



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:36 PM UTC

PDB ID : 4W4G / pdb_00004w4g
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

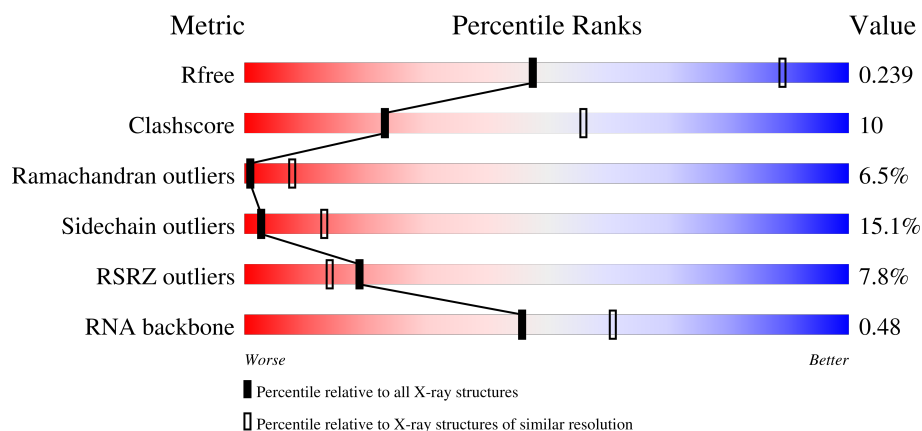
1 Overall quality at a glance

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 56% 33% 10%
1	XA	1522	2% 57% 35% 7%
2	QB	256	8% 52% 31% 9% 8%
2	XB	256	13% 50% 34% 8% 8%

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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
56	MG	RA	3405	-	-	-	X
56	MG	YA	3001	-	-	-	X
56	MG	YA	3167	-	-	-	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	140	Total 140	Mg 140	0	0
56	QE	1	Total 1	Mg 1	0	0
56	QL	1	Total 1	Mg 1	0	0
56	QV	5	Total 5	Mg 5	0	0
56	RA	413	Total 413	Mg 413	0	0
56	RB	4	Total 4	Mg 4	0	0
56	RD	2	Total 2	Mg 2	0	0
56	RE	1	Total 1	Mg 1	0	0
56	RF	1	Total 1	Mg 1	0	0
56	RP	2	Total 2	Mg 2	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	RY	1	Total 1	Mg 1	0	0
56	R0	2	Total 2	Mg 2	0	0
56	R2	1	Total 1	Mg 1	0	0
56	R5	3	Total 3	Mg 3	0	0
56	XA	160	Total 160	Mg 160	0	0
56	XD	1	Total 1	Mg 1	0	0
56	XF	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0

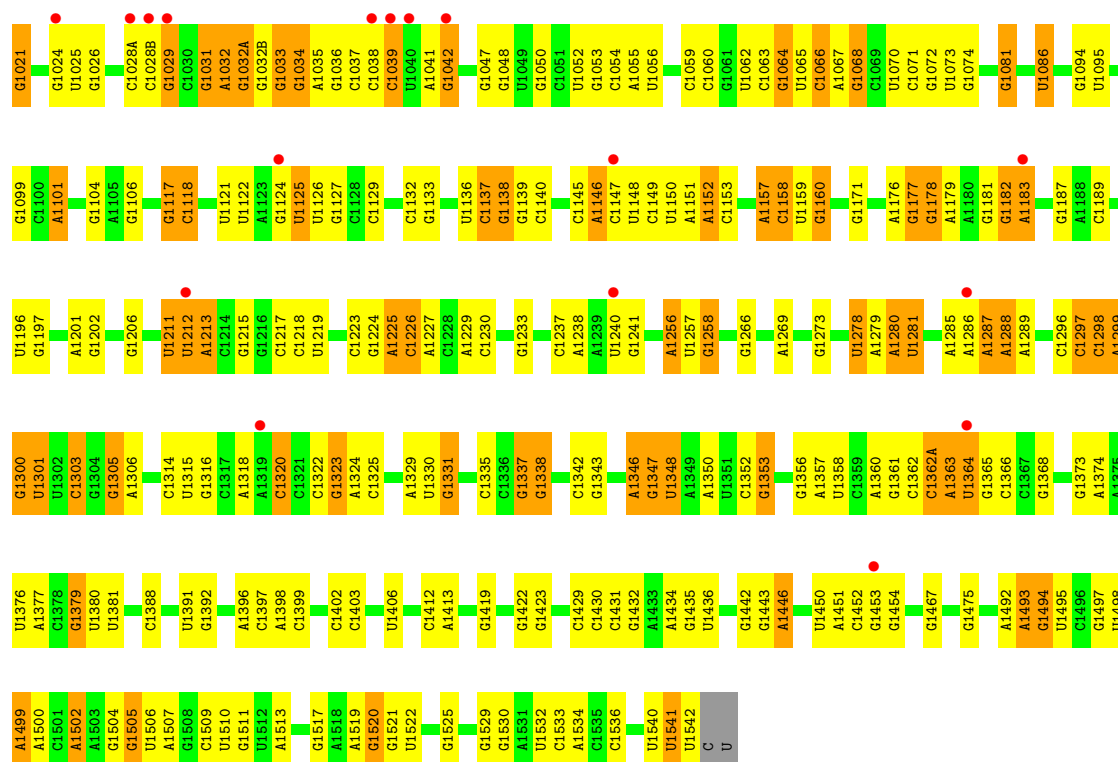
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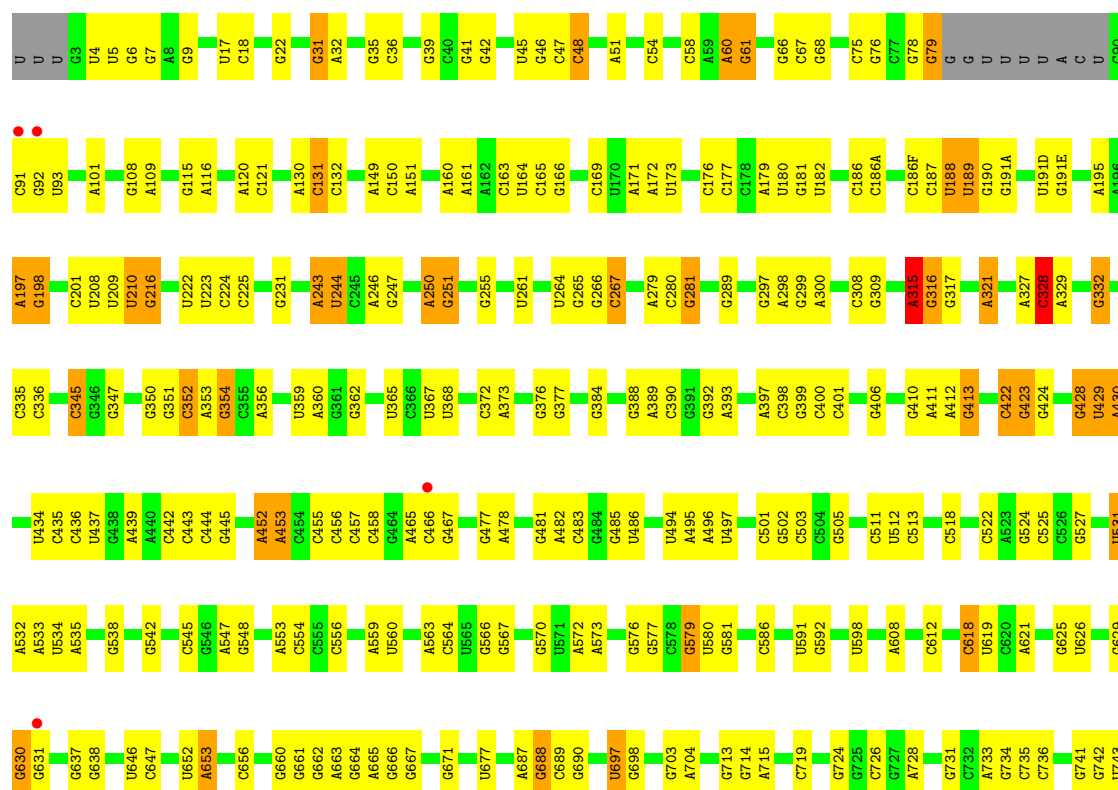
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XN	1	Total 1	Mg 1	0	0
56	XV	4	Total 4	Mg 4	0	0
56	YA	464	Total 464	Mg 464	0	0
56	YB	5	Total 5	Mg 5	0	0
56	YD	1	Total 1	Mg 1	0	0
56	YE	2	Total 2	Mg 2	0	0
56	YG	1	Total 1	Mg 1	0	0
56	YH	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	2	Total 2	Mg 2	0	0
56	YQ	2	Total 2	Mg 2	0	0
56	YR	1	Total 1	Mg 1	0	0
56	YU	1	Total 1	Mg 1	0	0
56	YV	1	Total 1	Mg 1	0	0
56	YY	1	Total 1	Mg 1	0	0
56	Y0	3	Total 3	Mg 3	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	Y5	2	Total 2	Mg 2	0	0
56	Y7	1	Total 1	Mg 1	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

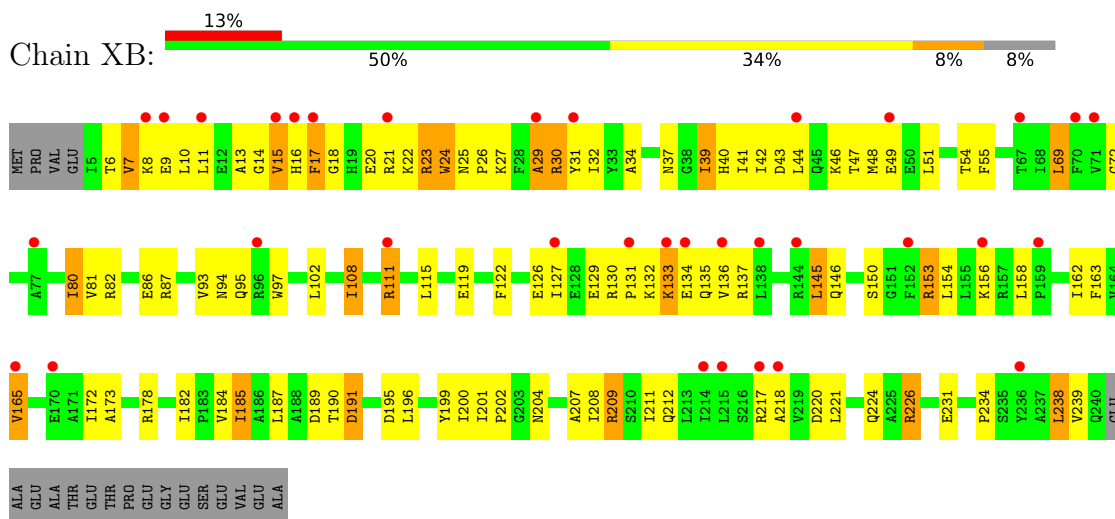
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QD	1	Total 1	Zn 1	0	0
57	QN	1	Total 1	Zn 1	0	0
57	XD	1	Total 1	Zn 1	0	0
57	XN	1	Total 1	Zn 1	0	0



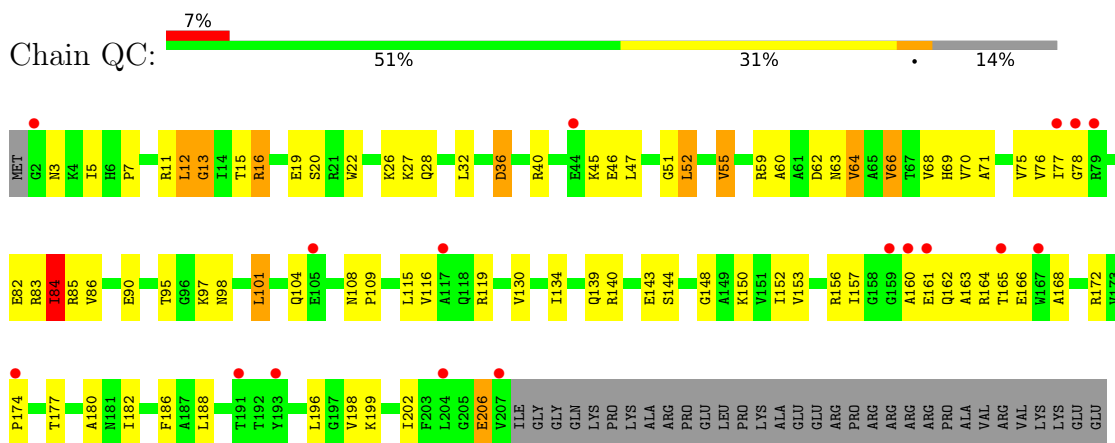
• Molecule 1: 16S rRNA



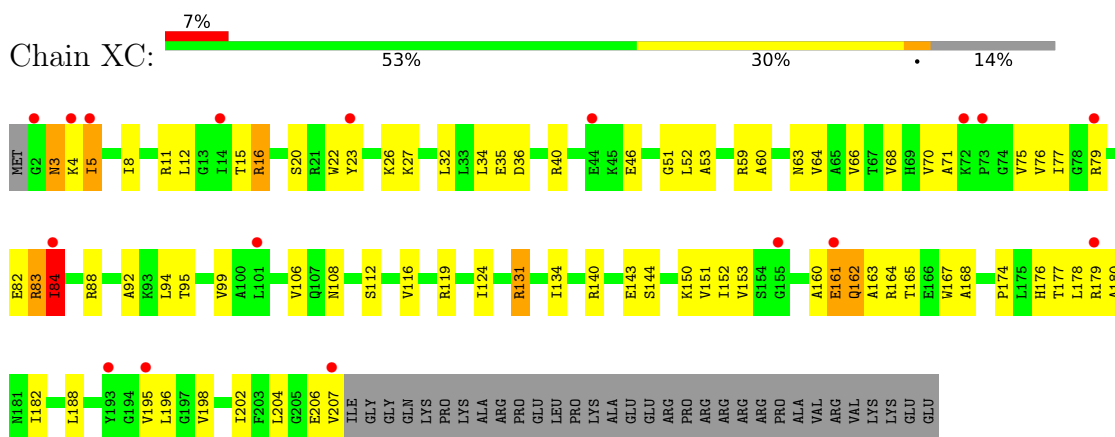
- Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

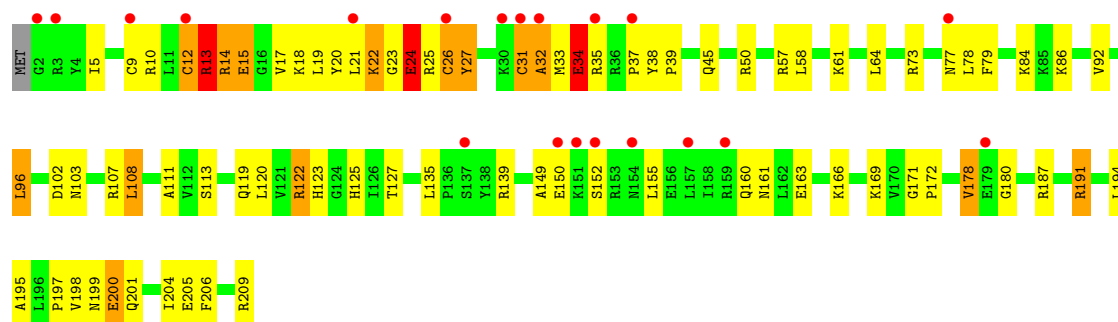


- Molecule 3: 30S ribosomal protein S3

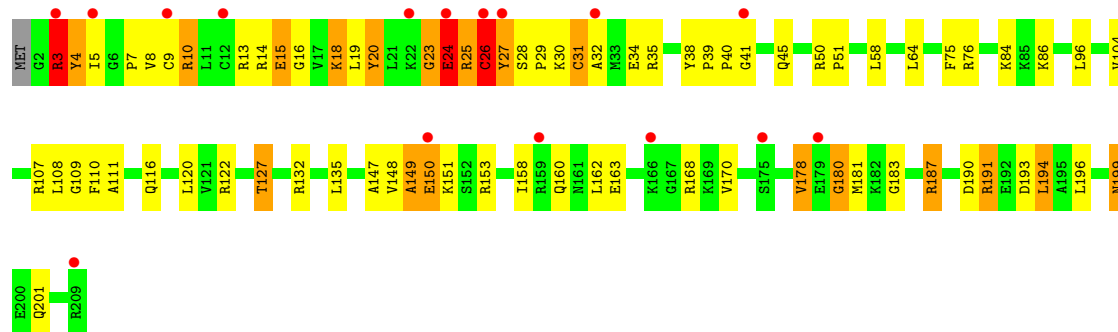


- Molecule 4: 30S ribosomal protein S4

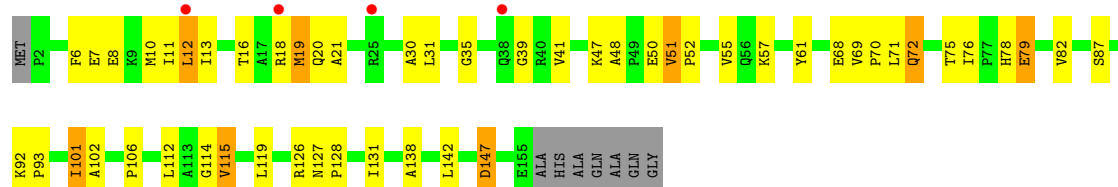




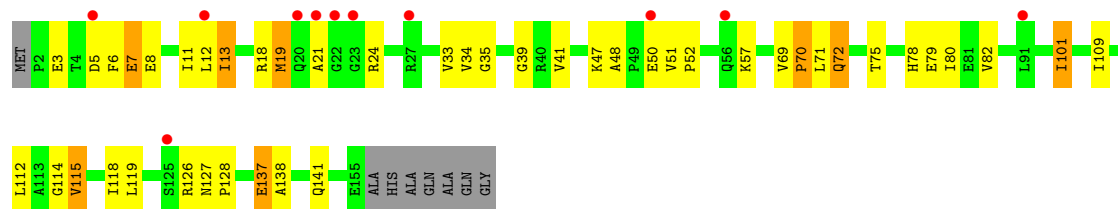
• Molecule 4: 30S ribosomal protein S4



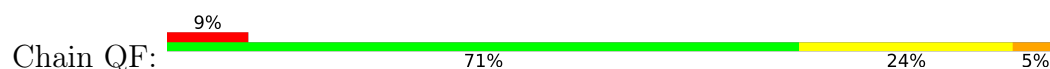
• Molecule 5: 30S ribosomal protein S5

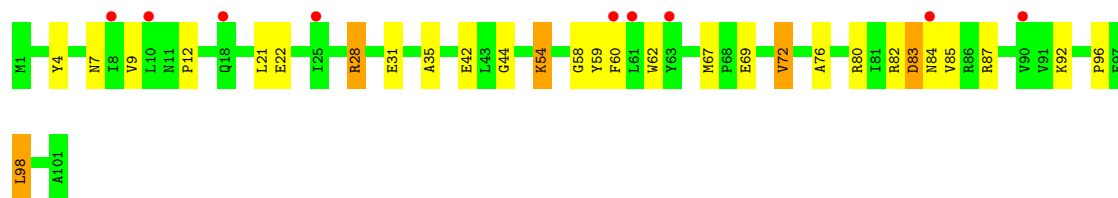


• Molecule 5: 30S ribosomal protein S5

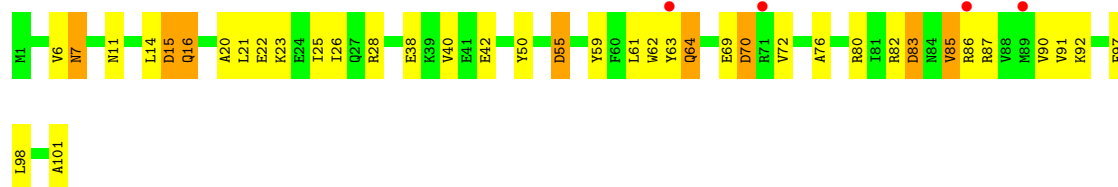


• Molecule 6: 30S ribosomal protein S6

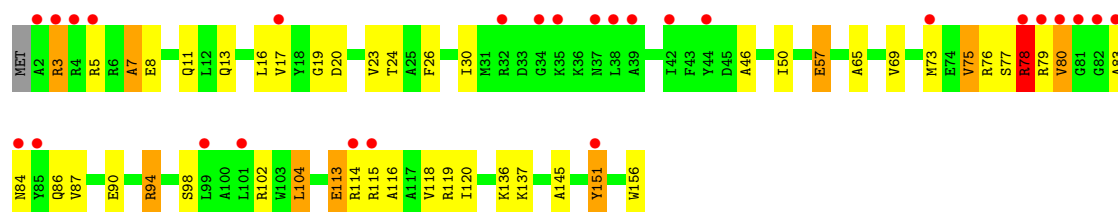




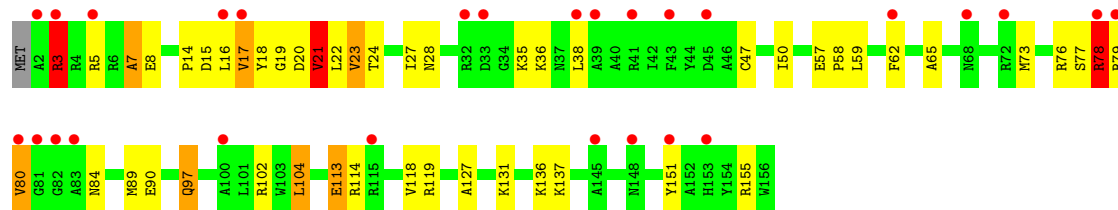
- Molecule 6: 30S ribosomal protein S6



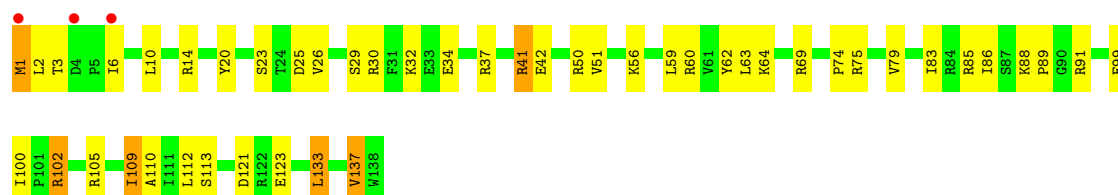
- Molecule 7: 30S ribosomal protein S7



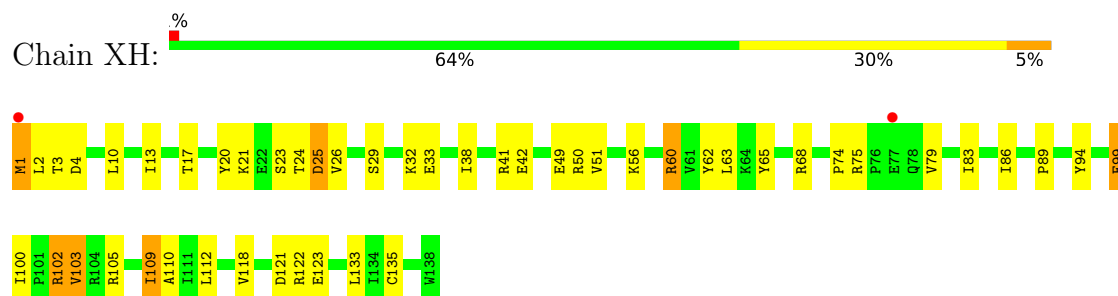
- Molecule 7: 30S ribosomal protein S7



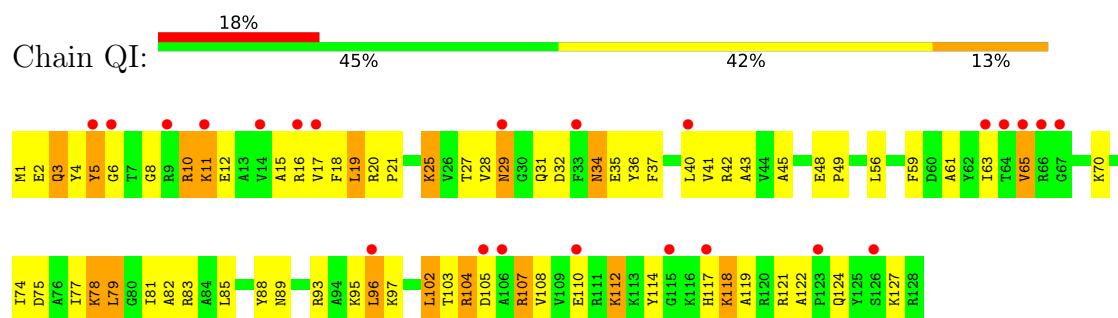
- Molecule 8: 30S ribosomal protein S8



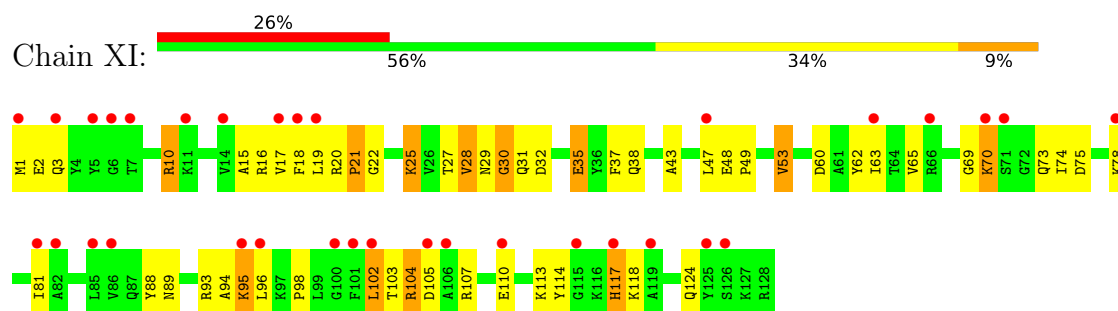
- Molecule 8: 30S ribosomal protein S8



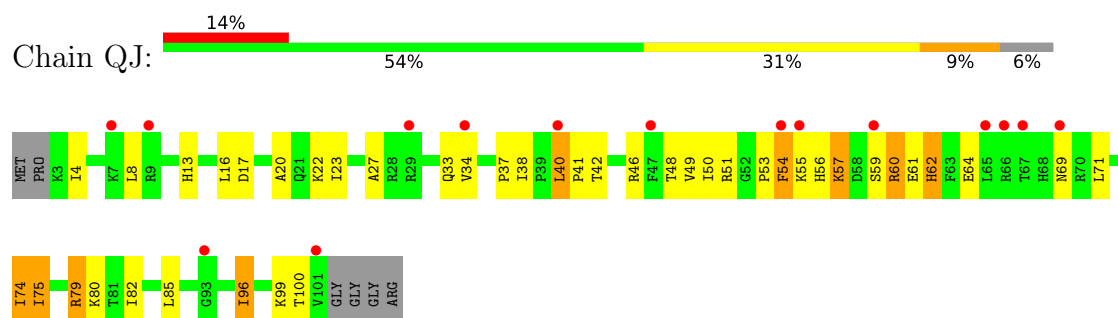
- Molecule 9: 30S ribosomal protein S9



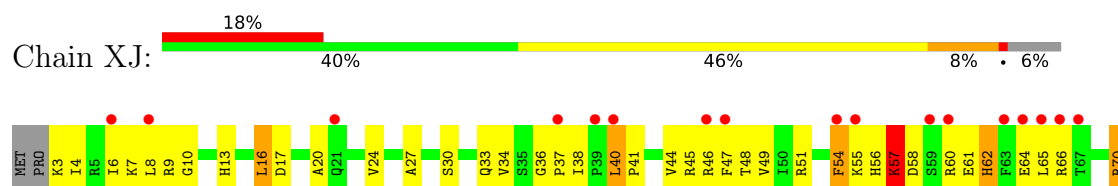
- Molecule 9: 30S ribosomal protein S9

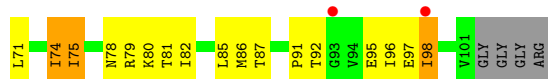


- Molecule 10: 30S ribosomal protein S10

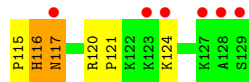


- Molecule 10: 30S ribosomal protein S10

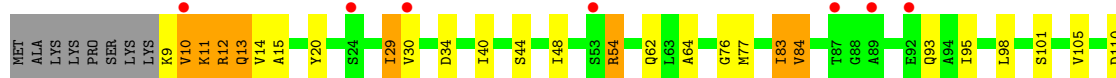




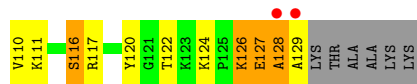
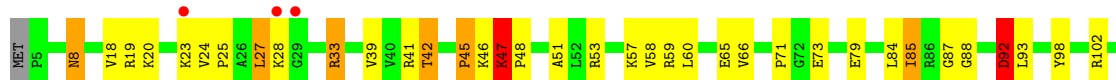
- Molecule 11: 30S ribosomal protein S11



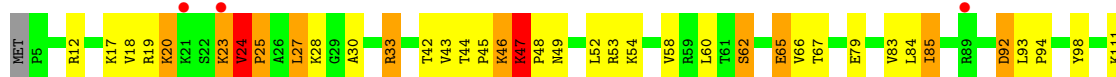
- Molecule 11: 30S ribosomal protein S11



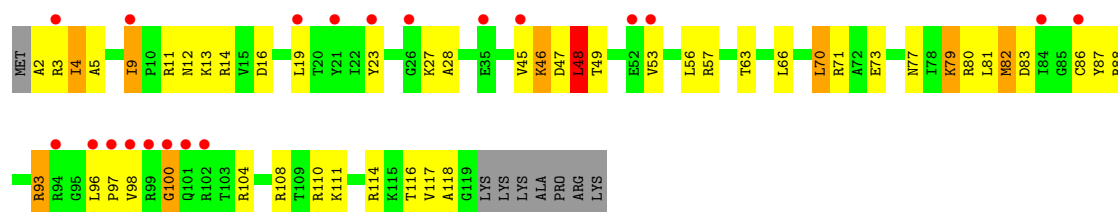
- Molecule 12: 30S ribosomal protein S12



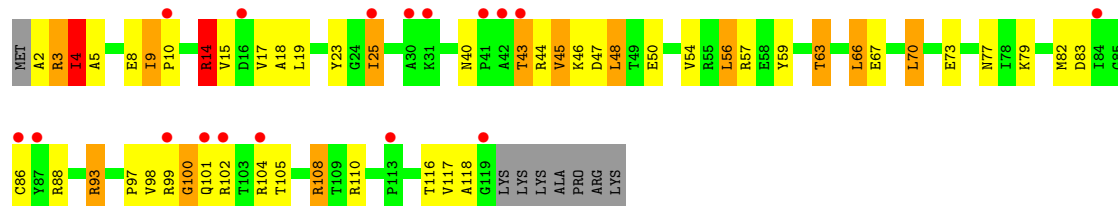
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13



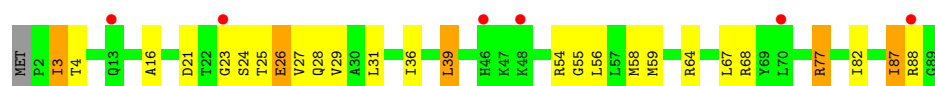
• Molecule 14: 30S ribosomal protein S14



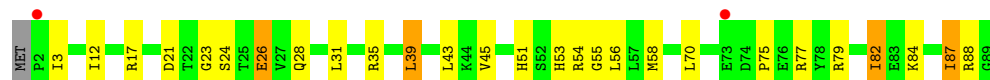
• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15

