71,71	0
56	MG	YA	3156	1/1	0.80	0.18	42,42,42,42	0
56	MG	XA	1724	1/1	0.80	0.62	64,64,64,64	0
56	MG	RA	3165	1/1	0.80	0.25	52,52,52,52	0
56	MG	XA	1692	1/1	0.80	0.24	102,102,102,102	0
56	MG	RA	3336	1/1	0.80	0.23	39,39,39,39	0
56	MG	RA	3050	1/1	0.80	0.71	57,57,57,57	0
56	MG	RA	3384	1/1	0.80	0.51	61,61,61,61	0
56	MG	YA	3389	1/1	0.80	0.70	59,59,59,59	0
56	MG	RA	3294	1/1	0.80	0.15	53,53,53,53	0
56	MG	YO	201	1/1	0.80	0.37	63,63,63,63	0
56	MG	RA	3160	1/1	0.80	0.21	36,36,36,36	0
56	MG	RA	3355	1/1	0.80	0.24	73,73,73,73	0
56	MG	QA	1710	1/1	0.80	0.37	54,54,54,54	0
56	MG	XA	1688	1/1	0.80	0.23	39,39,39,39	0
56	MG	YA	3258	1/1	0.80	0.36	60,60,60,60	0
56	MG	YA	3132	1/1	0.80	0.54	62,62,62,62	0
56	MG	YA	3180	1/1	0.81	0.27	61,61,61,61	0
56	MG	RA	3269	1/1	0.81	0.27	75,75,75,75	0
56	MG	XA	1652	1/1	0.81	0.21	38,38,38,38	0
56	MG	YA	3313	1/1	0.81	0.19	54,54,54,54	0
56	MG	RA	3271	1/1	0.81	0.38	55,55,55,55	0
56	MG	R0	102	1/1	0.81	0.79	53,53,53,53	0
56	MG	R5	103	1/1	0.81	0.13	60,60,60,60	0
56	MG	YA	3248	1/1	0.81	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3234	1/1	0.81	0.25	33,33,33,33	0
56	MG	RA	3278	1/1	0.81	0.12	67,67,67,67	0
56	MG	YA	3273	1/1	0.81	0.25	50,50,50,50	0
56	MG	YA	3287	1/1	0.81	0.34	62,62,62,62	0
56	MG	QA	1725	1/1	0.81	0.10	65,65,65,65	0
56	MG	YA	3393	1/1	0.81	0.36	62,62,62,62	0
56	MG	RA	3346	1/1	0.81	0.46	43,43,43,43	0
56	MG	XA	1759	1/1	0.81	0.26	69,69,69,69	0
56	MG	RA	3352	1/1	0.81	0.87	67,67,67,67	0
56	MG	RA	3303	1/1	0.82	0.69	55,55,55,55	0
56	MG	QA	1621	1/1	0.82	0.16	38,38,38,38	0
56	MG	QA	1738	1/1	0.82	0.19	67,67,67,67	0
56	MG	YA	3097	1/1	0.82	0.30	78,78,78,78	0
56	MG	YA	3264	1/1	0.82	0.31	66,66,66,66	0
56	MG	XA	1640	1/1	0.82	0.33	54,54,54,54	0
56	MG	RA	3250	1/1	0.82	0.42	55,55,55,55	0
56	MG	QV	101	1/1	0.82	0.29	35,35,35,35	0
56	MG	RA	3311	1/1	0.82	0.56	55,55,55,55	0
56	MG	YA	3067	1/1	0.82	0.30	40,40,40,40	0
56	MG	QA	1689	1/1	0.82	0.22	61,61,61,61	0
56	MG	YA	3305	1/1	0.82	0.19	57,57,57,57	0
56	MG	XA	1742	1/1	0.82	0.27	63,63,63,63	0
56	MG	RA	3208	1/1	0.82	0.37	48,48,48,48	0
56	MG	YU	3400	1/1	0.82	0.41	47,47,47,47	0
56	MG	RA	3304	1/1	0.82	0.31	76,76,76,76	0
56	MG	RA	3282	1/1	0.82	0.40	40,40,40,40	0
56	MG	YA	3319	1/1	0.82	0.48	54,54,54,54	0
56	MG	YA	3371	1/1	0.82	0.32	56,56,56,56	0
56	MG	XA	1720	1/1	0.82	0.36	53,53,53,53	0
56	MG	XA	1727	1/1	0.82	0.94	59,59,59,59	0
56	MG	QA	1612	1/1	0.82	0.36	51,51,51,51	0
56	MG	RA	3353	1/1	0.83	0.10	85,85,85,85	0
56	MG	QA	1658	1/1	0.83	0.33	46,46,46,46	0
56	MG	RA	3022	1/1	0.83	0.32	56,56,56,56	0
56	MG	RA	3035	1/1	0.83	0.27	40,40,40,40	0
56	MG	XA	1649	1/1	0.83	0.32	60,60,60,60	0
56	MG	YA	3384	1/1	0.83	0.28	58,58,58,58	0
56	MG	YA	3303	1/1	0.83	0.44	60,60,60,60	0
56	MG	YA	3235	1/1	0.83	0.22	54,54,54,54	0
56	MG	QA	1734	1/1	0.83	0.19	61,61,61,61	0
56	MG	XA	1705	1/1	0.83	0.52	53,53,53,53	0
56	MG	RA	3320	1/1	0.83	0.51	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1683	1/1	0.83	0.29	64,64,64,64	0
56	MG	YA	3419	1/1	0.83	0.46	59,59,59,59	0
56	MG	YA	3095	1/1	0.83	0.46	53,53,53,53	0
56	MG	RA	3302	1/1	0.83	0.35	51,51,51,51	0
56	MG	YA	3413	1/1	0.83	0.26	42,42,42,42	0
56	MG	XA	1687	1/1	0.83	0.65	49,49,49,49	0
56	MG	YA	3221	1/1	0.83	0.18	37,37,37,37	0
56	MG	XA	1684	1/1	0.83	0.39	48,48,48,48	0
56	MG	QA	1659	1/1	0.83	0.16	41,41,41,41	0
56	MG	RA	3368	1/1	0.83	0.31	51,51,51,51	0
56	MG	QA	1736	1/1	0.83	0.36	52,52,52,52	0
56	MG	QA	1701	1/1	0.84	0.61	77,77,77,77	0
56	MG	YA	3435	1/1	0.84	0.20	57,57,57,57	0
56	MG	RA	3209	1/1	0.84	0.22	24,24,24,24	0
56	MG	RA	3363	1/1	0.84	0.62	45,45,45,45	0
56	MG	XA	1620	1/1	0.84	0.29	33,33,33,33	0
56	MG	XA	1698	1/1	0.84	0.23	66,66,66,66	0
56	MG	RA	3203	1/1	0.84	0.36	42,42,42,42	0
56	MG	YA	3227	1/1	0.84	0.33	54,54,54,54	0
56	MG	RA	3169	1/1	0.84	0.41	53,53,53,53	0
56	MG	RA	3404	1/1	0.84	0.62	58,58,58,58	0
56	MG	XA	1613	1/1	0.84	0.21	43,43,43,43	0
56	MG	XA	1732	1/1	0.84	0.17	40,40,40,40	0
56	MG	XA	1615	1/1	0.84	0.23	39,39,39,39	0
56	MG	YA	3344	1/1	0.84	0.26	66,66,66,66	0
56	MG	QA	1670	1/1	0.84	0.23	62,62,62,62	0
56	MG	RA	3261	1/1	0.84	0.77	45,45,45,45	0
56	MG	YA	3278	1/1	0.84	0.28	75,75,75,75	0
56	MG	YA	3404	1/1	0.84	0.24	28,28,28,28	0
56	MG	YB	203	1/1	0.84	0.34	52,52,52,52	0
56	MG	YA	3354	1/1	0.84	0.55	79,79,79,79	0
56	MG	QA	1703	1/1	0.84	0.22	43,43,43,43	0
56	MG	YA	3455	1/1	0.84	0.18	68,68,68,68	0
56	MG	RA	3102	1/1	0.84	0.39	54,54,54,54	0
56	MG	QV	102	1/1	0.84	0.28	38,38,38,38	0
56	MG	YA	3252	1/1	0.84	0.51	93,93,93,93	0
56	MG	YA	3346	1/1	0.84	0.27	34,34,34,34	0
56	MG	YA	3295	1/1	0.84	0.64	56,56,56,56	0
56	MG	QA	1613	1/1	0.84	0.23	56,56,56,56	0
56	MG	YA	3340	1/1	0.84	0.57	48,48,48,48	0
56	MG	QA	1646	1/1	0.84	0.17	52,52,52,52	0
56	MG	RA	3180	1/1	0.84	0.28	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3459	1/1	0.84	0.44	57,57,57,57	0
56	MG	RA	3345	1/1	0.84	0.18	61,61,61,61	0
56	MG	YA	3299	1/1	0.84	0.33	67,67,67,67	0
56	MG	YA	3364	1/1	0.84	0.21	44,44,44,44	0
56	MG	RA	3266	1/1	0.84	0.37	42,42,42,42	0
56	MG	RA	3389	1/1	0.84	0.42	57,57,57,57	0
56	MG	XA	1726	1/1	0.84	0.37	55,55,55,55	0
56	MG	QA	1675	1/1	0.84	0.47	50,50,50,50	0
56	MG	YP	202	1/1	0.85	0.30	50,50,50,50	0
56	MG	YA	3370	1/1	0.85	0.28	62,62,62,62	0
56	MG	RA	3187	1/1	0.85	0.43	59,59,59,59	0
56	MG	XD	302	1/1	0.85	0.08	86,86,86,86	0
56	MG	YA	3249	1/1	0.85	0.53	40,40,40,40	0
56	MG	R5	102	1/1	0.85	0.34	63,63,63,63	0
56	MG	QA	1630	1/1	0.85	0.38	57,57,57,57	0
56	MG	YA	3129	1/1	0.85	0.30	41,41,41,41	0
56	MG	RA	3093	1/1	0.85	0.44	26,26,26,26	0
56	MG	RA	3173	1/1	0.85	0.21	52,52,52,52	0
56	MG	RA	3318	1/1	0.85	0.09	40,40,40,40	0
56	MG	RA	3184	1/1	0.85	0.48	71,71,71,71	0
56	MG	YA	3311	1/1	0.85	0.38	51,51,51,51	0
56	MG	YA	3399	1/1	0.85	0.25	61,61,61,61	0
56	MG	YA	3366	1/1	0.85	0.34	47,47,47,47	0
56	MG	XA	1704	1/1	0.85	0.22	55,55,55,55	0
56	MG	RA	3391	1/1	0.85	0.24	113,113,113,113	0
56	MG	YA	3290	1/1	0.85	0.20	78,78,78,78	0
56	MG	YA	3216	1/1	0.85	0.28	51,51,51,51	0
56	MG	QV	105	1/1	0.85	0.18	56,56,56,56	0
