



# wwPDB X-ray Structure Validation Summary Report

Sep 19, 2014 – 02:07 PM EDT

PDB ID : 4LSK  
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCG-G on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-07-22  
Resolution : 3.48 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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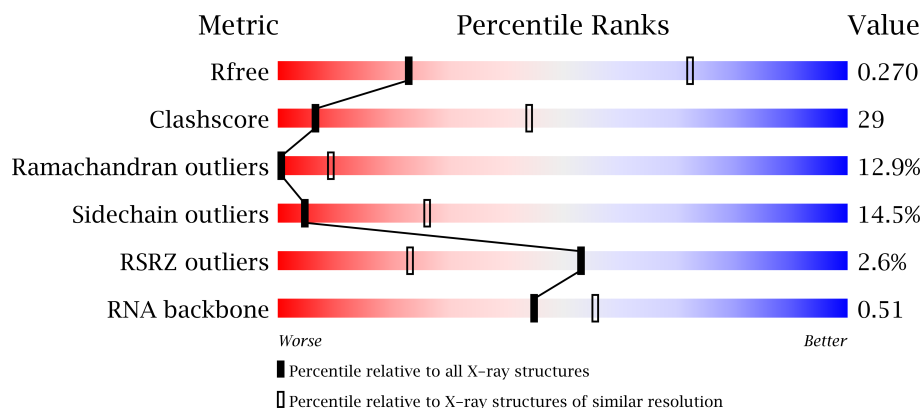
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 3.48 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))
$R_{free}$	66092	1175 (3.66-3.30)
Clashscore	79885	1001 (3.62-3.34)
Ramachandran outliers	78287	1001 (3.64-3.32)
Sidechain outliers	78261	1002 (3.64-3.32)
RSRZ outliers	66119	1175 (3.66-3.30)
RNA backbone	1838	1006 (4.20-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	

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Mol	Chain	Length	Quality of chain
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	
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QY	17	
23	XY	17	
24	QX	25	
24	XX	25	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	Z8	3	

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292002 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			
23	XY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			

- Molecule 24 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			
24	XX	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RE	2	Total	Mg	0	0
			2	2		
57	RR	2	Total	Mg	0	0
			2	2		
57	XA	74	Total	Mg	0	0
			74	74		
57	QA	65	Total	Mg	0	0
			65	65		
57	Y0	1	Total	Mg	0	0
			1	1		

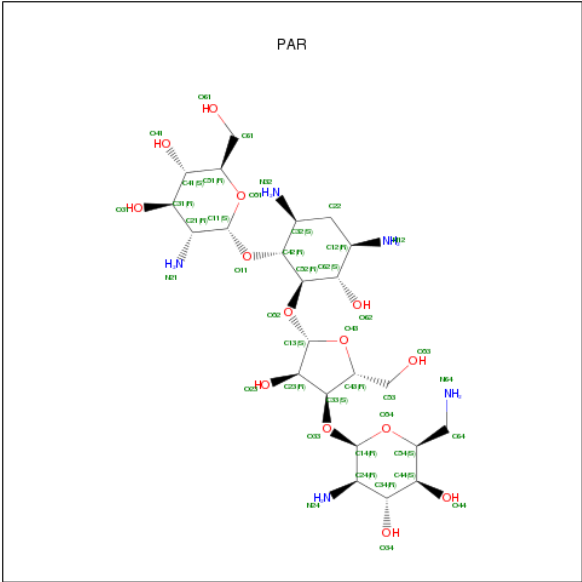
*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R0	1	Total 1	Mg 1	0	0
57	QX	1	Total 1	Mg 1	0	0
57	YA	268	Total 268	Mg 268	0	0
57	YB	4	Total 4	Mg 4	0	0
57	QF	1	Total 1	Mg 1	0	0
57	QM	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RA	241	Total 241	Mg 241	0	0
57	QH	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	YP	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	QV	1	Total 1	Mg 1	0	0
57	YE	1	Total 1	Mg 1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).

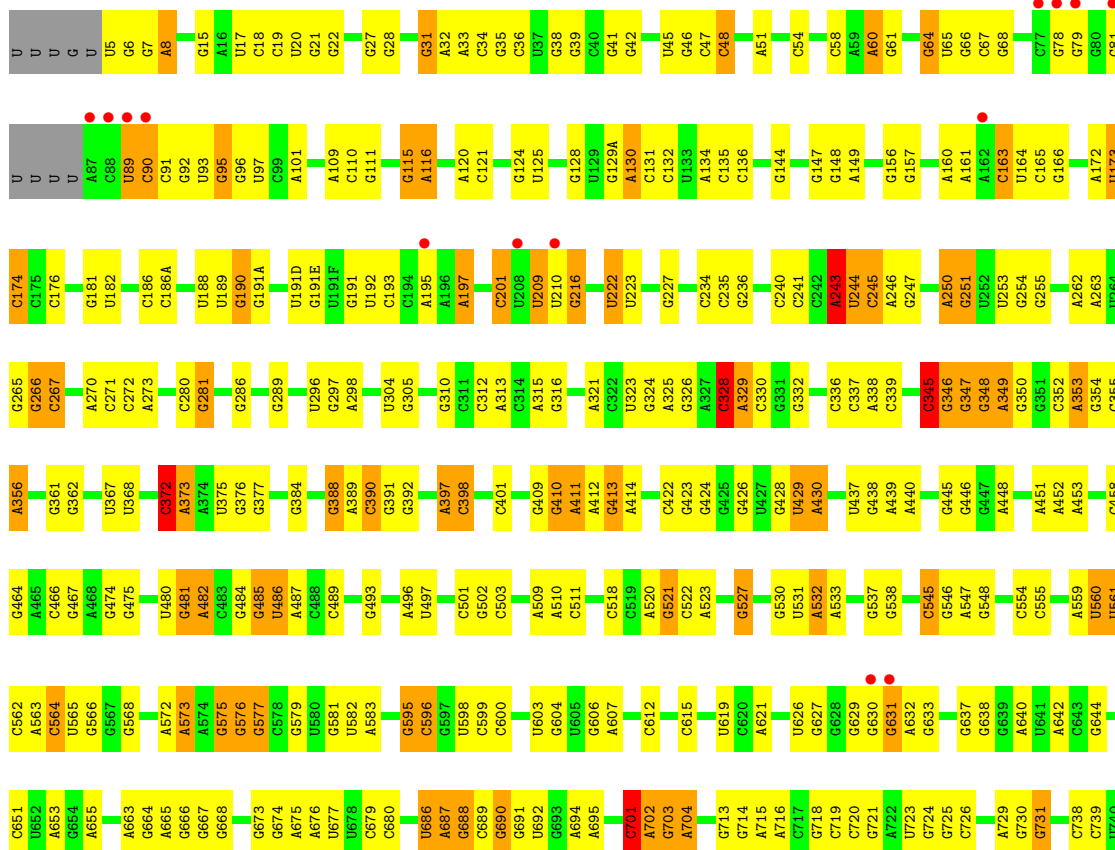


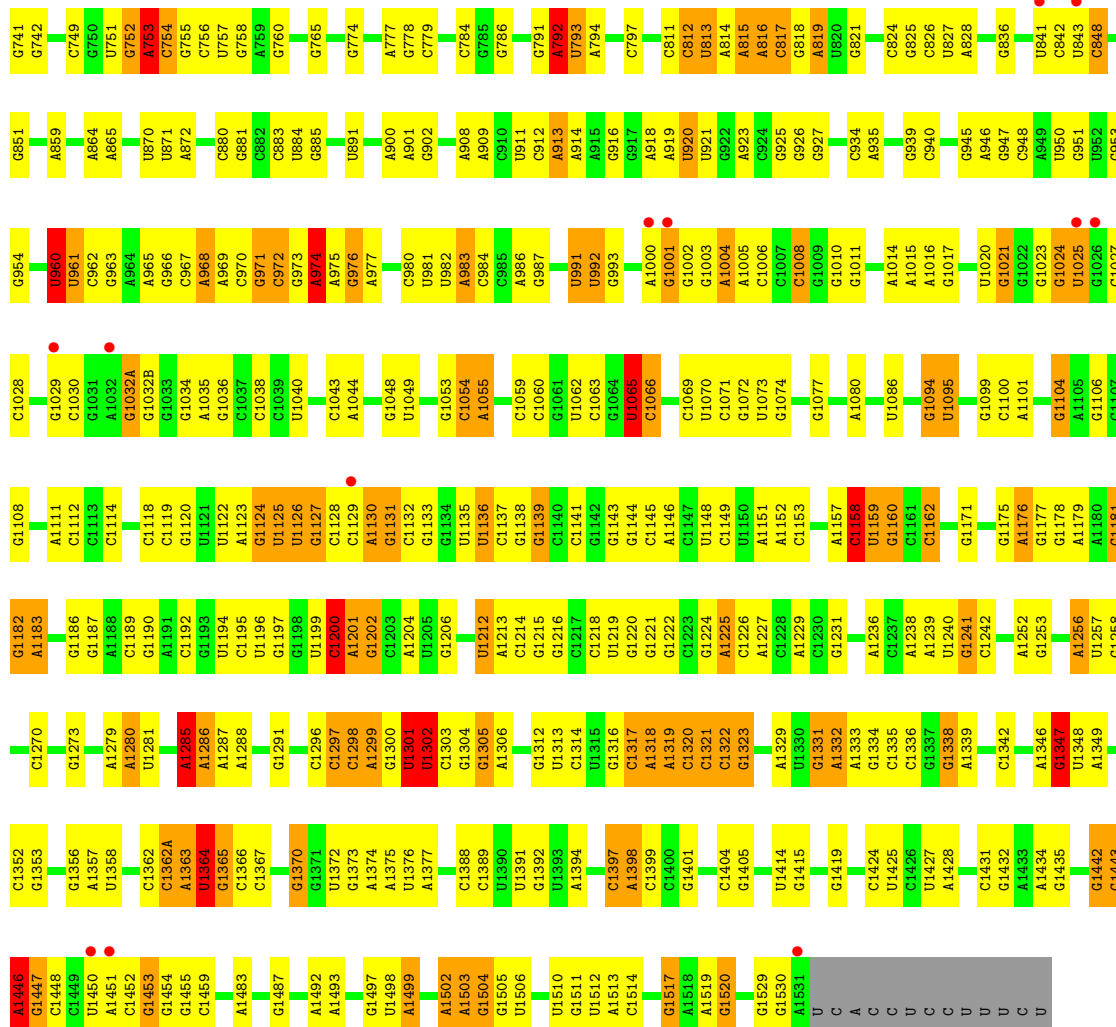
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total	C	N	O	0	0
			42	23	5	14		
58	XA	1	Total	C	N	O	0	0
			42	23	5	14		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	QD	1	Total	Zn	0	0
			1	1		
59	XD	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		