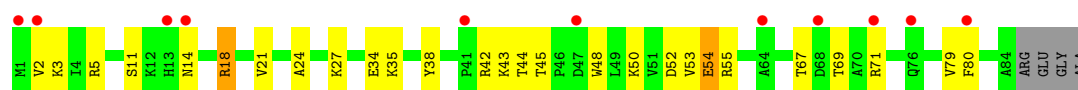


• Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

Chain QP: 



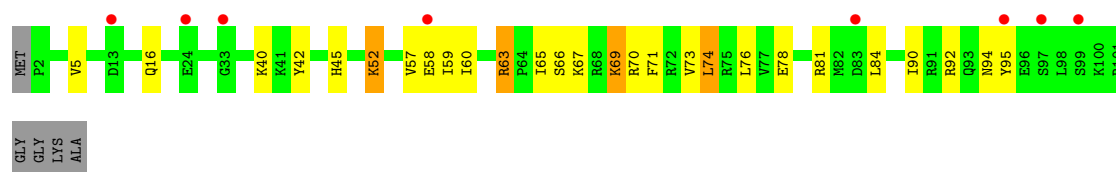
- Molecule 16: 30S ribosomal protein S16

Chain XP: 



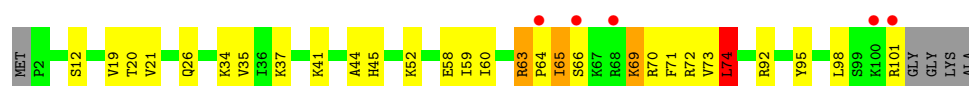
- Molecule 17: 30S ribosomal protein S17

Chain QQ: 



- Molecule 17: 30S ribosomal protein S17

Chain XQ: 



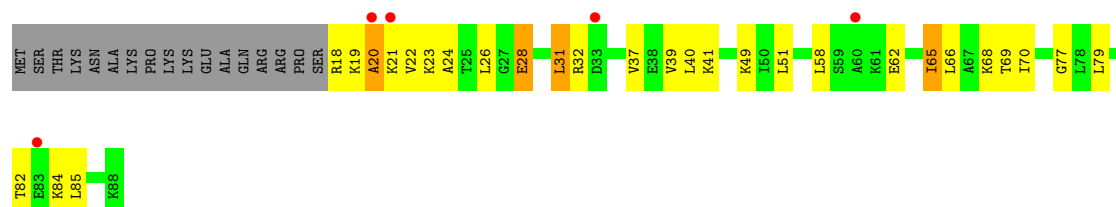
- Molecule 18: 30S ribosomal protein S18

Chain QR: 

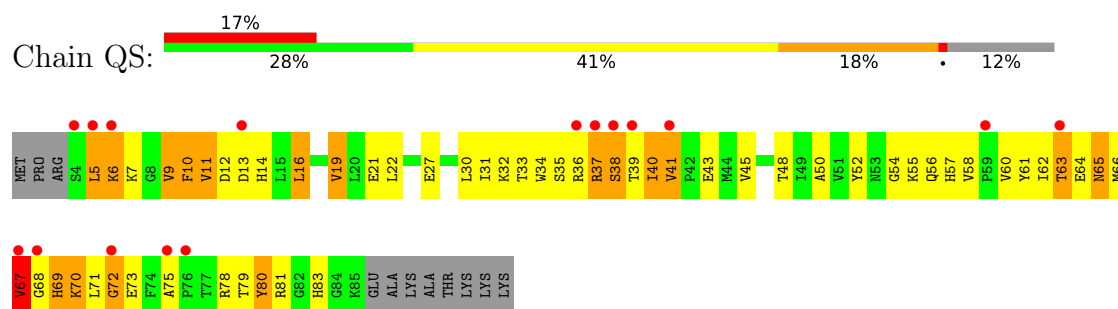


- Molecule 18: 30S ribosomal protein S18

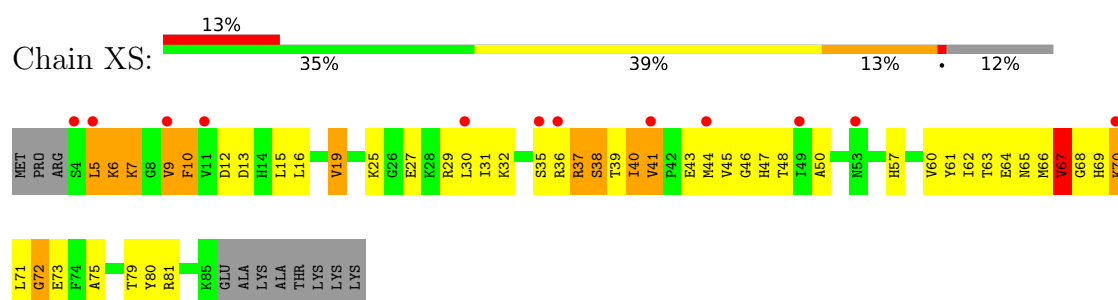
Chain XR: 



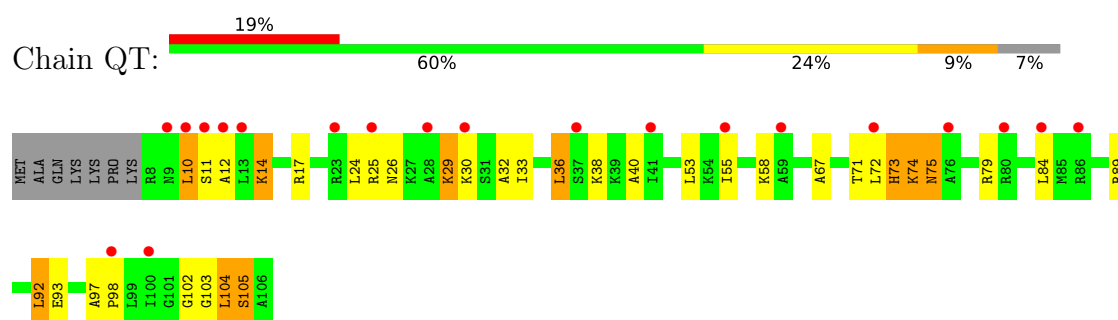
- Molecule 19: 30S ribosomal protein S19



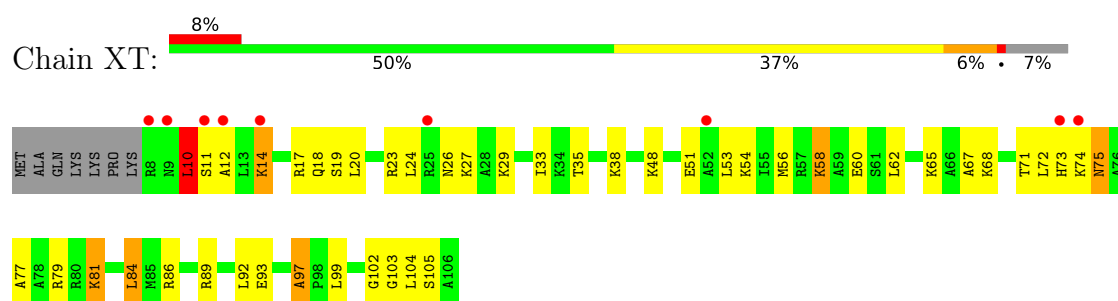
- Molecule 19: 30S ribosomal protein S19



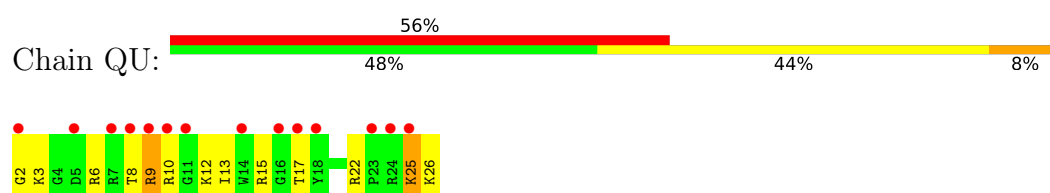
- Molecule 20: 30S ribosomal protein S20



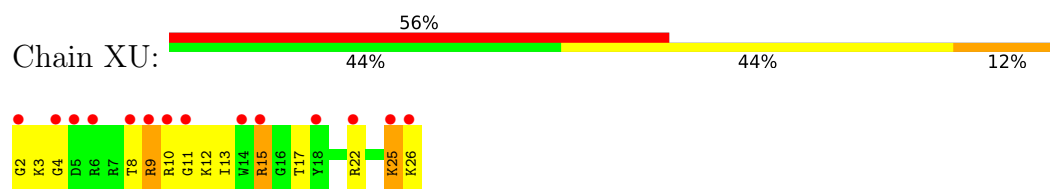
- Molecule 20: 30S ribosomal protein S20



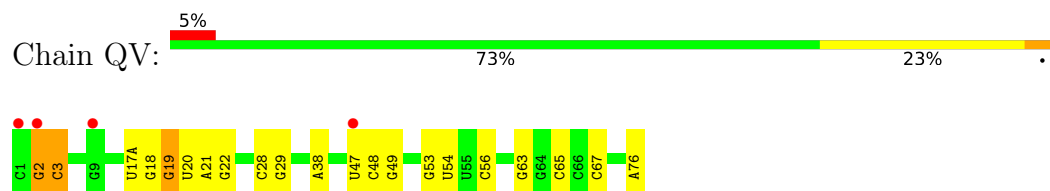
- Molecule 21: 30S ribosomal protein Thx



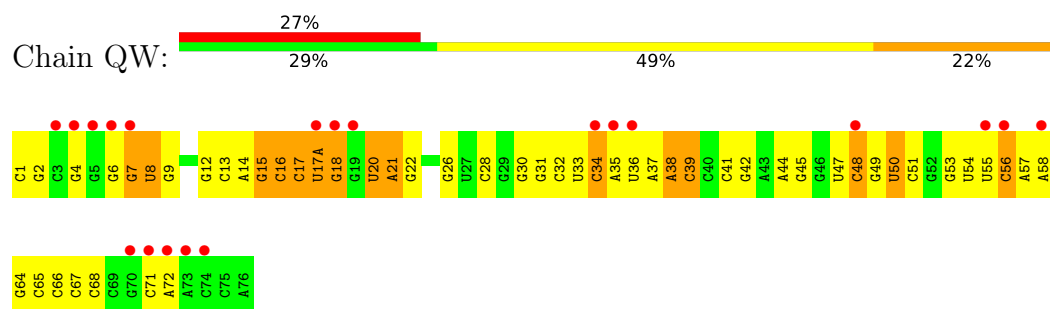
- Molecule 21: 30S ribosomal protein Thx



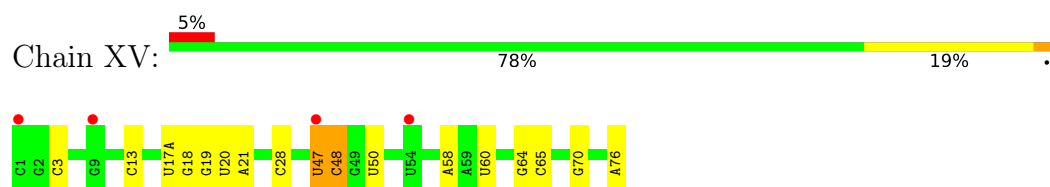
- Molecule 22: tRNA fMet



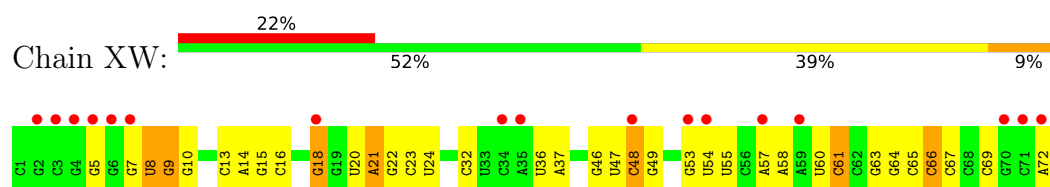
- Molecule 22: tRNA fMet



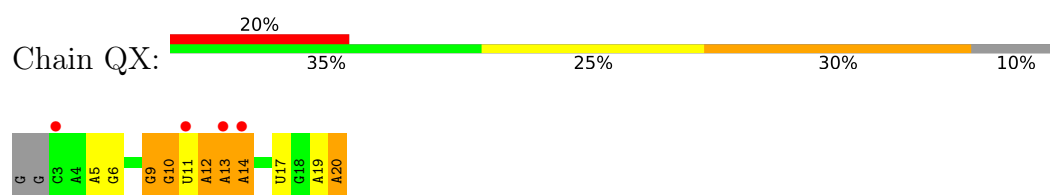
- Molecule 22: tRNA fMet



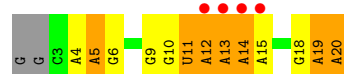
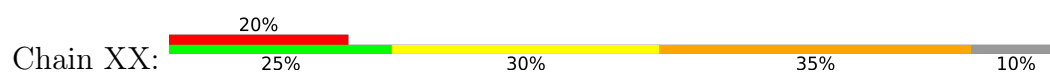
- Molecule 22: tRNA fMet



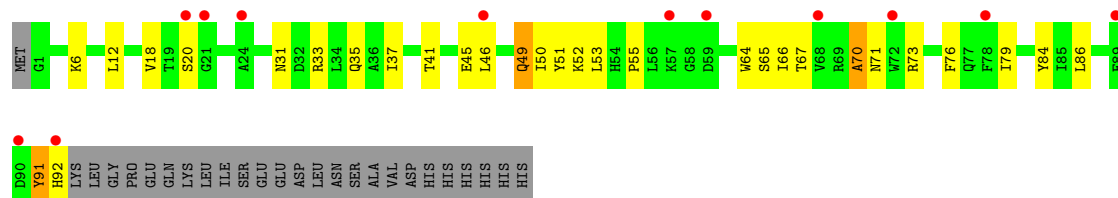
- Molecule 23: messenger RNA



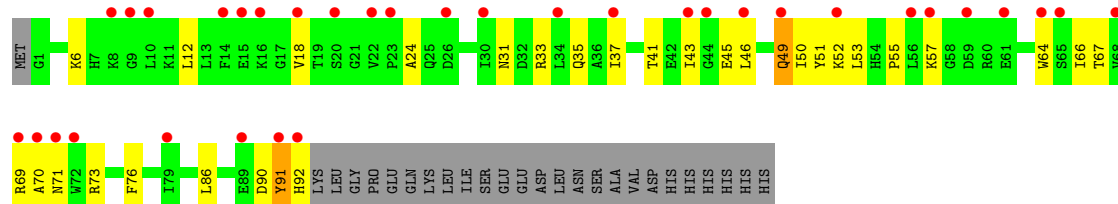
- Molecule 23: messenger RNA



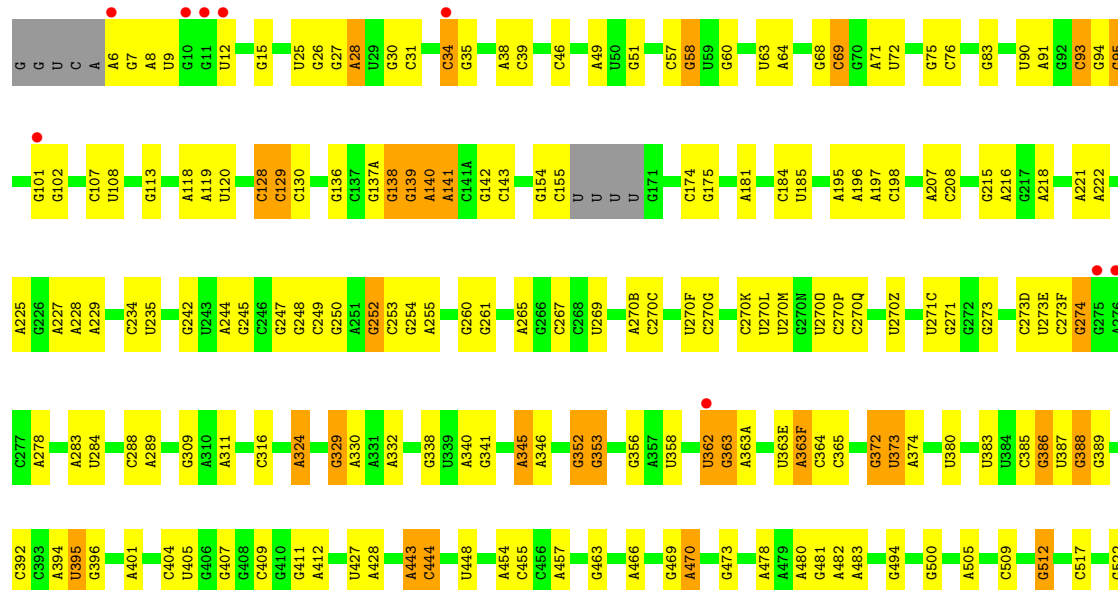
• Molecule 24: Host inhibition of growth B



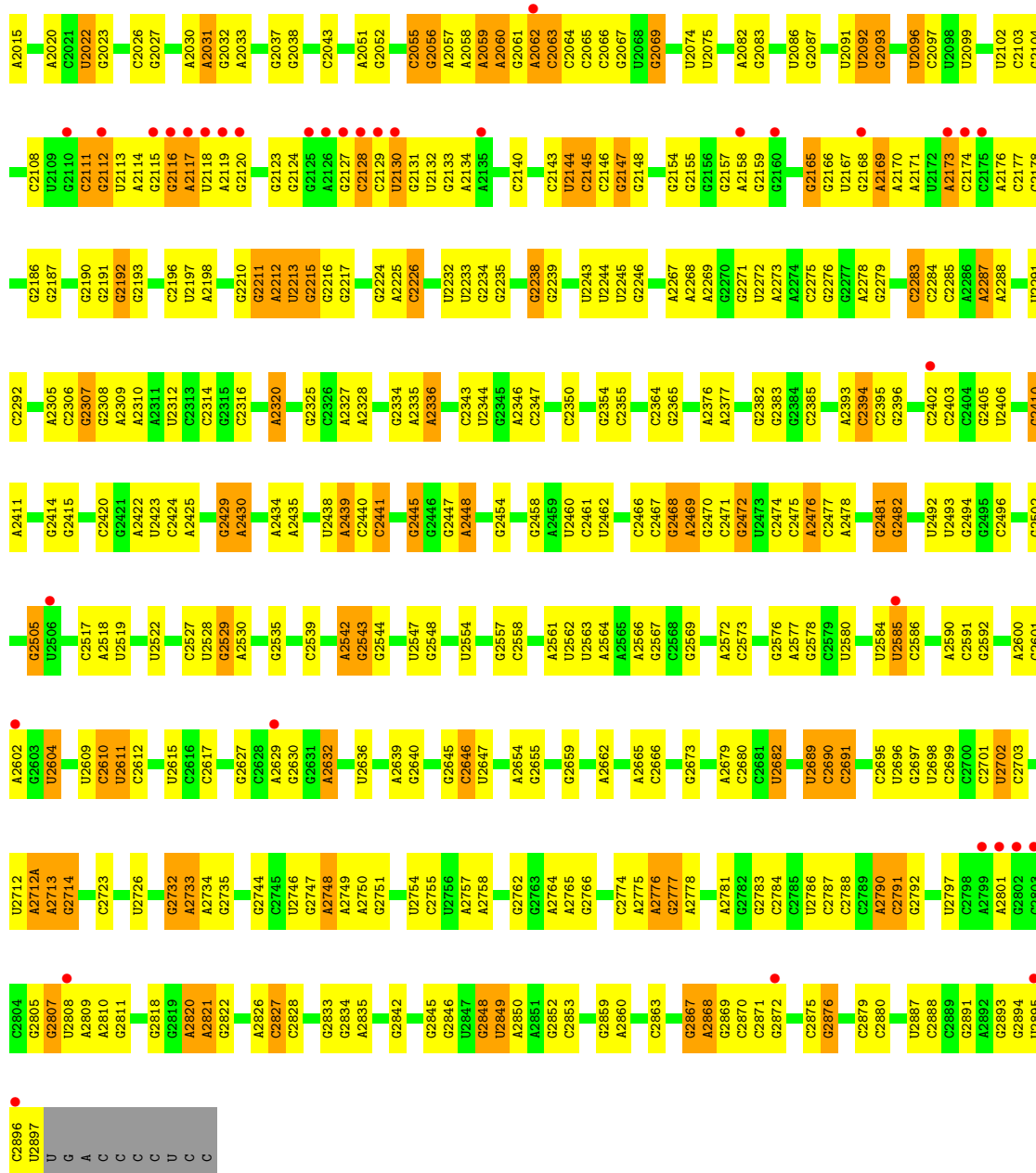
• Molecule 24: Host inhibition of growth B



• Molecule 25: 23S rRNA

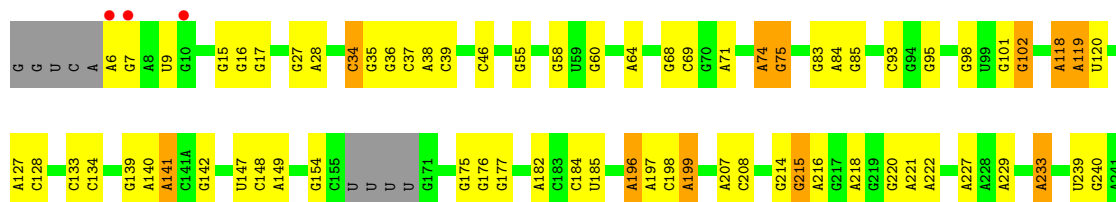


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G1903	C1790	G1647	G1522	G1421	G1310	A1204	G1093	C995	A896	C797	G886	A627	A528
G1906	A1791	C1648	G1525	A1427	U1312	A1210	U1094	A996	C897	G898	C628	G628	A529
A1912	U1794	A1652	G1526	C1428	U1313	A1213	A1095	C1006	A900	C805	C692	A631	G530
A1913	C1795	G1653	G1534	C1437	G1319	A1220	U1105	A1010	A901	C806	A632	A633	A532
U1916	U1796	A1654	U1535	G1441	G1328	C1225	G1106	G1011	C904	U811	G700	G636	G545
A1917	C1797	A1536	C1537	G1442	U1329	C1226	G1110	C1012	U905	C812	A706	A637	C546
A1918	U1799	A1665	G1538	G1444	U1341	A1227	A1111	C1013	G906	U813	G707	A638	A547
A1919	C1800	A1668	G1542	A1444A	U1342	G1228	G1112	A1020	U907	C814	C708	G639	A548
C1920	G1801	A1669	A1543	C1445	A1360	G1233	U1113	A1021	A909	U819	G710	C640	G549
G1929	U1805	G1674	A1544	A1449	A1354	G1236	G1114	U1022	A910	U827	A722	C641	G550
U1930	U1810	U1688	A1545	C1480	G1355	G1237	G1122	U1023	A911	U828	A723	C642	G556
U1931	A1811	A1689	C1547	G1451	G1356	G1238	G1125	G1024	C912	U829	U724	A643	G563
G1935	A1812	G1693	C1548	A1453	U1357	G1239	A1126	G1025	A917	U833	G725	C645	U666
A1936	G1813	U1694	C1549	U1454	G1358	G1240	A1130	U1026	A918	U839	G726	A646	G570
A1937	G1814	G1695	C1550	G1455	A1360	A1241	U1135	A1027	C921	C940	C730	G651	G574
A1938	A1815	G1696	A1554	G1459	G1364	G1244	C1135	G1030	G928	U839	C739	A652	A575
U1939	G1816	A1700	C1557	A1460	A1365	G1250	G1136	G1033	G929	G845	G746	A654	U576
U1946	A1819	A1701	A1558	C1462	A1366	G1251	G1137	G1044	G932	G848	U747	G854A	G577
G1948	U1820	G1701	C1559	C1463	A1367	C1252	G1138	A1045	A933	G855	G748	C854B	U578
G1949	C1827	G1718	A1566	C1464	G1368	A1253	C1140	A1046	G934	C856	G751	G854C	G579
G1950	G1828	G1725	A1567	C1467	A1373	A1254	U1141	G1047	A941	C857	A751	G854D	C581
U1951	A1829	U1726	G1568	C1471	U1255	G1256	U1142	C1048	G942	U858	A752	G854E	G582
A1952	U1727	G1728	A1569	A1471	U1257	C1257	A1142A	C1049	A945	C859	C753	C854F	G583
A1953	G1835	U1729	C1577	G1475	A1379	G1264	C1149	A1050	U946	U860	C754	G	A586
G1954	U1730	A1730	U1578	C1476	A1384	A1265	C1150	C1051	A957	U861	C755	C	C587
U1955	G1731	A1732	C1582	A1477	G1385	G1266	C1155	C1052	G956	G862	C756	C	U688
U1956	A1847	C1735	A1583	G1478	C1386	G1271	A1165	C1053	U958	A863	G759	G	A590
U1963	U1851	G1785	C1585	U1482	A1392	A1272	U1166	G1056	C961	A866	A761	G854N	G593
G1964	C1852	G1743	A1586	G1483	A1393	G1283	C1166	A1057	G968	G873	A764	G854O	U594
C1967	A1853	G1750	C1587	G1484	U1394	G1284	G1169	G1058	U969	G874	C772	C854P	G598
G1968	A1854	G1751	C1588	G1485	A1395	U1281	G1170	U1060	C974A	G875	U773	C854R	C601
A1969	G1863	G1752	G1595	U1488	U1396	G1282	G1171	G1061	G974	C876	A774	C854S	A603
A1970	U1864	G1753	C1598	U1489	G1400	G1283	G1172	G1062	C975	C877	G775	A654T	G604
A1971	G1869	C1754	A1599	A1490	G1401	G1285	A1173	G1063	G976	C878	G776	A654V	C605
A1972	C1870	A1759	A1603	C1493	C1402	A1286	G1175	A1070	G977	G880	U779	A655	U606
A1981	A1871	A1760	C1607	A1494	C1403	A1287	A1177	G1071	G978	G881	G779	U657	U607
C1982	G1878	C1761	A1608	A1495	G1404	U1288	C1178	C1075	G979	G882	A782	U658	G615
U1991	G1879	A1762	A1609	A1496	U1405	C1289	G1179	C1076	G980	C883	A783	C859	U613
G1992	C1880	G1763	A1614	A1497	U1406	C1290	C1180	A1077	G981	C884	A784	C859	U614
U1993	C1882	C1765	A1615	C1501	C1407	C1291	G1186	C1080	G982	C885	G785	C661	G616
G1999	G1883	G1622	G1625	C1505	U1415	C1293	G1187	A1084	G983	C888	A788	G668	A617
G2000	A1889	C1767	G1626	C1509	G1416	U1300	G1190	A1085	A989	C889	A789	C673	G617
G2010	A1890	A1773	A1510	A1510	C1417	A1301	G1195	A1086	C991	G892	G792	C678	G620
	G1899	A1780	C1640	A1510	A1419	A1308	G1195	G1087	G993	C894	A793		A621