56	MG	YY	201	1/1	0.85	0.33	42,42,42,42	0
56	MG	YA	3306	1/1	0.85	0.60	56,56,56,56	0
56	MG	XV	104	1/1	0.85	0.26	44,44,44,44	0
56	MG	YA	3436	1/1	0.85	0.65	52,52,52,52	0
56	MG	YA	3098	1/1	0.85	0.43	66,66,66,66	0
56	MG	XA	1723	1/1	0.85	0.18	47,47,47,47	0
56	MG	XA	1719	1/1	0.85	0.20	46,46,46,46	0
56	MG	YA	3437	1/1	0.85	0.26	56,56,56,56	0
56	MG	YA	3167	1/1	0.85	0.48	91,91,91,91	0
56	MG	RA	3167	1/1	0.86	0.33	52,52,52,52	0
56	MG	XA	1656	1/1	0.86	0.26	51,51,51,51	0
56	MG	YA	3324	1/1	0.86	0.45	33,33,33,33	0
56	MG	YA	3164	1/1	0.86	0.52	41,41,41,41	0
56	MG	QA	1632	1/1	0.86	0.65	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1606	1/1	0.86	0.35	27,27,27,27	0
56	MG	RA	3207	1/1	0.86	0.46	24,24,24,24	0
56	MG	Y0	103	1/1	0.86	0.44	57,57,57,57	0
56	MG	RA	3401	1/1	0.86	0.21	54,54,54,54	0
56	MG	YA	3360	1/1	0.86	0.16	57,57,57,57	0
56	MG	YA	3179	1/1	0.86	0.32	45,45,45,45	0
56	MG	YA	3100	1/1	0.86	0.45	33,33,33,33	0
56	MG	RA	3377	1/1	0.86	0.12	32,32,32,32	0
56	MG	XN	102	1/1	0.86	0.33	62,62,62,62	0
56	MG	RA	3124	1/1	0.86	0.25	29,29,29,29	0
56	MG	RB	203	1/1	0.86	0.38	52,52,52,52	0
56	MG	QA	1668	1/1	0.86	0.41	68,68,68,68	0
56	MG	QA	1667	1/1	0.86	0.28	52,52,52,52	0
56	MG	YA	3238	1/1	0.86	0.21	45,45,45,45	0
56	MG	YB	201	1/1	0.86	0.33	42,42,42,42	0
56	MG	YA	3439	1/1	0.86	0.29	32,32,32,32	0
56	MG	QA	1718	1/1	0.86	1.02	72,72,72,72	0
56	MG	YA	3143	1/1	0.86	0.27	80,80,80,80	0
56	MG	QA	1661	1/1	0.86	0.12	75,75,75,75	0
56	MG	YA	3109	1/1	0.86	0.32	39,39,39,39	0
56	MG	RA	3099	1/1	0.86	0.30	68,68,68,68	0
56	MG	RA	3313	1/1	0.86	0.36	50,50,50,50	0
56	MG	RA	3373	1/1	0.86	0.79	26,26,26,26	0
56	MG	YA	3280	1/1	0.86	0.07	38,38,38,38	0
56	MG	XA	1612	1/1	0.86	0.18	46,46,46,46	0
56	MG	YA	3191	1/1	0.87	0.80	32,32,32,32	0
56	MG	RA	3279	1/1	0.87	0.15	55,55,55,55	0
56	MG	RY	201	1/1	0.87	0.34	21,21,21,21	0
56	MG	RA	3273	1/1	0.87	0.16	51,51,51,51	0
56	MG	XA	1676	1/1	0.87	0.70	42,42,42,42	0
56	MG	YA	3410	1/1	0.87	0.37	61,61,61,61	0
56	MG	RA	3220	1/1	0.87	0.50	54,54,54,54	0
56	MG	QA	1650	1/1	0.87	0.14	34,34,34,34	0
56	MG	YA	3253	1/1	0.87	0.49	60,60,60,60	0
56	MG	XA	1629	1/1	0.87	0.17	83,83,83,83	0
56	MG	RA	3321	1/1	0.87	0.49	78,78,78,78	0
56	MG	RA	3386	1/1	0.87	0.25	44,44,44,44	0
56	MG	XA	1749	1/1	0.87	0.83	74,74,74,74	0
56	MG	RA	3322	1/1	0.87	0.18	61,61,61,61	0
56	MG	YA	3200	1/1	0.87	0.28	60,60,60,60	0
56	MG	YE	301	1/1	0.87	0.53	50,50,50,50	0
56	MG	YA	3155	1/1	0.87	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3118	1/1	0.87	0.58	56,56,56,56	0
56	MG	YA	3451	1/1	0.87	0.41	50,50,50,50	0
56	MG	RA	3204	1/1	0.87	0.33	33,33,33,33	0
56	MG	YA	3343	1/1	0.87	0.29	46,46,46,46	0
56	MG	RA	3096	1/1	0.87	0.47	74,74,74,74	0
56	MG	YA	3213	1/1	0.87	0.16	42,42,42,42	0
56	MG	RA	3403	1/1	0.87	0.18	52,52,52,52	0
56	MG	RA	3276	1/1	0.87	0.31	46,46,46,46	0
56	MG	QA	1685	1/1	0.87	0.32	38,38,38,38	0
56	MG	RA	3141	1/1	0.87	0.22	64,64,64,64	0
56	MG	YA	3416	1/1	0.87	0.24	79,79,79,79	0
56	MG	YA	3270	1/1	0.87	0.54	45,45,45,45	0
56	MG	RA	3354	1/1	0.87	0.19	71,71,71,71	0
56	MG	YA	3265	1/1	0.87	0.26	41,41,41,41	0
56	MG	YG	201	1/1	0.87	0.13	63,63,63,63	0
56	MG	XA	1608	1/1	0.87	0.53	52,52,52,52	0
56	MG	RA	3201	1/1	0.87	0.09	19,19,19,19	0
56	MG	RA	3170	1/1	0.87	0.55	49,49,49,49	0
56	MG	QA	1717	1/1	0.88	0.24	57,57,57,57	0
56	MG	YA	3182	1/1	0.88	0.38	55,55,55,55	0
56	MG	XA	1653	1/1	0.88	0.76	60,60,60,60	0
56	MG	RA	3238	1/1	0.88	0.27	44,44,44,44	0
56	MG	YB	204	1/1	0.88	0.12	63,63,63,63	0
56	MG	RD	301	1/1	0.88	0.17	34,34,34,34	0
56	MG	RA	3409	1/1	0.88	0.20	39,39,39,39	0
56	MG	YA	3382	1/1	0.88	0.51	47,47,47,47	0
56	MG	RQ	202	1/1	0.88	0.36	53,53,53,53	0
56	MG	XA	1750	1/1	0.88	0.25	57,57,57,57	0
56	MG	YA	3461	1/1	0.88	0.39	44,44,44,44	0
56	MG	YA	3112	1/1	0.88	0.26	32,32,32,32	0
56	MG	YA	3267	1/1	0.88	0.54	48,48,48,48	0
56	MG	XA	1618	1/1	0.88	0.62	34,34,34,34	0
56	MG	YA	3383	1/1	0.88	0.25	47,47,47,47	0
56	MG	RA	3091	1/1	0.88	0.27	48,48,48,48	0
56	MG	YA	3105	1/1	0.88	0.45	42,42,42,42	0
56	MG	QA	1624	1/1	0.88	0.17	72,72,72,72	0
56	MG	YA	3183	1/1	0.88	0.28	35,35,35,35	0
56	MG	YA	3190	1/1	0.88	0.47	39,39,39,39	0
56	MG	RA	3129	1/1	0.88	0.20	41,41,41,41	0
56	MG	YA	3301	1/1	0.88	0.38	30,30,30,30	0
56	MG	QA	1678	1/1	0.88	0.74	51,51,51,51	0
56	MG	RA	3119	1/1	0.88	0.16	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1667	1/1	0.88	0.26	50,50,50,50	0
56	MG	YA	3341	1/1	0.88	0.32	41,41,41,41	0
56	MG	QA	1627	1/1	0.88	0.17	104,104,104,104	0
56	MG	RA	3296	1/1	0.88	0.30	46,46,46,46	0
56	MG	QA	1727	1/1	0.88	0.39	61,61,61,61	0
56	MG	QA	1721	1/1	0.88	0.27	62,62,62,62	0
56	MG	YA	3304	1/1	0.88	0.25	38,38,38,38	0
56	MG	RA	3166	1/1	0.88	0.23	59,59,59,59	0
56	MG	RA	3252	1/1	0.88	0.17	43,43,43,43	0
56	MG	YA	3294	1/1	0.88	0.18	35,35,35,35	0
56	MG	XA	1627	1/1	0.88	0.17	44,44,44,44	0
56	MG	RA	3254	1/1	0.88	0.59	74,74,74,74	0
56	MG	RA	3246	1/1	0.88	0.42	47,47,47,47	0
56	MG	YA	3277	1/1	0.88	0.50	59,59,59,59	0
56	MG	Y1	101	1/1	0.88	0.32	26,26,26,26	0
56	MG	YA	3441	1/1	0.88	0.33	54,54,54,54	0
56	MG	QA	1679	1/1	0.88	0.54	61,61,61,61	0
56	MG	YA	3326	1/1	0.88	0.62	52,52,52,52	0
56	MG	RA	3098	1/1	0.88	0.27	22,22,22,22	0
56	MG	XA	1680	1/1	0.88	0.16	38,38,38,38	0
56	MG	YA	3332	1/1	0.88	0.68	43,43,43,43	0
56	MG	YA	3030	1/1	0.88	0.38	21,21,21,21	0
56	MG	YA	3230	1/1	0.88	1.01	69,69,69,69	0
56	MG	XA	1631	1/1	0.88	0.32	57,57,57,57	0
56	MG	RA	3151	1/1	0.88	0.19	35,35,35,35	0
56	MG	YA	3405	1/1	0.88	0.20	22,22,22,22	0
56	MG	YA	3362	1/1	0.88	0.45	48,48,48,48	0
56	MG	RA	3236	1/1	0.88	0.28	48,48,48,48	0
56	MG	YA	3103	1/1	0.88	0.21	62,62,62,62	0
56	MG	QA	1695	1/1	0.88	0.17	61,61,61,61	0
56	MG	YA	3449	1/1	0.89	0.35	60,60,60,60	0
56	MG	YA	3228	1/1	0.89	0.30	51,51,51,51	0
56	MG	XA	1738	1/1	0.89	0.21	30,30,30,30	0
56	MG	YA	3438	1/1	0.89	0.63	91,91,91,91	0
56	MG	XA	1757	1/1	0.89	0.63	58,58,58,58	0
56	MG	RA	3149	1/1	0.89	0.39	60,60,60,60	0
56	MG	YA	3292	1/1	0.89	0.13	45,45,45,45	0
56	MG	RA	3067	1/1	0.89	0.35	17,17,17,17	0