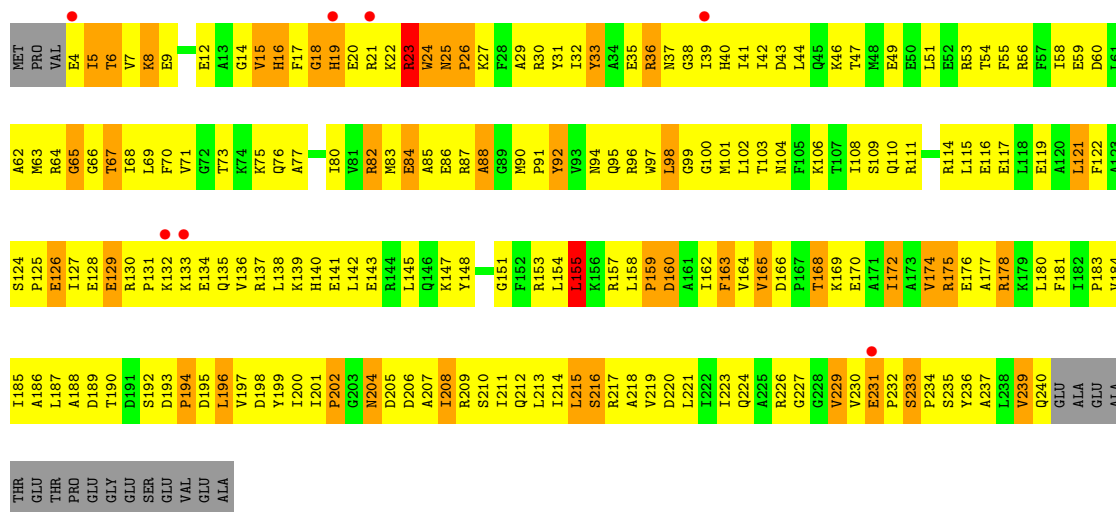




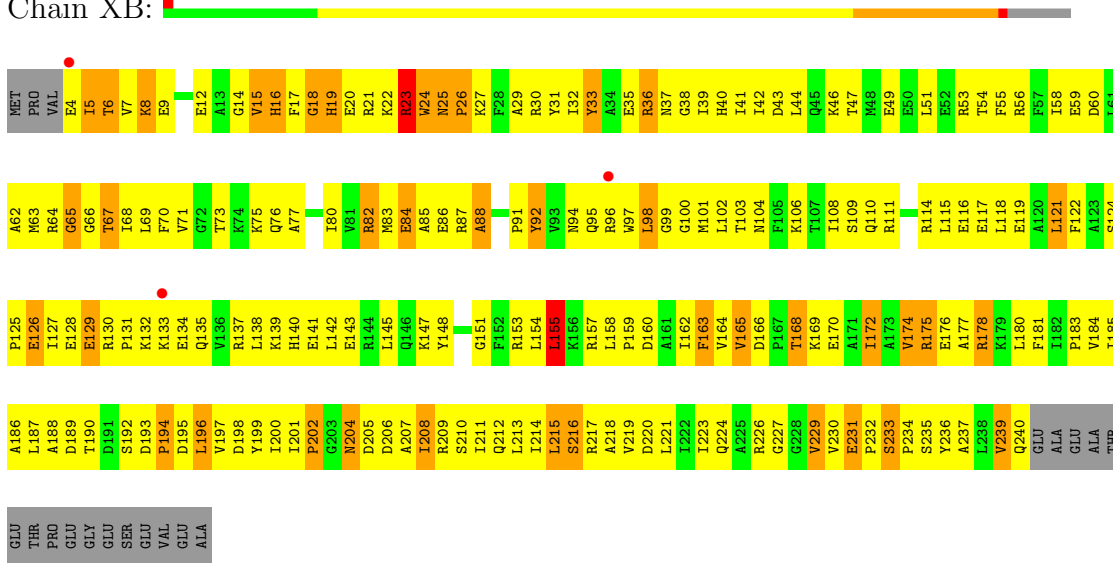


• Molecule 2: 30S ribosomal protein S2

Chain QB:



Chain XB:



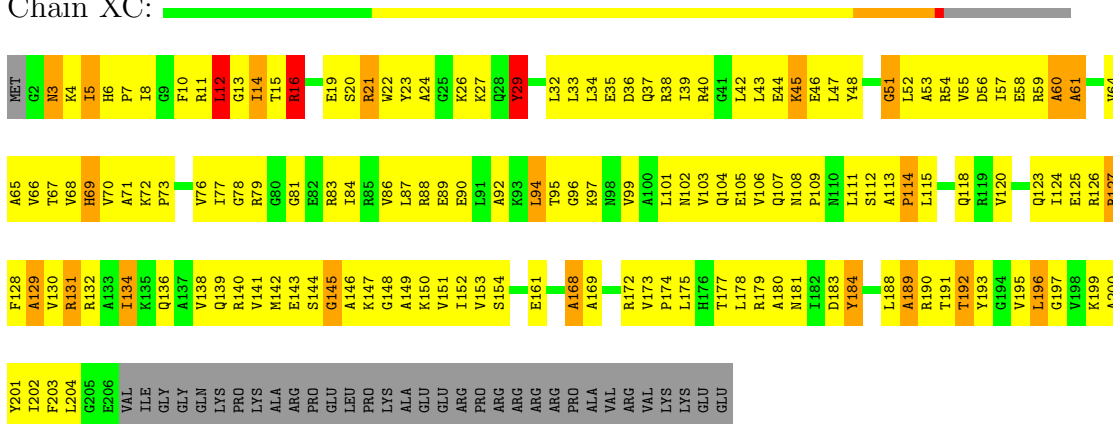
- Molecule 3: 30S ribosomal protein S3

Chain QC:



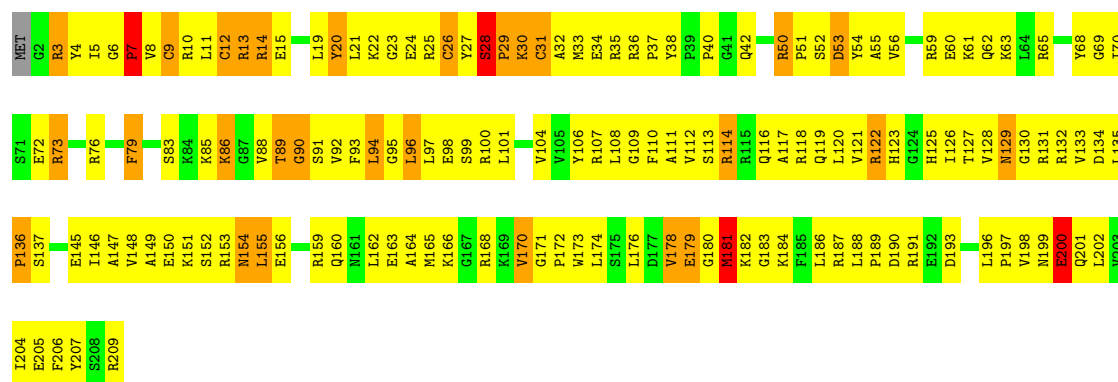
- Molecule 3: 30S ribosomal protein S3

Chain XC:



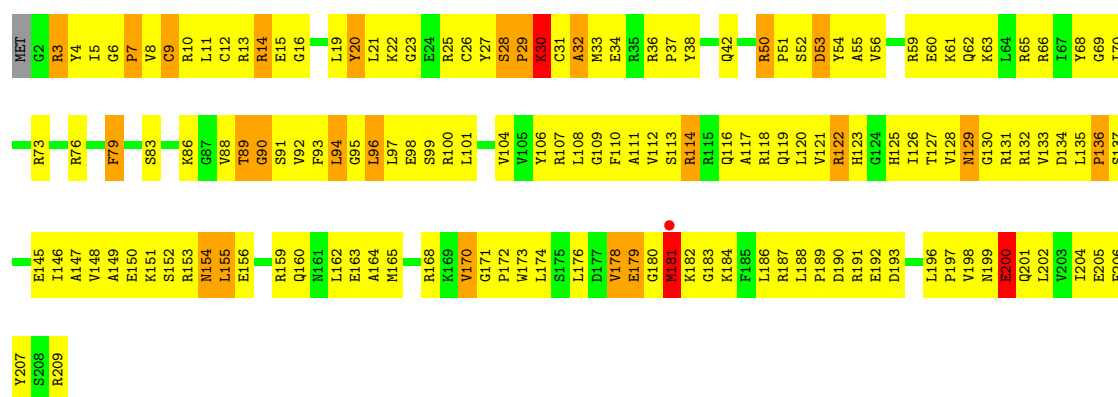
- Molecule 4: 30S ribosomal protein S4

Chain QD:



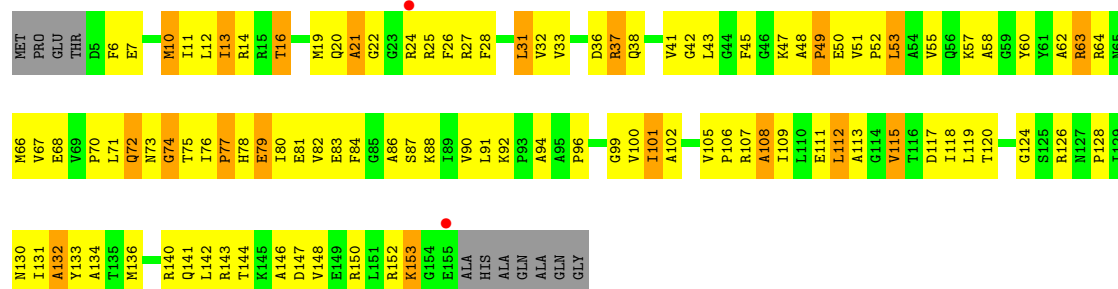
• Molecule 4: 30S ribosomal protein S4

Chain XD:



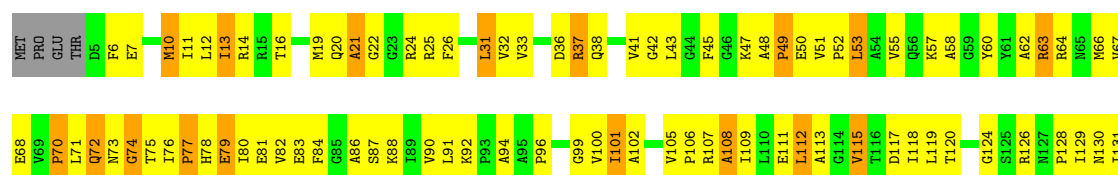
• Molecule 5: 30S ribosomal protein S5

Chain QE:



• Molecule 5: 30S ribosomal protein S5

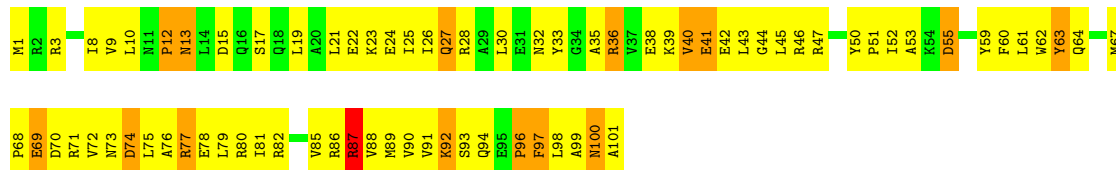
Chain XE:





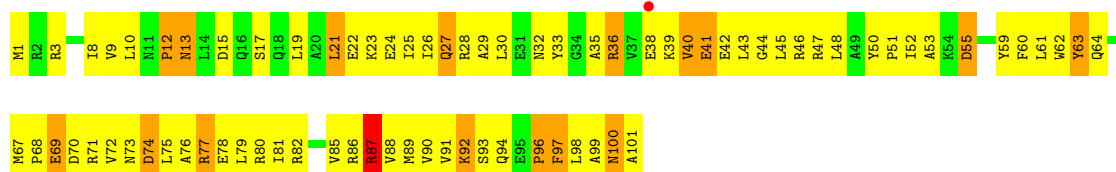
• Molecule 6: 30S ribosomal protein S6

Chain QF:



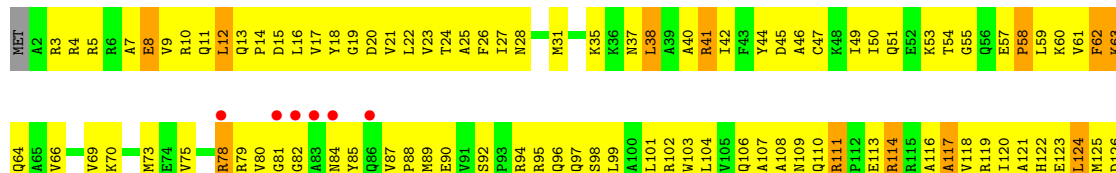
• Molecule 6: 30S ribosomal protein S6

Chain XF:



• Molecule 7: 30S ribosomal protein S7

Chain QG:



• Molecule 7: 30S ribosomal protein S7

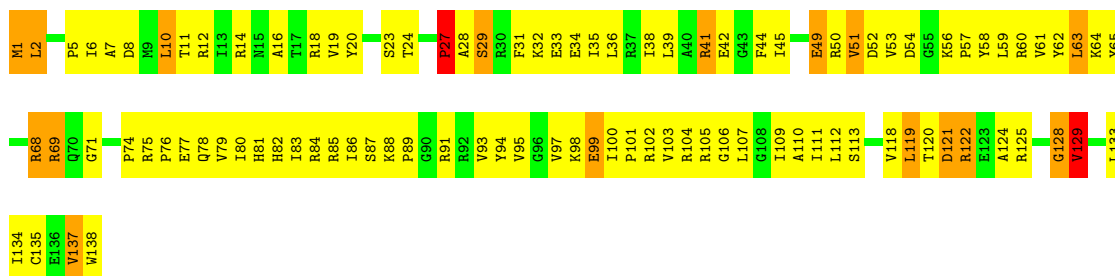
Chain XG:



• Molecule 8: 30S ribosomal protein S8

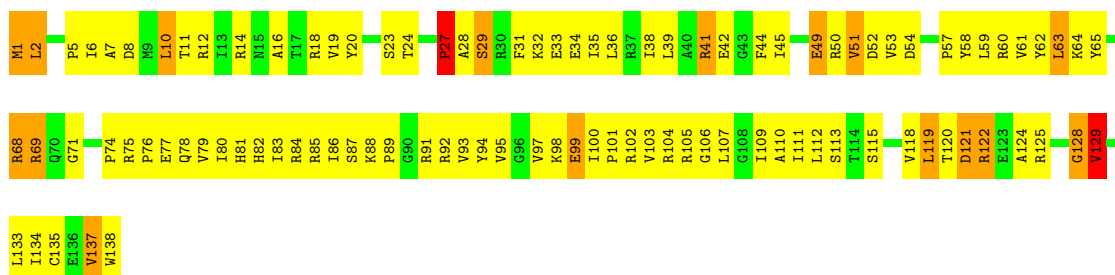
Chain QH:





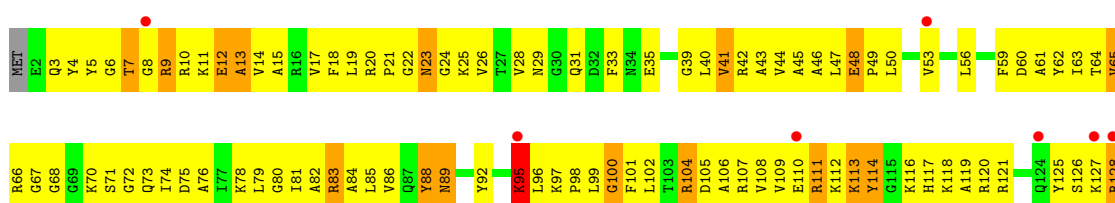
• Molecule 8: 30S ribosomal protein S8

Chain XH:



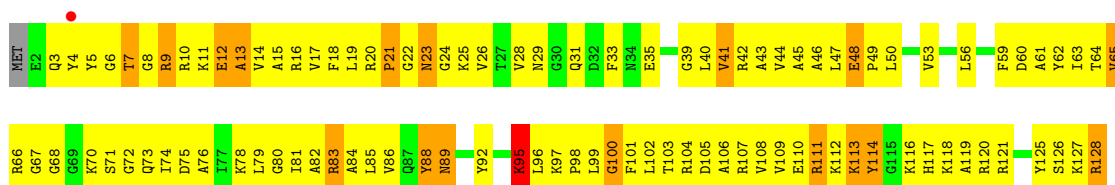
• Molecule 9: 30S ribosomal protein S9

Chain QI:



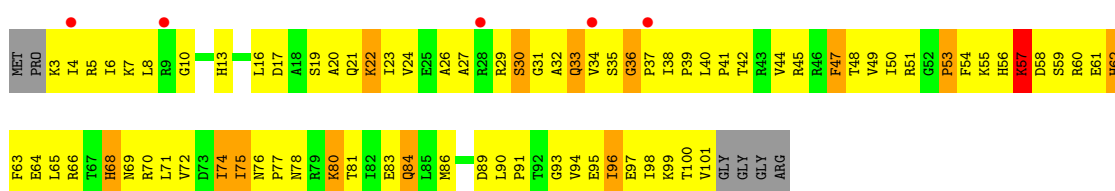
• Molecule 9: 30S ribosomal protein S9

Chain XI:

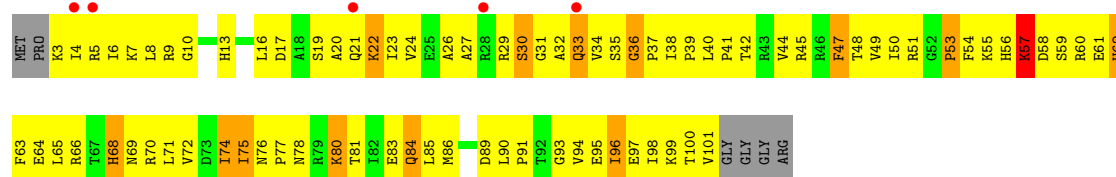


• Molecule 10: 30S ribosomal protein S10

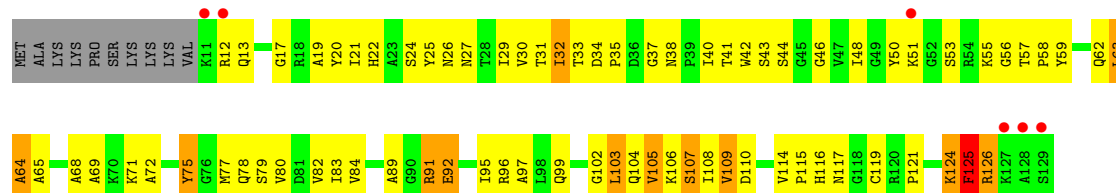
Chain QJ:



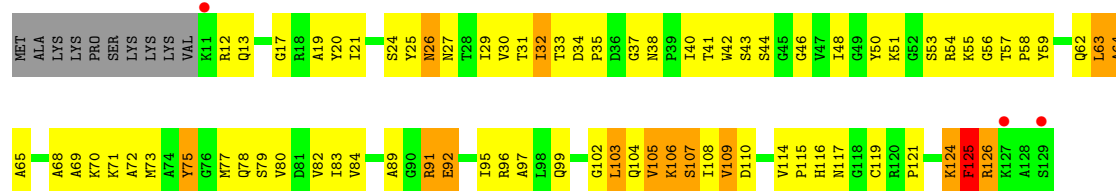
• Molecule 10: 30S ribosomal protein S10

Chain XJ: 

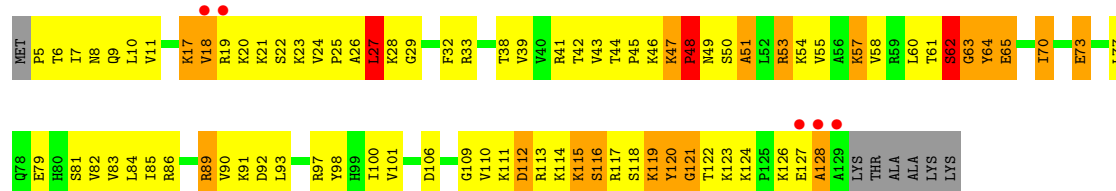
- Molecule 11: 30S ribosomal protein S11

Chain QK: 

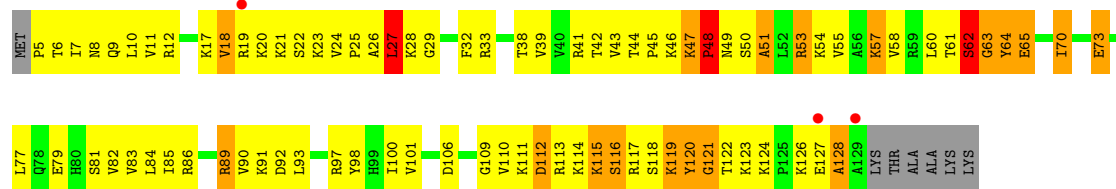
- Molecule 11: 30S ribosomal protein S11

Chain XK: 

- Molecule 12: 30S ribosomal protein S12

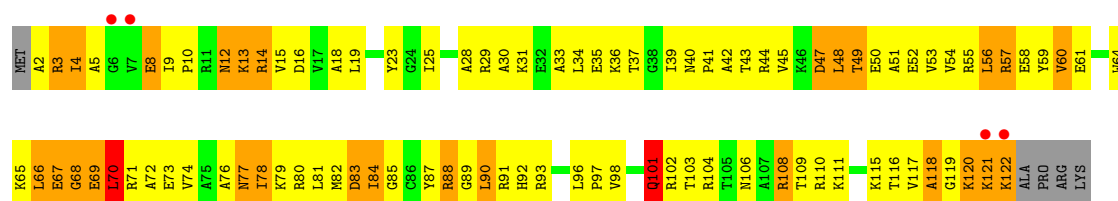
Chain QL: 

- Molecule 12: 30S ribosomal protein S12

Chain XL: 

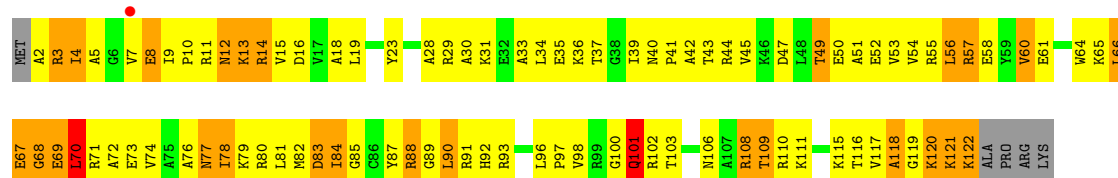
- Molecule 13: 30S ribosomal protein S13

Chain QM: 



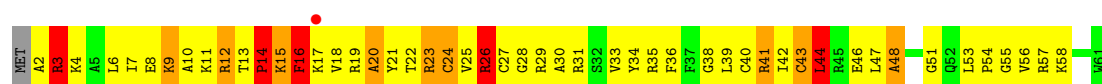
• Molecule 13: 30S ribosomal protein S13

Chain XM:



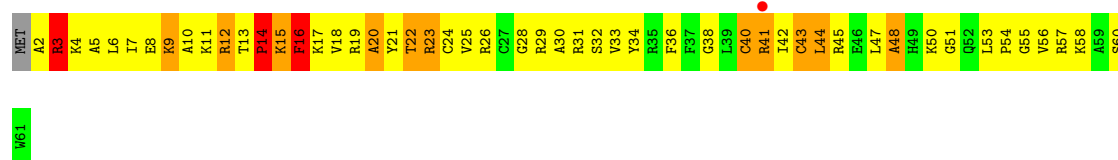
• Molecule 14: 30S ribosomal protein S14

Chain QN:



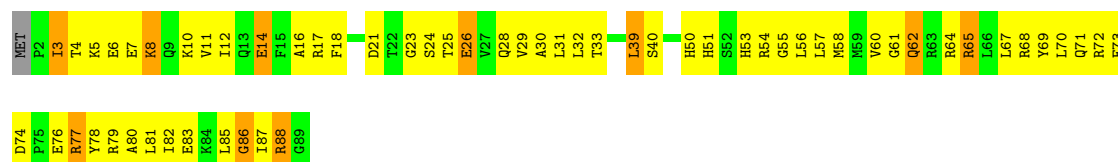
• Molecule 14: 30S ribosomal protein S14

Chain XN:



• Molecule 15: 30S ribosomal protein S15

Chain QO:



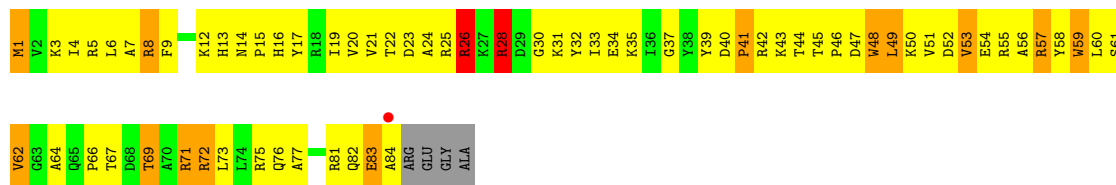
• Molecule 15: 30S ribosomal protein S15

Chain XO:



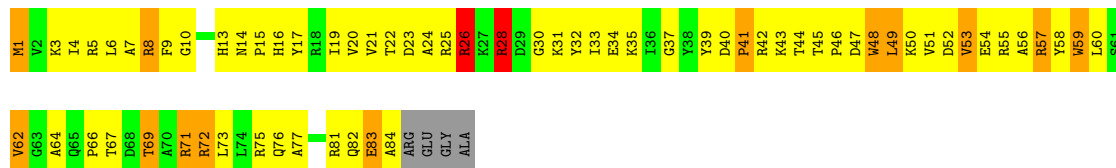
- Molecule 16: 30S ribosomal protein S16

Chain QP:



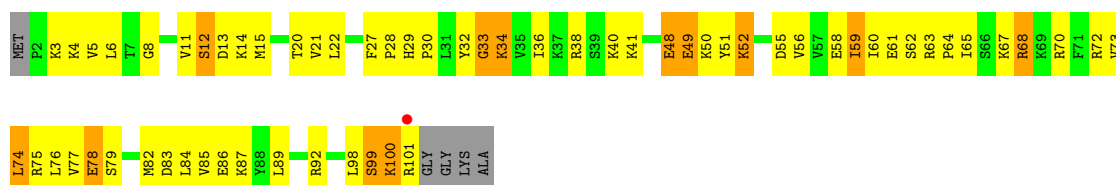
- Molecule 16: 30S ribosomal protein S16