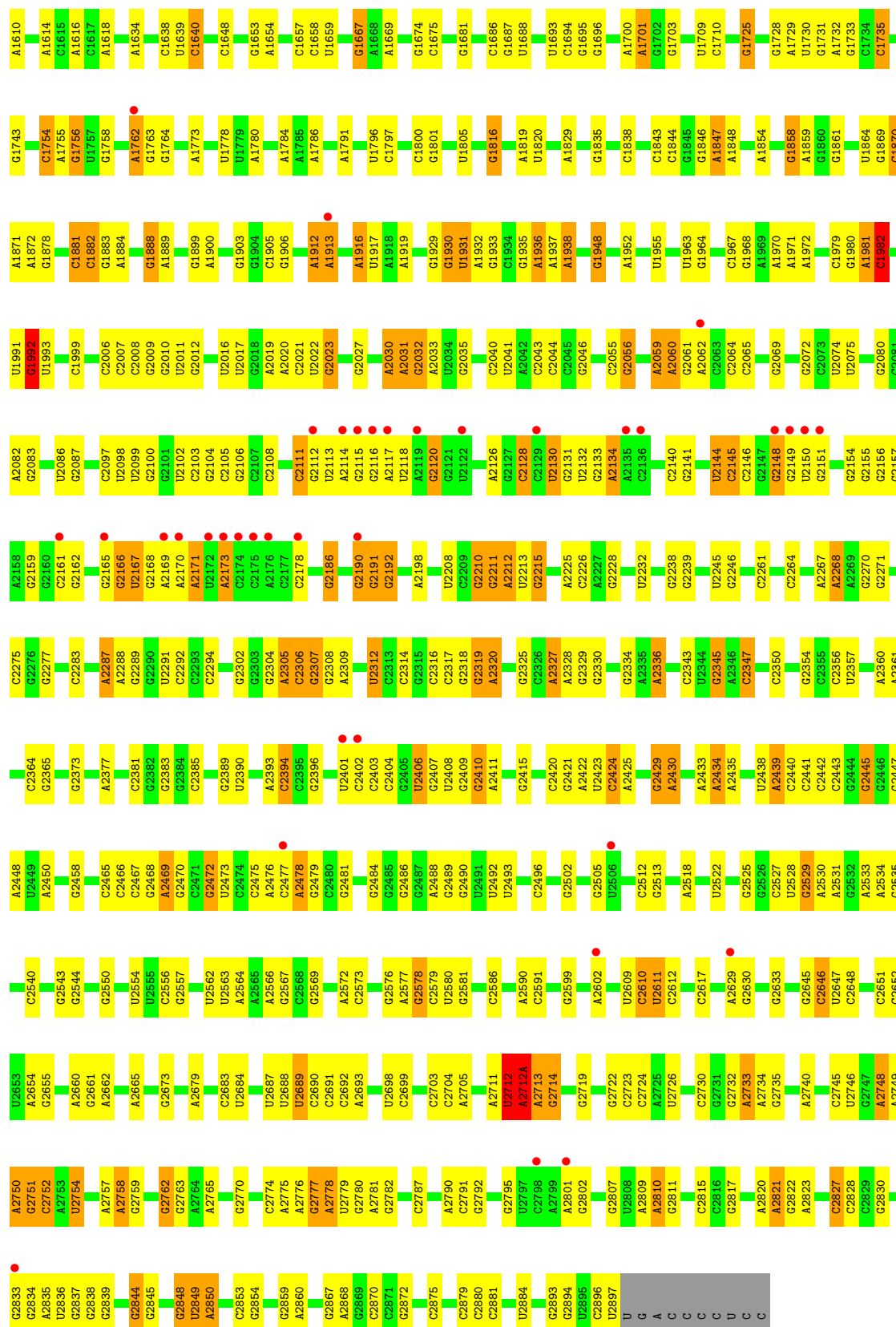


• Molecule 25: 23S rRNA

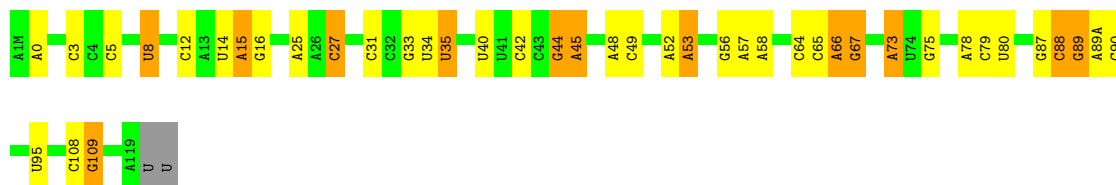
Chain YA: 2% 60% 31% 7%



G1519	G1522	G1526	G1527	A1528	G1534	A1536	C1537	U1541	G1542	A1543	C1544	A1545	C1547	C1548	C1549	A1554	A1558	G1559	A1566	A1567	G1568	A1569	A1570	G1573	C1574	C1575	U1576	U1577	U1578	A1579	A1580	G1581	C1585	A1586	A1587	C1588	G1591	C1592	G1595	C1598	C1599	A1608	A1609									
G1417	G1418	A1419	U1420	G1421	A1427	C1428	C1432	U1433	C1437	G1444	A1444A	C1445	G1448	A1449	G1449A	C1450	C1451	A1453	U1454	G1455	C1458	G1459	A1460	G1461	C1467	A1471	G1475	U1482	G1483	G1484	G1485	G1488	U1489	A1490	C1493	A1496	C1502	C1505	C1509	A1510	U1514	C1515										
C1297	U1300	A1301	A1302	G1309	C1314	U1315	U1316	A1317	C1318	G1319	A1322	G1328	U1329	C1330	C1333	A1336	G1339	U1340	U1341	C1345	U1352	G1358	A1359	A1360	A1365	G1368	A1379	G1380	A1384	G1385	U1391	G1400	G1401	C1402	C1403	C1404	U1405	U1406	C1407	C1408	U1514	C1515										
G1203	A1204	U1205	G1206	C1207	C1217	C1218	G1219	A1220	C1225	G1226	C1230	G1231	G1239	U1240	A1241	G1245	A1246	A1247	G1250	U1251	G1252	A1253	U1254	U1255	G1256	A1262	U1263	G1264	A1265	G1266	C1270	U1271	A1272	U1273	A1274	A1275	A1278	G1279	G1280	U1281	U1282	G1285	C1289	C1290	G1291	C1292	C1293					
G1110	A1111	G1112	U1113	G1114	G1115	C1116	G1117	G1120	C1121	G1122	G1125	A1126	A1127	A1128	U1130	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	A1143	A1155	U1165	C1166	U1167	G1168	G1169	G1170	G1171	G1173	A1174	U1175	A1177	C1178	C1179	C1180	G1183	U1188	A1189	G1190	G1191	G1195	C1201	C1202					
G1030	G1031	A1032	U1033	G1034	U1035	G1036	G1042	C1043	G1044	A1045	A1046	G1047	A1048	C1049	A1050	C1052	C1053	A1054	G1055	G1056	U1060	U1061	G1062	G1063	U1066	A1070	A1073	U1074	C1075	C1076	A1077	A1085	A1086	G1087	A1088	G1089	G1093	U1094	A1095	A1096	U1097	A1098	C1099	C1100	U1101	C1102	U1105	G1106	C1109			
A933	G934	A941	A945	G946	A953	G956	A957	U958	A959	A960	C961	U969	C970	C971	G972	A973	G974	C974A	A980	A983	G989	A990	C991	G992	G993	A996	G997	C998	U999	A1000	C1007	C1008	A1009	A1010	U1011	U1012	C1013	C1018	A1021	G1022	U1023	G1024	G1025	U1026	A1027	A1028	A1029					
G831	G832	U833	G848	C856	C857	U858	U859	U860	A861	G862	A866	C876	U877	A878	G879	G880	G881	G882	G883	C884	C885	C886	A887	C888	C889	A890	G892	C893	C894	U895	A896	C897	A901	C902	C903	G906	U907	A910	A911	C914	C915	G916	A918	U919	G919	U922	G928	C932				
G725	G726	C730	G738	G739	A746	A752	C753	C754	C755	C756	A761	A764	G768	G771	C772	U773	A774	G775	G776	A782	A783	G785	A788	A789	G792	A793	C796	C797	G798	G805	C806	U807	C812	C817	G818	U819	C825	U826	U827	U828												
C652	A653	A	C	G	G	C	C	C	C	C	A	C	G	G	C	C	C	C	C	C	C	A	A654V	A655	G656	U657	C658	C659	G660	G663	A784	C669	A670	C673	G674	A685	G686	C687	U688	C691	C692	G704	A705	A706	G707	C708	U709	G710	G717	A722	G723	U724
C537	G556	G561	U562	G563	G570	A571	A572	G573	C574	A575	U576	G577	A586	C587	U588	C589	A590	G593	A603	G604	C605	U606	U607	A608	A609	G609A	U614	G615	A616	G617	C624	G625	U626	A627	G630	A633	C634	C635	G636	A637	G642	A645	A646	G647	G651							
G298	U306	G307	G308	G309	A310	A311	G312	A320	A324	G329	C330	U331	A332	C335	A340	C342	G341	A345	A346	U350	G351	G352	G356	G361	U362	G363	A363A	G363B	G363C	U363E	A363F	C364	G386	G389	C392	G396	G407	G408	A409	G410	G411	A412	C413	C414								
G242	G247	G248	C249	G250	A251	G252	C253	G254	G261	A262	C263	A265	A270B	C270C	C270D	U270E	U270F	C270G	C270K	U270L	U270M	U270N	G270O	G270P	C270Q	G270R	G270S	U270T	C270U	U270Z	C271A	G271B	U271C	G271	G272	C273D	U273E	C273F	G274	C277	A278	C279	A283	C287	C288	A289	G290	C297				

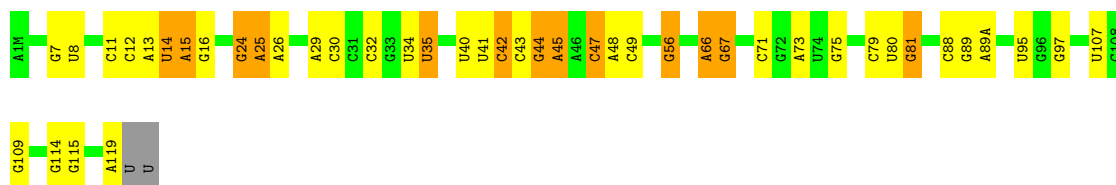


Chain RB:  65% 23% 10% .



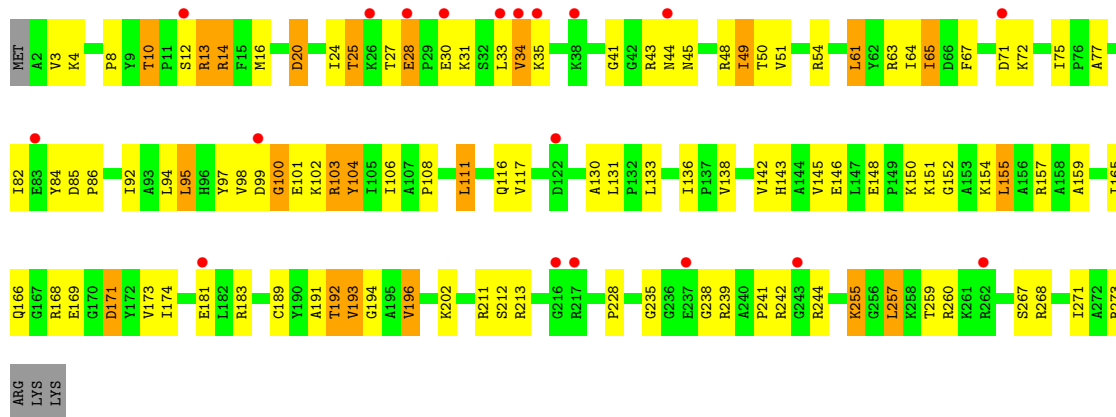
• Molecule 26: 5S rRNA

Chain YB:  63% 25% 10% .



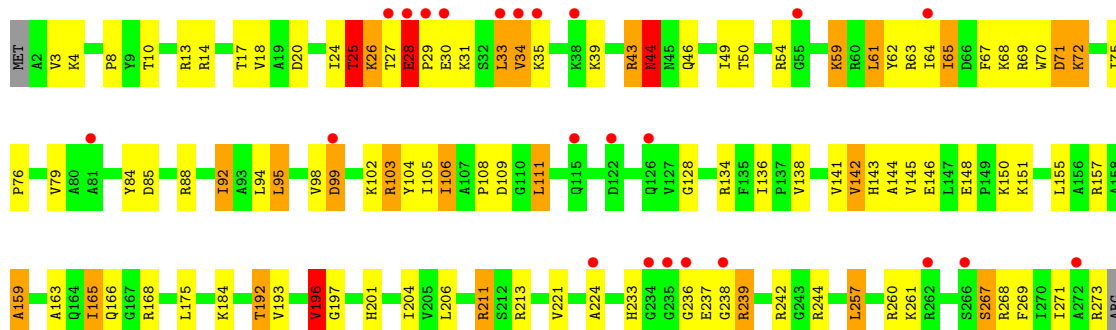
• Molecule 27: 50S ribosomal protein L2

Chain RD:  7% 60% 31% 8% .



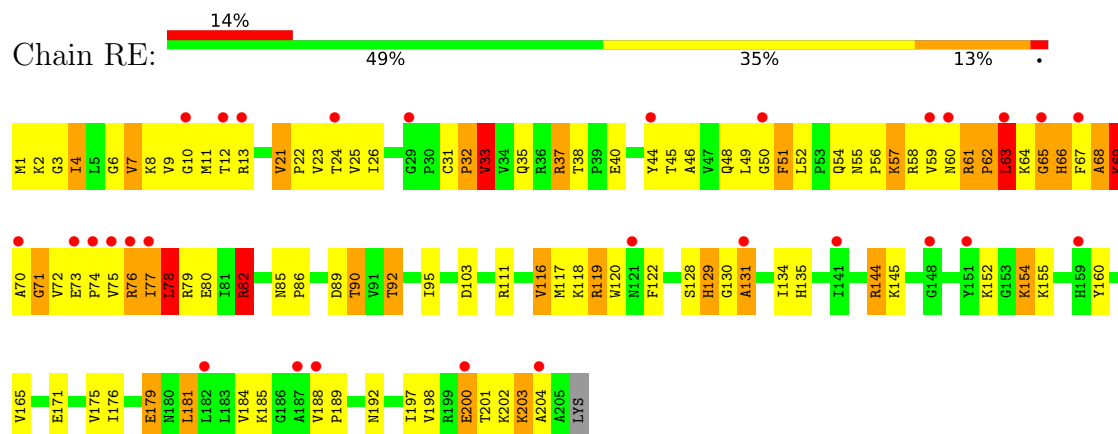
• Molecule 27: 50S ribosomal protein L2

Chain YD:  8% 60% 29% 8% ..

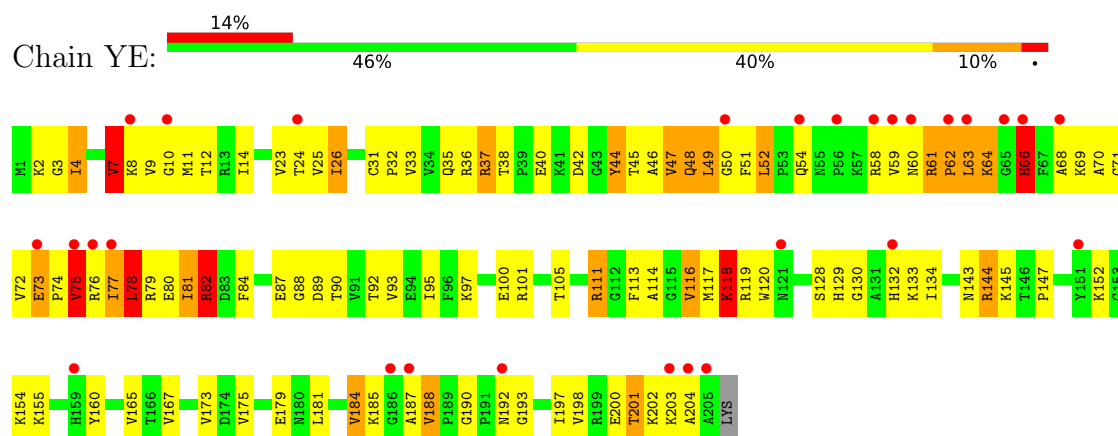


LYS
LYS

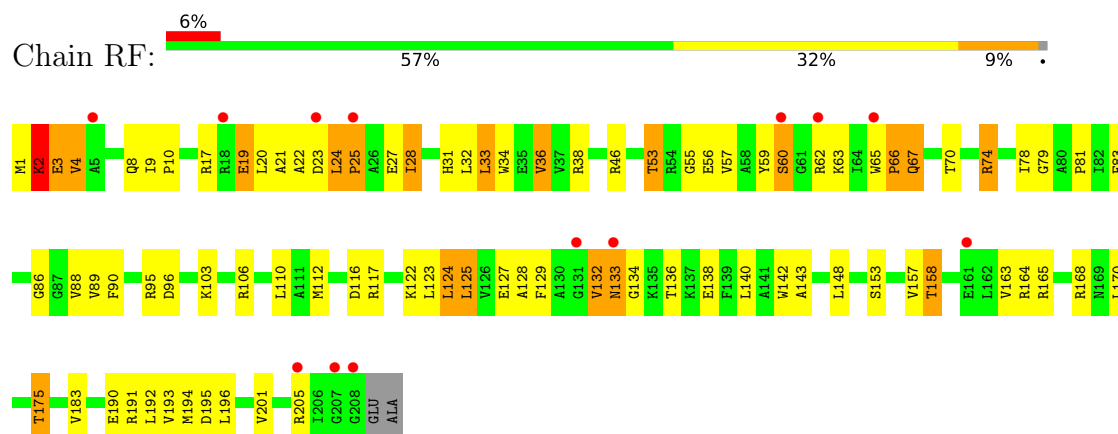
- Molecule 28: 50S ribosomal protein L3



- Molecule 28: 50S ribosomal protein L3

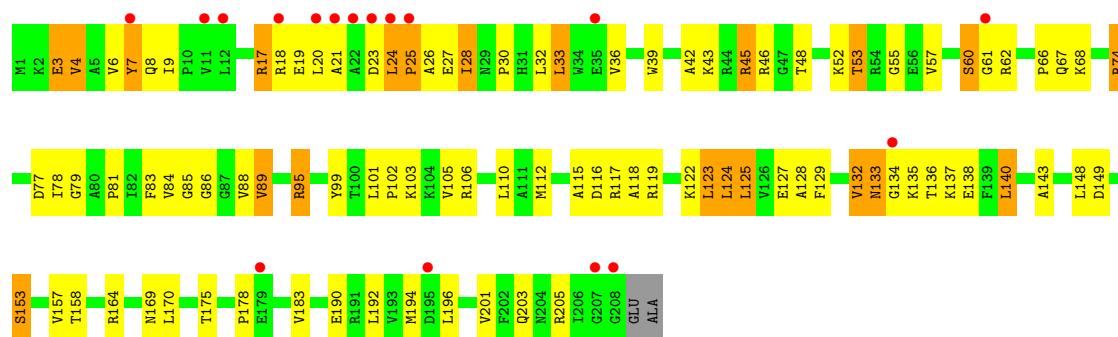


- Molecule 29: 50S ribosomal protein L4

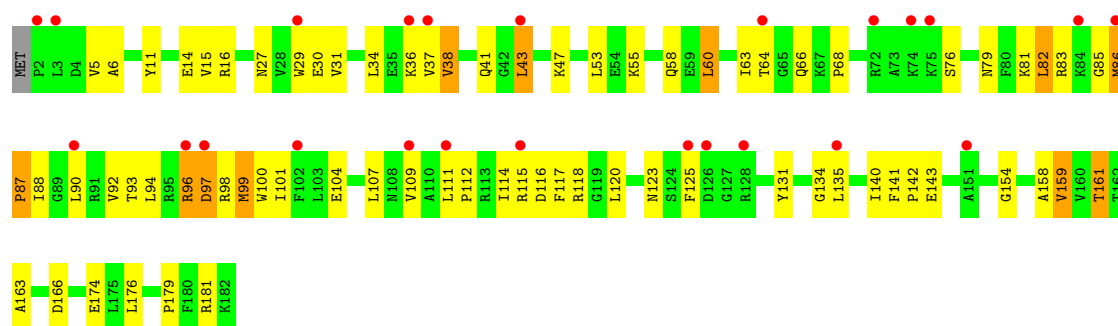


- Molecule 29: 50S ribosomal protein L4

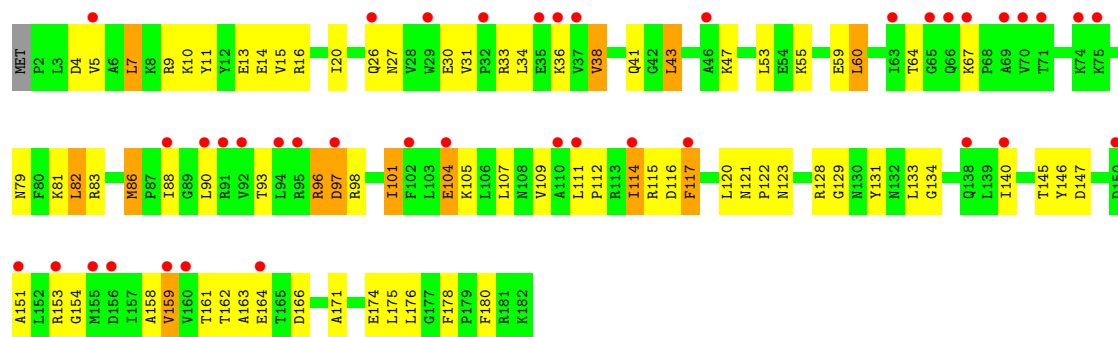




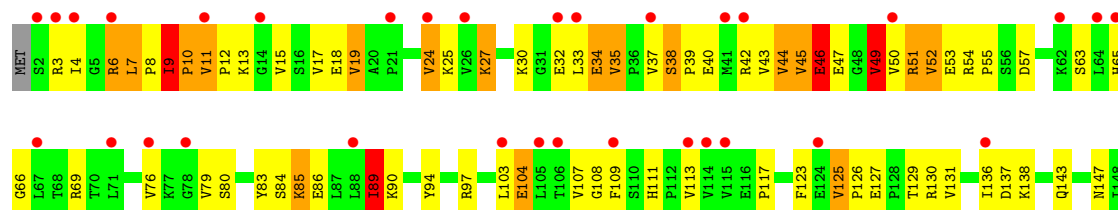
• Molecule 30: 50S ribosomal protein L5

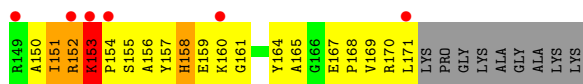


• Molecule 30: 50S ribosomal protein L5

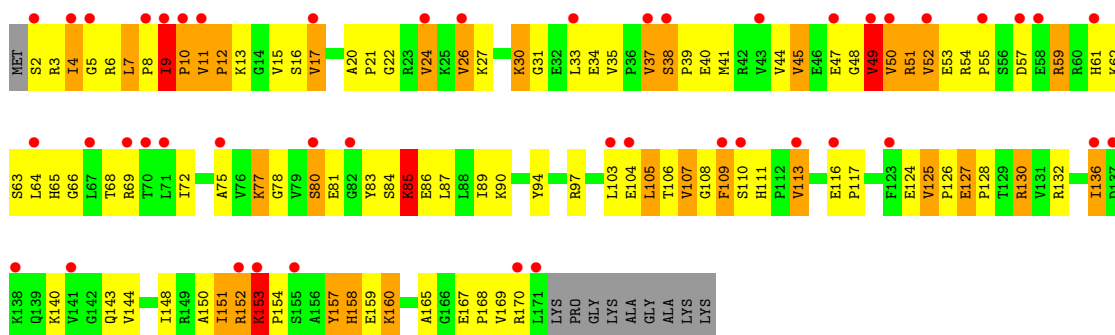


• Molecule 31: 50S ribosomal protein L6

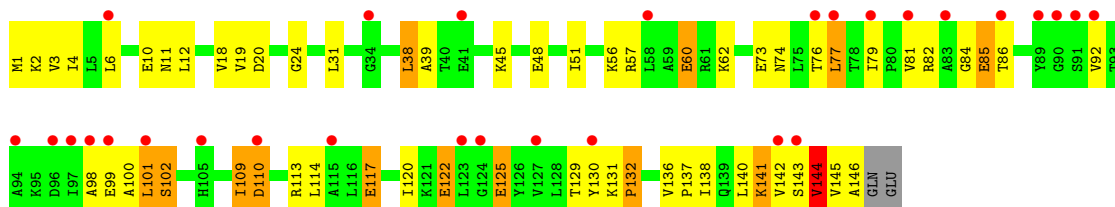




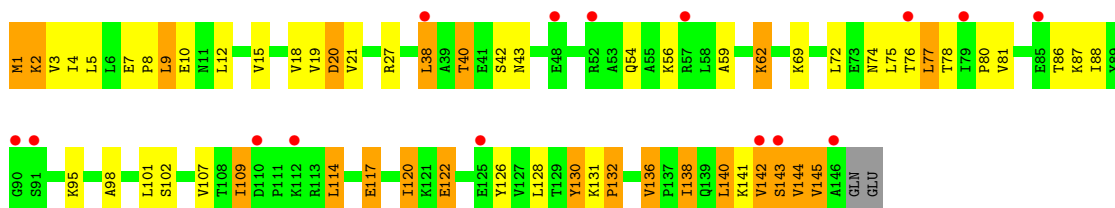
• Molecule 31: 50S ribosomal protein L6



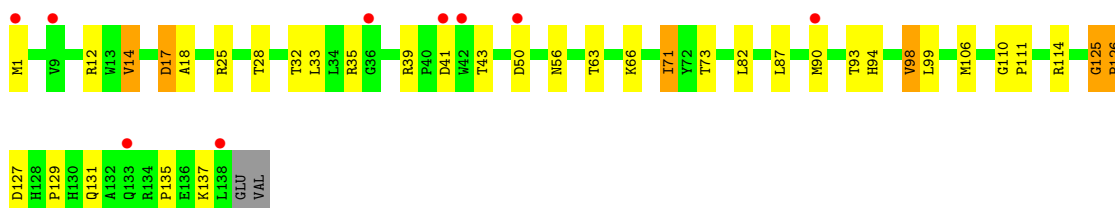
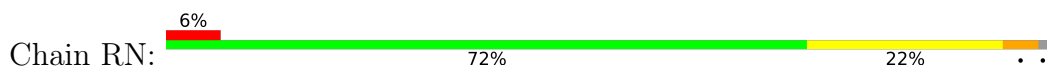
• Molecule 32: 50S ribosomal protein L9



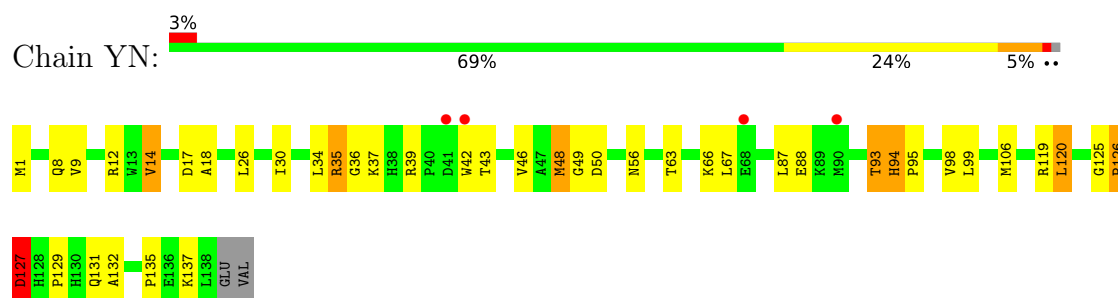
• Molecule 32: 50S ribosomal protein L9



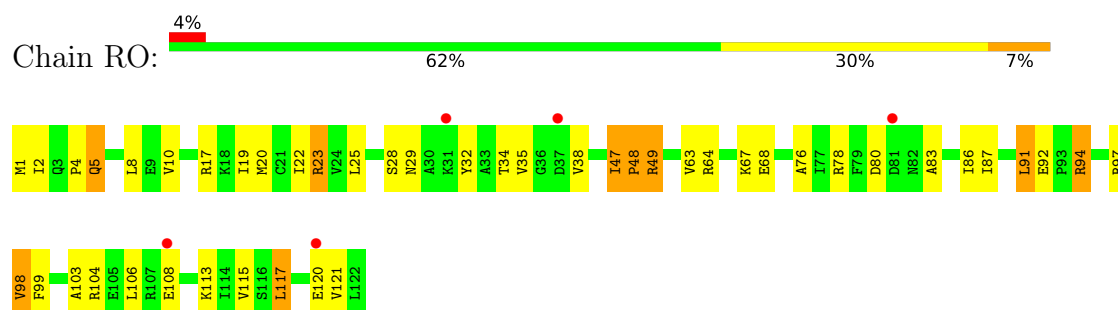
• Molecule 33: 50S ribosomal protein L13



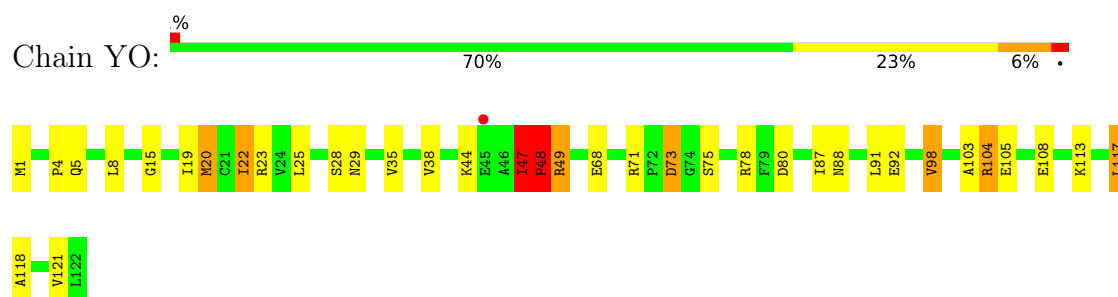
- Molecule 33: 50S ribosomal protein L13



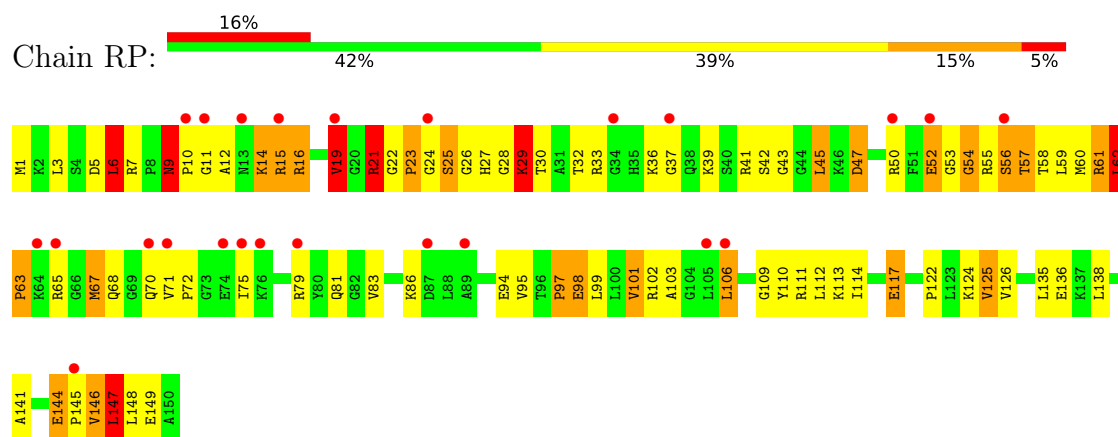
- Molecule 34: 50S ribosomal protein L14



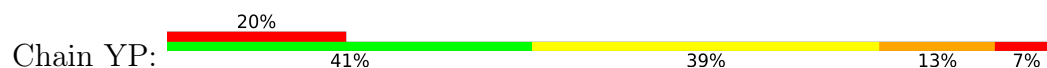
- Molecule 34: 50S ribosomal protein L14

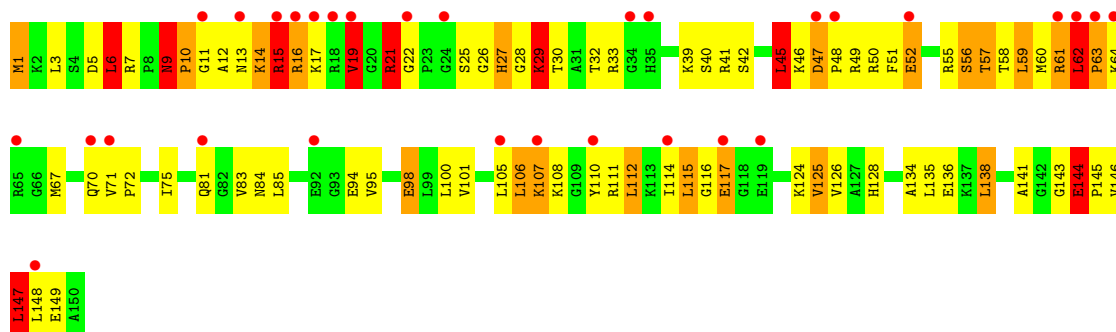


- Molecule 35: 50S ribosomal protein L15

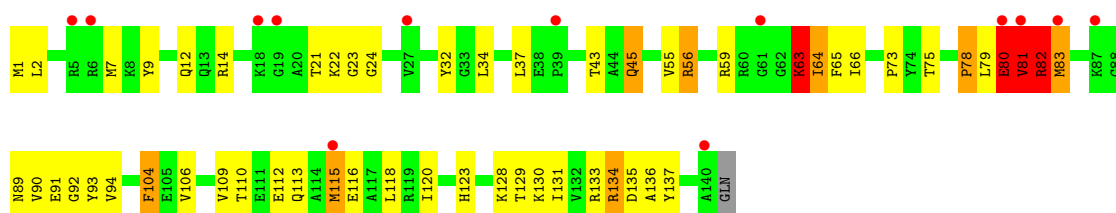


- Molecule 35: 50S ribosomal protein L15

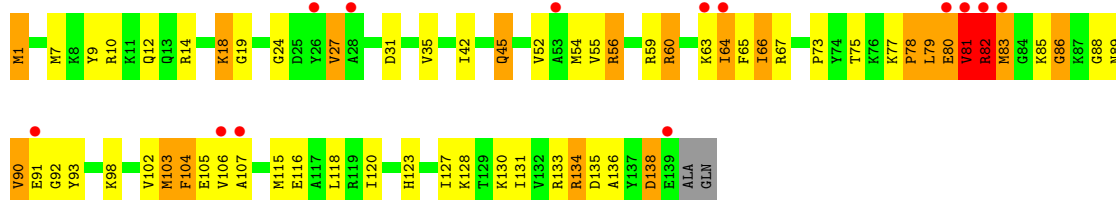




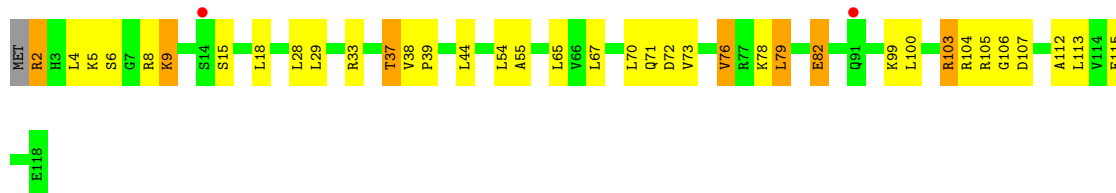
- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L17



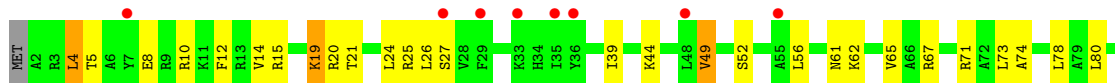
- Molecule 37: 50S ribosomal protein L17





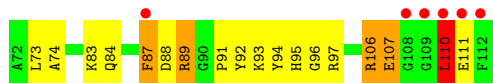
• Molecule 38: 50S ribosomal protein L18

Chain RS: 11% 59% 33% 5% ..