56	MG	YA	3268	1/1	0.89	0.17	53,53,53,53	0
56	MG	XA	1712	1/1	0.89	0.37	41,41,41,41	0
56	MG	QA	1657	1/1	0.89	0.27	36,36,36,36	0
56	MG	XA	1677	1/1	0.89	0.39	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1705	1/1	0.89	0.69	48,48,48,48	0
56	MG	YA	3321	1/1	0.89	0.35	71,71,71,71	0
56	MG	QA	1724	1/1	0.89	0.11	50,50,50,50	0
56	MG	RA	3307	1/1	0.89	0.95	60,60,60,60	0
56	MG	YA	3403	1/1	0.89	0.22	36,36,36,36	0
56	MG	XA	1718	1/1	0.89	0.54	48,48,48,48	0
56	MG	YA	3247	1/1	0.89	0.24	42,42,42,42	0
56	MG	QA	1629	1/1	0.89	0.15	56,56,56,56	0
56	MG	XA	1730	1/1	0.89	0.25	50,50,50,50	0
56	MG	QA	1603	1/1	0.89	0.23	83,83,83,83	0
56	MG	YA	3406	1/1	0.89	0.06	74,74,74,74	0
56	MG	RA	3398	1/1	0.89	0.25	55,55,55,55	0
56	MG	RA	3362	1/1	0.89	0.16	72,72,72,72	0
56	MG	YA	3251	1/1	0.89	0.18	82,82,82,82	0
56	MG	RA	3193	1/1	0.89	0.40	33,33,33,33	0
56	MG	RA	3412	1/1	0.89	0.15	34,34,34,34	0
56	MG	YA	3171	1/1	0.89	0.21	26,26,26,26	0
56	MG	YA	3423	1/1	0.89	0.20	47,47,47,47	0
56	MG	XA	1642	1/1	0.89	0.14	54,54,54,54	0
56	MG	QA	1702	1/1	0.89	0.50	60,60,60,60	0
56	MG	YA	3450	1/1	0.89	0.27	40,40,40,40	0
56	MG	QA	1636	1/1	0.89	0.22	62,62,62,62	0
56	MG	RA	3181	1/1	0.89	0.30	67,67,67,67	0
56	MG	YA	3099	1/1	0.89	0.26	51,51,51,51	0
56	MG	RA	3378	1/1	0.89	0.19	18,18,18,18	0
56	MG	YA	3440	1/1	0.89	0.31	59,59,59,59	0
56	MG	YA	3357	1/1	0.89	0.35	27,27,27,27	0
56	MG	YA	3197	1/1	0.89	0.16	15,15,15,15	0
56	MG	YA	3411	1/1	0.89	0.12	53,53,53,53	0
56	MG	YA	3429	1/1	0.89	0.19	38,38,38,38	0
56	MG	RA	3347	1/1	0.89	0.46	52,52,52,52	0
56	MG	RA	3068	1/1	0.89	0.33	39,39,39,39	0
56	MG	QA	1665	1/1	0.89	0.20	58,58,58,58	0
56	MG	QA	1610	1/1	0.89	0.10	64,64,64,64	0
56	MG	RA	3410	1/1	0.90	0.19	26,26,26,26	0
56	MG	QA	1691	1/1	0.90	0.18	44,44,44,44	0
56	MG	RA	3198	1/1	0.90	0.54	45,45,45,45	0
56	MG	QA	1637	1/1	0.90	0.33	59,59,59,59	0
56	MG	YA	3202	1/1	0.90	0.40	42,42,42,42	0
56	MG	YA	3160	1/1	0.90	0.26	50,50,50,50	0
56	MG	YA	3274	1/1	0.90	0.35	28,28,28,28	0
56	MG	XA	1708	1/1	0.90	0.34	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1744	1/1	0.90	0.54	50,50,50,50	0
56	MG	XA	1722	1/1	0.90	0.29	61,61,61,61	0
56	MG	RA	3290	1/1	0.90	0.21	59,59,59,59	0
56	MG	YA	3374	1/1	0.90	0.18	62,62,62,62	0
56	MG	XA	1626	1/1	0.90	0.51	51,51,51,51	0
56	MG	YA	3316	1/1	0.90	0.39	60,60,60,60	0
56	MG	Y5	102	1/1	0.90	0.40	39,39,39,39	0
56	MG	QA	1617	1/1	0.90	0.32	42,42,42,42	0
56	MG	YA	3424	1/1	0.90	0.24	56,56,56,56	0
56	MG	QA	1656	1/1	0.90	0.34	38,38,38,38	0
56	MG	YA	3339	1/1	0.90	0.27	40,40,40,40	0
56	MG	YA	3222	1/1	0.90	0.35	42,42,42,42	0
56	MG	RA	3382	1/1	0.90	0.19	49,49,49,49	0
56	MG	YA	3128	1/1	0.90	0.26	36,36,36,36	0
56	MG	YA	3146	1/1	0.90	0.10	70,70,70,70	0
56	MG	RA	3406	1/1	0.90	0.56	42,42,42,42	0
56	MG	RA	3411	1/1	0.90	0.18	35,35,35,35	0
56	MG	RA	3136	1/1	0.90	0.26	41,41,41,41	0
56	MG	YA	3358	1/1	0.90	0.23	60,60,60,60	0
56	MG	YA	3426	1/1	0.90	0.30	66,66,66,66	0
56	MG	YA	3233	1/1	0.90	0.43	45,45,45,45	0
56	MG	RA	3083	1/1	0.90	0.31	49,49,49,49	0
56	MG	YA	3445	1/1	0.90	0.38	55,55,55,55	0
56	MG	YA	3286	1/1	0.90	0.60	64,64,64,64	0
56	MG	RA	3343	1/1	0.90	0.10	57,57,57,57	0
56	MG	RA	3125	1/1	0.90	0.72	68,68,68,68	0
56	MG	YA	3372	1/1	0.90	0.32	45,45,45,45	0
56	MG	YA	3245	1/1	0.90	0.21	57,57,57,57	0
56	MG	YA	3145	1/1	0.90	0.40	46,46,46,46	0
56	MG	YA	3152	1/1	0.90	0.18	27,27,27,27	0
56	MG	YA	3170	1/1	0.90	0.32	45,45,45,45	0
56	MG	RA	3310	1/1	0.90	0.23	12,12,12,12	0
56	MG	RA	3390	1/1	0.90	0.30	53,53,53,53	0
56	MG	RA	3133	1/1	0.90	0.14	38,38,38,38	0
56	MG	RA	3185	1/1	0.90	0.26	36,36,36,36	0
56	MG	XA	1663	1/1	0.90	0.24	46,46,46,46	0
56	MG	YA	3162	1/1	0.90	0.16	48,48,48,48	0
56	MG	QA	1628	1/1	0.90	0.60	44,44,44,44	0
56	MG	RA	3101	1/1	0.90	0.36	31,31,31,31	0
56	MG	XA	1619	1/1	0.90	0.18	27,27,27,27	0
56	MG	YA	3376	1/1	0.90	0.46	41,41,41,41	0
56	MG	XA	1694	1/1	0.90	0.21	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3352	1/1	0.90	0.30	53,53,53,53	0
56	MG	RA	3128	1/1	0.90	0.22	33,33,33,33	0
56	MG	YB	202	1/1	0.90	0.29	49,49,49,49	0
56	MG	QA	1640	1/1	0.90	0.22	76,76,76,76	0
56	MG	YA	3178	1/1	0.90	0.52	40,40,40,40	0
56	MG	RA	3395	1/1	0.90	0.40	45,45,45,45	0
56	MG	YA	3288	1/1	0.90	0.53	39,39,39,39	0
56	MG	QA	1664	1/1	0.90	0.26	39,39,39,39	0
56	MG	RA	3059	1/1	0.90	0.13	15,15,15,15	0
56	MG	RA	3383	1/1	0.90	0.22	53,53,53,53	0
56	MG	QA	1716	1/1	0.90	0.41	68,68,68,68	0
56	MG	YA	3241	1/1	0.90	0.48	40,40,40,40	0
56	MG	RA	3183	1/1	0.90	0.17	56,56,56,56	0
56	MG	RR	201	1/1	0.91	0.42	44,44,44,44	0
56	MG	RA	3337	1/1	0.91	0.44	54,54,54,54	0
56	MG	XA	1671	1/1	0.91	0.51	56,56,56,56	0
56	MG	XA	1691	1/1	0.91	0.27	53,53,53,53	0
56	MG	YA	3284	1/1	0.91	0.26	52,52,52,52	0
56	MG	YA	3255	1/1	0.91	0.77	43,43,43,43	0
56	MG	RA	3065	1/1	0.91	0.37	39,39,39,39	0
56	MG	YA	3058	1/1	0.91	0.14	29,29,29,29	0
56	MG	QA	1625	1/1	0.91	0.11	35,35,35,35	0
56	MG	YA	3108	1/1	0.91	0.47	25,25,25,25	0
56	MG	XA	1632	1/1	0.91	0.55	39,39,39,39	0
56	MG	XA	1756	1/1	0.91	0.48	50,50,50,50	0
56	MG	RA	3112	1/1	0.91	0.26	38,38,38,38	0
56	MG	YA	3392	1/1	0.91	0.32	20,20,20,20	0
56	MG	YA	3149	1/1	0.91	0.22	34,34,34,34	0
56	MG	RA	3399	1/1	0.91	0.19	42,42,42,42	0
56	MG	YA	3068	1/1	0.91	0.20	30,30,30,30	0
56	MG	RA	3215	1/1	0.91	0.14	36,36,36,36	0
56	MG	XA	1664	1/1	0.91	0.38	59,59,59,59	0
56	MG	RA	3407	1/1	0.91	0.50	52,52,52,52	0
56	MG	YA	3363	1/1	0.91	0.23	69,69,69,69	0
56	MG	YA	3007	1/1	0.91	1.20	39,39,39,39	0
56	MG	RA	3113	1/1	0.91	0.53	74,74,74,74	0
56	MG	YA	3359	1/1	0.91	0.38	39,39,39,39	0
56	MG	YA	3163	1/1	0.91	0.23	33,33,33,33	0
56	MG	YA	3256	1/1	0.91	0.27	58,58,58,58	0
56	MG	YA	3463	1/1	0.91	0.19	46,46,46,46	0
56	MG	YA	3138	1/1	0.91	0.08	26,26,26,26	0
56	MG	QA	1739	1/1	0.91	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3443	1/1	0.91	0.27	54,54,54,54	0
56	MG	XA	1760	1/1	0.91	0.08	79,79,79,79	0
56	MG	RA	3235	1/1	0.91	0.26	25,25,25,25	0
56	MG	YA	3314	1/1	0.91	0.17	56,56,56,56	0
56	MG	QA	1666	1/1	0.91	0.28	63,63,63,63	0
56	MG	RA	3348	1/1	0.91	0.57	58,58,58,58	0