Chain XP:



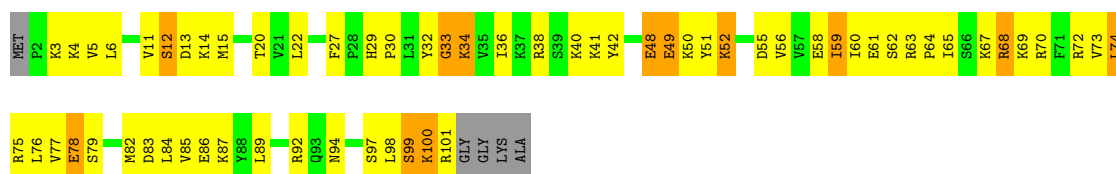
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



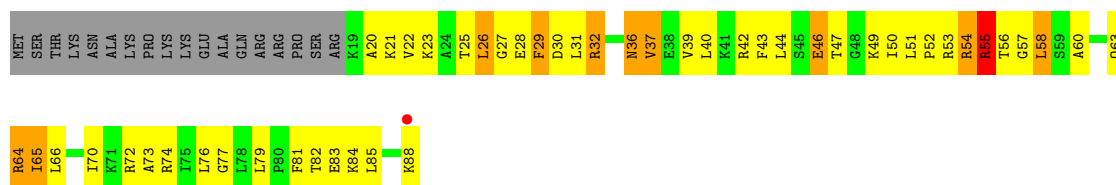
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



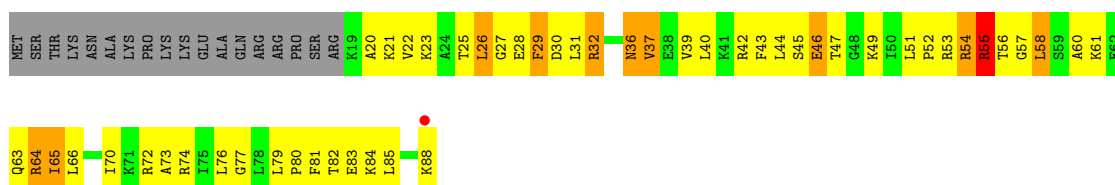
- Molecule 18: 30S ribosomal protein S18

Chain QR:



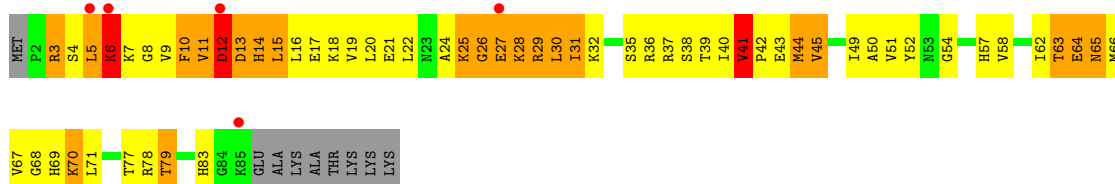
- Molecule 18: 30S ribosomal protein S18

Chain XR:



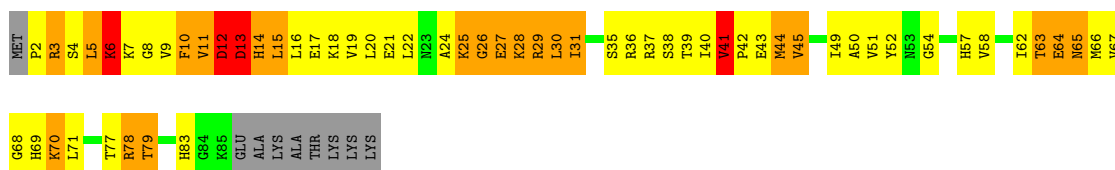
- Molecule 19: 30S ribosomal protein S19

Chain QS:



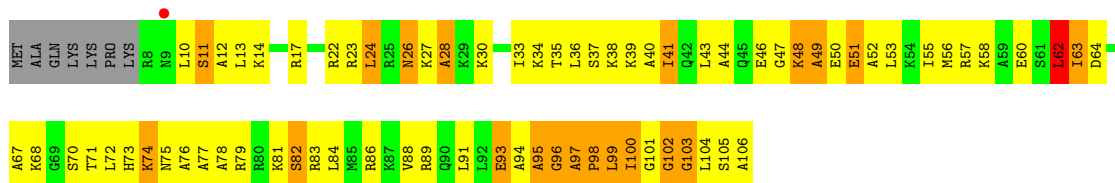
- Molecule 19: 30S ribosomal protein S19

Chain XS:



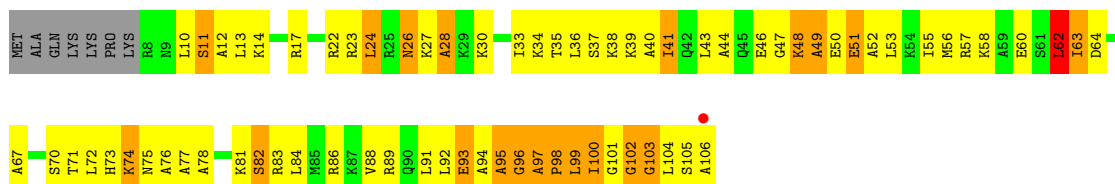
- Molecule 20: 30S ribosomal protein S20

Chain QT:



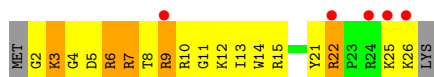
- Molecule 20: 30S ribosomal protein S20

Chain XT:



- Molecule 21: 30S ribosomal protein S21

Chain QU:



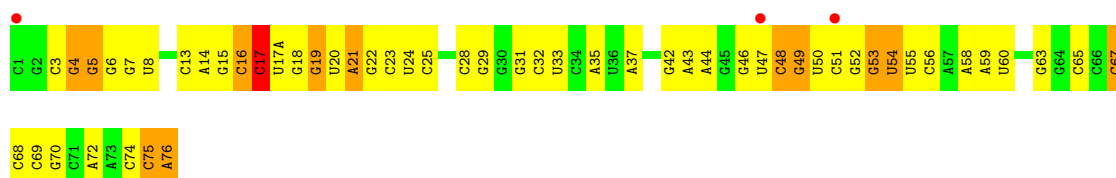
- Molecule 21: 30S ribosomal protein S21

Chain XU: 



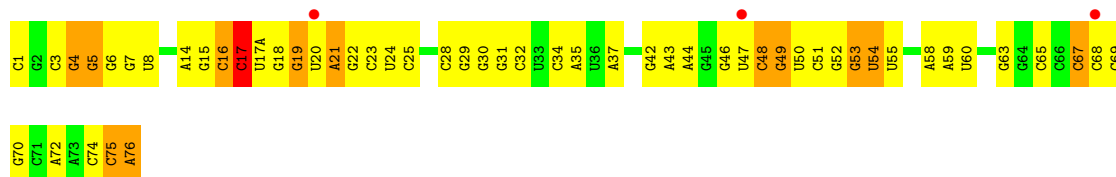
- Molecule 22: P-site tRNA fMet

Chain QV: 



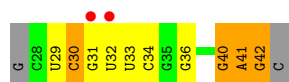
- Molecule 22: P-site tRNA fMet

Chain XV: 



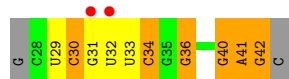
- Molecule 23: messenger RNA

Chain QY: 



- Molecule 23: messenger RNA

Chain XY: 



- Molecule 24: A-site ASL SufA6

Chain QX: 