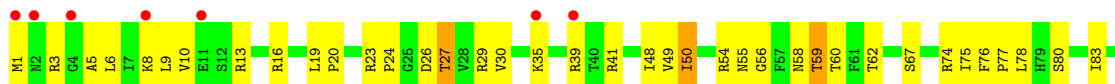
• Molecule 38: 50S ribosomal protein L18

Chain YS: 17% 54% 37% 8% ..



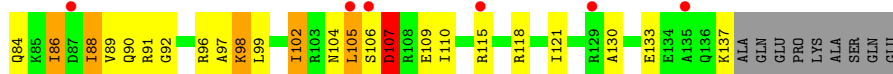
• Molecule 39: 50S ribosomal protein L19

Chain RT: 11% 50% 40% .. 6%



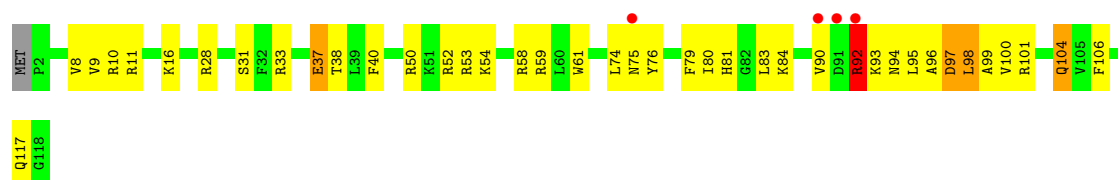
• Molecule 39: 50S ribosomal protein L19

Chain YT: 12% 53% 33% 7% • 6%

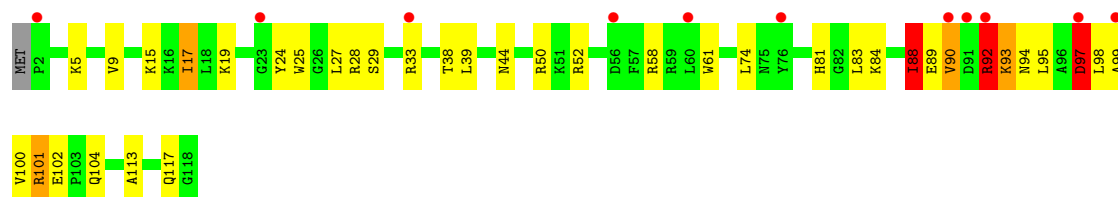


• Molecule 40: 50S ribosomal protein L20

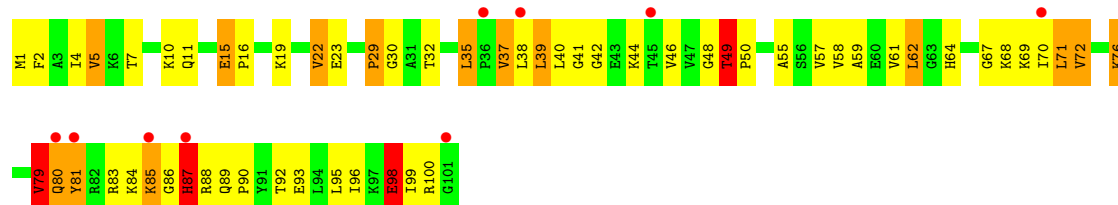
Chain RU: 3% 65% 30% ..



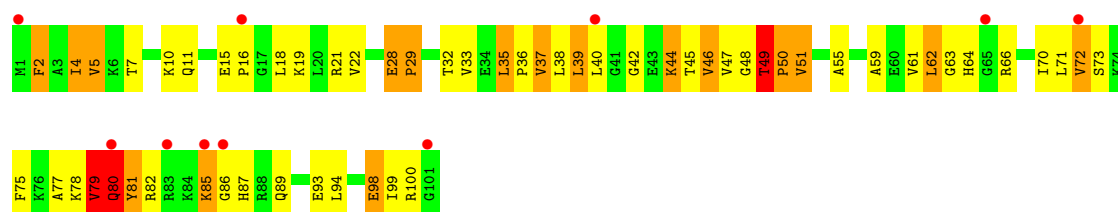
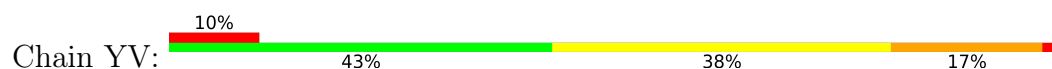
- Molecule 40: 50S ribosomal protein L20



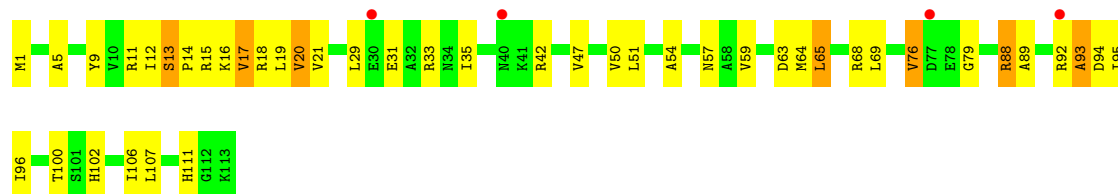
- Molecule 41: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L21

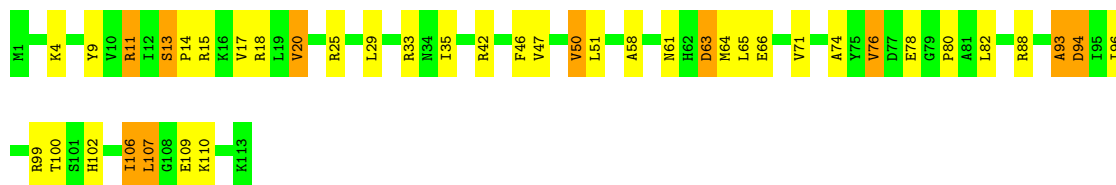


- Molecule 42: 50S ribosomal protein L22



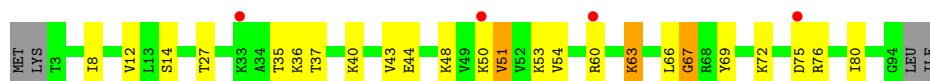
- Molecule 42: 50S ribosomal protein L22

Chain YW: 



- Molecule 43: 50S ribosomal protein L23

Chain RX: 



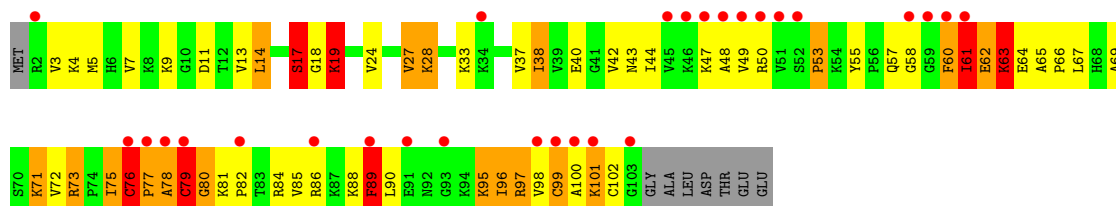
- Molecule 43: 50S ribosomal protein L23

Chain YX: 

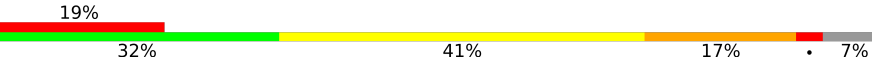


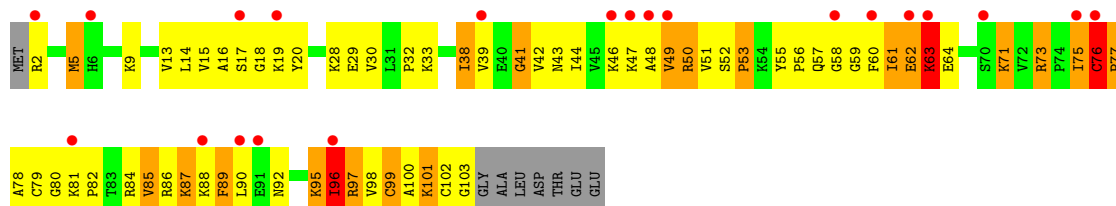
- Molecule 44: 50S ribosomal protein L24

Chain RY: 

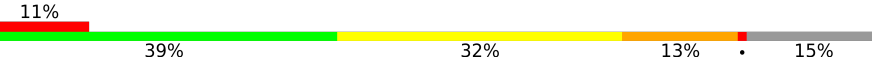


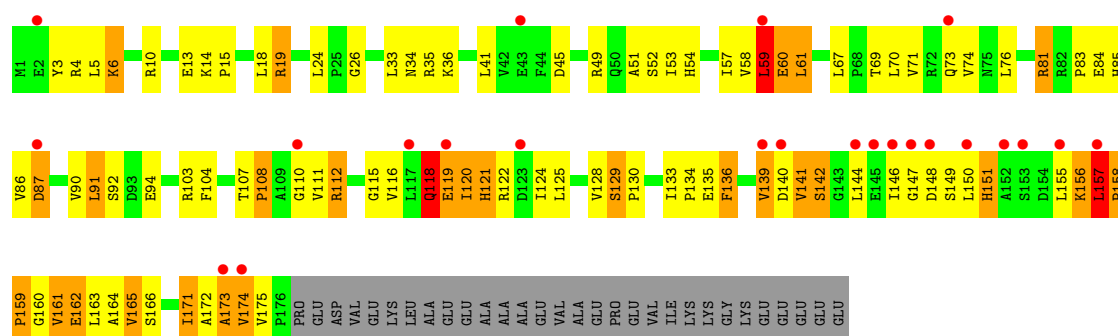
- Molecule 44: 50S ribosomal protein L24

Chain YY: 

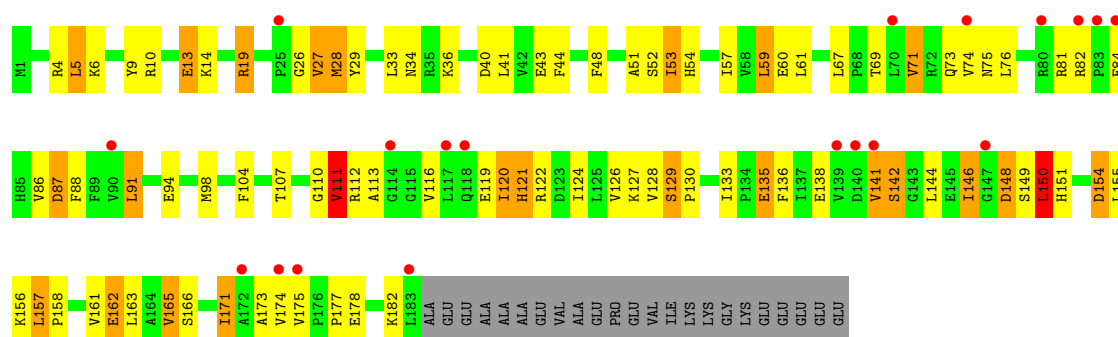


- Molecule 45: 50S ribosomal protein L25

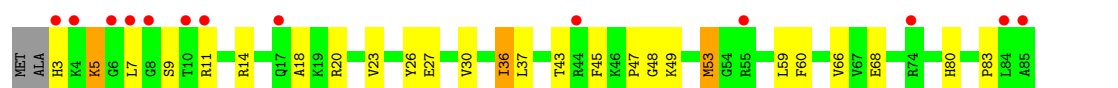
Chain RZ: 



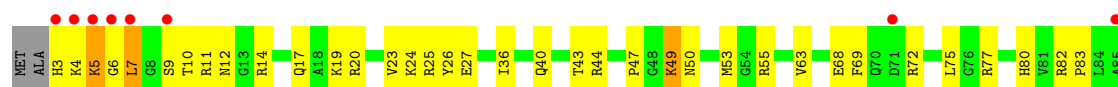
• Molecule 45: 50S ribosomal protein L25



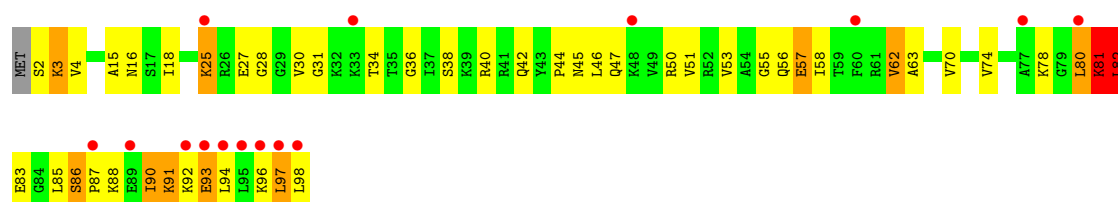
• Molecule 46: 50S ribosomal protein L27



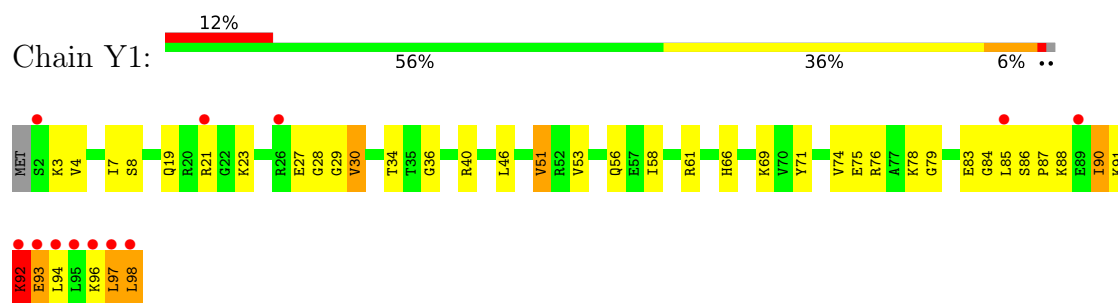
• Molecule 46: 50S ribosomal protein L27



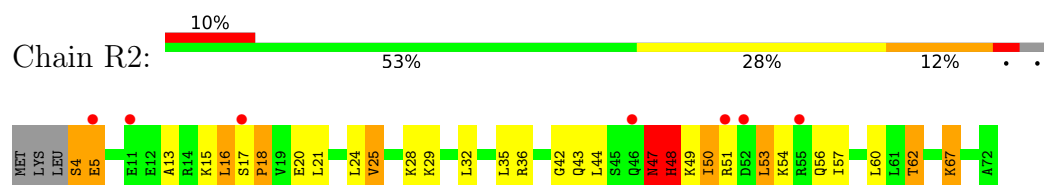
• Molecule 47: 50S ribosomal protein L28



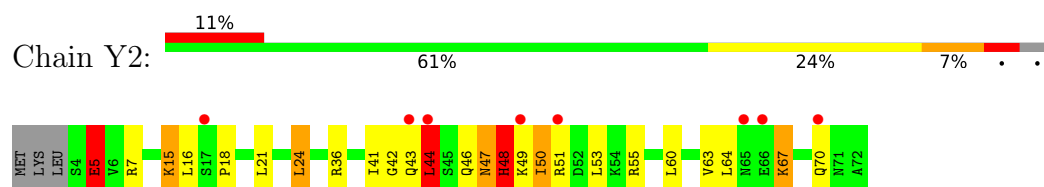
- Molecule 47: 50S ribosomal protein L28



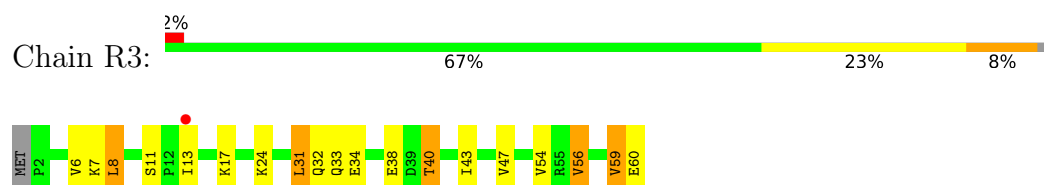
- Molecule 48: 50S ribosomal protein L29



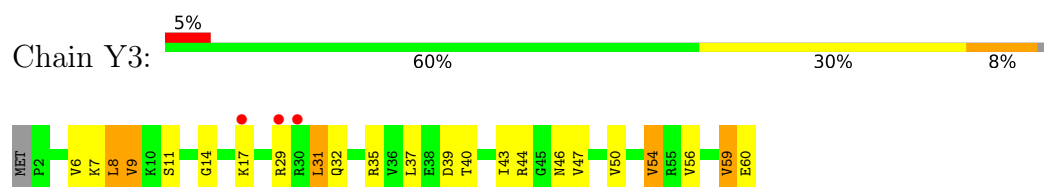
- Molecule 48: 50S ribosomal protein L29



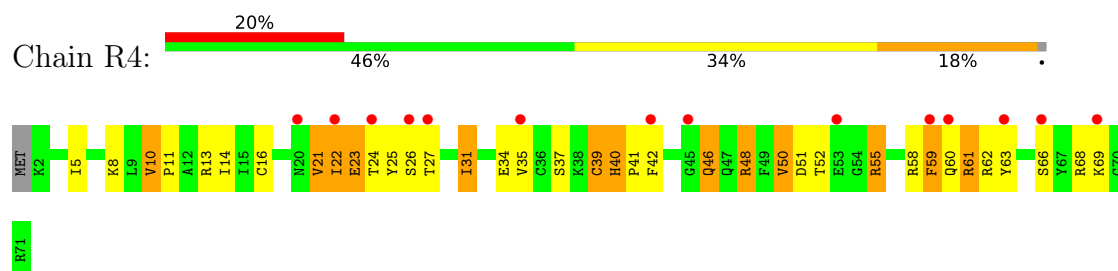
- Molecule 49: 50S ribosomal protein L30



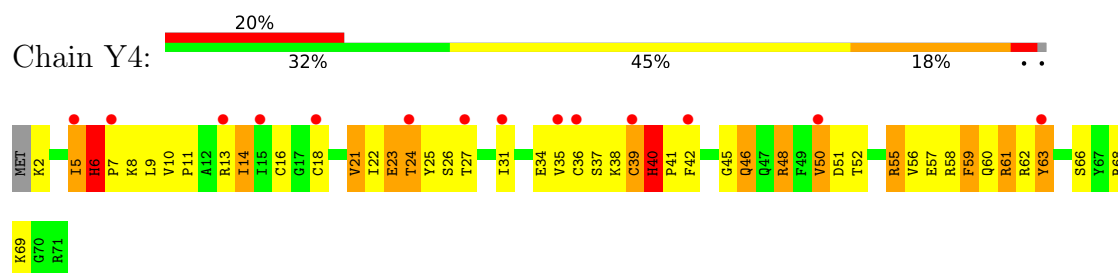
- Molecule 49: 50S ribosomal protein L30



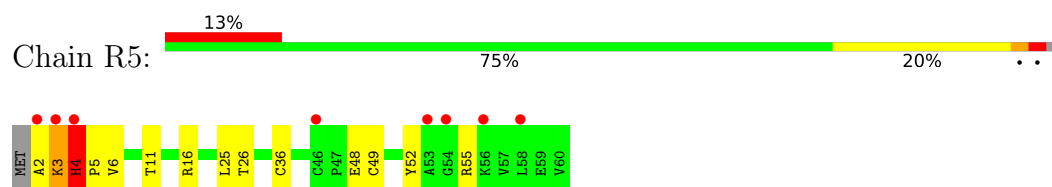
- Molecule 50: 50S ribosomal protein L31



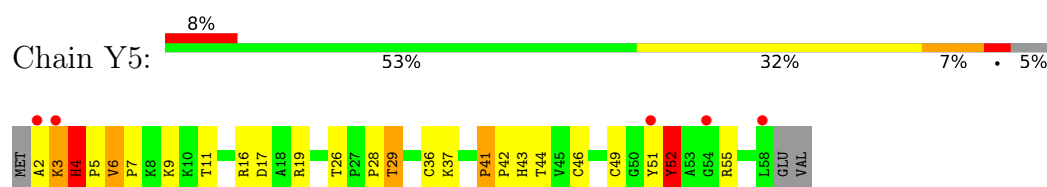
● Molecule 50: 50S ribosomal protein L31



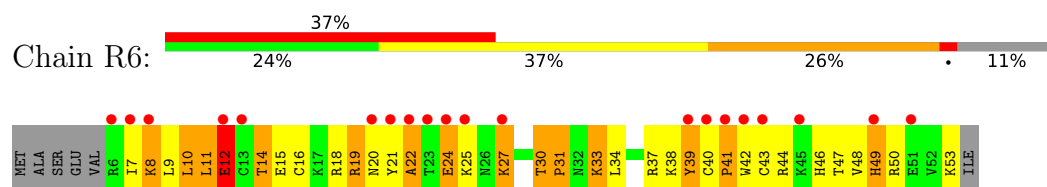
● Molecule 51: 50S ribosomal protein L32



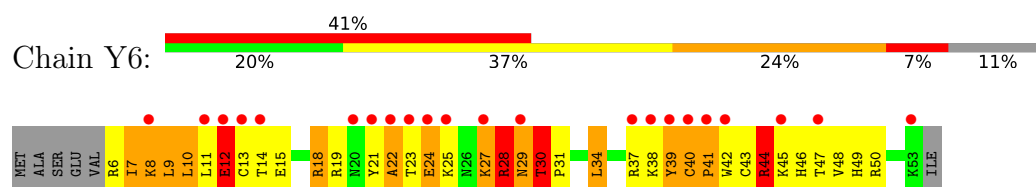
● Molecule 51: 50S ribosomal protein L32



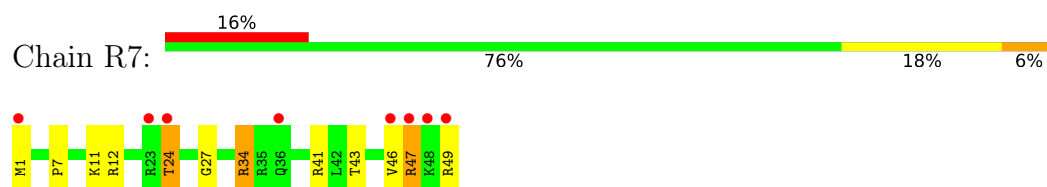
● Molecule 52: 50S ribosomal protein L33



● Molecule 52: 50S ribosomal protein L33



● Molecule 53: 50S ribosomal protein L34

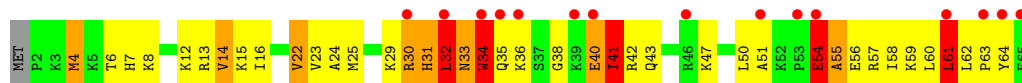


● Molecule 53: 50S ribosomal protein L34

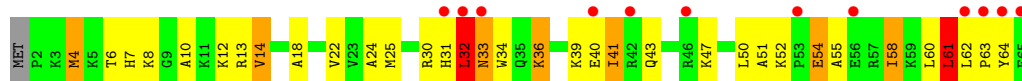




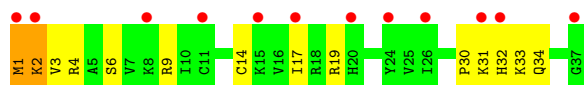
- Molecule 54: 50S ribosomal protein L35



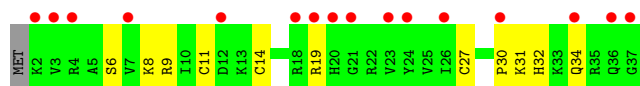
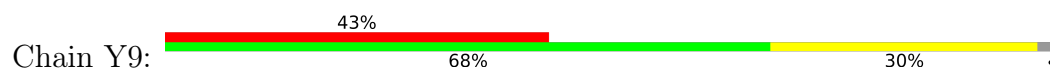
- Molecule 54: 50S ribosomal protein L35



- 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) 94.2 (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 0.210 , 0.239	Depositor DCC
R_{free} test set	38567 reflections (4.39%)	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 , 85.5	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	0.92	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, MG, A3P

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	0.18	0/36346	0.37	0/56724
1	XA	0.18	0/36276	0.37	6/56615 (0.0%)
2	QB	0.33	0/1950	0.81	2/2630 (0.1%)
2	XB	0.33	0/1950	0.82	2/2630 (0.1%)
3	QC	0.33	0/1636	0.77	0/2205
3	XC	0.36	0/1636	0.79	0/2205
4	QD	0.36	0/1733	0.85	2/2318 (0.1%)
4	XD	0.36	0/1733	0.83	3/2318 (0.1%)
5	QE	0.36	0/1195	0.86	0/1609
5	XE	0.41	0/1195	0.80	0/1609
6	QF	0.31	0/856	0.74	0/1154
6	XF	0.33	0/856	0.76	0/1154
7	QG	0.33	0/1276	0.80	2/1709 (0.1%)
7	XG	0.36	0/1276	0.85	2/1709 (0.1%)
8	QH	0.33	0/1136	0.82	0/1527
8	XH	0.36	0/1136	0.81	2/1527 (0.1%)
9	QI	0.34	0/1037	0.83	1/1389 (0.1%)
9	XI	0.35	0/1037	0.83	2/1389 (0.1%)
10	QJ	0.31	0/814	0.77	0/1095
10	XJ	0.32	0/814	0.78	0/1095
11	QK	0.42	0/916	0.85	2/1234 (0.2%)
11	XK	0.38	0/916	0.86	1/1234 (0.1%)
12	QL	0.39	0/991	0.88	2/1327 (0.2%)
12	XL	0.43	1/991 (0.1%)	0.92	8/1327 (0.6%)
13	QM	0.36	0/947	0.84	0/1270
13	XM	0.35	0/947	0.85	0/1270
14	QN	0.32	0/501	0.80	0/664
14	XN	0.35	0/501	0.79	0/664
15	QO	0.31	0/745	0.70	0/992
15	XO	0.35	0/745	0.75	0/992
16	QP	0.33	0/721	0.75	0/970
16	XP	0.34	0/721	0.75	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.32	0/847	0.79	0/1131
17	XQ	0.34	0/847	0.74	0/1131
18	QR	0.33	0/590	0.78	0/782
18	XR	0.33	0/590	0.78	0/782
19	QS	0.37	0/670	0.86	1/901 (0.1%)
19	XS	0.41	0/670	0.88	0/901
20	QT	0.35	0/765	0.80	1/1007 (0.1%)
20	XT	0.34	0/765	0.80	1/1007 (0.1%)
21	QU	0.28	0/221	0.77	0/288
21	XU	0.29	0/221	0.74	0/288
22	QV	0.17	0/1832	0.31	0/2855
22	QW	0.15	0/1832	0.32	0/2855
22	XV	0.18	0/1832	0.32	0/2855
22	XW	0.12	0/1832	0.28	0/2855
23	QX	0.27	0/420	0.48	0/654
23	XX	0.25	0/420	0.50	0/654
24	QY	0.46	0/773	0.75	1/1043 (0.1%)
24	XY	0.45	0/773	0.73	1/1043 (0.1%)
25	RA	0.22	0/69742	0.40	5/108874 (0.0%)
25	YA	0.22	0/69356	0.40	4/108271 (0.0%)
26	RB	0.16	0/2928	0.35	0/4568
26	YB	0.17	0/2928	0.34	0/4568
27	RD	0.43	0/2165	0.88	4/2919 (0.1%)
27	YD	0.47	0/2165	0.93	5/2919 (0.2%)
28	RE	0.41	0/1601	0.88	5/2160 (0.2%)
28	YE	0.48	0/1601	0.96	6/2160 (0.3%)
29	RF	0.44	0/1662	0.92	4/2249 (0.2%)
29	YF	0.41	0/1662	0.91	2/2249 (0.1%)
30	RG	0.34	0/1499	0.78	2/2016 (0.1%)
30	YG	0.35	0/1499	0.78	0/2016
31	RH	0.41	0/1332	1.06	10/1802 (0.6%)
31	YH	0.42	0/1332	1.01	6/1802 (0.3%)
32	RI	0.35	0/1151	0.83	1/1558 (0.1%)
32	YI	0.40	0/1151	0.93	5/1558 (0.3%)
33	RN	0.36	0/1131	0.85	3/1525 (0.2%)
33	YN	0.38	0/1131	0.87	2/1525 (0.1%)
34	RO	0.39	0/943	0.87	2/1269 (0.2%)
34	YO	0.42	0/943	0.87	2/1269 (0.2%)
35	RP	0.46	0/1162	0.98	6/1544 (0.4%)
35	YP	0.48	0/1162	0.99	4/1544 (0.3%)
36	RQ	0.45	0/1133	0.88	1/1515 (0.1%)
36	YQ	0.46	0/1128	0.91	2/1508 (0.1%)
37	RR	0.39	0/974	0.80	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.42	0/974	0.80	1/1302 (0.1%)
38	RS	0.32	0/892	0.77	1/1187 (0.1%)
38	YS	0.36	0/892	0.83	1/1187 (0.1%)
39	RT	0.35	0/1155	0.78	2/1542 (0.1%)
39	YT	0.39	0/1155	0.81	0/1542
40	RU	0.42	0/982	0.86	3/1306 (0.2%)
40	YU	0.41	0/982	0.91	4/1306 (0.3%)
41	RV	0.56	0/790	1.06	6/1057 (0.6%)
41	YV	0.52	0/790	1.06	7/1057 (0.7%)
42	RW	0.43	0/911	0.84	3/1220 (0.2%)
42	YW	0.42	0/911	0.82	2/1220 (0.2%)
43	RX	0.40	0/739	0.85	0/993
43	YX	0.45	0/739	0.89	1/993 (0.1%)
44	RY	0.45	0/798	0.95	0/1064
44	YY	0.47	0/798	0.99	2/1064 (0.2%)
45	RZ	0.49	3/1435 (0.2%)	0.97	5/1947 (0.3%)
45	YZ	0.44	0/1493	0.96	6/2026 (0.3%)
46	R0	0.40	0/666	0.85	0/885
46	Y0	0.40	0/666	0.87	1/885 (0.1%)
47	R1	0.42	0/770	0.85	0/1022
47	Y1	0.49	0/770	0.84	0/1022
48	R2	0.34	0/583	0.92	1/771 (0.1%)
48	Y2	0.41	0/583	0.90	1/771 (0.1%)
49	R3	0.37	0/474	0.77	0/635
49	Y3	0.37	0/474	0.80	0/635
50	R4	0.34	0/586	0.77	0/785
50	Y4	0.37	0/586	0.85	1/785 (0.1%)
51	R5	0.44	0/473	1.07	2/639 (0.3%)
51	Y5	0.67	3/456 (0.7%)	1.15	9/617 (1.5%)
52	R6	0.41	0/424	0.99	2/565 (0.4%)
52	Y6	0.57	0/424	1.15	3/565 (0.5%)
53	R7	0.42	0/438	0.80	0/575
53	Y7	0.44	0/438	0.83	2/575 (0.3%)
54	R8	0.56	0/525	1.13	5/691 (0.7%)
54	Y8	0.54	0/525	1.13	3/691 (0.4%)
55	R9	0.33	0/310	0.72	0/407
55	Y9	0.31	0/301	0.70	0/397
All	All	0.28	7/321819 (0.0%)	0.56	197/481178 (0.0%)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	RZ	157	LEU	C-N	6.41	1.41	1.33
51	Y5	4	HIS	C-N	6.37	1.41	1.33
51	Y5	6	VAL	C-N	5.54	1.41	1.33
45	RZ	158	PRO	N-CD	5.45	1.55	1.47
51	Y5	7	PRO	N-CD	5.38	1.55	1.47