56	MG	XA	1639	1/1	0.91	0.50	63,63,63,63	0
56	MG	RA	3218	1/1	0.91	0.24	45,45,45,45	0
56	MG	RA	3316	1/1	0.91	0.23	49,49,49,49	0
56	MG	RA	3134	1/1	0.91	0.24	50,50,50,50	0
56	MG	RA	3076	1/1	0.91	0.28	35,35,35,35	0
56	MG	QA	1651	1/1	0.91	0.24	30,30,30,30	0
56	MG	YA	3361	1/1	0.91	0.32	45,45,45,45	0
56	MG	YA	3123	1/1	0.91	0.22	34,34,34,34	0
56	MG	RA	3075	1/1	0.91	0.29	18,18,18,18	0
56	MG	QA	1697	1/1	0.91	0.11	54,54,54,54	0
56	MG	YA	3185	1/1	0.91	0.28	36,36,36,36	0
56	MG	QE	201	1/1	0.91	0.69	52,52,52,52	0
56	MG	YA	3388	1/1	0.91	0.12	49,49,49,49	0
56	MG	RA	3342	1/1	0.91	0.33	44,44,44,44	0
56	MG	RA	3379	1/1	0.91	0.39	44,44,44,44	0
56	MG	RA	3122	1/1	0.91	0.30	36,36,36,36	0
56	MG	RA	3376	1/1	0.91	0.41	26,26,26,26	0
56	MG	YA	3335	1/1	0.91	0.21	66,66,66,66	0
56	MG	RA	3339	1/1	0.91	0.62	55,55,55,55	0
56	MG	YA	3387	1/1	0.91	0.11	98,98,98,98	0
56	MG	YA	3223	1/1	0.91	0.41	34,34,34,34	0
56	MG	RA	3328	1/1	0.91	0.21	61,61,61,61	0
56	MG	RA	3301	1/1	0.91	0.42	53,53,53,53	0
56	MG	XA	1624	1/1	0.91	0.18	53,53,53,53	0
56	MG	RA	3178	1/1	0.91	0.59	38,38,38,38	0
56	MG	YA	3157	1/1	0.91	0.38	16,16,16,16	0
56	MG	YA	3408	1/1	0.91	0.31	41,41,41,41	0
56	MG	QA	1730	1/1	0.91	0.21	55,55,55,55	0
56	MG	QA	1729	1/1	0.91	0.25	48,48,48,48	0
56	MG	YA	3323	1/1	0.91	0.39	39,39,39,39	0
56	MG	YA	3090	1/1	0.91	0.28	35,35,35,35	0
56	MG	YA	3452	1/1	0.92	0.18	71,71,71,71	0
56	MG	YA	3317	1/1	0.92	0.21	41,41,41,41	0
56	MG	RA	3123	1/1	0.92	0.30	39,39,39,39	0
56	MG	RA	3168	1/1	0.92	0.49	79,79,79,79	0
56	MG	XA	1736	1/1	0.92	0.17	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1631	1/1	0.92	0.44	56,56,56,56	0
56	MG	YA	3047	1/1	0.92	0.39	20,20,20,20	0
56	MG	RA	3202	1/1	0.92	0.29	32,32,32,32	0
56	MG	YA	3208	1/1	0.92	0.15	31,31,31,31	0
56	MG	YA	3327	1/1	0.92	0.52	24,24,24,24	0
56	MG	YA	3125	1/1	0.92	0.39	48,48,48,48	0
56	MG	YR	201	1/1	0.92	0.32	39,39,39,39	0
56	MG	RA	3280	1/1	0.92	0.33	43,43,43,43	0
56	MG	RA	3263	1/1	0.92	0.26	62,62,62,62	0
56	MG	RA	3205	1/1	0.92	0.40	44,44,44,44	0
56	MG	RA	3116	1/1	0.92	0.33	45,45,45,45	0
56	MG	RA	3049	1/1	0.92	0.22	4,4,4,4	0
56	MG	XA	1661	1/1	0.92	0.51	39,39,39,39	0
56	MG	QA	1611	1/1	0.92	0.21	41,41,41,41	0
56	MG	YA	3246	1/1	0.92	0.45	61,61,61,61	0
56	MG	Y0	101	1/1	0.92	0.18	30,30,30,30	0
56	MG	RA	3142	1/1	0.92	0.33	44,44,44,44	0
56	MG	YA	3414	1/1	0.92	0.21	87,87,87,87	0
56	MG	QL	201	1/1	0.92	0.10	63,63,63,63	0
56	MG	RA	3260	1/1	0.92	0.16	57,57,57,57	0
56	MG	YA	3318	1/1	0.92	0.39	19,19,19,19	0
56	MG	YA	3417	1/1	0.92	0.15	53,53,53,53	0
56	MG	RA	3323	1/1	0.92	0.28	43,43,43,43	0
56	MG	YA	3046	1/1	0.92	0.54	32,32,32,32	0
56	MG	YA	3269	1/1	0.92	0.20	43,43,43,43	0
56	MG	RA	3145	1/1	0.92	0.28	54,54,54,54	0
56	MG	YA	3462	1/1	0.92	0.24	25,25,25,25	0
56	MG	YA	3158	1/1	0.92	0.32	53,53,53,53	0
56	MG	RA	3005	1/1	0.92	0.13	15,15,15,15	0
56	MG	RA	3126	1/1	0.92	0.20	53,53,53,53	0
56	MG	RD	302	1/1	0.92	0.38	27,27,27,27	0
56	MG	QA	1728	1/1	0.92	0.13	61,61,61,61	0
56	MG	YV	201	1/1	0.92	0.38	22,22,22,22	0
56	MG	XA	1695	1/1	0.92	0.13	46,46,46,46	0
56	MG	YA	3147	1/1	0.92	0.31	43,43,43,43	0
56	MG	YA	3309	1/1	0.92	0.16	76,76,76,76	0
56	MG	RB	204	1/1	0.92	0.10	61,61,61,61	0
56	MG	YA	3322	1/1	0.92	0.23	50,50,50,50	0
56	MG	RA	3234	1/1	0.92	0.30	38,38,38,38	0
57	ZN	QD	301	1/1	0.92	0.32	58,58,58,58	0
56	MG	YA	3281	1/1	0.92	0.24	34,34,34,34	0
56	MG	YA	3204	1/1	0.92	0.39	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3168	1/1	0.92	0.40	52,52,52,52	0
56	MG	YA	3013	1/1	0.92	0.22	11,11,11,11	0
56	MG	XA	1685	1/1	0.92	0.76	65,65,65,65	0
56	MG	XA	1741	1/1	0.92	0.21	56,56,56,56	0
56	MG	XA	1753	1/1	0.92	0.23	100,100,100,100	0
56	MG	RA	3118	1/1	0.92	1.11	63,63,63,63	0
56	MG	RA	3226	1/1	0.92	0.34	25,25,25,25	0
56	MG	YA	3044	1/1	0.92	0.34	14,14,14,14	0
56	MG	YA	3076	1/1	0.92	0.27	43,43,43,43	0
56	MG	RA	3366	1/1	0.92	0.47	33,33,33,33	0
56	MG	YA	3320	1/1	0.92	0.48	39,39,39,39	0
56	MG	XV	102	1/1	0.92	0.36	36,36,36,36	0
56	MG	YA	3430	1/1	0.92	0.46	17,17,17,17	0
56	MG	XA	1683	1/1	0.92	0.21	44,44,44,44	0
56	MG	YA	3260	1/1	0.92	0.23	61,61,61,61	0
56	MG	QA	1707	1/1	0.92	0.11	47,47,47,47	0
56	MG	YA	3262	1/1	0.92	0.43	39,39,39,39	0
56	MG	QA	1648	1/1	0.92	0.62	43,43,43,43	0
56	MG	XA	1669	1/1	0.92	0.58	35,35,35,35	0
56	MG	XA	1609	1/1	0.92	0.11	70,70,70,70	0
56	MG	RA	3190	1/1	0.92	0.30	38,38,38,38	0
56	MG	YA	3350	1/1	0.92	0.39	58,58,58,58	0
56	MG	QA	1614	1/1	0.92	0.15	55,55,55,55	0
56	MG	XA	1614	1/1	0.92	0.18	37,37,37,37	0
56	MG	RA	3387	1/1	0.92	0.38	41,41,41,41	0
56	MG	YA	3225	1/1	0.92	0.29	38,38,38,38	0
56	MG	XA	1668	1/1	0.92	0.34	44,44,44,44	0
56	MG	YA	3196	1/1	0.93	0.10	57,57,57,57	0
56	MG	YA	3244	1/1	0.93	0.32	76,76,76,76	0
56	MG	YA	3078	1/1	0.93	0.30	36,36,36,36	0
56	MG	YA	3458	1/1	0.93	0.24	45,45,45,45	0
56	MG	RA	3264	1/1	0.93	0.26	28,28,28,28	0
56	MG	YA	3094	1/1	0.93	0.43	58,58,58,58	0
56	MG	QA	1602	1/1	0.93	0.41	33,33,33,33	0
56	MG	QA	1669	1/1	0.93	0.60	52,52,52,52	0
56	MG	YA	3134	1/1	0.93	0.18	56,56,56,56	0
56	MG	YA	3239	1/1	0.93	0.31	26,26,26,26	0
56	MG	YA	3263	1/1	0.93	0.26	57,57,57,57	0
56	MG	XV	103	1/1	0.93	0.36	40,40,40,40	0
56	MG	RA	3070	1/1	0.93	0.35	27,27,27,27	0
56	MG	YA	3218	1/1	0.93	0.22	30,30,30,30	0
56	MG	YA	3421	1/1	0.93	0.51	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	Y0	102	1/1	0.93	0.25	46,46,46,46	0
56	MG	RA	3148	1/1	0.93	0.21	43,43,43,43	0
56	MG	YA	3189	1/1	0.93	0.41	40,40,40,40	0
56	MG	YA	3420	1/1	0.93	0.23	63,63,63,63	0
56	MG	YA	3037	1/1	0.93	0.45	33,33,33,33	0
56	MG	RA	3380	1/1	0.93	0.47	40,40,40,40	0
56	MG	RA	3227	1/1	0.93	0.22	43,43,43,43	0
56	MG	YA	3091	1/1	0.93	0.58	29,29,29,29	0
56	MG	QA	1647	1/1	0.93	0.24	56,56,56,56	0
56	MG	RA	3052	1/1	0.93	0.22	34,34,34,34	0
56	MG	QA	1731	1/1	0.93	0.41	37,37,37,37	0
56	MG	YA	3101	1/1	0.93	0.39	36,36,36,36	0
56	MG	RA	3212	1/1	0.93	0.26	44,44,44,44	0
56	MG	RA	3332	1/1	0.93	0.43	87,87,87,87	0
56	MG	RA	3375	1/1	0.93	0.28	39,39,39,39	0
56	MG	XA	1737	1/1	0.93	0.66	41,41,41,41	0