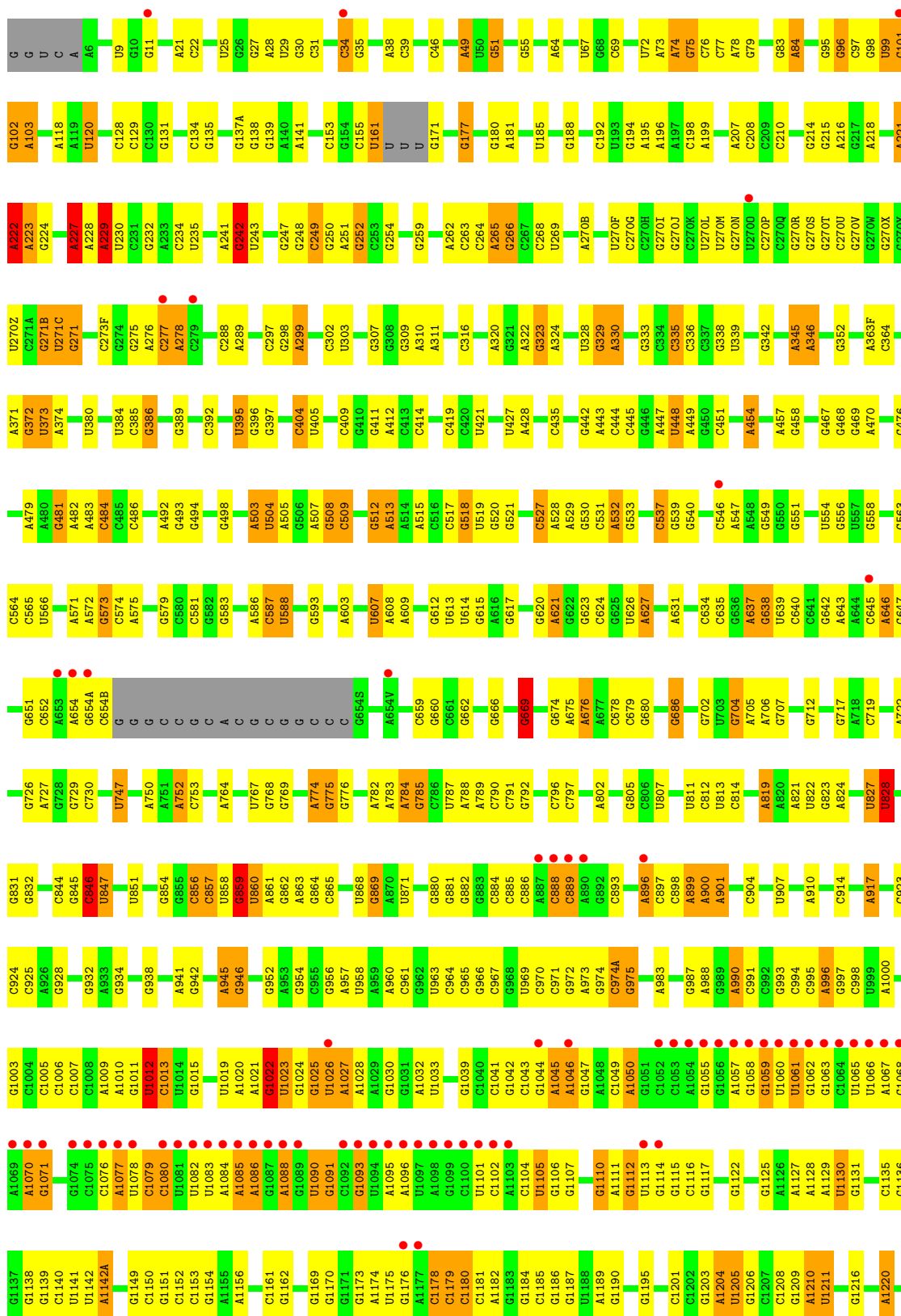
- Molecule 24: A-site ASL SufA6

Chain XX: 



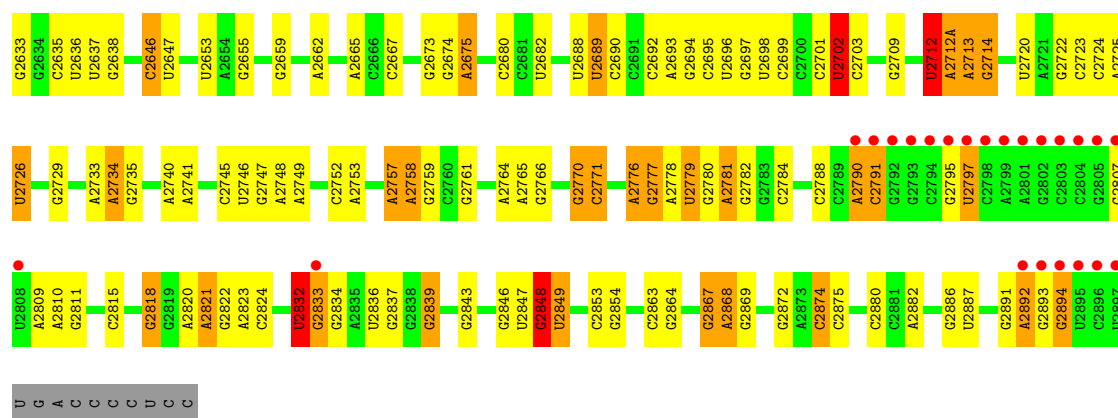
- Molecule 25: 23S rRNA

Chain RA:



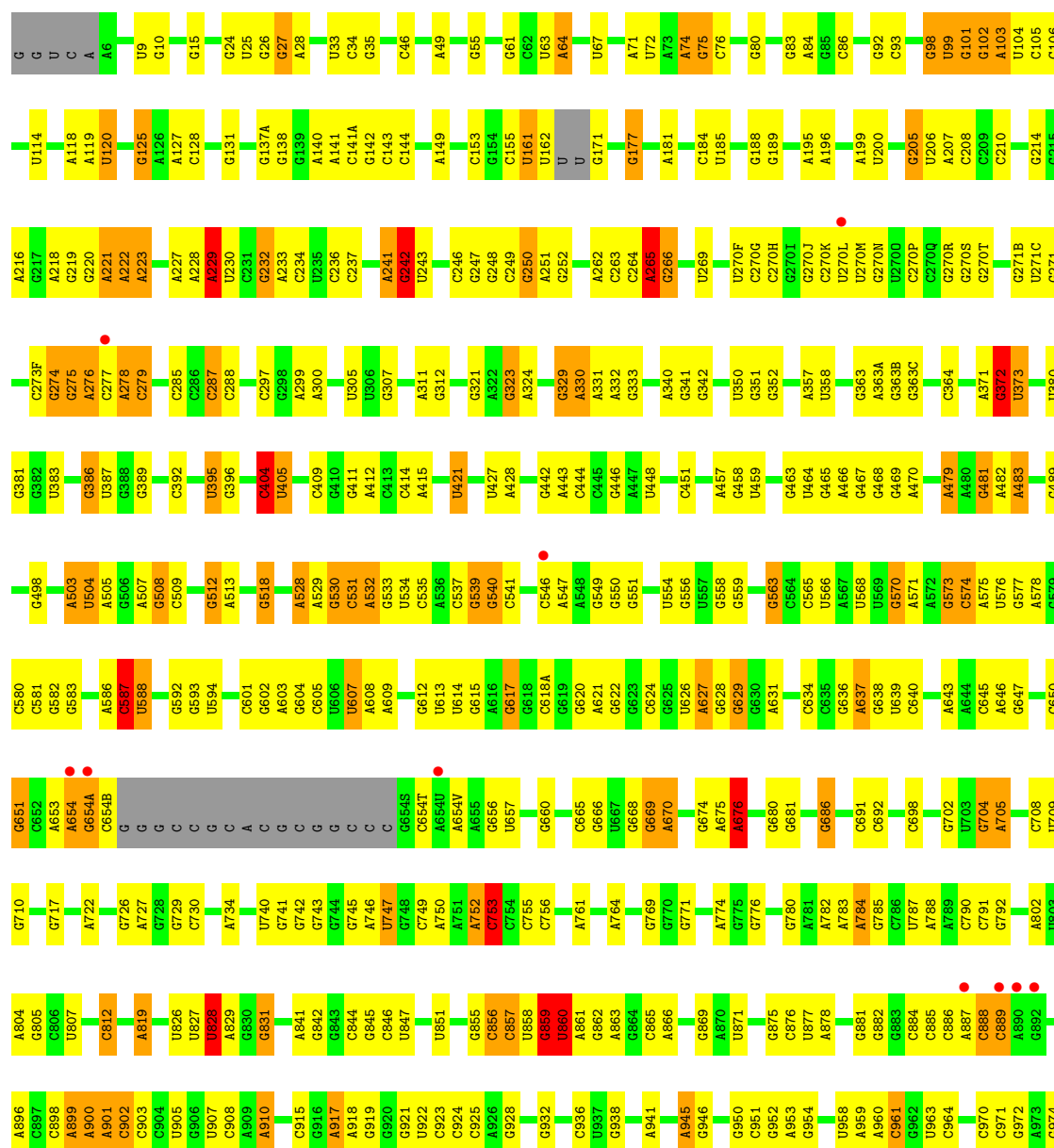
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G2553	A2450	A2199	C2291	A2117	U2117	U2022	A1829	G1743	A1608	C1505	G1421	U1329	G1228
U2554	C2452	G2372	C2292	A2119	A2118	G2023	G1829	C1754	A1609	C1506	G1422	G1332	G1236
C2560	G2455	A2376	C2293	C2205	A2120	C2024	G1835	C1755	A1610	U1507	G1426	A1237	G1237
A2561	G2458	A2377	C2294	C2206	G2122	C2025	C1836	G1756	A1614	C1508	A1427	G1336	G1238
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G2466	G2306	G2383	G2307	G2211	G2125	G2032	A1847	A1760	A1618	G1522	G1436	A1342	A1253
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A2598	G2330	G2246	G2330	G2246	G2155	C2065	C1891	C1797	G1678	G1568	C1474	U1292	U1292
G2502	G2331	G2250	G2331	G2250	G2156	U2068	C1892	U1798	U1688	A1569	G1475	U1391	G1297
A2503	G2332	G2251	A2332	G2251	A2157	G2069	G1893	G1799	A1689	C1577	A1477	U1394	U1300
U2504	G2333	G2252	A2333	G2252	A2158	G2070	A1894	U1799	C1694	A1578	U1482	A1395	A1301
G2505	A2334	G2253	A2334	G2253	C2161	A2071	C1895	U1799	G1695	A1580	G1483	U1397	C1304
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C2507	C2342	C2258	C2343	C2258	C2163	U2074	C1897	G1802	A1701	U1586	A1486	U1405	C1306
G2513	G2344	A2268	U2344	A2268	C2164	U2075	C1898	A1803	G1728	A1587	G1487	C1406	G1309
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C2517	G2345	U2272	A2346	U2272	U2167	U2096	G1900	G1813	U1730	C1589	G1492	G1412	U1313
U2518	G2346	A2273	A2347	A2273	A2168	G2102	C1901	G1814	U1497	U1590	C1493	G1413	C1314
U2519	G2347	G2274	G2348	G2274	A2171	C2103	G1902	A1815	A1731	U1591	G1496	G1416	G1320
G2527	G2349	C2275	G2350	C2275	A2172	G2104	G1903	G1816	A1732	U1592	A1497	C1417	A1321
U2528	G2351	G2276	A2352	G2276	C2174	G2105	G1904	G1817	U1733	U1593	C1498	G1418	
G2529	G2353	G2277	G2354	G2277	C2175	G2106	G1905	U1818	U1730	G1594			
A2530	G2354	C2283	G2355	C2283	A2176	G2110	G1906	U1819	U1731	G1595			
C2540	G2354	C2284	G2356	C2284	C2188	C2111	A1913	U1820	U1732				
A2541	G2358	G2285	A2358	G2285	U2189	G2112	A2014	G1821	A1732				
A2542	A2286	A2286	A2361	A2286	U2190	A2114	A2015	G1822					
G2543	A2287	A2288	A2361	A2287	G2191		A2019						