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Y8	41	ILE	N-CA-C	-12.64	101.70	113.71
31	YH	9	ILE	C-N-CD	-11.91	94.41	120.60
54	R8	41	ILE	N-CA-C	-11.85	102.45	113.71
36	YQ	82	ARG	N-CA-C	11.18	124.86	109.54
31	RH	9	ILE	C-N-CD	-10.87	96.68	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32472	0	16392	434	0
1	XA	32409	0	16360	369	0
2	QB	1915	0	1969	58	0
2	XB	1915	0	1969	63	0
3	QC	1612	0	1677	48	0
3	XC	1612	0	1677	39	0
4	QD	1703	0	1766	56	0
4	XD	1703	0	1766	36	0
5	QE	1178	0	1234	41	0
5	XE	1178	0	1234	24	0
6	QF	843	0	857	18	0
6	XF	843	0	857	30	0
7	QG	1257	0	1296	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	36	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	43	0
11	QK	901	0	926	26	0
11	XK	901	0	926	21	0
12	QL	975	0	1062	29	0
12	XL	975	0	1062	25	0
13	QM	937	0	995	29	0
13	XM	937	0	995	55	0
14	QN	492	0	530	20	0
14	XN	492	0	529	12	0
15	QO	734	0	771	16	0
15	XO	734	0	771	17	0
16	QP	705	0	725	16	0
16	XP	705	0	725	10	0
17	QQ	834	0	904	15	0
17	XQ	834	0	904	18	0
18	QR	585	0	657	10	0
18	XR	585	0	657	19	0
19	QS	656	0	678	47	0
19	XS	656	0	678	45	0
20	QT	763	0	861	24	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	27	0
23	QX	399	0	196	11	0
23	XX	399	0	196	17	0
24	QY	756	0	749	20	0
24	XY	756	0	749	19	0
25	RA	62269	0	31391	636	0
25	YA	61924	0	31215	620	0
26	RB	2617	0	1328	26	0
26	YB	2617	0	1328	30	0
27	RD	2115	0	2195	67	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	92	0
28	YE	1568	0	1634	73	0
29	RF	1627	0	1680	62	0
29	YF	1627	0	1680	58	0
30	RG	1474	0	1535	51	0
30	YG	1474	0	1535	46	0
31	RH	1307	0	1382	75	0
31	YH	1307	0	1382	71	0
32	RI	1136	0	1223	39	0
32	YI	1136	0	1223	68	0
33	RN	1104	0	1180	16	0
33	YN	1104	0	1180	22	0
34	RO	933	0	996	35	0
34	YO	933	0	996	26	0
35	RP	1145	0	1228	92	0
35	YP	1145	0	1228	85	0
36	RQ	1112	0	1170	39	0
36	YQ	1107	0	1165	42	0
37	RR	960	0	1021	16	0
37	YR	960	0	1021	24	0
38	RS	882	0	943	28	0
38	YS	882	0	943	31	0
39	RT	1141	0	1202	45	0
39	YT	1141	0	1202	39	0
40	RU	964	0	1022	37	0
40	YU	964	0	1022	31	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	14	0
43	YX	725	0	778	20	0
44	RY	785	0	878	64	0
44	YY	785	0	878	51	0
45	RZ	1404	0	1437	94	0
45	YZ	1461	0	1493	51	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	26	0
48	R2	581	0	629	20	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	11	0
49	Y3	469	0	518	10	0
50	R4	573	0	565	22	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	28	0
52	Y6	417	0	441	43	0
53	R7	430	0	480	6	0
53	Y7	430	0	480	11	0
54	R8	517	0	582	39	0
54	Y8	517	0	582	34	0
55	R9	307	0	338	14	0
55	Y9	298	0	326	9	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	4968	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 4968 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	5
2	XB	234/256 (91%)	189 (81%)	27 (12%)	18 (8%)	1	5
3	QC	204/239 (85%)	162 (79%)	26 (13%)	16 (8%)	1	5
3	XC	204/239 (85%)	160 (78%)	31 (15%)	13 (6%)	1	8
4	QD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	1	10
4	XD	206/209 (99%)	168 (82%)	22 (11%)	16 (8%)	1	5
5	QE	152/162 (94%)	136 (90%)	11 (7%)	5 (3%)	3	19
5	XE	152/162 (94%)	137 (90%)	9 (6%)	6 (4%)	2	16
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%)	4	23
7	XG	153/156 (98%)	133 (87%)	15 (10%)	5 (3%)	3	19
8	QH	136/138 (99%)	126 (93%)	7 (5%)	3 (2%)	5	26
8	XH	136/138 (99%)	123 (90%)	10 (7%)	3 (2%)	5	26
9	QI	126/128 (98%)	94 (75%)	24 (19%)	8 (6%)	1	8
9	XI	126/128 (98%)	96 (76%)	23 (18%)	7 (6%)	1	9
10	QJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	2	15
10	XJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	1	11
11	QK	119/129 (92%)	101 (85%)	13 (11%)	5 (4%)	2	14
11	XK	119/129 (92%)	105 (88%)	10 (8%)	4 (3%)	3	18
12	QL	123/132 (93%)	99 (80%)	16 (13%)	8 (6%)	1	8
12	XL	123/132 (93%)	97 (79%)	18 (15%)	8 (6%)	1	8
13	QM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	3
13	XM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	3
14	QN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1	11
14	XN	58/61 (95%)	50 (86%)	5 (9%)	3 (5%)	1	11
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%)	12	40
17	XQ	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	6	27
18	QR	69/88 (78%)	61 (88%)	8 (12%)	0	100	100
18	XR	69/88 (78%)	62 (90%)	6 (9%)	1 (1%)	9	33
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%)	3	20
20	XT	97/106 (92%)	80 (82%)	14 (14%)	3 (3%)	3	20
21	QU	23/25 (92%)	16 (70%)	6 (26%)	1 (4%)	2	14
21	XU	23/25 (92%)	18 (78%)	3 (13%)	2 (9%)	0	4
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%)	3	20
27	YD	270/276 (98%)	228 (84%)	32 (12%)	10 (4%)	2	17
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	8
29	YF	206/210 (98%)	168 (82%)	22 (11%)	16 (8%)	1	5
30	RG	179/182 (98%)	141 (79%)	26 (14%)	12 (7%)	1	7
30	YG	179/182 (98%)	147 (82%)	21 (12%)	11 (6%)	1	9
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%)	2	14
32	YI	144/148 (97%)	116 (81%)	24 (17%)	4 (3%)	4	21
33	RN	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	1	11
33	YN	136/140 (97%)	110 (81%)	19 (14%)	7 (5%)	1	11
34	RO	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	45
34	YO	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	45
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	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	YQ	137/141 (97%)	111 (81%)	15 (11%)	11 (8%)	1	5
37	RR	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	18
37	YR	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	4	23
38	RS	109/112 (97%)	84 (77%)	17 (16%)	8 (7%)	1	6
38	YS	109/112 (97%)	85 (78%)	13 (12%)	11 (10%)	0	3
39	RT	135/146 (92%)	109 (81%)	24 (18%)	2 (2%)	8	32
39	YT	135/146 (92%)	113 (84%)	17 (13%)	5 (4%)	2	17
40	RU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	7	30
40	YU	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	4	23
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%)	4	22
42	YW	111/113 (98%)	104 (94%)	3 (3%)	4 (4%)	2	17
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	26
43	YX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	26
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	3
46	R0	81/85 (95%)	73 (90%)	5 (6%)	3 (4%)	2	17
46	Y0	81/85 (95%)	67 (83%)	11 (14%)	3 (4%)	2	17
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	8
48	R2	67/72 (93%)	54 (81%)	8 (12%)	5 (8%)	1	6
48	Y2	67/72 (93%)	56 (84%)	5 (8%)	6 (9%)	0	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	0
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	18
51	Y5	55/60 (92%)	48 (87%)	4 (7%)	3 (6%)	1	10

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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%)	3	21
55	Y9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11649/12360 (94%)	9394 (81%)	1496 (13%)	759 (6%)	1	8

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%)	176 (86%)	28 (14%)	3	16
2	XB	204/220 (93%)	175 (86%)	29 (14%)	3	14
3	QC	160/188 (85%)	143 (89%)	17 (11%)	6	24
3	XC	160/188 (85%)	139 (87%)	21 (13%)	4	17
4	QD	180/181 (99%)	157 (87%)	23 (13%)	4	18
4	XD	180/181 (99%)	151 (84%)	29 (16%)	2	12
5	QE	119/123 (97%)	107 (90%)	12 (10%)	7	26
5	XE	119/123 (97%)	106 (89%)	13 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	QF	90/90 (100%)	84 (93%)	6 (7%)	15	42
6	XF	90/90 (100%)	75 (83%)	15 (17%)	2	11
7	QG	126/127 (99%)	112 (89%)	14 (11%)	6	22
7	XG	126/127 (99%)	107 (85%)	19 (15%)	3	13
8	QH	119/119 (100%)	108 (91%)	11 (9%)	8	30
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	23
9	QI	99/99 (100%)	78 (79%)	21 (21%)	1	5
9	XI	99/99 (100%)	83 (84%)	16 (16%)	2	11
10	QJ	89/92 (97%)	78 (88%)	11 (12%)	4	19
10	XJ	89/92 (97%)	76 (85%)	13 (15%)	3	14
11	QK	92/99 (93%)	83 (90%)	9 (10%)	7	28
11	XK	92/99 (93%)	83 (90%)	9 (10%)	7	28
12	QL	104/109 (95%)	89 (86%)	15 (14%)	3	14
12	XL	104/109 (95%)	82 (79%)	22 (21%)	1	5
13	QM	94/101 (93%)	79 (84%)	15 (16%)	2	11
13	XM	94/101 (93%)	83 (88%)	11 (12%)	5	20
14	QN	49/50 (98%)	46 (94%)	3 (6%)	17	45
14	XN	49/50 (98%)	45 (92%)	4 (8%)	10	35
15	QO	79/80 (99%)	71 (90%)	8 (10%)	7	26
15	XO	79/80 (99%)	72 (91%)	7 (9%)	9	32
16	QP	72/74 (97%)	65 (90%)	7 (10%)	8	28
16	XP	72/74 (97%)	65 (90%)	7 (10%)	8	28
17	QQ	95/97 (98%)	90 (95%)	5 (5%)	20	49
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	38
18	QR	62/77 (80%)	57 (92%)	5 (8%)	11	36
18	XR	62/77 (80%)	55 (89%)	7 (11%)	5	21
19	QS	71/80 (89%)	52 (73%)	19 (27%)	0	2
19	XS	71/80 (89%)	56 (79%)	15 (21%)	1	5
20	QT	76/82 (93%)	61 (80%)	15 (20%)	1	6
20	XT	76/82 (93%)	63 (83%)	13 (17%)	2	10
21	QU	20/20 (100%)	19 (95%)	1 (5%)	22	50

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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%)	75 (95%)	4 (5%)	21	50
24	XY	79/103 (77%)	75 (95%)	4 (5%)	21	50
27	RD	214/218 (98%)	175 (82%)	39 (18%)	2	8
27	YD	214/218 (98%)	172 (80%)	42 (20%)	1	6
28	RE	165/166 (99%)	135 (82%)	30 (18%)	2	8
28	YE	165/166 (99%)	131 (79%)	34 (21%)	1	6
29	RF	165/166 (99%)	139 (84%)	26 (16%)	2	12
29	YF	165/166 (99%)	141 (86%)	24 (14%)	3	14
30	RG	155/156 (99%)	143 (92%)	12 (8%)	12	37
30	YG	155/156 (99%)	138 (89%)	17 (11%)	6	23
31	RH	142/148 (96%)	121 (85%)	21 (15%)	3	13
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	6
32	RI	122/124 (98%)	99 (81%)	23 (19%)	1	7
32	YI	122/124 (98%)	100 (82%)	22 (18%)	2	8
33	RN	117/119 (98%)	104 (89%)	13 (11%)	6	22
33	YN	117/119 (98%)	105 (90%)	12 (10%)	7	25
34	RO	100/100 (100%)	88 (88%)	12 (12%)	5	20
34	YO	100/100 (100%)	86 (86%)	14 (14%)	3	15
35	RP	116/116 (100%)	84 (72%)	32 (28%)	0	2
35	YP	116/116 (100%)	82 (71%)	34 (29%)	0	2
36	RQ	110/111 (99%)	94 (86%)	16 (14%)	3	14
36	YQ	110/111 (99%)	90 (82%)	20 (18%)	2	8
37	RR	100/101 (99%)	81 (81%)	19 (19%)	1	7
37	YR	100/101 (99%)	84 (84%)	16 (16%)	2	11
38	RS	87/88 (99%)	78 (90%)	9 (10%)	7	25
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	13
39	RT	120/127 (94%)	99 (82%)	21 (18%)	2	9
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	9
40	RU	93/94 (99%)	85 (91%)	8 (9%)	10	33
40	YU	93/94 (99%)	84 (90%)	9 (10%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	RV	82/82 (100%)	68 (83%)	14 (17%)	2	10
41	YV	82/82 (100%)	63 (77%)	19 (23%)	1	4
42	RW	92/92 (100%)	78 (85%)	14 (15%)	3	13
42	YW	92/92 (100%)	79 (86%)	13 (14%)	3	14
43	RX	74/78 (95%)	64 (86%)	10 (14%)	4	16
43	YX	74/78 (95%)	66 (89%)	8 (11%)	6	23
44	RY	85/91 (93%)	61 (72%)	24 (28%)	0	2
44	YY	85/91 (93%)	62 (73%)	23 (27%)	0	2
45	RZ	155/179 (87%)	124 (80%)	31 (20%)	1	6
45	YZ	162/179 (90%)	132 (82%)	30 (18%)	1	7
46	R0	66/67 (98%)	60 (91%)	6 (9%)	9	31
46	Y0	66/67 (98%)	59 (89%)	7 (11%)	6	24
47	R1	82/83 (99%)	68 (83%)	14 (17%)	2	10
47	Y1	82/83 (99%)	71 (87%)	11 (13%)	4	16
48	R2	64/67 (96%)	52 (81%)	12 (19%)	1	7
48	Y2	64/67 (96%)	55 (86%)	9 (14%)	3	14
49	R3	51/52 (98%)	43 (84%)	8 (16%)	2	12
49	Y3	51/52 (98%)	41 (80%)	10 (20%)	1	6
50	R4	62/63 (98%)	49 (79%)	13 (21%)	1	5
50	Y4	62/63 (98%)	45 (73%)	17 (27%)	0	2
51	R5	51/52 (98%)	43 (84%)	8 (16%)	2	12
51	Y5	49/52 (94%)	43 (88%)	6 (12%)	5	19
52	R6	47/52 (90%)	34 (72%)	13 (28%)	0	2
52	Y6	47/52 (90%)	29 (62%)	18 (38%)	0	0
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2	11
53	Y7	42/42 (100%)	36 (86%)	6 (14%)	3	14
54	R8	54/55 (98%)	43 (80%)	11 (20%)	1	6
54	Y8	54/55 (98%)	44 (82%)	10 (18%)	1	7
55	R9	34/34 (100%)	32 (94%)	2 (6%)	18	46
55	Y9	33/34 (97%)	33 (100%)	0	100	100
All	All	9856/10268 (96%)	8370 (85%)	1486 (15%)	3	13

5 of 1486 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	XM	108	ARG
32	YI	54	GLN
18	XR	31	LEU
13	XM	93	ARG
28	YE	35	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
45	YZ	75	ASN
45	YZ	132	ASN
55	Y9	29	ASN
36	RQ	113	GLN
36	RQ	45	GLN

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%)	577 (19%)	52 (1%)
25	YA	2872/2916 (98%)	561 (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%)	1851 (19%)	178 (1%)

5 of 1851 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
1	XA	485	G
25	YA	587	C
1	XA	748	C
1	XA	1065	U
25	YA	1171	G

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	25,28,29	1.51	3 (12%)	37,42,45	2.05	10 (27%)
23	A3P	XX	20	23	25,28,29	1.46	4 (16%)	37,42,45	2.00	9 (24%)

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	-	5/12/30/31	0/3/3/3
23	A3P	XX	20	23	-	2/12/30/31	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	C5-C4	4.86	1.47	1.39
23	XX	20	A3P	C5-C4	4.72	1.47	1.39
23	QX	20	A3P	C5-C6	3.17	1.49	1.41
23	XX	20	A3P	C5-C6	2.72	1.48	1.41
23	QX	20	A3P	C8-N7	2.47	1.36	1.31

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	20	A3P	C5-C4-N3	-6.30	118.04	126.72
23	XX	20	A3P	C5-C4-N3	-6.08	118.35	126.72
23	XX	20	A3P	N3-C4-N9	4.72	135.19	127.17
23	QX	20	A3P	N3-C4-N9	4.67	135.11	127.17
23	QX	20	A3P	C4-C5-N7	-4.06	105.94	110.58

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	QX	20	A3P	C2'-C3'-O3'-P1
23	QX	20	A3P	C4'-C3'-O3'-P1
23	QX	20	A3P	C3'-O3'-P1-O1P
23	QX	20	A3P	C3'-C4'-C5'-O5'
23	QX	20	A3P	O4'-C1'-N9-C8

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 oligosaccharides 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%)	0.06	33 (2%) 62 43	47, 90, 193, 346	0
1	XA	1508/1522 (99%)	-0.04	30 (1%) 65 46	42, 85, 179, 385	0
2	QB	236/256 (92%)	0.79	21 (8%) 15 12	95, 145, 216, 283	0
2	XB	236/256 (92%)	1.05	34 (14%) 6 5	80, 127, 194, 248	0
3	QC	206/239 (86%)	0.75	17 (8%) 17 13	86, 129, 209, 279	0
3	XC	206/239 (86%)	0.72	17 (8%) 17 13	73, 111, 176, 256	0
4	QD	208/209 (99%)	0.69	20 (9%) 13 11	58, 81, 132, 231	0
4	XD	208/209 (99%)	0.69	16 (7%) 19 14	63, 92, 153, 186	0
5	QE	154/162 (95%)	0.35	4 (2%) 57 38	57, 83, 141, 207	0
5	XE	154/162 (95%)	0.54	11 (7%) 22 15	56, 83, 145, 244	0
6	QF	101/101 (100%)	0.97	9 (8%) 15 12	92, 138, 183, 203	0
6	XF	101/101 (100%)	0.44	4 (3%) 42 28	60, 90, 119, 171	0
7	QG	155/156 (99%)	1.10	27 (17%) 4 4	96, 144, 192, 282	0
7	XG	155/156 (99%)	0.97	27 (17%) 4 4	87, 115, 173, 226	0
8	QH	138/138 (100%)	0.37	3 (2%) 62 43	59, 91, 128, 188	0
8	XH	138/138 (100%)	0.36	2 (1%) 73 55	64, 88, 121, 174	0
9	QI	128/128 (100%)	1.25	23 (17%) 3 3	88, 168, 229, 293	0
9	XI	128/128 (100%)	1.32	33 (25%) 1 1	83, 136, 203, 246	0
10	QJ	99/105 (94%)	1.29	15 (15%) 5 5	92, 168, 228, 284	0
10	XJ	99/105 (94%)	1.30	19 (19%) 3 3	78, 141, 219, 279	0
11	QK	121/129 (93%)	0.97	12 (9%) 13 10	66, 117, 191, 242	0
11	XK	121/129 (93%)	0.97	9 (7%) 20 15	52, 84, 161, 197	0
12	QL	125/132 (94%)	0.46	5 (4%) 42 28	53, 71, 115, 232	0
12	XL	125/132 (94%)	0.44	4 (3%) 50 34	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%)	1.17	20 (16%) 4 4	93, 148, 218, 278	0
13	XM	118/126 (93%)	0.94	17 (14%) 6 5	82, 126, 181, 267	0
14	QN	60/61 (98%)	1.31	9 (15%) 5 5	98, 127, 180, 208	0
14	XN	60/61 (98%)	1.11	9 (15%) 5 5	81, 102, 132, 248	0
15	QO	88/89 (98%)	0.41	6 (6%) 23 16	63, 89, 143, 153	0
15	XO	88/89 (98%)	0.41	2 (2%) 61 42	54, 80, 125, 147	0
16	QP	84/88 (95%)	0.78	11 (13%) 7 6	61, 77, 115, 213	0
16	XP	84/88 (95%)	0.61	3 (3%) 46 31	75, 98, 139, 217	0
17	QQ	100/105 (95%)	0.66	8 (8%) 18 14	60, 85, 113, 137	0
17	XQ	100/105 (95%)	0.50	5 (5%) 34 23	58, 85, 117, 209	0
18	QR	71/88 (80%)	0.78	4 (5%) 30 20	92, 124, 204, 224	0
18	XR	71/88 (80%)	0.78	5 (7%) 22 15	63, 86, 179, 224	0
19	QS	82/93 (88%)	1.33	16 (19%) 3 3	96, 159, 239, 270	0
19	XS	82/93 (88%)	1.15	12 (14%) 6 5	91, 129, 221, 278	0
20	QT	99/106 (93%)	1.17	20 (20%) 3 2	65, 99, 158, 210	0
20	XT	99/106 (93%)	0.87	9 (9%) 15 11	79, 113, 174, 201	0
21	QU	25/25 (100%)	2.22	14 (56%) 0 0	109, 136, 171, 253	0
21	XU	25/25 (100%)	2.17	14 (56%) 0 0	95, 118, 171, 181	0
22	QV	77/77 (100%)	0.55	4 (5%) 33 22	47, 91, 145, 216	0
22	QW	77/77 (100%)	1.57	21 (27%) 1 1	60, 203, 273, 298	0
22	XV	77/77 (100%)	0.28	4 (5%) 33 22	47, 90, 138, 204	0
22	XW	77/77 (100%)	1.44	17 (22%) 2 2	71, 225, 299, 354	0
23	QX	17/20 (85%)	1.41	4 (23%) 2 2	59, 207, 269, 270	0
23	XX	17/20 (85%)	1.20	4 (23%) 2 2	52, 200, 283, 301	0
24	QY	92/118 (77%)	0.91	12 (13%) 7 6	66, 123, 158, 177	0
24	XY	92/118 (77%)	1.74	34 (36%) 1 1	79, 160, 201, 212	0
25	RA	2891/2916 (99%)	-0.14	64 (2%) 62 43	35, 64, 209, 371	0
25	YA	2875/2916 (98%)	-0.19	58 (2%) 65 46	33, 60, 231, 360	0
26	RB	122/124 (98%)	0.08	0 100 100	67, 110, 153, 202	0
26	YB	122/124 (98%)	0.13	0 100 100	74, 102, 152, 201	0
27	RD	272/276 (98%)	0.59	19 (6%) 22 15	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%)	0.41	23 (8%)	16 13	32, 48, 92, 192	0
28	RE	205/206 (99%)	0.92	29 (14%)	6 5	41, 79, 169, 273	0
28	YE	205/206 (99%)	0.88	28 (13%)	6 5	40, 78, 163, 260	0
29	RF	208/210 (99%)	0.51	13 (6%)	26 17	35, 60, 170, 262	0
29	YF	208/210 (99%)	0.55	17 (8%)	17 13	35, 73, 172, 250	0
30	RG	181/182 (99%)	0.97	24 (13%)	7 6	85, 125, 168, 187	0
30	YG	181/182 (99%)	1.24	40 (22%)	2 2	85, 122, 183, 239	0
31	RH	170/180 (94%)	1.45	38 (22%)	2 2	99, 169, 244, 283	0
31	YH	170/180 (94%)	1.58	46 (27%)	1 1	75, 147, 231, 277	0
32	RI	146/148 (98%)	1.24	29 (19%)	3 2	70, 125, 186, 284	0
32	YI	146/148 (98%)	0.87	15 (10%)	12 10	47, 100, 178, 253	0
33	RN	138/140 (98%)	0.48	9 (6%)	25 17	49, 78, 131, 230	0
33	YN	138/140 (98%)	0.63	4 (2%)	53 35	53, 85, 143, 177	0
34	RO	122/122 (100%)	0.55	5 (4%)	41 27	48, 68, 105, 143	0
34	YO	122/122 (100%)	0.14	1 (0%)	82 68	46, 64, 92, 136	0
35	RP	150/150 (100%)	1.03	24 (16%)	5 4	37, 78, 157, 260	0
35	YP	150/150 (100%)	1.18	30 (20%)	3 2	40, 75, 139, 253	0
36	RQ	140/141 (99%)	0.63	13 (9%)	14 11	47, 77, 136, 200	0
36	YQ	139/141 (98%)	0.76	13 (9%)	14 11	50, 79, 131, 251	0
37	RR	117/118 (99%)	0.38	2 (1%)	69 50	50, 73, 111, 146	0
37	YR	117/118 (99%)	0.58	6 (5%)	33 22	48, 68, 101, 145	0
38	RS	111/112 (99%)	0.84	12 (10%)	11 9	82, 114, 162, 217	0
38	YS	111/112 (99%)	1.17	19 (17%)	4 4	78, 102, 155, 196	0
39	RT	137/146 (93%)	0.87	16 (11%)	9 8	58, 83, 174, 271	0
39	YT	137/146 (93%)	0.69	17 (12%)	8 6	55, 79, 183, 256	0
40	RU	117/118 (99%)	0.48	4 (3%)	48 32	40, 63, 130, 250	0
40	YU	117/118 (99%)	0.71	11 (9%)	14 11	47, 76, 150, 184	0
41	RV	101/101 (100%)	0.59	9 (8%)	15 12	40, 83, 148, 266	0
41	YV	101/101 (100%)	0.82	10 (9%)	13 10	46, 103, 153, 191	0
42	RW	113/113 (100%)	0.28	4 (3%)	47 31	40, 61, 127, 192	0
42	YW	113/113 (100%)	0.42	0	100 100	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%)	0.38	4 (4%) 40 25	57, 77, 114, 151	0
43	YX	92/96 (95%)	0.28	2 (2%) 62 43	43, 62, 99, 124	0
44	RY	102/110 (92%)	1.48	28 (27%) 1 1	57, 88, 196, 277	0
44	YY	102/110 (92%)	1.41	21 (20%) 2 2	63, 102, 218, 267	0
45	RZ	176/206 (85%)	0.87	23 (13%) 7 6	76, 116, 207, 274	0
45	YZ	183/206 (88%)	0.95	19 (10%) 11 9	75, 120, 186, 245	0
46	R0	83/85 (97%)	0.65	13 (15%) 5 4	46, 72, 159, 246	0
46	Y0	83/85 (97%)	0.57	8 (9%) 13 11	46, 76, 141, 197	0
47	R1	97/98 (98%)	0.96	15 (15%) 5 4	44, 73, 173, 231	0
47	Y1	97/98 (98%)	0.81	12 (12%) 8 6	36, 57, 166, 259	0
48	R2	69/72 (95%)	0.70	7 (10%) 12 10	66, 99, 165, 209	0
48	Y2	69/72 (95%)	0.76	8 (11%) 9 8	52, 76, 141, 198	0
49	R3	59/60 (98%)	0.25	1 (1%) 69 50	54, 68, 118, 154	0
49	Y3	59/60 (98%)	0.53	3 (5%) 33 22	59, 86, 131, 188	0
50	R4	70/71 (98%)	1.36	14 (20%) 3 2	100, 181, 261, 319	0
50	Y4	70/71 (98%)	1.25	14 (20%) 3 2	108, 173, 248, 312	0
51	R5	59/60 (98%)	0.76	8 (13%) 7 6	32, 68, 183, 221	0
51	Y5	57/60 (95%)	1.03	5 (8%) 15 12	31, 77, 168, 220	0
52	R6	48/54 (88%)	2.30	20 (41%) 0 0	80, 144, 220, 264	0
52	Y6	48/54 (88%)	2.20	22 (45%) 0 0	84, 123, 179, 225	0
53	R7	49/49 (100%)	0.70	8 (16%) 4 4	29, 46, 128, 207	0
53	Y7	49/49 (100%)	0.69	6 (12%) 8 7	20, 42, 117, 204	0
54	R8	64/65 (98%)	1.25	15 (23%) 2 2	36, 60, 143, 194	0
54	Y8	64/65 (98%)	1.06	12 (18%) 3 3	29, 59, 98, 237	0
55	R9	37/37 (100%)	1.80	12 (32%) 1 1	97, 141, 178, 209	0
55	Y9	36/37 (97%)	1.99	16 (44%) 0 0	84, 133, 171, 215	0
All	All	21220/21832 (97%)	0.44	1647 (7%) 19 14	20, 85, 198, 385	0

The worst 5 of 1647 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	RY	103	GLY	11.4
52	R6	41	PRO	10.3

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Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	9.1
28	YE	59	VAL	8.6
52	Y6	41	PRO	7.8