56	MG	YA	3184	1/1	0.93	0.23	83,83,83,83	0
56	MG	YA	3431	1/1	0.93	0.18	36,36,36,36	0
56	MG	QA	1662	1/1	0.93	0.33	51,51,51,51	0
56	MG	YA	3329	1/1	0.93	0.16	40,40,40,40	0
56	MG	RA	3298	1/1	0.93	0.12	63,63,63,63	0
56	MG	RA	3110	1/1	0.93	0.31	25,25,25,25	0
56	MG	QA	1682	1/1	0.93	0.36	64,64,64,64	0
56	MG	YA	3240	1/1	0.93	0.26	47,47,47,47	0
56	MG	RA	3189	1/1	0.93	0.43	25,25,25,25	0
56	MG	YA	3133	1/1	0.93	0.37	40,40,40,40	0
56	MG	YA	3093	1/1	0.93	0.10	51,51,51,51	0
56	MG	XA	1747	1/1	0.93	0.21	88,88,88,88	0
56	MG	YA	3275	1/1	0.93	0.17	50,50,50,50	0
56	MG	YA	3333	1/1	0.93	0.30	63,63,63,63	0
56	MG	XA	1681	1/1	0.93	0.30	39,39,39,39	0
56	MG	XF	201	1/1	0.93	0.28	35,35,35,35	0
56	MG	YA	3186	1/1	0.93	0.22	58,58,58,58	0
56	MG	XA	1755	1/1	0.93	0.12	71,71,71,71	0
56	MG	YA	3039	1/1	0.93	0.41	22,22,22,22	0
56	MG	RA	3197	1/1	0.93	0.55	28,28,28,28	0
56	MG	RA	3177	1/1	0.93	0.20	42,42,42,42	0
56	MG	RA	3253	1/1	0.93	0.26	47,47,47,47	0
56	MG	RA	3293	1/1	0.93	0.30	38,38,38,38	0
56	MG	RA	3228	1/1	0.93	0.41	50,50,50,50	0
56	MG	YA	3193	1/1	0.93	0.60	35,35,35,35	0
56	MG	RA	3139	1/1	0.93	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3240	1/1	0.93	0.18	34,34,34,34	0
56	MG	RA	3357	1/1	0.93	0.31	47,47,47,47	0
56	MG	RA	3196	1/1	0.93	0.14	40,40,40,40	0
56	MG	RA	3291	1/1	0.93	0.23	26,26,26,26	0
56	MG	XA	1670	1/1	0.93	0.42	36,36,36,36	0
56	MG	QA	1652	1/1	0.93	0.19	60,60,60,60	0
56	MG	YA	3110	1/1	0.93	0.12	10,10,10,10	0
56	MG	YA	3428	1/1	0.93	0.23	50,50,50,50	0
56	MG	YA	3237	1/1	0.93	0.53	34,34,34,34	0
56	MG	YA	3353	1/1	0.93	0.50	53,53,53,53	0
56	MG	RA	3069	1/1	0.93	0.29	30,30,30,30	0
56	MG	RF	301	1/1	0.93	0.18	27,27,27,27	0
56	MG	QA	1713	1/1	0.93	0.73	46,46,46,46	0
56	MG	YA	3065	1/1	0.93	0.36	52,52,52,52	0
56	MG	YA	3175	1/1	0.93	0.18	70,70,70,70	0
56	MG	RA	3159	1/1	0.93	0.26	44,44,44,44	0
56	MG	QA	1686	1/1	0.93	0.32	49,49,49,49	0
56	MG	QA	1655	1/1	0.93	0.26	39,39,39,39	0
56	MG	RA	3257	1/1	0.93	0.16	47,47,47,47	0
56	MG	RA	3029	1/1	0.93	0.23	17,17,17,17	0
56	MG	YA	3398	1/1	0.93	0.45	34,34,34,34	0
56	MG	QA	1653	1/1	0.94	0.38	41,41,41,41	0
56	MG	RA	3154	1/1	0.94	0.09	35,35,35,35	0
56	MG	YA	3293	1/1	0.94	0.48	48,48,48,48	0
56	MG	RA	3002	1/1	0.94	0.16	15,15,15,15	0
56	MG	QA	1722	1/1	0.94	0.21	39,39,39,39	0
56	MG	YA	3130	1/1	0.94	0.18	18,18,18,18	0
56	MG	QA	1692	1/1	0.94	0.32	42,42,42,42	0
56	MG	RA	3221	1/1	0.94	0.31	40,40,40,40	0
56	MG	YA	3126	1/1	0.94	0.14	51,51,51,51	0
56	MG	XA	1699	1/1	0.94	0.13	84,84,84,84	0
56	MG	XA	1636	1/1	0.94	0.37	54,54,54,54	0
56	MG	RA	3413	1/1	0.94	0.35	24,24,24,24	0
56	MG	QA	1601	1/1	0.94	0.50	44,44,44,44	0
56	MG	RA	3247	1/1	0.94	0.24	41,41,41,41	0
56	MG	YA	3453	1/1	0.94	0.24	35,35,35,35	0
56	MG	RA	3224	1/1	0.94	0.36	37,37,37,37	0
56	MG	YA	3243	1/1	0.94	0.46	48,48,48,48	0
56	MG	QA	1673	1/1	0.94	0.31	62,62,62,62	0
56	MG	YA	3457	1/1	0.94	0.36	44,44,44,44	0
56	MG	YA	3308	1/1	0.94	0.47	31,31,31,31	0
56	MG	RA	3097	1/1	0.94	0.41	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1638	1/1	0.94	0.13	76,76,76,76	0
56	MG	YA	3203	1/1	0.94	0.40	39,39,39,39	0
56	MG	YA	3215	1/1	0.94	0.30	60,60,60,60	0
56	MG	QA	1635	1/1	0.94	0.39	64,64,64,64	0
56	MG	YA	3003	1/1	0.94	0.52	22,22,22,22	0
57	ZN	XN	101	1/1	0.94	0.11	67,67,67,67	0
56	MG	QA	1674	1/1	0.94	0.45	55,55,55,55	0
56	MG	RA	3340	1/1	0.94	0.12	79,79,79,79	0
56	MG	XA	1748	1/1	0.94	0.16	57,57,57,57	0
56	MG	YA	3201	1/1	0.94	0.20	32,32,32,32	0
56	MG	YA	3050	1/1	0.94	0.76	52,52,52,52	0
56	MG	YA	3057	1/1	0.94	0.13	37,37,37,37	0
56	MG	RA	3300	1/1	0.94	0.29	49,49,49,49	0
56	MG	YA	3229	1/1	0.94	0.27	32,32,32,32	0
56	MG	YA	3072	1/1	0.94	0.42	42,42,42,42	0
56	MG	YA	3348	1/1	0.94	0.27	35,35,35,35	0
56	MG	YA	3115	1/1	0.94	0.41	33,33,33,33	0
56	MG	RA	3338	1/1	0.94	0.33	51,51,51,51	0
56	MG	Y7	101	1/1	0.94	0.22	51,51,51,51	0
56	MG	RA	3156	1/1	0.94	0.15	63,63,63,63	0
56	MG	YA	3017	1/1	0.94	0.33	10,10,10,10	0
56	MG	YA	3122	1/1	0.94	0.37	21,21,21,21	0
56	MG	RA	3104	1/1	0.94	0.28	40,40,40,40	0
56	MG	YA	3088	1/1	0.94	0.50	21,21,21,21	0
56	MG	YA	3024	1/1	0.94	0.46	21,21,21,21	0
56	MG	RA	3393	1/1	0.94	0.24	28,28,28,28	0
56	MG	RA	3163	1/1	0.94	0.25	51,51,51,51	0
56	MG	RA	3305	1/1	0.94	0.21	68,68,68,68	0
56	MG	XA	1717	1/1	0.94	0.38	39,39,39,39	0
56	MG	RA	3258	1/1	0.94	0.41	46,46,46,46	0
56	MG	RA	3150	1/1	0.94	0.56	37,37,37,37	0
56	MG	YA	3254	1/1	0.94	0.44	47,47,47,47	0
56	MG	QA	1708	1/1	0.94	0.31	50,50,50,50	0
56	MG	RA	3146	1/1	0.94	0.31	28,28,28,28	0
56	MG	YA	3289	1/1	0.94	0.29	43,43,43,43	0
56	MG	YA	3236	1/1	0.94	0.44	30,30,30,30	0
56	MG	YA	3053	1/1	0.94	0.47	31,31,31,31	0
56	MG	YA	3367	1/1	0.94	0.33	43,43,43,43	0
56	MG	RA	3040	1/1	0.94	0.34	24,24,24,24	0
56	MG	YA	3104	1/1	0.94	0.13	36,36,36,36	0
56	MG	XA	1703	1/1	0.94	0.54	50,50,50,50	0
56	MG	YA	3409	1/1	0.94	0.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3231	1/1	0.94	0.28	40,40,40,40	0
56	MG	XA	1622	1/1	0.94	0.54	44,44,44,44	0
56	MG	RA	3397	1/1	0.94	0.46	55,55,55,55	0
56	MG	RA	3186	1/1	0.94	0.33	44,44,44,44	0
56	MG	YA	3045	1/1	0.94	0.32	22,22,22,22	0
56	MG	RA	3394	1/1	0.94	0.23	57,57,57,57	0
56	MG	YA	3049	1/1	0.94	0.15	29,29,29,29	0
56	MG	YA	3315	1/1	0.94	0.25	47,47,47,47	0
56	MG	RA	3385	1/1	0.94	0.20	44,44,44,44	0
56	MG	YA	3194	1/1	0.94	0.14	39,39,39,39	0
56	MG	RA	3027	1/1	0.94	0.43	24,24,24,24	0
56	MG	RA	3371	1/1	0.94	0.64	57,57,57,57	0
56	MG	RA	3105	1/1	0.94	0.14	36,36,36,36	0
56	MG	YA	3296	1/1	0.94	0.34	66,66,66,66	0
56	MG	XA	1673	1/1	0.94	0.21	49,49,49,49	0
56	MG	XA	1715	1/1	0.94	0.16	43,43,43,43	0
56	MG	RA	3084	1/1	0.94	0.08	23,23,23,23	0
56	MG	XA	1700	1/1	0.94	0.16	87,87,87,87	0
56	MG	QA	1740	1/1	0.94	0.17	43,43,43,43	0
56	MG	RA	3206	1/1	0.94	0.46	44,44,44,44	0
56	MG	RA	3285	1/1	0.94	0.28	60,60,60,60	0
56	MG	XA	1752	1/1	0.94	0.23	83,83,83,83	0
56	MG	YA	3031	1/1	0.94	0.30	29,29,29,29	0
56	MG	YA	3062	1/1	0.94	0.15	38,38,38,38	0
56	MG	QA	1684	1/1	0.94	0.13	46,46,46,46	0
56	MG	YA	3207	1/1	0.94	0.16	29,29,29,29	0
56	MG	RA	3063	1/1	0.94	0.26	33,33,33,33	0