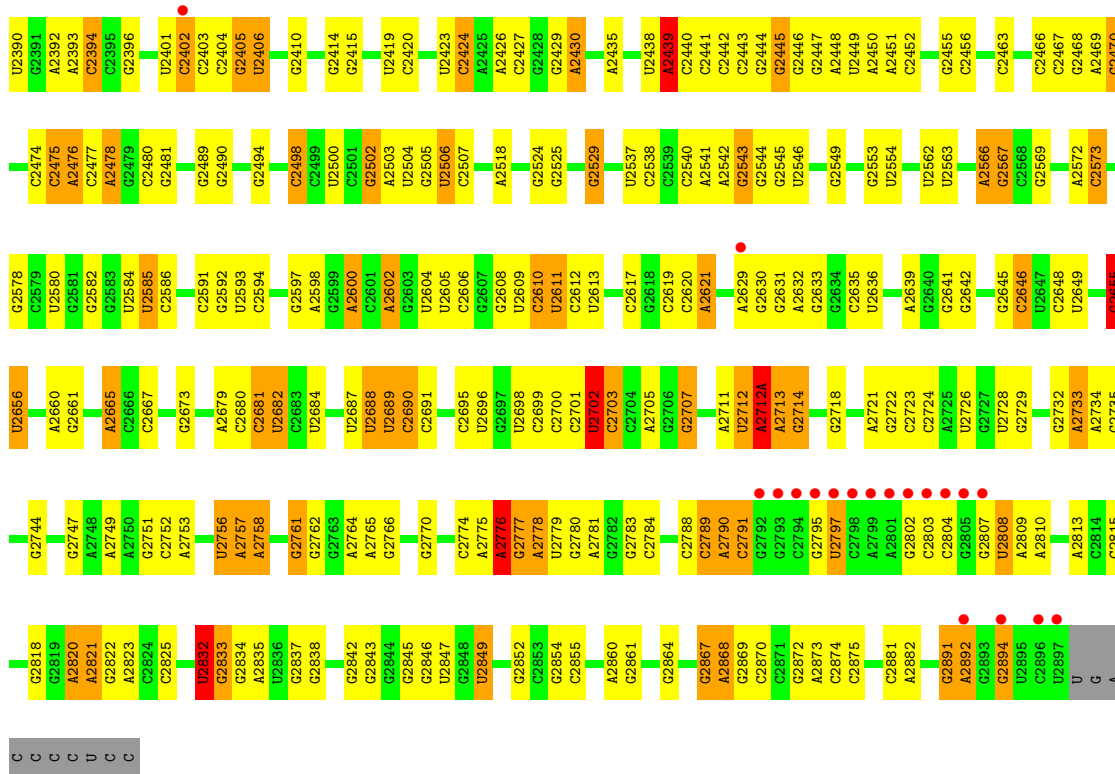


# Molecule 25: 23S rRNA

Chain YA:

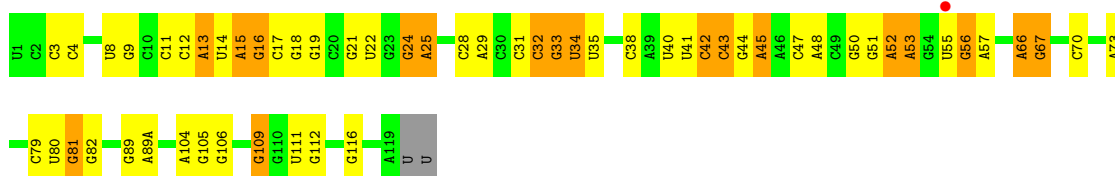






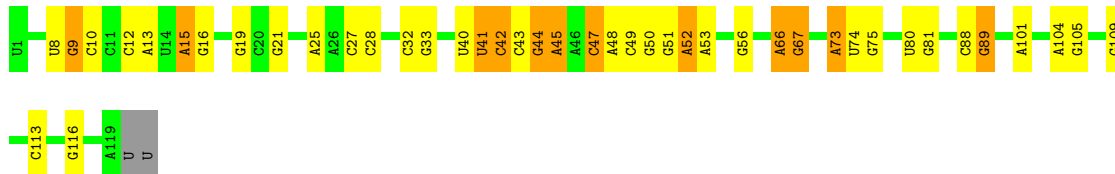
• Molecule 26: 5S rRNA

Chain RB:



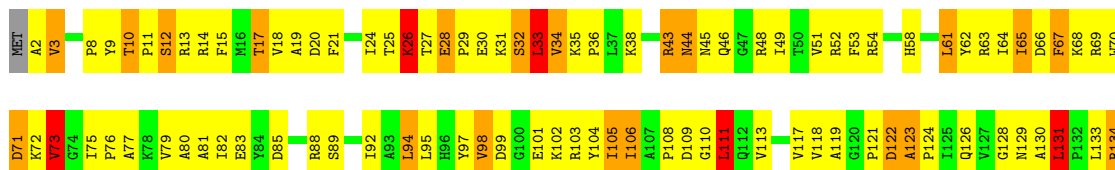
• Molecule 26: 5S rRNA

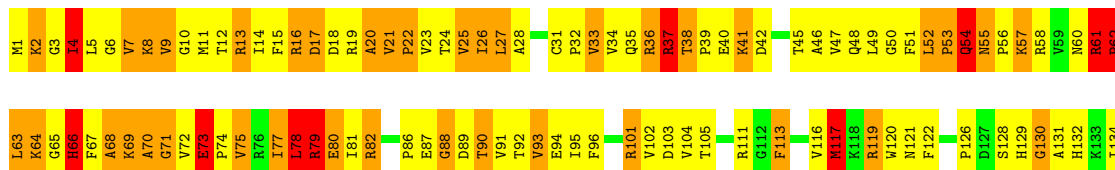
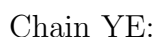
Chain YB:



• Molecule 27: 50S ribosomal protein L2

Chain RD:

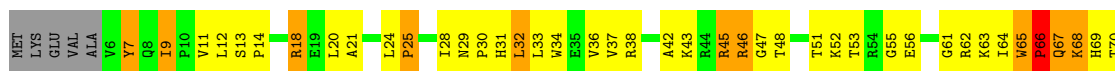






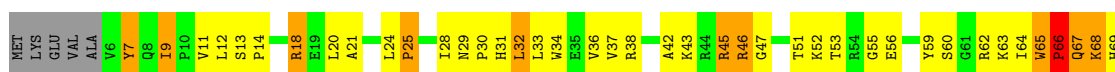
• Molecule 29: 50S ribosomal protein L4

Chain RF:



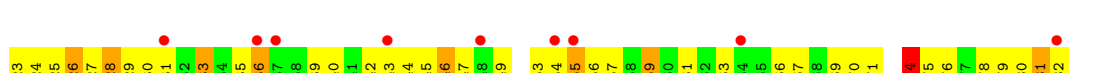
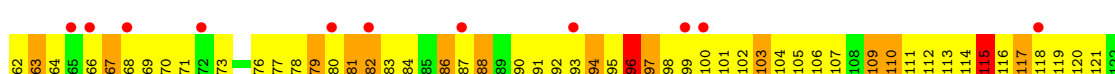
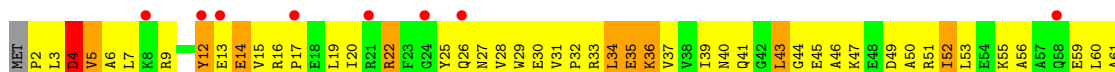
• Molecule 29: 50S ribosomal protein L4

Chain YF:



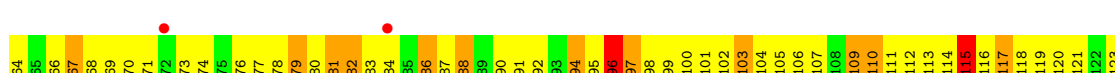
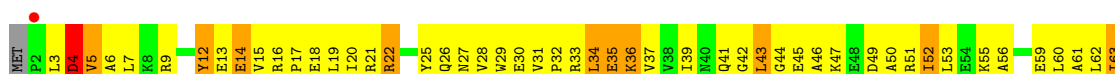
• Molecule 30: 50S ribosomal protein L5