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	0.66	0.19	222,222,222,222	0
23	A3P	QX	20	26/27	0.80	0.13	175,175,175,175	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	YA	3401	1/1	-0.45	0.39	166,166,166,166	0
56	MG	XA	1745	1/1	0.19	0.20	99,99,99,99	0
56	MG	XA	1692	1/1	0.25	0.22	102,102,102,102	0
56	MG	QA	1690	1/1	0.27	0.26	80,80,80,80	0
56	MG	XA	1754	1/1	0.31	0.27	119,119,119,119	0
56	MG	XA	1702	1/1	0.38	0.32	101,101,101,101	0
56	MG	YQ	202	1/1	0.46	0.18	66,66,66,66	0
56	MG	YA	3397	1/1	0.47	0.18	58,58,58,58	0
56	MG	XA	1657	1/1	0.49	0.31	59,59,59,59	0
56	MG	YA	3278	1/1	0.50	0.32	75,75,75,75	0
56	MG	XA	1625	1/1	0.53	0.18	87,87,87,87	0
56	MG	YA	3224	1/1	0.53	0.21	63,63,63,63	0
56	MG	QA	1694	1/1	0.54	0.22	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3460	1/1	0.55	0.19	82,82,82,82	0
56	MG	XD	302	1/1	0.55	0.18	86,86,86,86	0
56	MG	RA	3391	1/1	0.56	0.17	113,113,113,113	0
56	MG	RA	3259	1/1	0.56	0.19	57,57,57,57	0
56	MG	YA	3452	1/1	0.59	0.20	71,71,71,71	0
56	MG	RA	3405	1/1	0.59	0.40	74,74,74,74	0
56	MG	QA	1733	1/1	0.59	0.15	65,65,65,65	0
56	MG	RA	3216	1/1	0.60	0.30	67,67,67,67	0
56	MG	RA	3269	1/1	0.60	0.18	75,75,75,75	0
56	MG	YA	3390	1/1	0.61	0.20	92,92,92,92	0
56	MG	RA	3055	1/1	0.61	0.06	15,15,15,15	0
56	MG	YA	3438	1/1	0.63	0.22	91,91,91,91	0
56	MG	RA	3155	1/1	0.63	0.23	55,55,55,55	0
56	MG	XA	1751	1/1	0.64	0.26	58,58,58,58	0
56	MG	QA	1735	1/1	0.64	0.22	75,75,75,75	0
56	MG	RA	3165	1/1	0.64	0.18	52,52,52,52	0
56	MG	R2	101	1/1	0.65	0.25	74,74,74,74	0
56	MG	RA	3132	1/1	0.66	0.28	58,58,58,58	0
56	MG	YA	3167	1/1	0.67	0.41	91,91,91,91	0
56	MG	YA	3336	1/1	0.67	0.28	75,75,75,75	0
56	MG	RA	3126	1/1	0.67	0.09	53,53,53,53	0
56	MG	YA	3099	1/1	0.68	0.23	51,51,51,51	0
56	MG	QA	1672	1/1	0.68	0.16	49,49,49,49	0
56	MG	RA	3082	1/1	0.68	0.14	15,15,15,15	0
56	MG	YA	3461	1/1	0.68	0.27	44,44,44,44	0
56	MG	RA	3090	1/1	0.68	0.13	61,61,61,61	0
56	MG	QA	1709	1/1	0.69	0.21	59,59,59,59	0
56	MG	YA	3232	1/1	0.69	0.20	57,57,57,57	0
56	MG	RA	3262	1/1	0.69	0.12	38,38,38,38	0
56	MG	YA	3406	1/1	0.70	0.20	74,74,74,74	0
56	MG	YA	3103	1/1	0.70	0.36	62,62,62,62	0
56	MG	XA	1659	1/1	0.71	0.21	76,76,76,76	0
56	MG	YA	3351	1/1	0.71	0.19	74,74,74,74	0
56	MG	YA	3387	1/1	0.71	0.16	98,98,98,98	0
56	MG	XA	1714	1/1	0.71	0.14	81,81,81,81	0
56	MG	QA	1698	1/1	0.71	0.16	101,101,101,101	0
56	MG	YA	3335	1/1	0.71	0.14	66,66,66,66	0
56	MG	XA	1739	1/1	0.72	0.14	57,57,57,57	0
56	MG	QA	1670	1/1	0.72	0.30	62,62,62,62	0
56	MG	YA	3422	1/1	0.72	0.24	63,63,63,63	0
56	MG	YA	3181	1/1	0.72	0.24	64,64,64,64	0
56	MG	RA	3331	1/1	0.73	0.23	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3311	1/1	0.73	0.12	51,51,51,51	0
56	MG	XA	1656	1/1	0.73	0.24	51,51,51,51	0
56	MG	YA	3121	1/1	0.73	0.22	40,40,40,40	0
56	MG	RA	3336	1/1	0.73	0.16	39,39,39,39	0
56	MG	QA	1682	1/1	0.73	0.21	64,64,64,64	0
56	MG	RA	3074	1/1	0.73	0.15	33,33,33,33	0
56	MG	RA	3320	1/1	0.73	0.23	63,63,63,63	0
56	MG	QA	1683	1/1	0.74	0.14	64,64,64,64	0
56	MG	QV	105	1/1	0.74	0.25	56,56,56,56	0
56	MG	YA	3227	1/1	0.74	0.26	54,54,54,54	0
56	MG	YA	3446	1/1	0.74	0.35	68,68,68,68	0
56	MG	RA	3035	1/1	0.74	0.19	40,40,40,40	0
56	MG	XA	1694	1/1	0.74	0.17	66,66,66,66	0
56	MG	YA	3279	1/1	0.74	0.24	66,66,66,66	0
56	MG	RA	3295	1/1	0.74	0.17	58,58,58,58	0
56	MG	YA	3441	1/1	0.75	0.10	54,54,54,54	0
56	MG	RA	3208	1/1	0.76	0.16	48,48,48,48	0
56	MG	YA	3429	1/1	0.76	0.18	38,38,38,38	0
56	MG	RA	3156	1/1	0.76	0.14	63,63,63,63	0
56	MG	YA	3363	1/1	0.76	0.22	69,69,69,69	0
56	MG	RA	3223	1/1	0.76	0.19	67,67,67,67	0
56	MG	RA	3227	1/1	0.76	0.09	43,43,43,43	0
56	MG	RA	3233	1/1	0.76	0.24	50,50,50,50	0
56	MG	RA	3333	1/1	0.76	0.14	52,52,52,52	0
56	MG	QA	1725	1/1	0.76	0.17	65,65,65,65	0
56	MG	YA	3140	1/1	0.77	0.11	64,64,64,64	0
56	MG	RA	3334	1/1	0.77	0.13	55,55,55,55	0
56	MG	XA	1736	1/1	0.77	0.11	24,24,24,24	0
56	MG	YA	3221	1/1	0.77	0.19	37,37,37,37	0
56	MG	XA	1699	1/1	0.77	0.15	84,84,84,84	0
56	MG	RA	3173	1/1	0.77	0.11	52,52,52,52	0
56	MG	XA	1706	1/1	0.77	0.28	81,81,81,81	0
56	MG	YA	3374	1/1	0.78	0.18	62,62,62,62	0
56	MG	YA	3380	1/1	0.78	0.12	65,65,65,65	0
56	MG	XA	1612	1/1	0.78	0.09	46,46,46,46	0
56	MG	QA	1726	1/1	0.78	0.20	56,56,56,56	0
56	MG	YA	3129	1/1	0.78	0.21	41,41,41,41	0
56	MG	QA	1629	1/1	0.78	0.20	56,56,56,56	0
56	MG	YA	3404	1/1	0.78	0.13	28,28,28,28	0
56	MG	YA	3303	1/1	0.78	0.20	60,60,60,60	0
56	MG	YA	3463	1/1	0.78	0.16	46,46,46,46	0
56	MG	YA	3420	1/1	0.78	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3216	1/1	0.79	0.25	51,51,51,51	0
56	MG	XA	1674	1/1	0.79	0.11	50,50,50,50	0
56	MG	XA	1678	1/1	0.79	0.14	70,70,70,70	0
56	MG	RA	3050	1/1	0.79	0.31	57,57,57,57	0
56	MG	YA	3134	1/1	0.79	0.23	56,56,56,56	0
56	MG	RA	3161	1/1	0.79	0.36	71,71,71,71	0
56	MG	YA	3001	1/1	0.79	0.46	70,70,70,70	0
56	MG	RA	3327	1/1	0.79	0.26	69,69,69,69	0
56	MG	QA	1676	1/1	0.80	0.15	56,56,56,56	0
56	MG	QA	1640	1/1	0.80	0.20	76,76,76,76	0
56	MG	YA	3251	1/1	0.80	0.23	82,82,82,82	0
56	MG	YA	3354	1/1	0.80	0.29	79,79,79,79	0
56	MG	YA	3189	1/1	0.80	0.31	40,40,40,40	0
56	MG	XA	1720	1/1	0.80	0.13	53,53,53,53	0
56	MG	QA	1673	1/1	0.80	0.17	62,62,62,62	0
56	MG	YH	201	1/1	0.80	0.10	105,105,105,105	0
56	MG	YA	3150	1/1	0.80	0.41	69,69,69,69	0
56	MG	YA	3067	1/1	0.81	0.17	40,40,40,40	0
56	MG	YA	3081	1/1	0.81	0.24	35,35,35,35	0
56	MG	QA	1722	1/1	0.81	0.14	39,39,39,39	0
56	MG	RA	3400	1/1	0.81	0.24	59,59,59,59	0
56	MG	XA	1743	1/1	0.81	0.13	39,39,39,39	0
56	MG	RA	3402	1/1	0.81	0.12	61,61,61,61	0
56	MG	YA	3131	1/1	0.81	0.21	48,48,48,48	0
56	MG	RA	3101	1/1	0.81	0.18	31,31,31,31	0
56	MG	YA	3386	1/1	0.81	0.11	48,48,48,48	0
56	MG	RA	3324	1/1	0.81	0.17	62,62,62,62	0
56	MG	RA	3254	1/1	0.81	0.30	74,74,74,74	0
56	MG	XA	1689	1/1	0.81	0.14	55,55,55,55	0
56	MG	YA	3307	1/1	0.81	0.21	101,101,101,101	0
56	MG	YA	3403	1/1	0.81	0.22	36,36,36,36	0
56	MG	RA	3349	1/1	0.82	0.16	80,80,80,80	0
56	MG	RA	3355	1/1	0.82	0.13	73,73,73,73	0
56	MG	QA	1665	1/1	0.82	0.12	58,58,58,58	0
56	MG	YA	3290	1/1	0.82	0.14	78,78,78,78	0
56	MG	QA	1631	1/1	0.82	0.28	56,56,56,56	0
56	MG	RA	3068	1/1	0.82	0.20	39,39,39,39	0
56	MG	XA	1750	1/1	0.82	0.15	57,57,57,57	0
56	MG	RA	3284	1/1	0.82	0.15	35,35,35,35	0
56	MG	RA	3292	1/1	0.82	0.11	38,38,38,38	0
56	MG	YA	3173	1/1	0.82	0.14	41,41,41,41	0
56	MG	XA	1604	1/1	0.82	0.22	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3294	1/1	0.82	0.09	53,53,53,53	0
56	MG	RA	3042	1/1	0.82	0.27	48,48,48,48	0
56	MG	XA	1630	1/1	0.82	0.17	35,35,35,35	0
56	MG	YA	3088	1/1	0.82	0.21	21,21,21,21	0
56	MG	YB	204	1/1	0.82	0.18	63,63,63,63	0
56	MG	YA	3089	1/1	0.82	0.13	42,42,42,42	0
56	MG	XA	1635	1/1	0.82	0.11	45,45,45,45	0
56	MG	QA	1679	1/1	0.83	0.25	61,61,61,61	0
56	MG	YA	3180	1/1	0.83	0.21	61,61,61,61	0
56	MG	YA	3437	1/1	0.83	0.17	56,56,56,56	0
56	MG	RA	3099	1/1	0.83	0.21	68,68,68,68	0
56	MG	QA	1641	1/1	0.83	0.15	50,50,50,50	0
56	MG	YA	3057	1/1	0.83	0.11	37,37,37,37	0
56	MG	QA	1661	1/1	0.83	0.13	75,75,75,75	0
56	MG	RA	3177	1/1	0.83	0.16	42,42,42,42	0
56	MG	QA	1662	1/1	0.83	0.20	51,51,51,51	0
56	MG	YA	3340	1/1	0.83	0.22	48,48,48,48	0
56	MG	YA	3343	1/1	0.83	0.16	46,46,46,46	0
56	MG	QA	1603	1/1	0.83	0.14	83,83,83,83	0
56	MG	YA	3095	1/1	0.83	0.18	53,53,53,53	0
56	MG	RQ	201	1/1	0.84	0.12	52,52,52,52	0
56	MG	YA	3146	1/1	0.84	0.16	70,70,70,70	0
56	MG	RU	201	1/1	0.84	0.26	63,63,63,63	0
56	MG	YA	3030	1/1	0.84	0.23	21,21,21,21	0
56	MG	YA	3407	1/1	0.84	0.09	44,44,44,44	0
56	MG	YA	3331	1/1	0.84	0.14	56,56,56,56	0
56	MG	RA	3170	1/1	0.84	0.27	49,49,49,49	0
56	MG	RA	3129	1/1	0.84	0.17	41,41,41,41	0
56	MG	QA	1636	1/1	0.84	0.16	62,62,62,62	0
56	MG	RA	3141	1/1	0.84	0.08	64,64,64,64	0
56	MG	QA	1608	1/1	0.84	0.37	35,35,35,35	0
56	MG	YA	3444	1/1	0.84	0.18	56,56,56,56	0
56	MG	QA	1699	1/1	0.84	0.29	60,60,60,60	0
56	MG	RA	3125	1/1	0.84	0.34	68,68,68,68	0
56	MG	RA	3359	1/1	0.84	0.20	56,56,56,56	0
56	MG	QV	101	1/1	0.84	0.09	35,35,35,35	0
56	MG	YA	3245	1/1	0.84	0.22	57,57,57,57	0
56	MG	RA	3321	1/1	0.84	0.20	78,78,78,78	0
56	MG	RA	3166	1/1	0.84	0.24	59,59,59,59	0
56	MG	RA	3325	1/1	0.84	0.17	56,56,56,56	0
56	MG	XA	1654	1/1	0.85	0.16	48,48,48,48	0
56	MG	RA	3357	1/1	0.85	0.30	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1753	1/1	0.85	0.18	100,100,100,100	0
56	MG	RA	3048	1/1	0.85	0.13	21,21,21,21	0
56	MG	RA	3373	1/1	0.85	0.28	26,26,26,26	0
56	MG	XF	201	1/1	0.85	0.15	35,35,35,35	0
56	MG	QA	1738	1/1	0.85	0.09	67,67,67,67	0
56	MG	RA	3110	1/1	0.85	0.18	25,25,25,25	0
56	MG	YA	3393	1/1	0.85	0.22	62,62,62,62	0
56	MG	RA	3238	1/1	0.85	0.22	44,44,44,44	0
56	MG	RA	3122	1/1	0.85	0.18	36,36,36,36	0
56	MG	YA	3231	1/1	0.85	0.28	64,64,64,64	0
56	MG	YA	3078	1/1	0.85	0.20	36,36,36,36	0
56	MG	YA	3238	1/1	0.85	0.09	45,45,45,45	0
56	MG	RA	3412	1/1	0.85	0.20	34,34,34,34	0
56	MG	QA	1706	1/1	0.85	0.28	50,50,50,50	0
56	MG	YA	3252	1/1	0.85	0.29	93,93,93,93	0
56	MG	YA	3258	1/1	0.85	0.22	60,60,60,60	0
56	MG	YA	3432	1/1	0.85	0.23	53,53,53,53	0
56	MG	RA	3328	1/1	0.85	0.17	61,61,61,61	0
56	MG	QV	104	1/1	0.85	0.24	68,68,68,68	0
56	MG	QA	1724	1/1	0.85	0.10	50,50,50,50	0
56	MG	YA	3296	1/1	0.85	0.22	66,66,66,66	0
56	MG	XA	1607	1/1	0.85	0.19	37,37,37,37	0
56	MG	QA	1697	1/1	0.85	0.08	54,54,54,54	0
56	MG	YA	3458	1/1	0.85	0.10	45,45,45,45	0
56	MG	XA	1738	1/1	0.85	0.09	30,30,30,30	0
56	MG	RA	3289	1/1	0.85	0.34	27,27,27,27	0
56	MG	XA	1742	1/1	0.85	0.19	63,63,63,63	0
56	MG	RA	3133	1/1	0.85	0.09	38,38,38,38	0
56	MG	QA	1737	1/1	0.85	0.14	93,93,93,93	0
56	MG	YA	3147	1/1	0.85	0.17	43,43,43,43	0
56	MG	YY	201	1/1	0.85	0.11	42,42,42,42	0
56	MG	XA	1724	1/1	0.86	0.17	64,64,64,64	0
56	MG	RA	3304	1/1	0.86	0.24	76,76,76,76	0
56	MG	RA	3237	1/1	0.86	0.24	70,70,70,70	0
56	MG	YA	3097	1/1	0.86	0.15	78,78,78,78	0
56	MG	RA	3389	1/1	0.86	0.12	57,57,57,57	0
56	MG	YA	3101	1/1	0.86	0.25	36,36,36,36	0
56	MG	RA	3116	1/1	0.86	0.28	45,45,45,45	0
56	MG	YA	3253	1/1	0.86	0.20	60,60,60,60	0
56	MG	RA	3247	1/1	0.86	0.10	41,41,41,41	0
56	MG	YA	3269	1/1	0.86	0.11	43,43,43,43	0
56	MG	YA	3276	1/1	0.86	0.24	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3175	1/1	0.86	0.22	57,57,57,57	0
56	MG	XA	1671	1/1	0.86	0.25	56,56,56,56	0
56	MG	QA	1701	1/1	0.86	0.26	77,77,77,77	0
56	MG	RA	3206	1/1	0.86	0.26	44,44,44,44	0
56	MG	YA	3435	1/1	0.86	0.10	57,57,57,57	0
56	MG	XA	1684	1/1	0.86	0.13	48,48,48,48	0
56	MG	YA	3305	1/1	0.86	0.09	57,57,57,57	0
56	MG	QA	1702	1/1	0.86	0.20	60,60,60,60	0
56	MG	RA	3274	1/1	0.86	0.21	64,64,64,64	0
56	MG	XL	201	1/1	0.86	0.10	60,60,60,60	0
56	MG	YA	3447	1/1	0.86	0.27	97,97,97,97	0
56	MG	RA	3209	1/1	0.86	0.13	24,24,24,24	0
56	MG	YA	3174	1/1	0.86	0.14	66,66,66,66	0
56	MG	R5	103	1/1	0.86	0.07	60,60,60,60	0
56	MG	YA	3045	1/1	0.86	0.17	22,22,22,22	0
56	MG	QA	1612	1/1	0.86	0.28	51,51,51,51	0
56	MG	QA	1630	1/1	0.86	0.19	57,57,57,57	0
56	MG	QA	1644	1/1	0.86	0.21	58,58,58,58	0
56	MG	YA	3364	1/1	0.86	0.17	44,44,44,44	0
56	MG	RA	3001	1/1	0.86	0.18	73,73,73,73	0
56	MG	RA	3144	1/1	0.87	0.16	51,51,51,51	0
56	MG	XA	1615	1/1	0.87	0.17	39,39,39,39	0
56	MG	XA	1621	1/1	0.87	0.23	47,47,47,47	0
56	MG	YA	3342	1/1	0.87	0.11	54,54,54,54	0
56	MG	XA	1740	1/1	0.87	0.28	50,50,50,50	0
56	MG	XA	1622	1/1	0.87	0.28	44,44,44,44	0
56	MG	RA	3337	1/1	0.87	0.13	54,54,54,54	0
56	MG	XA	1629	1/1	0.87	0.11	83,83,83,83	0
56	MG	RA	3288	1/1	0.87	0.24	39,39,39,39	0
56	MG	RA	3094	1/1	0.87	0.30	46,46,46,46	0
56	MG	XA	1636	1/1	0.87	0.21	54,54,54,54	0
56	MG	XA	1639	1/1	0.87	0.26	63,63,63,63	0
56	MG	XA	1758	1/1	0.87	0.23	60,60,60,60	0
56	MG	RA	3065	1/1	0.87	0.20	39,39,39,39	0
56	MG	RA	3293	1/1	0.87	0.13	38,38,38,38	0
56	MG	YA	3222	1/1	0.87	0.18	42,42,42,42	0
56	MG	RA	3180	1/1	0.87	0.15	74,74,74,74	0
56	MG	RA	3182	1/1	0.87	0.20	38,38,38,38	0
56	MG	YA	3228	1/1	0.87	0.18	51,51,51,51	0
56	MG	RA	3240	1/1	0.87	0.12	34,34,34,34	0
56	MG	XA	1672	1/1	0.87	0.10	12,12,12,12	0
56	MG	YA	3414	1/1	0.87	0.17	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3314	1/1	0.87	0.21	60,60,60,60	0
56	MG	YA	3058	1/1	0.87	0.07	29,29,29,29	0
56	MG	YA	3427	1/1	0.87	0.21	99,99,99,99	0
56	MG	YA	3062	1/1	0.87	0.18	38,38,38,38	0
56	MG	RA	3190	1/1	0.87	0.11	38,38,38,38	0
56	MG	YA	3073	1/1	0.87	0.22	36,36,36,36	0
56	MG	RA	3196	1/1	0.87	0.17	40,40,40,40	0
56	MG	YA	3263	1/1	0.87	0.20	57,57,57,57	0
56	MG	QA	1632	1/1	0.87	0.23	36,36,36,36	0
56	MG	QA	1633	1/1	0.87	0.23	68,68,68,68	0
56	MG	RR	201	1/1	0.87	0.30	44,44,44,44	0
56	MG	RA	3266	1/1	0.87	0.15	42,42,42,42	0
56	MG	YA	3281	1/1	0.87	0.13	34,34,34,34	0
56	MG	QA	1732	1/1	0.87	0.28	63,63,63,63	0
56	MG	R5	102	1/1	0.87	0.22	63,63,63,63	0
56	MG	YA	3301	1/1	0.87	0.17	30,30,30,30	0
56	MG	RA	3271	1/1	0.87	0.25	55,55,55,55	0
56	MG	YB	202	1/1	0.87	0.19	49,49,49,49	0
56	MG	XA	1719	1/1	0.87	0.17	46,46,46,46	0
56	MG	YA	3114	1/1	0.87	0.12	22,22,22,22	0
56	MG	RA	3273	1/1	0.87	0.14	51,51,51,51	0
56	MG	QA	1650	1/1	0.87	0.15	34,34,34,34	0
56	MG	RA	3239	1/1	0.88	0.24	52,52,52,52	0
56	MG	RA	3393	1/1	0.88	0.20	28,28,28,28	0
56	MG	XA	1631	1/1	0.88	0.12	57,57,57,57	0
56	MG	YA	3379	1/1	0.88	0.20	87,87,87,87	0
56	MG	YA	3235	1/1	0.88	0.13	54,54,54,54	0
56	MG	YA	3382	1/1	0.88	0.10	47,47,47,47	0
56	MG	YA	3090	1/1	0.88	0.22	35,35,35,35	0
56	MG	YA	3244	1/1	0.88	0.29	76,76,76,76	0
56	MG	QA	1734	1/1	0.88	0.10	61,61,61,61	0
56	MG	RA	3040	1/1	0.88	0.13	24,24,24,24	0
56	MG	YA	3394	1/1	0.88	0.18	21,21,21,21	0
56	MG	RA	3251	1/1	0.88	0.28	59,59,59,59	0
56	MG	RA	3095	1/1	0.88	0.12	62,62,62,62	0
56	MG	YA	3256	1/1	0.88	0.26	58,58,58,58	0
56	MG	RB	204	1/1	0.88	0.17	61,61,61,61	0
56	MG	YA	3260	1/1	0.88	0.22	61,61,61,61	0
56	MG	YA	3104	1/1	0.88	0.12	36,36,36,36	0
56	MG	YA	3411	1/1	0.88	0.10	53,53,53,53	0
56	MG	YA	3413	1/1	0.88	0.10	42,42,42,42	0
56	MG	YA	3265	1/1	0.88	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3258	1/1	0.88	0.14	46,46,46,46	0
56	MG	XA	1747	1/1	0.88	0.17	88,88,88,88	0
56	MG	QA	1729	1/1	0.88	0.17	48,48,48,48	0
56	MG	QA	1606	1/1	0.88	0.20	27,27,27,27	0
56	MG	RA	3183	1/1	0.88	0.10	56,56,56,56	0
56	MG	XA	1673	1/1	0.88	0.11	49,49,49,49	0
56	MG	RA	3309	1/1	0.88	0.33	69,69,69,69	0
56	MG	RA	3079	1/1	0.88	0.20	37,37,37,37	0
56	MG	XA	1682	1/1	0.88	0.19	33,33,33,33	0
56	MG	RA	3270	1/1	0.88	0.17	49,49,49,49	0
56	MG	RA	3363	1/1	0.88	0.21	45,45,45,45	0
56	MG	RA	3368	1/1	0.88	0.12	51,51,51,51	0
56	MG	YA	3450	1/1	0.88	0.16	40,40,40,40	0
56	MG	YA	3321	1/1	0.88	0.20	71,71,71,71	0
56	MG	YA	3454	1/1	0.88	0.12	59,59,59,59	0
56	MG	RA	3191	1/1	0.88	0.20	18,18,18,18	0
56	MG	XA	1696	1/1	0.88	0.19	56,56,56,56	0
56	MG	RA	3375	1/1	0.88	0.22	39,39,39,39	0
56	MG	RA	3380	1/1	0.88	0.15	40,40,40,40	0
56	MG	XA	1623	1/1	0.88	0.10	36,36,36,36	0
56	MG	XA	1624	1/1	0.88	0.13	53,53,53,53	0
56	MG	YG	201	1/1	0.88	0.08	63,63,63,63	0
56	MG	YA	3344	1/1	0.88	0.14	66,66,66,66	0
56	MG	QA	1715	1/1	0.88	0.21	74,74,74,74	0
56	MG	YV	201	1/1	0.88	0.20	22,22,22,22	0
56	MG	YA	3079	1/1	0.88	0.33	33,33,33,33	0
56	MG	Y0	102	1/1	0.88	0.23	46,46,46,46	0
56	MG	RA	3146	1/1	0.89	0.17	28,28,28,28	0
56	MG	YA	3309	1/1	0.89	0.07	76,76,76,76	0
56	MG	YA	3116	1/1	0.89	0.22	58,58,58,58	0
56	MG	RA	3150	1/1	0.89	0.31	37,37,37,37	0
56	MG	YA	3122	1/1	0.89	0.23	21,21,21,21	0
56	MG	XA	1730	1/1	0.89	0.11	50,50,50,50	0
56	MG	RA	3153	1/1	0.89	0.14	31,31,31,31	0
56	MG	YA	3133	1/1	0.89	0.19	40,40,40,40	0
56	MG	RA	3297	1/1	0.89	0.18	68,68,68,68	0
56	MG	XA	1627	1/1	0.89	0.16	44,44,44,44	0
56	MG	YA	3145	1/1	0.89	0.16	46,46,46,46	0
56	MG	RA	3300	1/1	0.89	0.14	49,49,49,49	0
56	MG	QA	1717	1/1	0.89	0.14	57,57,57,57	0
56	MG	RA	3386	1/1	0.89	0.07	44,44,44,44	0
56	MG	YA	3155	1/1	0.89	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3156	1/1	0.89	0.07	42,42,42,42	0
56	MG	RA	3305	1/1	0.89	0.12	68,68,68,68	0
56	MG	RA	3307	1/1	0.89	0.31	60,60,60,60	0
56	MG	RA	3201	1/1	0.89	0.07	19,19,19,19	0
56	MG	YA	3177	1/1	0.89	0.11	57,57,57,57	0
56	MG	YA	3178	1/1	0.89	0.22	40,40,40,40	0
56	MG	XA	1649	1/1	0.89	0.17	60,60,60,60	0
56	MG	XA	1653	1/1	0.89	0.33	60,60,60,60	0
56	MG	RA	3009	1/1	0.89	0.21	24,24,24,24	0
56	MG	YA	3395	1/1	0.89	0.25	25,25,25,25	0
56	MG	RA	3260	1/1	0.89	0.14	57,57,57,57	0
56	MG	XA	1759	1/1	0.89	0.19	69,69,69,69	0
56	MG	RA	3015	1/1	0.89	0.17	30,30,30,30	0
56	MG	QA	1721	1/1	0.89	0.15	62,62,62,62	0
56	MG	RA	3413	1/1	0.89	0.20	24,24,24,24	0
56	MG	RB	203	1/1	0.89	0.27	52,52,52,52	0
56	MG	RA	3268	1/1	0.89	0.07	48,48,48,48	0
56	MG	YA	3036	1/1	0.89	0.22	45,45,45,45	0
56	MG	YA	3234	1/1	0.89	0.12	33,33,33,33	0
56	MG	RA	3212	1/1	0.89	0.10	44,44,44,44	0
56	MG	YA	3055	1/1	0.89	0.24	18,18,18,18	0
56	MG	QA	1619	1/1	0.89	0.12	27,27,27,27	0
56	MG	RA	3070	1/1	0.89	0.27	27,27,27,27	0
56	MG	YA	3249	1/1	0.89	0.19	40,40,40,40	0
56	MG	XA	1683	1/1	0.89	0.15	44,44,44,44	0
56	MG	RA	3071	1/1	0.89	0.24	50,50,50,50	0
56	MG	XA	1687	1/1	0.89	0.16	49,49,49,49	0
56	MG	RA	3230	1/1	0.89	0.12	41,41,41,41	0
56	MG	YA	3257	1/1	0.89	0.16	44,44,44,44	0
56	MG	RA	3278	1/1	0.89	0.10	67,67,67,67	0
56	MG	XA	1693	1/1	0.89	0.15	59,59,59,59	0
56	MG	YA	3082	1/1	0.89	0.15	36,36,36,36	0
56	MG	RA	3136	1/1	0.89	0.20	41,41,41,41	0
56	MG	XA	1695	1/1	0.89	0.15	46,46,46,46	0
56	MG	RA	3139	1/1	0.89	0.10	35,35,35,35	0
56	MG	RA	3353	1/1	0.89	0.16	85,85,85,85	0
56	MG	XA	1613	1/1	0.89	0.10	43,43,43,43	0
56	MG	YA	3098	1/1	0.89	0.25	66,66,66,66	0
56	MG	YA	3287	1/1	0.89	0.26	62,62,62,62	0
56	MG	QA	1620	1/1	0.89	0.09	52,52,52,52	0
56	MG	YA	3295	1/1	0.89	0.28	56,56,56,56	0
56	MG	XA	1620	1/1	0.89	0.09	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3298	1/1	0.89	0.45	82,82,82,82	0
56	MG	YA	3102	1/1	0.89	0.13	12,12,12,12	0
56	MG	XA	1716	1/1	0.89	0.27	58,58,58,58	0
56	MG	RA	3113	1/1	0.89	0.31	74,74,74,74	0
56	MG	YA	3338	1/1	0.90	0.18	63,63,63,63	0
56	MG	RA	3063	1/1	0.90	0.16	33,33,33,33	0
56	MG	XA	1685	1/1	0.90	0.26	65,65,65,65	0
56	MG	YA	3047	1/1	0.90	0.12	20,20,20,20	0
56	MG	YA	3185	1/1	0.90	0.21	36,36,36,36	0
56	MG	YA	3347	1/1	0.90	0.28	74,74,74,74	0
56	MG	YA	3048	1/1	0.90	0.20	12,12,12,12	0
56	MG	YA	3352	1/1	0.90	0.09	53,53,53,53	0
56	MG	YA	3197	1/1	0.90	0.13	15,15,15,15	0
56	MG	YA	3203	1/1	0.90	0.15	39,39,39,39	0
56	MG	YA	3212	1/1	0.90	0.14	17,17,17,17	0
56	MG	RA	3350	1/1	0.90	0.42	61,61,61,61	0
56	MG	XA	1609	1/1	0.90	0.08	70,70,70,70	0
56	MG	QA	1646	1/1	0.90	0.13	52,52,52,52	0
56	MG	RA	3243	1/1	0.90	0.08	54,54,54,54	0
56	MG	XA	1614	1/1	0.90	0.14	37,37,37,37	0