56	MG	RA	3188	1/1	0.94	0.35	8,8,8,8	0
56	MG	QA	1712	1/1	0.94	0.29	34,34,34,34	0
56	MG	YA	3355	1/1	0.94	0.24	34,34,34,34	0
56	MG	RA	3356	1/1	0.94	0.32	54,54,54,54	0
56	MG	RA	3109	1/1	0.94	0.52	21,21,21,21	0
56	MG	RA	3219	1/1	0.94	0.26	48,48,48,48	0
56	MG	YA	3456	1/1	0.94	0.28	50,50,50,50	0
56	MG	YA	3188	1/1	0.94	0.21	24,24,24,24	0
56	MG	RA	3242	1/1	0.94	0.44	34,34,34,34	0
56	MG	YA	3177	1/1	0.95	0.09	57,57,57,57	0
56	MG	RA	3041	1/1	0.95	0.19	31,31,31,31	0
56	MG	RA	3275	1/1	0.95	0.34	44,44,44,44	0
56	MG	RA	3164	1/1	0.95	0.41	30,30,30,30	0
56	MG	YA	3259	1/1	0.95	0.30	50,50,50,50	0
56	MG	XA	1701	1/1	0.95	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3226	1/1	0.95	0.35	39,39,39,39	0
56	MG	YA	3342	1/1	0.95	0.15	54,54,54,54	0
56	MG	QA	1681	1/1	0.95	0.16	35,35,35,35	0
56	MG	QA	1639	1/1	0.95	0.33	52,52,52,52	0
56	MG	RA	3200	1/1	0.95	0.11	65,65,65,65	0
56	MG	YA	3394	1/1	0.95	0.42	21,21,21,21	0
56	MG	YA	3113	1/1	0.95	0.35	56,56,56,56	0
56	MG	RA	3019	1/1	0.95	0.39	13,13,13,13	0
56	MG	RA	3194	1/1	0.95	0.36	37,37,37,37	0
56	MG	RA	3268	1/1	0.95	0.21	48,48,48,48	0
56	MG	RA	3171	1/1	0.95	0.30	32,32,32,32	0
56	MG	RA	3349	1/1	0.95	0.15	80,80,80,80	0
56	MG	XA	1645	1/1	0.95	0.22	47,47,47,47	0
56	MG	RA	3256	1/1	0.95	0.16	59,59,59,59	0
56	MG	QA	1642	1/1	0.95	0.26	28,28,28,28	0
56	MG	RA	3100	1/1	0.95	0.58	56,56,56,56	0
56	MG	YA	3169	1/1	0.95	0.31	42,42,42,42	0
56	MG	RA	3143	1/1	0.95	0.24	23,23,23,23	0
56	MG	RA	3053	1/1	0.95	0.34	35,35,35,35	0
56	MG	YA	3019	1/1	0.95	0.34	17,17,17,17	0
56	MG	QA	1677	1/1	0.95	0.47	42,42,42,42	0
56	MG	QA	1633	1/1	0.95	0.38	68,68,68,68	0
56	MG	YA	3083	1/1	0.95	0.09	30,30,30,30	0
56	MG	YA	3261	1/1	0.95	0.53	67,67,67,67	0
56	MG	XA	1672	1/1	0.95	0.18	12,12,12,12	0
56	MG	YA	3153	1/1	0.95	0.17	19,19,19,19	0
56	MG	YA	3137	1/1	0.95	0.27	21,21,21,21	0
56	MG	YA	3395	1/1	0.95	0.38	25,25,25,25	0
56	MG	XA	1648	1/1	0.95	0.16	71,71,71,71	0
56	MG	RA	3281	1/1	0.95	0.29	39,39,39,39	0
56	MG	YA	3211	1/1	0.95	0.32	22,22,22,22	0
56	MG	QA	1608	1/1	0.95	0.48	35,35,35,35	0
56	MG	RA	3364	1/1	0.95	0.39	17,17,17,17	0
56	MG	YA	3217	1/1	0.95	0.28	24,24,24,24	0
56	MG	QA	1676	1/1	0.95	0.19	56,56,56,56	0
56	MG	QA	1638	1/1	0.95	0.33	58,58,58,58	0
56	MG	XA	1623	1/1	0.95	0.07	36,36,36,36	0
56	MG	RA	3055	1/1	0.95	0.20	15,15,15,15	0
56	MG	YA	3073	1/1	0.95	0.51	36,36,36,36	0
56	MG	YA	3092	1/1	0.95	0.28	22,22,22,22	0
56	MG	RA	3241	1/1	0.95	0.22	68,68,68,68	0
56	MG	RA	3344	1/1	0.95	0.05	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RE	301	1/1	0.95	0.35	21,21,21,21	0
56	MG	XA	1665	1/1	0.95	0.38	37,37,37,37	0
56	MG	RA	3195	1/1	0.95	0.40	26,26,26,26	0
56	MG	XA	1674	1/1	0.95	0.11	50,50,50,50	0
56	MG	QA	1609	1/1	0.95	0.43	50,50,50,50	0
56	MG	RA	3292	1/1	0.95	0.21	38,38,38,38	0
56	MG	RA	3138	1/1	0.95	0.32	21,21,21,21	0
56	MG	RA	3115	1/1	0.95	0.35	42,42,42,42	0
56	MG	RA	3361	1/1	0.95	0.37	40,40,40,40	0
56	MG	RA	3217	1/1	0.95	0.14	7,7,7,7	0
56	MG	QA	1654	1/1	0.95	0.40	43,43,43,43	0
56	MG	RA	3317	1/1	0.95	0.22	33,33,33,33	0
56	MG	YQ	201	1/1	0.95	0.28	35,35,35,35	0
56	MG	RA	3359	1/1	0.95	0.30	56,56,56,56	0
56	MG	QA	1696	1/1	0.95	0.65	33,33,33,33	0
56	MG	RA	3152	1/1	0.95	0.25	37,37,37,37	0
56	MG	RA	3046	1/1	0.95	0.22	14,14,14,14	0
56	MG	YA	3142	1/1	0.95	0.48	45,45,45,45	0
56	MG	RA	3249	1/1	0.95	0.14	39,39,39,39	0
56	MG	YA	3140	1/1	0.95	0.12	64,64,64,64	0
56	MG	QA	1714	1/1	0.95	0.32	33,33,33,33	0
56	MG	RA	3244	1/1	0.95	0.34	42,42,42,42	0
56	MG	YA	3051	1/1	0.95	0.27	15,15,15,15	0
56	MG	QA	1719	1/1	0.95	0.17	38,38,38,38	0
56	MG	YA	3096	1/1	0.95	0.32	24,24,24,24	0
56	MG	XA	1641	1/1	0.95	0.38	57,57,57,57	0
56	MG	RA	3060	1/1	0.95	0.23	26,26,26,26	0
56	MG	YA	3111	1/1	0.95	0.28	36,36,36,36	0
56	MG	RA	3117	1/1	0.95	0.30	33,33,33,33	0
56	MG	XA	1611	1/1	0.95	0.28	38,38,38,38	0
56	MG	RA	3222	1/1	0.96	0.30	19,19,19,19	0
56	MG	RA	3106	1/1	0.96	0.30	23,23,23,23	0
56	MG	RA	3011	1/1	0.96	0.46	4,4,4,4	0
56	MG	RA	3064	1/1	0.96	0.47	18,18,18,18	0
56	MG	RA	3288	1/1	0.96	0.33	39,39,39,39	0
56	MG	YA	3345	1/1	0.96	0.36	34,34,34,34	0
56	MG	YA	3114	1/1	0.96	0.30	22,22,22,22	0
56	MG	XA	1713	1/1	0.96	0.29	27,27,27,27	0
56	MG	QA	1622	1/1	0.96	0.68	39,39,39,39	0
56	MG	RA	3079	1/1	0.96	0.21	37,37,37,37	0
56	MG	XA	1686	1/1	0.96	0.11	40,40,40,40	0
56	MG	YA	3025	1/1	0.96	0.29	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3014	1/1	0.96	0.32	25,25,25,25	0
56	MG	YA	3136	1/1	0.96	0.20	31,31,31,31	0
56	MG	YA	3034	1/1	0.96	0.10	31,31,31,31	0
56	MG	YA	3396	1/1	0.96	0.15	45,45,45,45	0
56	MG	RA	3094	1/1	0.96	0.48	46,46,46,46	0
56	MG	YA	3198	1/1	0.96	0.26	27,27,27,27	0
56	MG	RA	3374	1/1	0.96	0.10	34,34,34,34	0
56	MG	YA	3412	1/1	0.96	0.16	38,38,38,38	0
56	MG	YA	3082	1/1	0.96	0.24	36,36,36,36	0
56	MG	RA	3013	1/1	0.96	0.38	10,10,10,10	0
56	MG	RA	3230	1/1	0.96	0.30	41,41,41,41	0
56	MG	RA	3255	1/1	0.96	0.32	64,64,64,64	0
56	MG	RA	3408	1/1	0.96	0.21	28,28,28,28	0
56	MG	YA	3148	1/1	0.96	0.70	18,18,18,18	0
56	MG	RA	3370	1/1	0.96	0.30	41,41,41,41	0
56	MG	QA	1634	1/1	0.96	0.45	33,33,33,33	0
56	MG	YA	3075	1/1	0.96	0.31	23,23,23,23	0
56	MG	YA	3206	1/1	0.96	0.40	38,38,38,38	0
56	MG	RA	3367	1/1	0.96	0.16	39,39,39,39	0
56	MG	RA	3058	1/1	0.96	0.14	41,41,41,41	0
56	MG	RA	3038	1/1	0.96	0.29	47,47,47,47	0
56	MG	RA	3089	1/1	0.96	0.55	16,16,16,16	0
56	MG	RB	202	1/1	0.96	0.29	35,35,35,35	0
56	MG	XA	1655	1/1	0.96	0.26	42,42,42,42	0
56	MG	YA	3356	1/1	0.96	0.42	48,48,48,48	0
56	MG	YA	3141	1/1	0.96	0.35	41,41,41,41	0
57	ZN	XD	301	1/1	0.96	0.33	69,69,69,69	0
56	MG	YA	3084	1/1	0.96	0.43	33,33,33,33	0
56	MG	XA	1658	1/1	0.96	0.27	40,40,40,40	0
56	MG	YA	3432	1/1	0.96	0.39	53,53,53,53	0
56	MG	YA	3212	1/1	0.96	0.32	17,17,17,17	0
56	MG	RA	3299	1/1	0.96	0.09	44,44,44,44	0
56	MG	YA	3106	1/1	0.96	0.39	17,17,17,17	0
56	MG	YA	3121	1/1	0.96	0.57	40,40,40,40	0
56	MG	RA	3312	1/1	0.96	0.52	39,39,39,39	0
56	MG	YA	3448	1/1	0.96	0.16	51,51,51,51	0
56	MG	RA	3214	1/1	0.96	0.25	40,40,40,40	0