56	MG	RA	3244	1/1	0.90	0.13	42,42,42,42	0
56	MG	QA	1727	1/1	0.90	0.23	61,61,61,61	0
56	MG	QA	1601	1/1	0.90	0.26	44,44,44,44	0
56	MG	RA	3118	1/1	0.90	0.26	63,63,63,63	0
56	MG	XA	1705	1/1	0.90	0.12	53,53,53,53	0
56	MG	YA	3084	1/1	0.90	0.15	33,33,33,33	0
56	MG	YA	3399	1/1	0.90	0.14	61,61,61,61	0
56	MG	RA	3200	1/1	0.90	0.16	65,65,65,65	0
56	MG	RA	3154	1/1	0.90	0.07	35,35,35,35	0
56	MG	RA	3377	1/1	0.90	0.08	32,32,32,32	0
56	MG	RA	3203	1/1	0.90	0.11	42,42,42,42	0
56	MG	QA	1655	1/1	0.90	0.15	39,39,39,39	0
56	MG	RA	3319	1/1	0.90	0.57	96,96,96,96	0
56	MG	XA	1728	1/1	0.90	0.20	73,73,73,73	0
56	MG	QA	1660	1/1	0.90	0.18	40,40,40,40	0
56	MG	YA	3418	1/1	0.90	0.24	52,52,52,52	0
56	MG	XA	1632	1/1	0.90	0.17	39,39,39,39	0
56	MG	XA	1634	1/1	0.90	0.17	39,39,39,39	0
56	MG	YA	3424	1/1	0.90	0.08	56,56,56,56	0
56	MG	QA	1718	1/1	0.90	0.27	72,72,72,72	0
56	MG	RA	3128	1/1	0.90	0.16	33,33,33,33	0
56	MG	YA	3268	1/1	0.90	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1741	1/1	0.90	0.18	56,56,56,56	0
56	MG	YA	3118	1/1	0.90	0.21	56,56,56,56	0
56	MG	QA	1613	1/1	0.90	0.11	56,56,56,56	0
56	MG	XA	1648	1/1	0.90	0.06	71,71,71,71	0
56	MG	RA	3131	1/1	0.90	0.34	65,65,65,65	0
56	MG	YA	3284	1/1	0.90	0.17	52,52,52,52	0
56	MG	RA	3226	1/1	0.90	0.17	25,25,25,25	0
56	MG	RA	3329	1/1	0.90	0.11	60,60,60,60	0
56	MG	QA	1736	1/1	0.90	0.14	52,52,52,52	0
56	MG	RA	3332	1/1	0.90	0.30	87,87,87,87	0
56	MG	RE	301	1/1	0.90	0.22	21,21,21,21	0
56	MG	QA	1678	1/1	0.90	0.23	51,51,51,51	0
56	MG	QA	1621	1/1	0.90	0.15	38,38,38,38	0
56	MG	QA	1664	1/1	0.90	0.15	39,39,39,39	0
56	MG	RA	3181	1/1	0.90	0.10	67,67,67,67	0
56	MG	RA	3340	1/1	0.90	0.15	79,79,79,79	0
56	MG	YA	3158	1/1	0.90	0.29	53,53,53,53	0
56	MG	RA	3345	1/1	0.90	0.11	61,61,61,61	0
56	MG	YA	3328	1/1	0.90	0.20	27,27,27,27	0
56	MG	YA	3003	1/1	0.90	0.27	22,22,22,22	0
56	MG	YA	3013	1/1	0.90	0.18	11,11,11,11	0
56	MG	XA	1603	1/1	0.90	0.18	19,19,19,19	0
56	MG	Y0	103	1/1	0.90	0.23	57,57,57,57	0
56	MG	YA	3175	1/1	0.91	0.15	70,70,70,70	0
56	MG	RA	3002	1/1	0.91	0.12	15,15,15,15	0
56	MG	RA	3100	1/1	0.91	0.29	56,56,56,56	0
56	MG	YA	3341	1/1	0.91	0.19	41,41,41,41	0
56	MG	QA	1666	1/1	0.91	0.26	63,63,63,63	0
56	MG	RA	3395	1/1	0.91	0.10	45,45,45,45	0
56	MG	YA	3060	1/1	0.91	0.22	13,13,13,13	0
56	MG	RA	3012	1/1	0.91	0.20	12,12,12,12	0
56	MG	YA	3196	1/1	0.91	0.10	57,57,57,57	0
56	MG	XA	1708	1/1	0.91	0.24	41,41,41,41	0
56	MG	RA	3275	1/1	0.91	0.12	44,44,44,44	0
56	MG	RA	3330	1/1	0.91	0.17	45,45,45,45	0
56	MG	YA	3215	1/1	0.91	0.26	60,60,60,60	0
56	MG	YA	3371	1/1	0.91	0.10	56,56,56,56	0
56	MG	RA	3013	1/1	0.91	0.26	10,10,10,10	0
56	MG	RA	3279	1/1	0.91	0.15	55,55,55,55	0
56	MG	QA	1645	1/1	0.91	0.26	75,75,75,75	0
56	MG	XA	1642	1/1	0.91	0.13	54,54,54,54	0
56	MG	XA	1646	1/1	0.91	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1731	1/1	0.91	0.10	59,59,59,59	0
56	MG	YA	3388	1/1	0.91	0.10	49,49,49,49	0
56	MG	XA	1647	1/1	0.91	0.35	67,67,67,67	0
56	MG	RA	3148	1/1	0.91	0.13	43,43,43,43	0
56	MG	QA	1654	1/1	0.91	0.25	43,43,43,43	0
56	MG	RA	3290	1/1	0.91	0.13	59,59,59,59	0
56	MG	YA	3396	1/1	0.91	0.07	45,45,45,45	0
56	MG	YA	3236	1/1	0.91	0.20	30,30,30,30	0
56	MG	QA	1623	1/1	0.91	0.11	52,52,52,52	0
56	MG	YA	3100	1/1	0.91	0.27	33,33,33,33	0
56	MG	RA	3342	1/1	0.91	0.13	44,44,44,44	0
56	MG	YA	3248	1/1	0.91	0.07	43,43,43,43	0
56	MG	RA	3124	1/1	0.91	0.11	29,29,29,29	0
56	MG	QA	1658	1/1	0.91	0.15	46,46,46,46	0
56	MG	RA	3245	1/1	0.91	0.29	41,41,41,41	0
56	MG	RA	3045	1/1	0.91	0.17	18,18,18,18	0
56	MG	RA	3083	1/1	0.91	0.20	49,49,49,49	0
56	MG	RA	3046	1/1	0.91	0.11	14,14,14,14	0
56	MG	YA	3119	1/1	0.91	0.16	71,71,71,71	0
56	MG	QA	1659	1/1	0.91	0.07	41,41,41,41	0
56	MG	RA	3362	1/1	0.91	0.18	72,72,72,72	0
56	MG	YA	3128	1/1	0.91	0.28	36,36,36,36	0
56	MG	RA	3168	1/1	0.91	0.13	79,79,79,79	0
56	MG	QA	1713	1/1	0.91	0.23	46,46,46,46	0
56	MG	YA	3132	1/1	0.91	0.12	62,62,62,62	0
56	MG	RA	3370	1/1	0.91	0.23	41,41,41,41	0
56	MG	XA	1616	1/1	0.91	0.15	36,36,36,36	0
56	MG	XV	104	1/1	0.91	0.06	44,44,44,44	0
56	MG	YA	3142	1/1	0.91	0.36	45,45,45,45	0
56	MG	YA	3286	1/1	0.91	0.27	64,64,64,64	0
56	MG	XA	1688	1/1	0.91	0.10	39,39,39,39	0
56	MG	RA	3214	1/1	0.91	0.10	40,40,40,40	0
56	MG	YA	3011	1/1	0.91	0.33	26,26,26,26	0
56	MG	XA	1691	1/1	0.91	0.09	53,53,53,53	0
56	MG	YA	3154	1/1	0.91	0.20	25,25,25,25	0
56	MG	YA	3299	1/1	0.91	0.21	67,67,67,67	0
56	MG	YA	3027	1/1	0.91	0.12	28,28,28,28	0
56	MG	RA	3318	1/1	0.91	0.12	40,40,40,40	0
56	MG	YA	3464	1/1	0.91	0.24	31,31,31,31	0
56	MG	RA	3215	1/1	0.91	0.13	36,36,36,36	0
56	MG	YB	203	1/1	0.91	0.35	52,52,52,52	0
56	MG	YA	3160	1/1	0.91	0.24	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3165	1/1	0.91	0.08	50,50,50,50	0
56	MG	YA	3166	1/1	0.91	0.19	41,41,41,41	0
56	MG	YA	3042	1/1	0.91	0.20	30,30,30,30	0
56	MG	YA	3325	1/1	0.91	0.18	39,39,39,39	0
56	MG	YA	3168	1/1	0.91	0.15	52,52,52,52	0
56	MG	RA	3171	1/1	0.91	0.11	32,32,32,32	0
56	MG	RA	3221	1/1	0.91	0.17	40,40,40,40	0
56	MG	YA	3337	1/1	0.92	0.15	46,46,46,46	0
56	MG	QA	1716	1/1	0.92	0.25	68,68,68,68	0
56	MG	XA	1666	1/1	0.92	0.17	28,28,28,28	0
56	MG	RA	3356	1/1	0.92	0.21	54,54,54,54	0
56	MG	XA	1746	1/1	0.92	0.23	67,67,67,67	0
56	MG	YA	3217	1/1	0.92	0.18	24,24,24,24	0
56	MG	RA	3117	1/1	0.92	0.14	33,33,33,33	0
56	MG	XA	1605	1/1	0.92	0.19	23,23,23,23	0
56	MG	QA	1695	1/1	0.92	0.07	61,61,61,61	0
56	MG	QA	1728	1/1	0.92	0.16	61,61,61,61	0
56	MG	YA	3109	1/1	0.92	0.29	39,39,39,39	0
56	MG	YA	3355	1/1	0.92	0.16	34,34,34,34	0
56	MG	YA	3360	1/1	0.92	0.14	57,57,57,57	0
56	MG	XA	1611	1/1	0.92	0.20	38,38,38,38	0
56	MG	XA	1755	1/1	0.92	0.07	71,71,71,71	0
56	MG	YA	3370	1/1	0.92	0.10	62,62,62,62	0
56	MG	RA	3207	1/1	0.92	0.20	24,24,24,24	0
56	MG	RA	3021	1/1	0.92	0.25	23,23,23,23	0
56	MG	YA	3375	1/1	0.92	0.27	68,68,68,68	0
56	MG	RA	3163	1/1	0.92	0.16	51,51,51,51	0
56	MG	RA	3371	1/1	0.92	0.25	57,57,57,57	0
56	MG	YA	3125	1/1	0.92	0.23	48,48,48,48	0
56	MG	YA	3384	1/1	0.92	0.16	58,58,58,58	0
56	MG	RA	3033	1/1	0.92	0.16	32,32,32,32	0
56	MG	QA	1740	1/1	0.92	0.11	43,43,43,43	0
56	MG	RA	3167	1/1	0.92	0.12	52,52,52,52	0
56	MG	QE	201	1/1	0.92	0.27	52,52,52,52	0
56	MG	RA	3220	1/1	0.92	0.27	54,54,54,54	0
56	MG	RA	3388	1/1	0.92	0.25	84,84,84,84	0
56	MG	YA	3255	1/1	0.92	0.26	43,43,43,43	0
56	MG	RA	3080	1/1	0.92	0.15	18,18,18,18	0
56	MG	QA	1705	1/1	0.92	0.25	48,48,48,48	0
56	MG	QA	1730	1/1	0.92	0.08	55,55,55,55	0
56	MG	YA	3259	1/1	0.92	0.14	50,50,50,50	0
56	MG	YA	3039	1/1	0.92	0.17	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1701	1/1	0.92	0.16	53,53,53,53	0
56	MG	QA	1635	1/1	0.92	0.18	64,64,64,64	0
56	MG	YA	3152	1/1	0.92	0.09	27,27,27,27	0
56	MG	YA	3409	1/1	0.92	0.08	47,47,47,47	0
56	MG	RA	3135	1/1	0.92	0.25	86,86,86,86	0
56	MG	YA	3275	1/1	0.92	0.17	50,50,50,50	0
56	MG	RA	3282	1/1	0.92	0.17	40,40,40,40	0
56	MG	YA	3415	1/1	0.92	0.13	41,41,41,41	0
56	MG	YA	3277	1/1	0.92	0.47	59,59,59,59	0
56	MG	RA	3047	1/1	0.92	0.25	24,24,24,24	0
56	MG	RA	3286	1/1	0.92	0.17	43,43,43,43	0
56	MG	YA	3280	1/1	0.92	0.06	38,38,38,38	0
56	MG	QA	1689	1/1	0.92	0.22	61,61,61,61	0
56	MG	YA	3164	1/1	0.92	0.21	41,41,41,41	0
56	MG	XA	1717	1/1	0.92	0.22	39,39,39,39	0
56	MG	XA	1637	1/1	0.92	0.14	48,48,48,48	0
56	MG	YA	3288	1/1	0.92	0.18	39,39,39,39	0
56	MG	YA	3066	1/1	0.92	0.25	25,25,25,25	0
56	MG	RB	202	1/1	0.92	0.19	35,35,35,35	0
56	MG	YA	3170	1/1	0.92	0.27	45,45,45,45	0
56	MG	YA	3171	1/1	0.92	0.05	26,26,26,26	0
56	MG	YA	3068	1/1	0.92	0.10	30,30,30,30	0
56	MG	YA	3300	1/1	0.92	0.28	74,74,74,74	0
56	MG	XA	1721	1/1	0.92	0.10	46,46,46,46	0
56	MG	RA	3049	1/1	0.92	0.16	4,4,4,4	0
56	MG	YA	3304	1/1	0.92	0.14	38,38,38,38	0
56	MG	QA	1624	1/1	0.92	0.14	72,72,72,72	0
56	MG	RA	3185	1/1	0.92	0.26	36,36,36,36	0
56	MG	RA	3242	1/1	0.92	0.16	34,34,34,34	0
56	MG	RQ	202	1/1	0.92	0.14	53,53,53,53	0
56	MG	YB	201	1/1	0.92	0.16	42,42,42,42	0
56	MG	YA	3316	1/1	0.92	0.34	60,60,60,60	0
56	MG	YA	3320	1/1	0.92	0.29	39,39,39,39	0
56	MG	YA	3182	1/1	0.92	0.22	55,55,55,55	0
56	MG	YA	3323	1/1	0.92	0.13	39,39,39,39	0
56	MG	YA	3183	1/1	0.92	0.20	35,35,35,35	0
56	MG	RA	3053	1/1	0.92	0.17	35,35,35,35	0
56	MG	QA	1657	1/1	0.92	0.20	36,36,36,36	0
56	MG	YA	3334	1/1	0.92	0.16	65,65,65,65	0
56	MG	RA	3352	1/1	0.92	0.87	67,67,67,67	0
56	MG	RA	3060	1/1	0.92	0.19	26,26,26,26	0
56	MG	RA	3204	1/1	0.93	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3317	1/1	0.93	0.10	41,41,41,41	0
56	MG	YA	3318	1/1	0.93	0.18	19,19,19,19	0
56	MG	RP	202	1/1	0.93	0.10	31,31,31,31	0
56	MG	YA	3020	1/1	0.93	0.20	32,32,32,32	0
56	MG	RA	3149	1/1	0.93	0.21	60,60,60,60	0
56	MG	RA	3104	1/1	0.93	0.21	40,40,40,40	0
56	MG	YA	3326	1/1	0.93	0.20	52,52,52,52	0
56	MG	YA	3031	1/1	0.93	0.19	29,29,29,29	0
56	MG	RA	3106	1/1	0.93	0.14	23,23,23,23	0
56	MG	RA	3107	1/1	0.93	0.42	50,50,50,50	0
56	MG	YA	3041	1/1	0.93	0.18	14,14,14,14	0
56	MG	RA	3109	1/1	0.93	0.29	21,21,21,21	0
56	MG	QA	1638	1/1	0.93	0.21	58,58,58,58	0
56	MG	RA	3343	1/1	0.93	0.08	57,57,57,57	0
56	MG	QA	1611	1/1	0.93	0.14	41,41,41,41	0
56	MG	YA	3052	1/1	0.93	0.22	40,40,40,40	0
56	MG	QA	1614	1/1	0.93	0.08	55,55,55,55	0
56	MG	RA	3164	1/1	0.93	0.19	30,30,30,30	0
56	MG	RA	3351	1/1	0.93	0.17	54,54,54,54	0
56	MG	YA	3188	1/1	0.93	0.12	24,24,24,24	0
56	MG	QA	1615	1/1	0.93	0.15	44,44,44,44	0
56	MG	YA	3190	1/1	0.93	0.20	39,39,39,39	0
56	MG	YA	3353	1/1	0.93	0.23	53,53,53,53	0
56	MG	QA	1617	1/1	0.93	0.12	42,42,42,42	0
56	MG	XA	1697	1/1	0.93	0.17	50,50,50,50	0
56	MG	YA	3358	1/1	0.93	0.15	60,60,60,60	0
56	MG	YA	3201	1/1	0.93	0.12	32,32,32,32	0
56	MG	RA	3354	1/1	0.93	0.23	71,71,71,71	0
56	MG	YA	3209	1/1	0.93	0.13	25,25,25,25	0
56	MG	XA	1700	1/1	0.93	0.08	87,87,87,87	0
56	MG	YA	3069	1/1	0.93	0.23	17,17,17,17	0
56	MG	RA	3120	1/1	0.93	0.24	20,20,20,20	0
56	MG	YA	3077	1/1	0.93	0.14	17,17,17,17	0
56	MG	RA	3043	1/1	0.93	0.27	28,28,28,28	0
56	MG	RA	3123	1/1	0.93	0.11	39,39,39,39	0
56	MG	RA	3075	1/1	0.93	0.11	18,18,18,18	0
56	MG	YA	3225	1/1	0.93	0.27	38,38,38,38	0
56	MG	XA	1617	1/1	0.93	0.27	50,50,50,50	0
56	MG	XA	1711	1/1	0.93	0.20	53,53,53,53	0
56	MG	YA	3086	1/1	0.93	0.14	37,37,37,37	0
56	MG	RA	3076	1/1	0.93	0.15	35,35,35,35	0
56	MG	XA	1715	1/1	0.93	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1628	1/1	0.93	0.27	44,44,44,44	0
56	MG	RA	3366	1/1	0.93	0.25	33,33,33,33	0
56	MG	YA	3237	1/1	0.93	0.28	34,34,34,34	0
56	MG	YA	3096	1/1	0.93	0.17	24,24,24,24	0
56	MG	YA	3243	1/1	0.93	0.18	48,48,48,48	0
56	MG	RA	3367	1/1	0.93	0.14	39,39,39,39	0
56	MG	RA	3296	1/1	0.93	0.19	46,46,46,46	0
56	MG	QA	1647	1/1	0.93	0.27	56,56,56,56	0
56	MG	XA	1723	1/1	0.93	0.12	47,47,47,47	0
56	MG	RA	3178	1/1	0.93	0.20	38,38,38,38	0
56	MG	QA	1687	1/1	0.93	0.12	33,33,33,33	0
56	MG	YA	3410	1/1	0.93	0.18	61,61,61,61	0
56	MG	QA	1649	1/1	0.93	0.15	32,32,32,32	0
56	MG	RA	3089	1/1	0.93	0.17	16,16,16,16	0
56	MG	YA	3108	1/1	0.93	0.23	25,25,25,25	0
56	MG	XA	1735	1/1	0.93	0.26	27,27,27,27	0
56	MG	YA	3417	1/1	0.93	0.09	53,53,53,53	0
56	MG	YA	3110	1/1	0.93	0.10	10,10,10,10	0
56	MG	YA	3113	1/1	0.93	0.16	56,56,56,56	0
56	MG	YA	3421	1/1	0.93	0.16	38,38,38,38	0
56	MG	QA	1602	1/1	0.93	0.27	33,33,33,33	0
56	MG	XA	1633	1/1	0.93	0.17	50,50,50,50	0
56	MG	RA	3381	1/1	0.93	0.10	37,37,37,37	0
56	MG	YA	3266	1/1	0.93	0.31	71,71,71,71	0
56	MG	RA	3383	1/1	0.93	0.17	53,53,53,53	0
56	MG	YA	3434	1/1	0.93	0.43	67,67,67,67	0
56	MG	RA	3313	1/1	0.93	0.21	50,50,50,50	0
56	MG	YA	3436	1/1	0.93	0.23	52,52,52,52	0
56	MG	QA	1652	1/1	0.93	0.15	60,60,60,60	0
56	MG	QA	1667	1/1	0.93	0.14	52,52,52,52	0
56	MG	RA	3252	1/1	0.93	0.10	43,43,43,43	0
56	MG	YA	3442	1/1	0.93	0.18	77,77,77,77	0
56	MG	RA	3098	1/1	0.93	0.17	22,22,22,22	0
56	MG	RA	3255	1/1	0.93	0.09	64,64,64,64	0
56	MG	XA	1749	1/1	0.93	0.28	74,74,74,74	0
56	MG	RA	3396	1/1	0.93	0.12	49,49,49,49	0
56	MG	RA	3256	1/1	0.93	0.10	59,59,59,59	0
56	MG	YA	3136	1/1	0.93	0.15	31,31,31,31	0
56	MG	YA	3456	1/1	0.93	0.12	50,50,50,50	0
56	MG	RA	3193	1/1	0.93	0.17	33,33,33,33	0
56	MG	YA	3141	1/1	0.93	0.20	41,41,41,41	0
56	MG	RA	3404	1/1	0.93	0.28	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3291	1/1	0.93	0.23	63,63,63,63	0
56	MG	RA	3326	1/1	0.93	0.12	52,52,52,52	0
56	MG	RA	3411	1/1	0.93	0.10	35,35,35,35	0
56	MG	XA	1658	1/1	0.93	0.13	40,40,40,40	0
56	MG	QA	1637	1/1	0.93	0.17	59,59,59,59	0
56	MG	XA	1660	1/1	0.93	0.32	60,60,60,60	0
56	MG	YB	205	1/1	0.93	0.07	62,62,62,62	0
56	MG	YE	301	1/1	0.93	0.16	50,50,50,50	0
56	MG	RA	3198	1/1	0.93	0.24	45,45,45,45	0
56	MG	XV	102	1/1	0.93	0.12	36,36,36,36	0
56	MG	RA	3017	1/1	0.93	0.15	9,9,9,9	0
56	MG	YR	201	1/1	0.93	0.15	39,39,39,39	0
56	MG	RA	3061	1/1	0.93	0.20	25,25,25,25	0
56	MG	YA	3159	1/1	0.93	0.15	58,58,58,58	0
56	MG	RA	3102	1/1	0.93	0.23	54,54,54,54	0
56	MG	YA	3163	1/1	0.93	0.10	33,33,33,33	0
57	ZN	QD	301	1/1	0.93	0.24	58,58,58,58	0
56	MG	RA	3283	1/1	0.94	0.18	40,40,40,40	0
56	MG	XA	1601	1/1	0.94	0.22	43,43,43,43	0
56	MG	YA	3044	1/1	0.94	0.17	14,14,14,14	0
56	MG	YA	3322	1/1	0.94	0.10	50,50,50,50	0
56	MG	QA	1642	1/1	0.94	0.15	28,28,28,28	0
56	MG	QA	1625	1/1	0.94	0.08	35,35,35,35	0
56	MG	RA	3287	1/1	0.94	0.09	64,64,64,64	0
56	MG	RA	3041	1/1	0.94	0.12	31,31,31,31	0
56	MG	XA	1608	1/1	0.94	0.31	52,52,52,52	0
56	MG	YA	3333	1/1	0.94	0.18	63,63,63,63	0
56	MG	YA	3179	1/1	0.94	0.15	45,45,45,45	0
56	MG	RA	3119	1/1	0.94	0.07	33,33,33,33	0
56	MG	XA	1610	1/1	0.94	0.16	46,46,46,46	0
56	MG	YA	3059	1/1	0.94	0.20	23,23,23,23	0
56	MG	QA	1668	1/1	0.94	0.21	68,68,68,68	0
56	MG	YA	3184	1/1	0.94	0.17	83,83,83,83	0
56	MG	RA	3291	1/1	0.94	0.06	26,26,26,26	0
56	MG	RA	3225	1/1	0.94	0.08	51,51,51,51	0
56	MG	RA	3121	1/1	0.94	0.16	14,14,14,14	0
56	MG	XA	1704	1/1	0.94	0.29	55,55,55,55	0
56	MG	YA	3345	1/1	0.94	0.21	34,34,34,34	0
56	MG	QA	1626	1/1	0.94	0.26	59,59,59,59	0
56	MG	YA	3349	1/1	0.94	0.22	58,58,58,58	0
56	MG	YA	3071	1/1	0.94	0.15	24,24,24,24	0
56	MG	YA	3072	1/1	0.94	0.22	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3202	1/1	0.94	0.26	42,42,42,42	0
56	MG	RA	3044	1/1	0.94	0.18	13,13,13,13	0
56	MG	YA	3207	1/1	0.94	0.13	29,29,29,29	0
56	MG	QA	1671	1/1	0.94	0.07	36,36,36,36	0
56	MG	RA	3006	1/1	0.94	0.11	11,11,11,11	0
56	MG	XA	1712	1/1	0.94	0.13	41,41,41,41	0
56	MG	RA	3298	1/1	0.94	0.05	63,63,63,63	0
56	MG	YA	3366	1/1	0.94	0.14	47,47,47,47	0
56	MG	YA	3368	1/1	0.94	0.16	53,53,53,53	0
56	MG	RA	3174	1/1	0.94	0.32	64,64,64,64	0
56	MG	YA	3083	1/1	0.94	0.08	30,30,30,30	0
56	MG	YA	3372	1/1	0.94	0.15	45,45,45,45	0
56	MG	RA	3301	1/1	0.94	0.28	53,53,53,53	0
56	MG	RA	3007	1/1	0.94	0.30	40,40,40,40	0
56	MG	QA	1688	1/1	0.94	0.21	26,26,26,26	0
56	MG	RA	3378	1/1	0.94	0.07	18,18,18,18	0
56	MG	QA	1627	1/1	0.94	0.08	104,104,104,104	0
56	MG	YA	3094	1/1	0.94	0.27	58,58,58,58	0
56	MG	XA	1722	1/1	0.94	0.09	61,61,61,61	0
56	MG	YA	3233	1/1	0.94	0.29	45,45,45,45	0
56	MG	RA	3091	1/1	0.94	0.07	48,48,48,48	0
56	MG	QA	1610	1/1	0.94	0.07	64,64,64,64	0
56	MG	YA	3392	1/1	0.94	0.18	20,20,20,20	0
56	MG	XA	1727	1/1	0.94	0.28	59,59,59,59	0
56	MG	RA	3384	1/1	0.94	0.30	61,61,61,61	0
56	MG	XA	1729	1/1	0.94	0.10	37,37,37,37	0
56	MG	YA	3241	1/1	0.94	0.16	40,40,40,40	0
56	MG	RA	3052	1/1	0.94	0.12	34,34,34,34	0
56	MG	RA	3387	1/1	0.94	0.20	41,41,41,41	0
56	MG	RA	3315	1/1	0.94	0.17	62,62,62,62	0
56	MG	YA	3246	1/1	0.94	0.24	61,61,61,61	0
56	MG	YA	3247	1/1	0.94	0.07	42,42,42,42	0
56	MG	QA	1692	1/1	0.94	0.13	42,42,42,42	0
56	MG	YA	3106	1/1	0.94	0.18	17,17,17,17	0
56	MG	RA	3390	1/1	0.94	0.16	53,53,53,53	0
56	MG	XA	1638	1/1	0.94	0.11	76,76,76,76	0
56	MG	RA	3184	1/1	0.94	0.28	71,71,71,71	0
56	MG	YA	3412	1/1	0.94	0.07	38,38,38,38	0
56	MG	XA	1640	1/1	0.94	0.21	54,54,54,54	0
56	MG	QA	1710	1/1	0.94	0.35	54,54,54,54	0
56	MG	YA	3115	1/1	0.94	0.14	33,33,33,33	0
56	MG	XA	1643	1/1	0.94	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1644	1/1	0.94	0.13	34,34,34,34	0
56	MG	RA	3137	1/1	0.94	0.11	47,47,47,47	0
56	MG	YA	3262	1/1	0.94	0.27	39,39,39,39	0
56	MG	RA	3323	1/1	0.94	0.10	43,43,43,43	0
56	MG	RA	3138	1/1	0.94	0.13	21,21,21,21	0
56	MG	RA	3059	1/1	0.94	0.12	15,15,15,15	0
56	MG	YA	3428	1/1	0.94	0.10	50,50,50,50	0
56	MG	RA	3195	1/1	0.94	0.22	26,26,26,26	0
56	MG	YA	3431	1/1	0.94	0.16	36,36,36,36	0
56	MG	XA	1752	1/1	0.94	0.12	83,83,83,83	0
56	MG	YA	3270	1/1	0.94	0.20	45,45,45,45	0
56	MG	YA	3273	1/1	0.94	0.21	50,50,50,50	0
56	MG	RA	3019	1/1	0.94	0.21	13,13,13,13	0
56	MG	XA	1655	1/1	0.94	0.14	42,42,42,42	0
56	MG	RA	3408	1/1	0.94	0.20	28,28,28,28	0
56	MG	QA	1609	1/1	0.94	0.25	50,50,50,50	0
56	MG	YA	3135	1/1	0.94	0.17	29,29,29,29	0
56	MG	YA	3443	1/1	0.94	0.10	54,54,54,54	0
56	MG	RA	3199	1/1	0.94	0.25	37,37,37,37	0
56	MG	RA	3145	1/1	0.94	0.14	54,54,54,54	0
56	MG	RA	3022	1/1	0.94	0.07	56,56,56,56	0
56	MG	YA	3449	1/1	0.94	0.24	60,60,60,60	0
56	MG	YA	3285	1/1	0.94	0.13	68,68,68,68	0
56	MG	YA	3451	1/1	0.94	0.15	50,50,50,50	0
56	MG	XA	1662	1/1	0.94	0.14	34,34,34,34	0
56	MG	YA	3453	1/1	0.94	0.06	35,35,35,35	0
56	MG	YA	3143	1/1	0.94	0.13	80,80,80,80	0
56	MG	XN	102	1/1	0.94	0.09	62,62,62,62	0
56	MG	RA	3202	1/1	0.94	0.20	32,32,32,32	0
56	MG	RA	3105	1/1	0.94	0.10	36,36,36,36	0
56	MG	YA	3294	1/1	0.94	0.09	35,35,35,35	0
56	MG	YA	3149	1/1	0.94	0.07	34,34,34,34	0
56	MG	RA	3064	1/1	0.94	0.24	18,18,18,18	0
56	MG	RA	3032	1/1	0.94	0.29	25,25,25,25	0
56	MG	YA	3007	1/1	0.94	0.22	39,39,39,39	0
56	MG	RA	3151	1/1	0.94	0.13	35,35,35,35	0
56	MG	RA	3066	1/1	0.94	0.14	38,38,38,38	0
56	MG	XA	1681	1/1	0.94	0.18	39,39,39,39	0
56	MG	YA	3021	1/1	0.94	0.26	24,24,24,24	0
56	MG	QL	201	1/1	0.94	0.09	63,63,63,63	0
56	MG	YA	3306	1/1	0.94	0.34	56,56,56,56	0
56	MG	YN	201	1/1	0.94	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YO	201	1/1	0.94	0.13	63,63,63,63	0
56	MG	YQ	201	1/1	0.94	0.10	35,35,35,35	0
56	MG	RA	3069	1/1	0.94	0.18	30,30,30,30	0
56	MG	RY	201	1/1	0.94	0.08	21,21,21,21	0
56	MG	YA	3033	1/1	0.94	0.16	19,19,19,19	0
56	MG	YA	3312	1/1	0.94	0.29	52,52,52,52	0
56	MG	Y0	101	1/1	0.94	0.11	30,30,30,30	0
56	MG	YA	3313	1/1	0.94	0.14	54,54,54,54	0
56	MG	RA	3280	1/1	0.94	0.22	43,43,43,43	0
56	MG	Y5	102	1/1	0.94	0.10	39,39,39,39	0
56	MG	RA	3115	1/1	0.94	0.17	42,42,42,42	0
57	ZN	QN	100	1/1	0.94	0.09	100,100,100,100	0
56	MG	RA	3004	1/1	0.95	0.24	10,10,10,10	0
56	MG	YA	3034	1/1	0.95	0.11	31,31,31,31	0
56	MG	YA	3035	1/1	0.95	0.17	24,24,24,24	0
56	MG	RA	3236	1/1	0.95	0.16	48,48,48,48	0