56	MG	XA	1601	1/1	0.96	0.29	43,43,43,43	0
56	MG	XA	1662	1/1	0.96	0.28	34,34,34,34	0
56	MG	YA	3159	1/1	0.96	0.36	58,58,58,58	0
56	MG	YA	3021	1/1	0.96	0.35	24,24,24,24	0
56	MG	YA	3415	1/1	0.96	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3025	1/1	0.96	0.51	34,34,34,34	0
56	MG	YA	3283	1/1	0.96	0.19	31,31,31,31	0
56	MG	YA	3328	1/1	0.96	0.37	27,27,27,27	0
56	MG	RA	3157	1/1	0.96	0.43	14,14,14,14	0
56	MG	RA	3077	1/1	0.96	0.36	36,36,36,36	0
56	MG	QA	1660	1/1	0.96	0.21	40,40,40,40	0
56	MG	XA	1634	1/1	0.96	0.29	39,39,39,39	0
56	MG	QA	1643	1/1	0.96	0.12	47,47,47,47	0
56	MG	YA	3447	1/1	0.96	0.43	97,97,97,97	0
56	MG	YA	3231	1/1	0.96	0.41	64,64,64,64	0
56	MG	YA	3214	1/1	0.96	0.39	34,34,34,34	0
56	MG	YA	3070	1/1	0.96	0.33	39,39,39,39	0
56	MG	YN	201	1/1	0.96	0.22	30,30,30,30	0
56	MG	RA	3191	1/1	0.96	0.33	18,18,18,18	0
56	MG	QA	1623	1/1	0.96	0.10	52,52,52,52	0
56	MG	RA	3042	1/1	0.96	0.60	48,48,48,48	0
56	MG	XA	1675	1/1	0.96	0.21	33,33,33,33	0
56	MG	XA	1603	1/1	0.96	0.18	19,19,19,19	0
56	MG	YA	3402	1/1	0.96	0.46	18,18,18,18	0
56	MG	YA	3016	1/1	0.96	0.10	18,18,18,18	0
56	MG	RP	201	1/1	0.96	0.13	38,38,38,38	0
56	MG	YA	3166	1/1	0.96	0.23	41,41,41,41	0
56	MG	R0	101	1/1	0.96	0.28	43,43,43,43	0
56	MG	YA	3020	1/1	0.96	0.24	32,32,32,32	0
56	MG	XA	1711	1/1	0.96	0.18	53,53,53,53	0
56	MG	RA	3308	1/1	0.96	0.43	38,38,38,38	0
56	MG	Y5	101	1/1	0.96	0.25	20,20,20,20	0
56	MG	RA	3004	1/1	0.96	0.38	10,10,10,10	0
56	MG	XA	1751	1/1	0.96	0.58	58,58,58,58	0
56	MG	YA	3008	1/1	0.96	0.13	8,8,8,8	0
56	MG	RA	3107	1/1	0.96	0.50	50,50,50,50	0
56	MG	XA	1709	1/1	0.96	0.62	45,45,45,45	0
56	MG	YA	3119	1/1	0.96	0.18	71,71,71,71	0
56	MG	QA	1620	1/1	0.96	0.27	52,52,52,52	0
56	MG	RA	3127	1/1	0.96	0.07	23,23,23,23	0
56	MG	QV	104	1/1	0.96	0.26	68,68,68,68	0
56	MG	RB	201	1/1	0.96	0.31	26,26,26,26	0
56	MG	YA	3120	1/1	0.96	0.39	32,32,32,32	0
56	MG	RA	3179	1/1	0.96	0.24	61,61,61,61	0
56	MG	YA	3272	1/1	0.96	0.32	49,49,49,49	0
56	MG	YA	3209	1/1	0.96	0.56	25,25,25,25	0
56	MG	RA	3044	1/1	0.96	0.29	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1621	1/1	0.96	0.21	47,47,47,47	0
56	MG	RA	3014	1/1	0.96	0.45	36,36,36,36	0
56	MG	YA	3069	1/1	0.96	0.33	17,17,17,17	0
56	MG	XA	1734	1/1	0.97	0.07	44,44,44,44	0
56	MG	YA	3400	1/1	0.97	0.07	11,11,11,11	0
56	MG	YE	302	1/1	0.97	0.19	12,12,12,12	0
56	MG	XA	1666	1/1	0.97	0.33	28,28,28,28	0
56	MG	RA	3121	1/1	0.97	0.32	14,14,14,14	0
56	MG	YA	3059	1/1	0.97	0.23	23,23,23,23	0
56	MG	RA	3381	1/1	0.97	0.24	37,37,37,37	0
56	MG	XA	1733	1/1	0.97	0.14	33,33,33,33	0
56	MG	YA	3107	1/1	0.97	0.18	22,22,22,22	0
56	MG	YA	3199	1/1	0.97	0.14	28,28,28,28	0
56	MG	YA	3066	1/1	0.97	0.58	25,25,25,25	0
56	MG	RA	3021	1/1	0.97	0.38	23,23,23,23	0
56	MG	YA	3080	1/1	0.97	0.44	12,12,12,12	0
56	MG	YA	3365	1/1	0.97	0.22	45,45,45,45	0
56	MG	RA	3120	1/1	0.97	0.29	20,20,20,20	0
56	MG	YA	3433	1/1	0.97	0.15	31,31,31,31	0
56	MG	RA	3092	1/1	0.97	0.27	31,31,31,31	0
56	MG	YA	3064	1/1	0.97	0.27	15,15,15,15	0
56	MG	YA	3391	1/1	0.97	0.41	26,26,26,26	0
56	MG	RA	3036	1/1	0.97	0.34	14,14,14,14	0
56	MG	YA	3005	1/1	0.97	0.31	6,6,6,6	0
56	MG	RA	3248	1/1	0.97	0.41	35,35,35,35	0
56	MG	RA	3028	1/1	0.97	0.24	24,24,24,24	0
56	MG	YP	201	1/1	0.97	0.20	25,25,25,25	0
56	MG	XA	1682	1/1	0.97	0.38	33,33,33,33	0
56	MG	RA	3137	1/1	0.97	0.19	47,47,47,47	0
56	MG	RA	3153	1/1	0.97	0.21	31,31,31,31	0
56	MG	QA	1687	1/1	0.97	0.14	33,33,33,33	0
56	MG	XA	1604	1/1	0.97	0.33	25,25,25,25	0
56	MG	YA	3043	1/1	0.97	0.28	21,21,21,21	0
56	MG	RA	3047	1/1	0.97	0.45	24,24,24,24	0
56	MG	RA	3045	1/1	0.97	0.39	18,18,18,18	0
56	MG	YA	3079	1/1	0.97	0.55	33,33,33,33	0
56	MG	QA	1607	1/1	0.97	0.32	33,33,33,33	0
56	MG	RA	3088	1/1	0.97	0.34	24,24,24,24	0
56	MG	XA	1643	1/1	0.97	0.09	51,51,51,51	0
56	MG	RA	3061	1/1	0.97	0.44	25,25,25,25	0
56	MG	YA	3464	1/1	0.97	0.37	31,31,31,31	0
56	MG	YA	3060	1/1	0.97	0.44	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YD	301	1/1	0.97	0.32	20,20,20,20	0
56	MG	XA	1646	1/1	0.97	0.46	50,50,50,50	0
56	MG	RA	3265	1/1	0.97	0.34	38,38,38,38	0
56	MG	RA	3211	1/1	0.97	0.23	16,16,16,16	0
56	MG	YA	3028	1/1	0.97	0.12	17,17,17,17	0
56	MG	YA	3378	1/1	0.97	0.30	34,34,34,34	0
56	MG	XA	1605	1/1	0.97	0.35	23,23,23,23	0
56	MG	RA	3277	1/1	0.97	0.12	18,18,18,18	0
56	MG	RA	3335	1/1	0.97	0.17	18,18,18,18	0
56	MG	XA	1693	1/1	0.97	0.43	59,59,59,59	0
56	MG	RA	3358	1/1	0.97	0.55	33,33,33,33	0
56	MG	XA	1610	1/1	0.97	0.18	46,46,46,46	0
56	MG	RA	3056	1/1	0.97	0.50	13,13,13,13	0
56	MG	XA	1697	1/1	0.97	0.32	50,50,50,50	0
56	MG	RA	3372	1/1	0.97	0.14	21,21,21,21	0
56	MG	YA	3027	1/1	0.97	0.29	28,28,28,28	0
56	MG	RA	3237	1/1	0.97	0.28	70,70,70,70	0
56	MG	XA	1721	1/1	0.97	0.22	46,46,46,46	0
56	MG	YA	3242	1/1	0.97	0.24	41,41,41,41	0
56	MG	YA	3087	1/1	0.97	0.25	14,14,14,14	0
56	MG	QA	1644	1/1	0.97	0.52	58,58,58,58	0
56	MG	YA	3124	1/1	0.97	0.36	33,33,33,33	0
56	MG	XA	1633	1/1	0.97	0.27	50,50,50,50	0
56	MG	YA	3127	1/1	0.97	0.09	20,20,20,20	0
56	MG	YA	3381	1/1	0.97	0.14	58,58,58,58	0
56	MG	YA	3297	1/1	0.97	0.48	37,37,37,37	0
56	MG	YA	3032	1/1	0.97	0.21	8,8,8,8	0
56	MG	XV	101	1/1	0.97	0.26	51,51,51,51	0
56	MG	YA	3041	1/1	0.97	0.34	14,14,14,14	0
56	MG	YA	3035	1/1	0.97	0.41	24,24,24,24	0
56	MG	YA	3302	1/1	0.97	0.19	36,36,36,36	0
56	MG	YA	3012	1/1	0.97	0.34	20,20,20,20	0
56	MG	RA	3232	1/1	0.97	0.29	39,39,39,39	0
56	MG	YA	3187	1/1	0.97	0.44	26,26,26,26	0
56	MG	RA	3213	1/1	0.97	0.26	31,31,31,31	0
56	MG	XA	1607	1/1	0.97	0.33	37,37,37,37	0
56	MG	RA	3062	1/1	0.97	0.34	11,11,11,11	0
56	MG	XA	1729	1/1	0.97	0.39	37,37,37,37	0
56	MG	RA	3012	1/1	0.97	0.29	12,12,12,12	0
56	MG	RA	3032	1/1	0.97	0.43	25,25,25,25	0
56	MG	YA	3310	1/1	0.97	0.14	56,56,56,56	0
56	MG	RA	3360	1/1	0.97	0.30	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3139	1/1	0.97	0.18	50,50,50,50	0
56	MG	YA	3023	1/1	0.97	0.29	12,12,12,12	0
56	MG	YA	3385	1/1	0.97	0.44	67,67,67,67	0
56	MG	RA	3365	1/1	0.97	0.39	43,43,43,43	0
56	MG	YA	3144	1/1	0.97	0.13	21,21,21,21	0
56	MG	RA	3199	1/1	0.97	0.38	37,37,37,37	0
56	MG	RA	3286	1/1	0.97	0.33	43,43,43,43	0
56	MG	XA	1650	1/1	0.97	0.27	21,21,21,21	0
56	MG	RA	3172	1/1	0.97	0.46	16,16,16,16	0
56	MG	RA	3008	1/1	0.97	0.17	17,17,17,17	0
56	MG	RA	3009	1/1	0.97	0.48	24,24,24,24	0
56	MG	R5	101	1/1	0.97	0.33	27,27,27,27	0
56	MG	QA	1604	1/1	0.97	0.17	33,33,33,33	0
56	MG	RA	3071	1/1	0.97	0.31	50,50,50,50	0
56	MG	QA	1711	1/1	0.97	0.30	33,33,33,33	0
56	MG	QA	1700	1/1	0.97	0.42	53,53,53,53	0
56	MG	YA	3330	1/1	0.97	0.51	20,20,20,20	0
56	MG	RA	3284	1/1	0.97	0.21	35,35,35,35	0
56	MG	RA	3015	1/1	0.97	0.32	30,30,30,30	0
56	MG	YA	3282	1/1	0.97	0.29	44,44,44,44	0
56	MG	RA	3066	1/1	0.97	0.44	38,38,38,38	0
56	MG	YA	3036	1/1	0.97	0.34	45,45,45,45	0
56	MG	YA	3116	1/1	0.97	0.32	58,58,58,58	0
56	MG	YA	3220	1/1	0.97	0.36	48,48,48,48	0
56	MG	RA	3006	1/1	0.97	0.29	11,11,11,11	0
56	MG	RA	3369	1/1	0.98	0.57	19,19,19,19	0
56	MG	YA	3002	1/1	0.98	0.12	6,6,6,6	0
56	MG	QA	1615	1/1	0.98	0.19	44,44,44,44	0
56	MG	YA	3257	1/1	0.98	0.07	44,44,44,44	0
56	MG	YA	3135	1/1	0.98	0.29	29,29,29,29	0
56	MG	RA	3111	1/1	0.98	0.13	39,39,39,39	0
56	MG	YA	3161	1/1	0.98	0.17	41,41,41,41	0
56	MG	RA	3192	1/1	0.98	0.32	16,16,16,16	0
56	MG	XA	1710	1/1	0.98	0.33	63,63,63,63	0
56	MG	YA	3192	1/1	0.98	0.60	25,25,25,25	0
56	MG	YA	3102	1/1	0.98	0.37	12,12,12,12	0
56	MG	YA	3377	1/1	0.98	0.21	31,31,31,31	0
56	MG	YA	3085	1/1	0.98	0.18	33,33,33,33	0
56	MG	RA	3031	1/1	0.98	0.28	15,15,15,15	0
56	MG	RA	3051	1/1	0.98	0.23	11,11,11,11	0
56	MG	RA	3225	1/1	0.98	0.09	51,51,51,51	0
56	MG	RA	3087	1/1	0.98	0.23	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3052	1/1	0.98	0.46	40,40,40,40	0
56	MG	RA	3086	1/1	0.98	0.17	23,23,23,23	0
56	MG	YA	3054	1/1	0.98	0.33	19,19,19,19	0
56	MG	RA	3023	1/1	0.98	0.49	12,12,12,12	0
56	MG	RA	3034	1/1	0.98	0.19	33,33,33,33	0
56	MG	YA	3086	1/1	0.98	0.27	37,37,37,37	0
56	MG	QA	1649	1/1	0.98	0.17	32,32,32,32	0
56	MG	YA	3033	1/1	0.98	0.27	19,19,19,19	0
56	MG	RA	3039	1/1	0.98	0.56	14,14,14,14	0
56	MG	YA	3071	1/1	0.98	0.34	24,24,24,24	0
56	MG	XA	1628	1/1	0.98	0.42	48,48,48,48	0
56	MG	RA	3003	1/1	0.98	0.26	10,10,10,10	0
56	MG	RA	3140	1/1	0.98	0.17	30,30,30,30	0
56	MG	YA	3176	1/1	0.98	0.08	12,12,12,12	0
56	MG	RA	3330	1/1	0.98	0.19	45,45,45,45	0
56	MG	RA	3289	1/1	0.98	0.59	27,27,27,27	0
56	MG	YA	3010	1/1	0.98	0.23	3,3,3,3	0
56	MG	XA	1606	1/1	0.98	0.34	31,31,31,31	0
56	MG	RA	3026	1/1	0.98	0.25	13,13,13,13	0
56	MG	RA	3108	1/1	0.98	0.47	10,10,10,10	0
56	MG	RA	3103	1/1	0.98	0.27	44,44,44,44	0
56	MG	QA	1663	1/1	0.98	0.22	38,38,38,38	0
56	MG	RA	3020	1/1	0.98	0.26	15,15,15,15	0
56	MG	XA	1651	1/1	0.98	0.40	30,30,30,30	0
56	MG	RA	3017	1/1	0.98	0.28	9,9,9,9	0
56	MG	YA	3074	1/1	0.98	0.42	34,34,34,34	0
56	MG	YA	3154	1/1	0.98	0.30	25,25,25,25	0
56	MG	QA	1737	1/1	0.98	0.25	93,93,93,93	0
56	MG	RA	3033	1/1	0.98	0.40	32,32,32,32	0
56	MG	RA	3114	1/1	0.98	0.33	12,12,12,12	0
56	MG	RA	3030	1/1	0.98	0.23	35,35,35,35	0
56	MG	RA	3392	1/1	0.98	0.36	16,16,16,16	0
56	MG	YA	3042	1/1	0.98	0.35	30,30,30,30	0
56	MG	YA	3063	1/1	0.98	0.40	29,29,29,29	0
56	MG	QA	1720	1/1	0.98	0.17	49,49,49,49	0
56	MG	YA	3026	1/1	0.98	0.38	10,10,10,10	0
56	MG	QA	1605	1/1	0.98	0.29	36,36,36,36	0
56	MG	RA	3080	1/1	0.98	0.27	18,18,18,18	0
56	MG	XA	1654	1/1	0.98	0.16	48,48,48,48	0
56	MG	YA	3205	1/1	0.98	0.11	22,22,22,22	0
56	MG	RA	3130	1/1	0.98	0.10	27,27,27,27	0
56	MG	YA	3011	1/1	0.98	0.65	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1616	1/1	0.98	0.26	36,36,36,36	0
56	MG	YA	3038	1/1	0.98	0.54	12,12,12,12	0
56	MG	RA	3287	1/1	0.98	0.13	64,64,64,64	0
56	MG	YA	3325	1/1	0.98	0.40	39,39,39,39	0
56	MG	YA	3018	1/1	0.98	0.26	18,18,18,18	0
56	MG	XA	1735	1/1	0.98	0.32	27,27,27,27	0
56	MG	YA	3117	1/1	0.98	0.25	36,36,36,36	0
56	MG	XA	1690	1/1	0.98	0.38	40,40,40,40	0
56	MG	YA	3061	1/1	0.98	0.43	15,15,15,15	0
56	MG	YA	3040	1/1	0.98	0.25	21,21,21,21	0
56	MG	YA	3022	1/1	0.98	0.57	23,23,23,23	0
56	MG	RA	3081	1/1	0.98	0.50	17,17,17,17	0
56	MG	RA	3229	1/1	0.98	0.14	31,31,31,31	0
56	MG	QA	1671	1/1	0.98	0.21	36,36,36,36	0
56	MG	RA	3010	1/1	0.98	0.16	16,16,16,16	0
56	MG	YA	3055	1/1	0.98	0.54	18,18,18,18	0
56	MG	XA	1644	1/1	0.98	0.36	34,34,34,34	0
56	MG	YA	3006	1/1	0.98	0.40	23,23,23,23	0
56	MG	RA	3054	1/1	0.98	0.46	21,21,21,21	0
56	MG	QA	1693	1/1	0.98	0.37	30,30,30,30	0
56	MG	YA	3195	1/1	0.98	0.24	21,21,21,21	0
56	MG	RA	3176	1/1	0.98	0.24	25,25,25,25	0
56	MG	YA	3015	1/1	0.98	0.26	16,16,16,16	0
56	MG	QA	1723	1/1	0.98	0.12	98,98,98,98	0
56	MG	RA	3016	1/1	0.98	0.14	6,6,6,6	0
56	MG	YA	3004	1/1	0.99	0.35	5,5,5,5	0
56	MG	XA	1679	1/1	0.99	0.35	32,32,32,32	0
56	MG	XA	1707	1/1	0.99	0.68	31,31,31,31	0
56	MG	RA	3270	1/1	0.99	0.39	49,49,49,49	0
56	MG	RA	3162	1/1	0.99	0.26	43,43,43,43	0
56	MG	YA	3250	1/1	0.99	0.22	24,24,24,24	0
56	MG	RA	3043	1/1	0.99	0.52	28,28,28,28	0
56	MG	QA	1688	1/1	0.99	0.41	26,26,26,26	0
56	MG	RA	3072	1/1	0.99	0.35	6,6,6,6	0
56	MG	YA	3271	1/1	0.99	0.19	22,22,22,22	0
56	MG	YA	3210	1/1	0.99	0.23	4,4,4,4	0
56	MG	QA	1616	1/1	0.99	0.21	46,46,46,46	0
56	MG	RA	3057	1/1	0.99	0.33	22,22,22,22	0
56	MG	RP	202	1/1	0.99	0.14	31,31,31,31	0
56	MG	RA	3158	1/1	0.99	0.10	38,38,38,38	0
56	MG	YA	3009	1/1	0.99	0.33	14,14,14,14	0
56	MG	YA	3172	1/1	0.99	0.40	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3037	1/1	0.99	0.30	22,22,22,22	0
56	MG	YA	3077	1/1	0.99	0.48	17,17,17,17	0
56	MG	RA	3306	1/1	0.99	0.13	40,40,40,40	0
56	MG	RA	3073	1/1	0.99	0.35	31,31,31,31	0
56	MG	QA	1680	1/1	0.99	0.21	24,24,24,24	0
56	MG	YA	3029	1/1	0.99	0.32	15,15,15,15	0
56	MG	YA	3048	1/1	0.99	0.50	12,12,12,12	0
56	MG	RA	3085	1/1	0.99	0.33	16,16,16,16	0
56	MG	RA	3018	1/1	0.99	0.27	16,16,16,16	0
56	MG	QA	1618	1/1	0.99	0.39	24,24,24,24	0
56	MG	RA	3024	1/1	0.99	0.28	28,28,28,28	0
56	MG	RA	3147	1/1	0.99	0.64	15,15,15,15	0
56	MG	RA	3078	1/1	0.99	0.34	13,13,13,13	0
56	MG	XA	1602	1/1	0.99	0.39	13,13,13,13	0
56	MG	YA	3056	1/1	0.99	0.31	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.