56	MG	YA	3332	1/1	0.95	0.31	43,43,43,43	0
56	MG	XA	1690	1/1	0.95	0.12	40,40,40,40	0
56	MG	QA	1675	1/1	0.95	0.13	50,50,50,50	0
56	MG	RA	3142	1/1	0.95	0.32	44,44,44,44	0
56	MG	RA	3360	1/1	0.95	0.17	31,31,31,31	0
56	MG	RA	3143	1/1	0.95	0.09	23,23,23,23	0
56	MG	YA	3046	1/1	0.95	0.16	32,32,32,32	0
56	MG	YA	3339	1/1	0.95	0.15	40,40,40,40	0
56	MG	RA	3073	1/1	0.95	0.14	31,31,31,31	0
56	MG	RA	3364	1/1	0.95	0.17	17,17,17,17	0
56	MG	YA	3049	1/1	0.95	0.06	29,29,29,29	0
56	MG	YA	3186	1/1	0.95	0.14	58,58,58,58	0
56	MG	RA	3365	1/1	0.95	0.28	43,43,43,43	0
56	MG	XA	1698	1/1	0.95	0.14	66,66,66,66	0
56	MG	YA	3346	1/1	0.95	0.10	34,34,34,34	0
56	MG	RA	3241	1/1	0.95	0.16	68,68,68,68	0
56	MG	YA	3194	1/1	0.95	0.21	39,39,39,39	0
56	MG	YA	3350	1/1	0.95	0.24	58,58,58,58	0
56	MG	RA	3188	1/1	0.95	0.16	8,8,8,8	0
56	MG	QA	1669	1/1	0.95	0.20	52,52,52,52	0
56	MG	YA	3198	1/1	0.95	0.25	27,27,27,27	0
56	MG	RA	3111	1/1	0.95	0.13	39,39,39,39	0
56	MG	QA	1703	1/1	0.95	0.18	43,43,43,43	0
56	MG	YA	3063	1/1	0.95	0.19	29,29,29,29	0
56	MG	YA	3359	1/1	0.95	0.07	39,39,39,39	0
56	MG	RA	3372	1/1	0.95	0.09	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3011	1/1	0.95	0.17	4,4,4,4	0
56	MG	RA	3308	1/1	0.95	0.22	38,38,38,38	0
56	MG	YA	3213	1/1	0.95	0.07	42,42,42,42	0
56	MG	XA	1710	1/1	0.95	0.13	63,63,63,63	0
56	MG	YA	3070	1/1	0.95	0.17	39,39,39,39	0
56	MG	RA	3250	1/1	0.95	0.23	55,55,55,55	0
56	MG	YA	3218	1/1	0.95	0.07	30,30,30,30	0
56	MG	RA	3078	1/1	0.95	0.15	13,13,13,13	0
56	MG	QA	1723	1/1	0.95	0.09	98,98,98,98	0
56	MG	YA	3376	1/1	0.95	0.10	41,41,41,41	0
56	MG	QA	1656	1/1	0.95	0.16	38,38,38,38	0
56	MG	XA	1626	1/1	0.95	0.33	51,51,51,51	0
56	MG	YA	3381	1/1	0.95	0.07	58,58,58,58	0
56	MG	YA	3226	1/1	0.95	0.31	39,39,39,39	0
56	MG	YA	3383	1/1	0.95	0.17	47,47,47,47	0
56	MG	RA	3382	1/1	0.95	0.10	49,49,49,49	0
56	MG	YA	3385	1/1	0.95	0.12	67,67,67,67	0
56	MG	RA	3317	1/1	0.95	0.07	33,33,33,33	0
56	MG	YA	3230	1/1	0.95	0.29	69,69,69,69	0
56	MG	RA	3081	1/1	0.95	0.20	17,17,17,17	0
56	MG	QA	1739	1/1	0.95	0.06	49,49,49,49	0
56	MG	QA	1691	1/1	0.95	0.05	44,44,44,44	0
56	MG	RA	3160	1/1	0.95	0.06	36,36,36,36	0
56	MG	RA	3088	1/1	0.95	0.16	24,24,24,24	0
56	MG	XA	1725	1/1	0.95	0.18	51,51,51,51	0
56	MG	XA	1726	1/1	0.95	0.29	55,55,55,55	0
56	MG	YA	3093	1/1	0.95	0.10	51,51,51,51	0
56	MG	YA	3240	1/1	0.95	0.24	47,47,47,47	0
56	MG	RA	3205	1/1	0.95	0.20	44,44,44,44	0
56	MG	QA	1707	1/1	0.95	0.10	47,47,47,47	0
56	MG	RA	3267	1/1	0.95	0.19	63,63,63,63	0
56	MG	RA	3394	1/1	0.95	0.06	57,57,57,57	0
56	MG	QA	1639	1/1	0.95	0.06	52,52,52,52	0
56	MG	XA	1732	1/1	0.95	0.14	40,40,40,40	0
56	MG	XA	1734	1/1	0.95	0.08	44,44,44,44	0
56	MG	QA	1681	1/1	0.95	0.11	35,35,35,35	0
56	MG	XA	1641	1/1	0.95	0.14	57,57,57,57	0
56	MG	RA	3092	1/1	0.95	0.17	31,31,31,31	0
56	MG	RA	3401	1/1	0.95	0.07	54,54,54,54	0
56	MG	YA	3105	1/1	0.95	0.28	42,42,42,42	0
56	MG	RA	3025	1/1	0.95	0.21	34,34,34,34	0
56	MG	RA	3272	1/1	0.95	0.29	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3419	1/1	0.95	0.21	59,59,59,59	0
56	MG	RA	3213	1/1	0.95	0.19	31,31,31,31	0
56	MG	RA	3030	1/1	0.95	0.22	35,35,35,35	0
56	MG	YA	3111	1/1	0.95	0.22	36,36,36,36	0
56	MG	YA	3261	1/1	0.95	0.13	67,67,67,67	0
56	MG	YA	3425	1/1	0.95	0.13	43,43,43,43	0
56	MG	XA	1744	1/1	0.95	0.16	50,50,50,50	0
56	MG	RA	3410	1/1	0.95	0.13	26,26,26,26	0
56	MG	YA	3264	1/1	0.95	0.15	66,66,66,66	0
56	MG	YA	3430	1/1	0.95	0.18	17,17,17,17	0
56	MG	QV	103	1/1	0.95	0.15	55,55,55,55	0
56	MG	QA	1605	1/1	0.95	0.17	36,36,36,36	0
56	MG	YA	3267	1/1	0.95	0.23	48,48,48,48	0
56	MG	RA	3219	1/1	0.95	0.22	48,48,48,48	0
56	MG	RB	201	1/1	0.95	0.15	26,26,26,26	0
56	MG	YA	3120	1/1	0.95	0.26	32,32,32,32	0
56	MG	RA	3339	1/1	0.95	0.20	55,55,55,55	0
56	MG	YA	3439	1/1	0.95	0.15	32,32,32,32	0
56	MG	YA	3440	1/1	0.95	0.17	59,59,59,59	0
56	MG	QA	1651	1/1	0.95	0.19	30,30,30,30	0
56	MG	YA	3124	1/1	0.95	0.21	33,33,33,33	0
56	MG	RA	3341	1/1	0.95	0.18	41,41,41,41	0
56	MG	YA	3126	1/1	0.95	0.05	51,51,51,51	0
56	MG	YA	3445	1/1	0.95	0.28	55,55,55,55	0
56	MG	RD	301	1/1	0.95	0.09	34,34,34,34	0
56	MG	XA	1661	1/1	0.95	0.11	39,39,39,39	0
56	MG	XA	1756	1/1	0.95	0.18	50,50,50,50	0
56	MG	YA	3283	1/1	0.95	0.10	31,31,31,31	0
56	MG	XA	1757	1/1	0.95	0.13	58,58,58,58	0
56	MG	RA	3134	1/1	0.95	0.26	50,50,50,50	0
56	MG	XA	1663	1/1	0.95	0.17	46,46,46,46	0
56	MG	RP	201	1/1	0.95	0.07	38,38,38,38	0
56	MG	XA	1670	1/1	0.95	0.21	36,36,36,36	0
56	MG	YA	3139	1/1	0.95	0.14	50,50,50,50	0
56	MG	RA	3036	1/1	0.95	0.18	14,14,14,14	0
56	MG	RA	3224	1/1	0.95	0.17	37,37,37,37	0
56	MG	RA	3347	1/1	0.95	0.23	52,52,52,52	0
56	MG	XV	103	1/1	0.95	0.25	40,40,40,40	0
56	MG	RA	3037	1/1	0.95	0.16	22,22,22,22	0
56	MG	XA	1675	1/1	0.95	0.12	33,33,33,33	0
56	MG	YA	3002	1/1	0.95	0.11	6,6,6,6	0
56	MG	XA	1676	1/1	0.95	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3005	1/1	0.95	0.17	6,6,6,6	0
56	MG	YA	3006	1/1	0.95	0.14	23,23,23,23	0
56	MG	XA	1677	1/1	0.95	0.07	49,49,49,49	0
56	MG	YA	3009	1/1	0.95	0.14	14,14,14,14	0
56	MG	YA	3010	1/1	0.95	0.16	3,3,3,3	0
56	MG	YA	3157	1/1	0.95	0.16	16,16,16,16	0
56	MG	QA	1685	1/1	0.95	0.24	38,38,38,38	0
56	MG	YA	3012	1/1	0.95	0.21	20,20,20,20	0
56	MG	RA	3179	1/1	0.95	0.25	61,61,61,61	0
56	MG	YU	3400	1/1	0.95	0.09	47,47,47,47	0
56	MG	YA	3315	1/1	0.95	0.12	47,47,47,47	0
56	MG	YA	3016	1/1	0.95	0.08	18,18,18,18	0
56	MG	R0	101	1/1	0.95	0.16	43,43,43,43	0
56	MG	RA	3228	1/1	0.95	0.40	50,50,50,50	0
56	MG	YA	3024	1/1	0.95	0.18	21,21,21,21	0
56	MG	Y1	101	1/1	0.95	0.15	26,26,26,26	0
56	MG	R5	101	1/1	0.95	0.15	27,27,27,27	0
56	MG	RA	3229	1/1	0.95	0.12	31,31,31,31	0
56	MG	QA	1674	1/1	0.95	0.13	55,55,55,55	0
56	MG	XA	1664	1/1	0.96	0.19	59,59,59,59	0
56	MG	RA	3197	1/1	0.96	0.11	28,28,28,28	0
56	MG	YA	3365	1/1	0.96	0.11	45,45,45,45	0
56	MG	XA	1669	1/1	0.96	0.14	35,35,35,35	0
56	MG	YA	3254	1/1	0.96	0.21	47,47,47,47	0
56	MG	RA	3234	1/1	0.96	0.20	38,38,38,38	0
56	MG	YA	3051	1/1	0.96	0.20	15,15,15,15	0
56	MG	QV	102	1/1	0.96	0.10	38,38,38,38	0
56	MG	YA	3373	1/1	0.96	0.19	41,41,41,41	0
56	MG	YA	3054	1/1	0.96	0.14	19,19,19,19	0
56	MG	RA	3038	1/1	0.96	0.18	47,47,47,47	0
56	MG	RA	3140	1/1	0.96	0.12	30,30,30,30	0
56	MG	RA	3054	1/1	0.96	0.26	21,21,21,21	0
56	MG	RA	3285	1/1	0.96	0.20	60,60,60,60	0
56	MG	RA	3039	1/1	0.96	0.16	14,14,14,14	0
56	MG	QA	1712	1/1	0.96	0.16	34,34,34,34	0
56	MG	RA	3172	1/1	0.96	0.28	16,16,16,16	0
56	MG	XA	1680	1/1	0.96	0.05	38,38,38,38	0
56	MG	RA	3024	1/1	0.96	0.14	28,28,28,28	0
56	MG	RA	3392	1/1	0.96	0.21	16,16,16,16	0
56	MG	YA	3162	1/1	0.96	0.07	48,48,48,48	0
56	MG	RA	3103	1/1	0.96	0.14	44,44,44,44	0
56	MG	YA	3272	1/1	0.96	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1748	1/1	0.96	0.16	57,57,57,57	0
56	MG	YA	3274	1/1	0.96	0.13	28,28,28,28	0
56	MG	QA	1677	1/1	0.96	0.25	42,42,42,42	0
56	MG	RA	3246	1/1	0.96	0.23	47,47,47,47	0
56	MG	XA	1686	1/1	0.96	0.09	40,40,40,40	0
56	MG	YA	3075	1/1	0.96	0.16	23,23,23,23	0
56	MG	RA	3176	1/1	0.96	0.11	25,25,25,25	0
56	MG	RA	3397	1/1	0.96	0.30	55,55,55,55	0
56	MG	RA	3399	1/1	0.96	0.07	42,42,42,42	0
56	MG	YA	3282	1/1	0.96	0.17	44,44,44,44	0
56	MG	YA	3405	1/1	0.96	0.11	22,22,22,22	0
56	MG	RA	3248	1/1	0.96	0.22	35,35,35,35	0
56	MG	RA	3344	1/1	0.96	0.07	43,43,43,43	0
56	MG	RA	3062	1/1	0.96	0.13	11,11,11,11	0
56	MG	RA	3403	1/1	0.96	0.09	52,52,52,52	0
56	MG	YA	3085	1/1	0.96	0.09	33,33,33,33	0
56	MG	RA	3211	1/1	0.96	0.15	16,16,16,16	0
56	MG	YA	3289	1/1	0.96	0.22	43,43,43,43	0
56	MG	XA	1760	1/1	0.96	0.05	79,79,79,79	0
56	MG	RA	3127	1/1	0.96	0.06	23,23,23,23	0
56	MG	YA	3416	1/1	0.96	0.20	79,79,79,79	0
56	MG	YA	3292	1/1	0.96	0.10	45,45,45,45	0
56	MG	YA	3293	1/1	0.96	0.26	48,48,48,48	0
56	MG	RA	3407	1/1	0.96	0.24	52,52,52,52	0
56	MG	YA	3091	1/1	0.96	0.29	29,29,29,29	0
56	MG	YA	3092	1/1	0.96	0.19	22,22,22,22	0
56	MG	RA	3253	1/1	0.96	0.18	47,47,47,47	0
56	MG	RA	3409	1/1	0.96	0.05	39,39,39,39	0
56	MG	XV	101	1/1	0.96	0.18	51,51,51,51	0
56	MG	RA	3027	1/1	0.96	0.22	24,24,24,24	0
56	MG	YA	3302	1/1	0.96	0.14	36,36,36,36	0
56	MG	YA	3192	1/1	0.96	0.22	25,25,25,25	0
56	MG	RA	3028	1/1	0.96	0.10	24,24,24,24	0
56	MG	RA	3303	1/1	0.96	0.24	55,55,55,55	0
56	MG	RA	3152	1/1	0.96	0.16	37,37,37,37	0
56	MG	RA	3130	1/1	0.96	0.16	27,27,27,27	0
56	MG	YA	3200	1/1	0.96	0.27	60,60,60,60	0
56	MG	YA	3310	1/1	0.96	0.09	56,56,56,56	0
56	MG	RA	3306	1/1	0.96	0.15	40,40,40,40	0
56	MG	QA	1616	1/1	0.96	0.09	46,46,46,46	0
56	MG	XA	1707	1/1	0.96	0.23	31,31,31,31	0
56	MG	YA	3204	1/1	0.96	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3206	1/1	0.96	0.14	38,38,38,38	0
56	MG	RA	3031	1/1	0.96	0.12	15,15,15,15	0
56	MG	YA	3008	1/1	0.96	0.06	8,8,8,8	0
56	MG	YA	3211	1/1	0.96	0.15	22,22,22,22	0
56	MG	XA	1709	1/1	0.96	0.23	45,45,45,45	0
56	MG	QA	1684	1/1	0.96	0.13	46,46,46,46	0
56	MG	RA	3310	1/1	0.96	0.05	12,12,12,12	0
56	MG	YA	3448	1/1	0.96	0.09	51,51,51,51	0
56	MG	YA	3324	1/1	0.96	0.21	33,33,33,33	0
56	MG	XA	1645	1/1	0.96	0.17	47,47,47,47	0
56	MG	XA	1713	1/1	0.96	0.20	27,27,27,27	0
56	MG	YA	3327	1/1	0.96	0.21	24,24,24,24	0
56	MG	YA	3014	1/1	0.96	0.20	25,25,25,25	0
56	MG	YA	3329	1/1	0.96	0.08	40,40,40,40	0
56	MG	YA	3330	1/1	0.96	0.22	20,20,20,20	0
56	MG	YA	3457	1/1	0.96	0.15	44,44,44,44	0
56	MG	YA	3219	1/1	0.96	0.05	38,38,38,38	0
56	MG	YA	3459	1/1	0.96	0.17	57,57,57,57	0
56	MG	RF	301	1/1	0.96	0.06	27,27,27,27	0
56	MG	YA	3019	1/1	0.96	0.18	17,17,17,17	0
56	MG	RA	3187	1/1	0.96	0.19	59,59,59,59	0
56	MG	YA	3117	1/1	0.96	0.16	36,36,36,36	0
56	MG	RA	3158	1/1	0.96	0.10	38,38,38,38	0
56	MG	RA	3159	1/1	0.96	0.20	44,44,44,44	0
56	MG	XA	1718	1/1	0.96	0.20	48,48,48,48	0
56	MG	YA	3229	1/1	0.96	0.14	32,32,32,32	0
56	MG	YA	3029	1/1	0.96	0.15	15,15,15,15	0
56	MG	YD	301	1/1	0.96	0.07	20,20,20,20	0
56	MG	RA	3316	1/1	0.96	0.12	49,49,49,49	0
56	MG	YA	3123	1/1	0.96	0.07	34,34,34,34	0
56	MG	QA	1663	1/1	0.96	0.15	38,38,38,38	0
56	MG	RA	3192	1/1	0.96	0.18	16,16,16,16	0
56	MG	QA	1686	1/1	0.96	0.17	49,49,49,49	0
56	MG	YP	201	1/1	0.96	0.06	25,25,25,25	0
56	MG	RA	3093	1/1	0.96	0.25	26,26,26,26	0
56	MG	QA	1653	1/1	0.96	0.18	41,41,41,41	0
56	MG	YA	3348	1/1	0.96	0.09	35,35,35,35	0
56	MG	YA	3130	1/1	0.96	0.15	18,18,18,18	0
56	MG	YA	3038	1/1	0.96	0.15	12,12,12,12	0
56	MG	RA	3322	1/1	0.96	0.19	61,61,61,61	0
56	MG	RA	3374	1/1	0.96	0.05	34,34,34,34	0
56	MG	RA	3231	1/1	0.96	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3043	1/1	0.96	0.26	21,21,21,21	0
56	MG	RA	3232	1/1	0.96	0.11	39,39,39,39	0
56	MG	YA	3137	1/1	0.96	0.09	21,21,21,21	0
56	MG	YA	3138	1/1	0.96	0.05	26,26,26,26	0
56	MG	RA	3276	1/1	0.96	0.05	46,46,46,46	0
57	ZN	XD	301	1/1	0.96	0.25	69,69,69,69	0
56	MG	YA	3400	1/1	0.97	0.08	11,11,11,11	0
56	MG	RA	3265	1/1	0.97	0.21	38,38,38,38	0
56	MG	RA	3005	1/1	0.97	0.04	15,15,15,15	0
56	MG	YA	3314	1/1	0.97	0.14	56,56,56,56	0
56	MG	QA	1604	1/1	0.97	0.09	33,33,33,33	0
56	MG	YA	3239	1/1	0.97	0.18	26,26,26,26	0
56	MG	YA	3161	1/1	0.97	0.10	41,41,41,41	0
56	MG	YA	3408	1/1	0.97	0.23	41,41,41,41	0
56	MG	QA	1719	1/1	0.97	0.06	38,38,38,38	0
56	MG	YA	3319	1/1	0.97	0.24	54,54,54,54	0
56	MG	YA	3242	1/1	0.97	0.10	41,41,41,41	0
56	MG	RA	3235	1/1	0.97	0.16	25,25,25,25	0
56	MG	YA	3037	1/1	0.97	0.16	33,33,33,33	0
56	MG	RA	3008	1/1	0.97	0.06	17,17,17,17	0
56	MG	XA	1651	1/1	0.97	0.23	30,30,30,30	0
56	MG	YA	3040	1/1	0.97	0.13	21,21,21,21	0
56	MG	XA	1652	1/1	0.97	0.12	38,38,38,38	0
56	MG	RA	3097	1/1	0.97	0.29	54,54,54,54	0
56	MG	RA	3029	1/1	0.97	0.14	17,17,17,17	0
56	MG	YA	3172	1/1	0.97	0.17	15,15,15,15	0
56	MG	RA	3072	1/1	0.97	0.15	6,6,6,6	0
56	MG	YA	3107	1/1	0.97	0.13	22,22,22,22	0
56	MG	RA	3312	1/1	0.97	0.26	39,39,39,39	0
56	MG	YA	3176	1/1	0.97	0.05	12,12,12,12	0
56	MG	YA	3426	1/1	0.97	0.20	66,66,66,66	0
56	MG	QA	1731	1/1	0.97	0.18	37,37,37,37	0
56	MG	RA	3398	1/1	0.97	0.05	55,55,55,55	0
56	MG	RA	3010	1/1	0.97	0.08	16,16,16,16	0
56	MG	YA	3112	1/1	0.97	0.11	32,32,32,32	0
56	MG	QA	1680	1/1	0.97	0.11	24,24,24,24	0
56	MG	YA	3050	1/1	0.97	0.23	52,52,52,52	0
56	MG	QA	1711	1/1	0.97	0.18	33,33,33,33	0
56	MG	RA	3077	1/1	0.97	0.22	36,36,36,36	0
56	MG	QA	1704	1/1	0.97	0.22	60,60,60,60	0
56	MG	RA	3281	1/1	0.97	0.10	39,39,39,39	0
56	MG	YA	3187	1/1	0.97	0.22	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1665	1/1	0.97	0.30	37,37,37,37	0
56	MG	RA	3361	1/1	0.97	0.19	40,40,40,40	0
56	MG	XA	1619	1/1	0.97	0.20	27,27,27,27	0
56	MG	YA	3271	1/1	0.97	0.10	22,22,22,22	0
56	MG	RA	3406	1/1	0.97	0.22	42,42,42,42	0
56	MG	YA	3193	1/1	0.97	0.24	35,35,35,35	0
56	MG	YA	3061	1/1	0.97	0.13	15,15,15,15	0
56	MG	RA	3014	1/1	0.97	0.28	36,36,36,36	0
56	MG	RA	3056	1/1	0.97	0.24	13,13,13,13	0
56	MG	QA	1643	1/1	0.97	0.08	47,47,47,47	0
56	MG	RA	3249	1/1	0.97	0.03	39,39,39,39	0
56	MG	RA	3162	1/1	0.97	0.10	43,43,43,43	0
56	MG	YA	3004	1/1	0.97	0.14	5,5,5,5	0
56	MG	RA	3222	1/1	0.97	0.15	19,19,19,19	0
56	MG	YA	3361	1/1	0.97	0.05	45,45,45,45	0
56	MG	YA	3362	1/1	0.97	0.19	48,48,48,48	0
56	MG	YA	3455	1/1	0.97	0.19	68,68,68,68	0
56	MG	QA	1714	1/1	0.97	0.16	33,33,33,33	0
56	MG	RA	3018	1/1	0.97	0.13	16,16,16,16	0
56	MG	RA	3112	1/1	0.97	0.14	38,38,38,38	0
56	MG	YA	3208	1/1	0.97	0.05	31,31,31,31	0
56	MG	YA	3367	1/1	0.97	0.17	43,43,43,43	0
56	MG	YA	3074	1/1	0.97	0.15	34,34,34,34	0
56	MG	YA	3369	1/1	0.97	0.41	83,83,83,83	0
56	MG	RA	3087	1/1	0.97	0.12	19,19,19,19	0
56	MG	YA	3076	1/1	0.97	0.28	43,43,43,43	0
56	MG	RA	3114	1/1	0.97	0.16	12,12,12,12	0
56	MG	YA	3214	1/1	0.97	0.16	34,34,34,34	0
56	MG	RA	3257	1/1	0.97	0.17	47,47,47,47	0
56	MG	QA	1634	1/1	0.97	0.15	33,33,33,33	0
56	MG	YA	3080	1/1	0.97	0.12	12,12,12,12	0
56	MG	RA	3020	1/1	0.97	0.20	15,15,15,15	0
56	MG	QA	1622	1/1	0.97	0.27	39,39,39,39	0
56	MG	YA	3144	1/1	0.97	0.04	21,21,21,21	0
56	MG	YA	3297	1/1	0.97	0.21	37,37,37,37	0
56	MG	RA	3379	1/1	0.97	0.18	44,44,44,44	0
56	MG	RA	3335	1/1	0.97	0.04	18,18,18,18	0
56	MG	YP	202	1/1	0.97	0.10	50,50,50,50	0
56	MG	XA	1737	1/1	0.97	0.27	41,41,41,41	0
56	MG	YA	3148	1/1	0.97	0.20	18,18,18,18	0
56	MG	RA	3261	1/1	0.97	0.26	45,45,45,45	0
56	MG	QA	1708	1/1	0.97	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3389	1/1	0.97	0.20	59,59,59,59	0
56	MG	YA	3151	1/1	0.97	0.24	26,26,26,26	0
56	MG	YA	3391	1/1	0.97	0.18	26,26,26,26	0
56	MG	YA	3025	1/1	0.97	0.08	13,13,13,13	0
56	MG	YA	3153	1/1	0.97	0.07	19,19,19,19	0
56	MG	RA	3338	1/1	0.97	0.24	51,51,51,51	0
56	MG	Y5	101	1/1	0.97	0.06	20,20,20,20	0
56	MG	YA	3308	1/1	0.97	0.17	31,31,31,31	0
56	MG	YA	3028	1/1	0.97	0.05	17,17,17,17	0
56	MG	RA	3299	1/1	0.97	0.08	44,44,44,44	0
56	MG	RA	3263	1/1	0.97	0.23	62,62,62,62	0
57	ZN	XN	101	1/1	0.97	0.05	67,67,67,67	0
56	MG	RA	3186	1/1	0.98	0.32	44,44,44,44	0
56	MG	RA	3169	1/1	0.98	0.26	53,53,53,53	0
56	MG	QA	1618	1/1	0.98	0.15	24,24,24,24	0
56	MG	YA	3205	1/1	0.98	0.07	22,22,22,22	0
56	MG	RA	3277	1/1	0.98	0.05	18,18,18,18	0
56	MG	XA	1650	1/1	0.98	0.09	21,21,21,21	0
56	MG	YA	3377	1/1	0.98	0.10	31,31,31,31	0
56	MG	YA	3378	1/1	0.98	0.13	34,34,34,34	0
56	MG	RA	3385	1/1	0.98	0.07	44,44,44,44	0
56	MG	RA	3189	1/1	0.98	0.19	25,25,25,25	0
56	MG	YA	3210	1/1	0.98	0.13	4,4,4,4	0
56	MG	YA	3053	1/1	0.98	0.25	31,31,31,31	0
56	MG	RA	3210	1/1	0.98	0.18	41,41,41,41	0
56	MG	XA	1733	1/1	0.98	0.11	33,33,33,33	0
56	MG	XA	1618	1/1	0.98	0.31	34,34,34,34	0
56	MG	RA	3096	1/1	0.98	0.30	74,74,74,74	0
56	MG	RD	302	1/1	0.98	0.10	27,27,27,27	0
56	MG	RA	3358	1/1	0.98	0.18	33,33,33,33	0
56	MG	QA	1648	1/1	0.98	0.24	43,43,43,43	0
56	MG	RA	3084	1/1	0.98	0.07	23,23,23,23	0
56	MG	YA	3220	1/1	0.98	0.23	48,48,48,48	0
56	MG	RA	3157	1/1	0.98	0.18	14,14,14,14	0
56	MG	YA	3064	1/1	0.98	0.08	15,15,15,15	0
56	MG	YA	3065	1/1	0.98	0.07	52,52,52,52	0
56	MG	RA	3194	1/1	0.98	0.19	37,37,37,37	0
56	MG	YA	3015	1/1	0.98	0.10	16,16,16,16	0
56	MG	YA	3169	1/1	0.98	0.16	42,42,42,42	0
56	MG	YA	3398	1/1	0.98	0.28	34,34,34,34	0
56	MG	RA	3085	1/1	0.98	0.10	16,16,16,16	0
56	MG	YA	3018	1/1	0.98	0.14	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3311	1/1	0.98	0.25	55,55,55,55	0
56	MG	XA	1703	1/1	0.98	0.18	50,50,50,50	0
56	MG	XA	1628	1/1	0.98	0.25	48,48,48,48	0
56	MG	YA	3022	1/1	0.98	0.31	23,23,23,23	0
56	MG	RA	3218	1/1	0.98	0.10	45,45,45,45	0
56	MG	RA	3086	1/1	0.98	0.10	23,23,23,23	0
56	MG	YA	3026	1/1	0.98	0.13	10,10,10,10	0
56	MG	XA	1667	1/1	0.98	0.25	50,50,50,50	0
56	MG	YE	302	1/1	0.98	0.08	12,12,12,12	0
56	MG	XA	1668	1/1	0.98	0.18	44,44,44,44	0
56	MG	RA	3264	1/1	0.98	0.07	28,28,28,28	0
56	MG	R0	102	1/1	0.98	0.30	53,53,53,53	0
56	MG	QA	1700	1/1	0.98	0.15	53,53,53,53	0
56	MG	YA	3032	1/1	0.98	0.07	8,8,8,8	0
56	MG	RA	3016	1/1	0.98	0.08	6,6,6,6	0
56	MG	QA	1696	1/1	0.98	0.26	33,33,33,33	0
56	MG	YA	3356	1/1	0.98	0.14	48,48,48,48	0
56	MG	RA	3147	1/1	0.98	0.28	15,15,15,15	0
56	MG	RA	3067	1/1	0.98	0.07	17,17,17,17	0
56	MG	YA	3087	1/1	0.98	0.12	14,14,14,14	0
56	MG	XA	1602	1/1	0.98	0.17	13,13,13,13	0
56	MG	RA	3058	1/1	0.98	0.13	41,41,41,41	0
56	MG	YA	3423	1/1	0.98	0.09	47,47,47,47	0
56	MG	RA	3346	1/1	0.98	0.18	43,43,43,43	0
56	MG	XA	1679	1/1	0.98	0.14	32,32,32,32	0
56	MG	RA	3376	1/1	0.98	0.21	26,26,26,26	0
56	MG	QA	1693	1/1	0.98	0.14	30,30,30,30	0
56	MG	Y7	101	1/1	0.98	0.09	51,51,51,51	0
56	MG	RA	3348	1/1	0.98	0.23	58,58,58,58	0
56	MG	YA	3199	1/1	0.98	0.14	28,28,28,28	0
56	MG	RA	3026	1/1	0.98	0.08	13,13,13,13	0
56	MG	RA	3034	1/1	0.98	0.12	33,33,33,33	0
56	MG	QA	1720	1/1	0.99	0.05	49,49,49,49	0
56	MG	RA	3051	1/1	0.99	0.10	11,11,11,11	0
56	MG	RA	3369	1/1	0.99	0.20	19,19,19,19	0
56	MG	XA	1606	1/1	0.99	0.34	31,31,31,31	0
56	MG	RA	3217	1/1	0.99	0.03	7,7,7,7	0
56	MG	YA	3433	1/1	0.99	0.04	31,31,31,31	0
56	MG	RA	3057	1/1	0.99	0.14	22,22,22,22	0
56	MG	YA	3056	1/1	0.99	0.13	15,15,15,15	0
56	MG	YA	3127	1/1	0.99	0.03	20,20,20,20	0
56	MG	YA	3017	1/1	0.99	0.14	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3223	1/1	0.99	0.12	34,34,34,34	0
56	MG	RA	3023	1/1	0.99	0.21	12,12,12,12	0
56	MG	YA	3462	1/1	0.99	0.04	25,25,25,25	0
56	MG	YA	3357	1/1	0.99	0.12	27,27,27,27	0
56	MG	QA	1607	1/1	0.99	0.24	33,33,33,33	0
56	MG	YA	3191	1/1	0.99	0.26	32,32,32,32	0
56	MG	RA	3108	1/1	0.99	0.14	10,10,10,10	0
56	MG	RA	3302	1/1	0.99	0.22	51,51,51,51	0
56	MG	YA	3402	1/1	0.99	0.19	18,18,18,18	0
56	MG	RA	3003	1/1	0.99	0.12	10,10,10,10	0
56	MG	YA	3195	1/1	0.99	0.11	21,21,21,21	0
56	MG	YA	3023	1/1	0.99	0.09	12,12,12,12	0
56	MG	YA	3250	1/1	0.99	0.12	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.