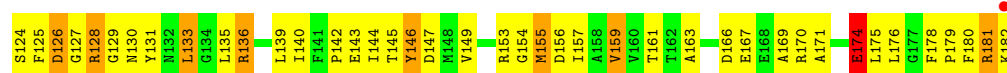
Chain RG:



• Molecule 30: 50S ribosomal protein L5

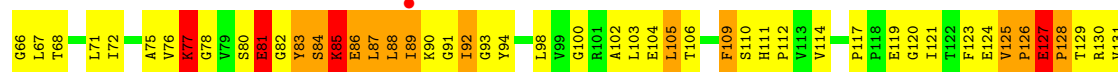
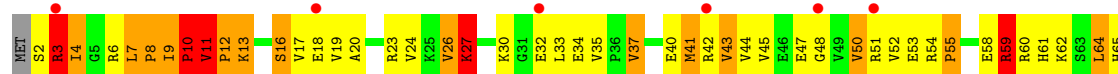
Chain YG:





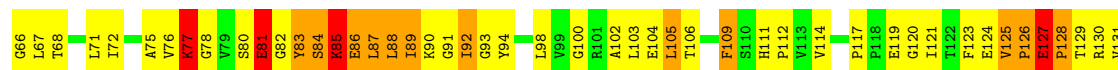
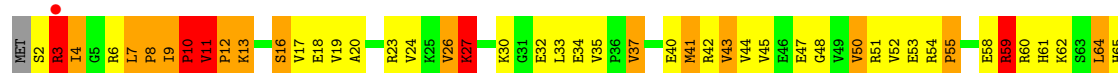
• Molecule 31: 50S ribosomal protein L6

Chain RH:



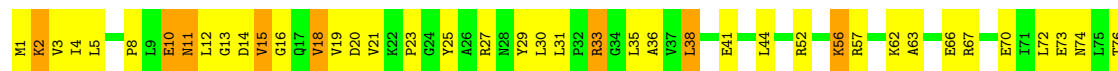
• Molecule 31: 50S ribosomal protein L6

Chain YH:



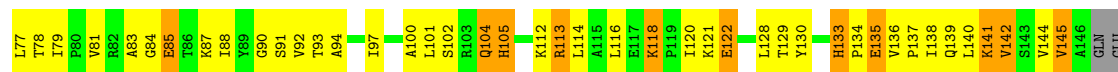
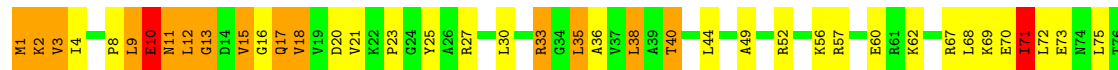
• Molecule 32: 50S ribosomal protein L9

Chain RI:



• Molecule 32: 50S ribosomal protein L9

Chain YI:



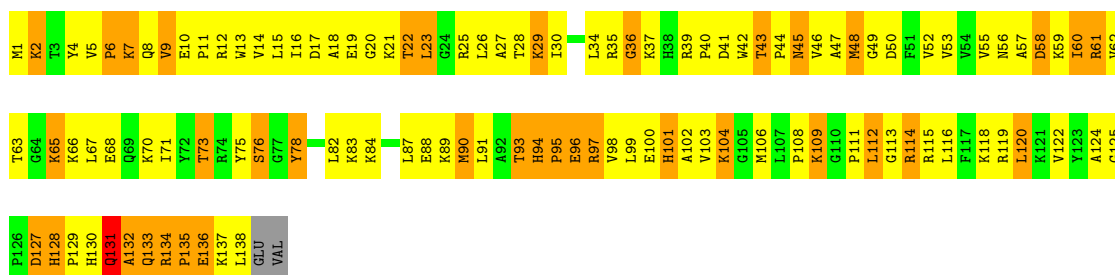
• Molecule 33: 50S ribosomal protein L13

Chain RN:



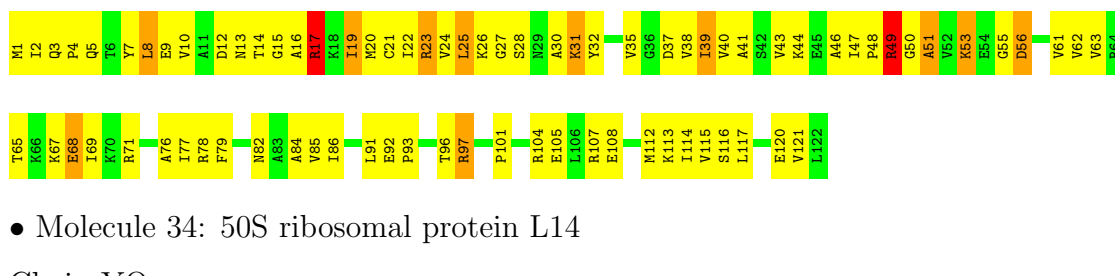
• Molecule 33: 50S ribosomal protein L13

Chain YN:



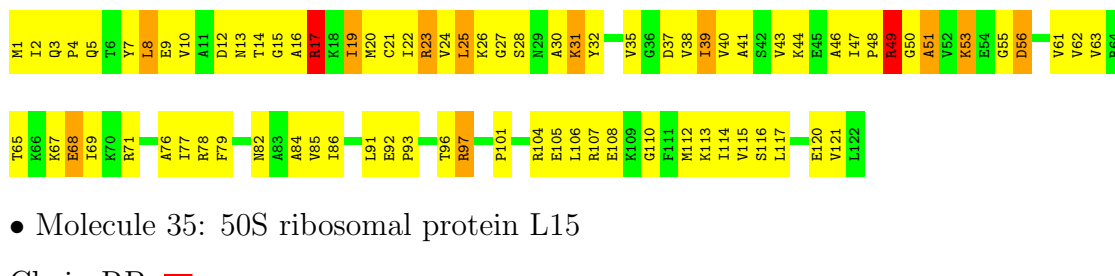
• Molecule 34: 50S ribosomal protein L14

Chain RO:



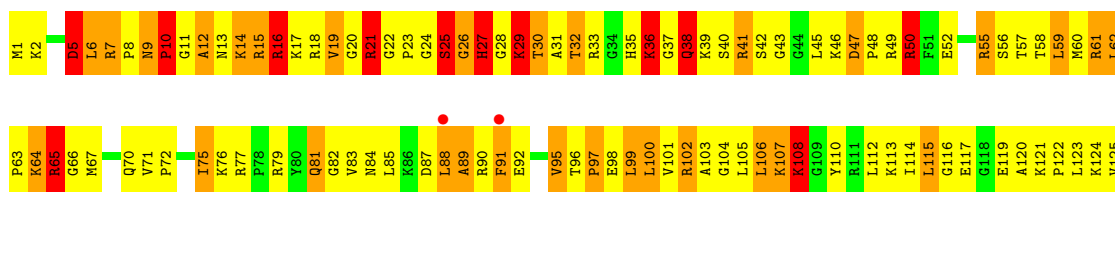
• Molecule 34: 50S ribosomal protein L14

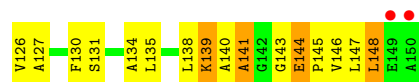
Chain YO:



• Molecule 35: 50S ribosomal protein L15

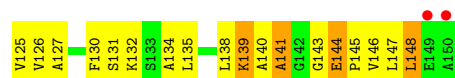
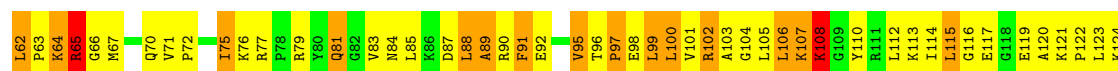
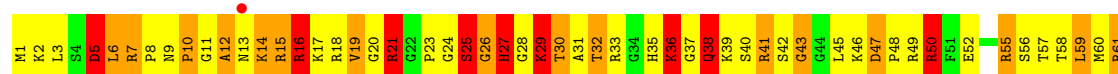
Chain RP:





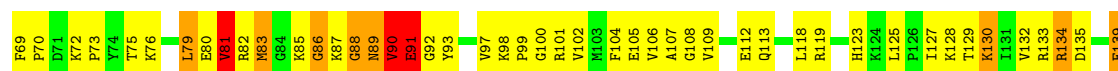
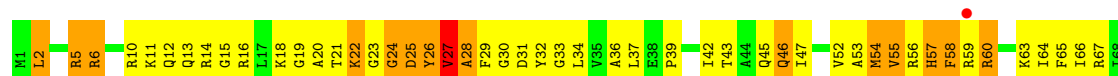
- Molecule 35: 50S ribosomal protein L15

Chain YP:



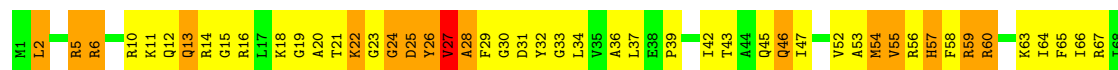
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



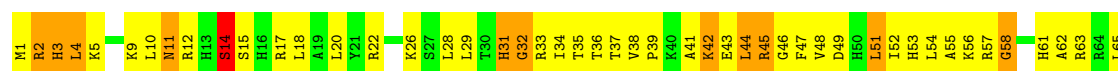
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



- Molecule 37: 50S ribosomal protein L17

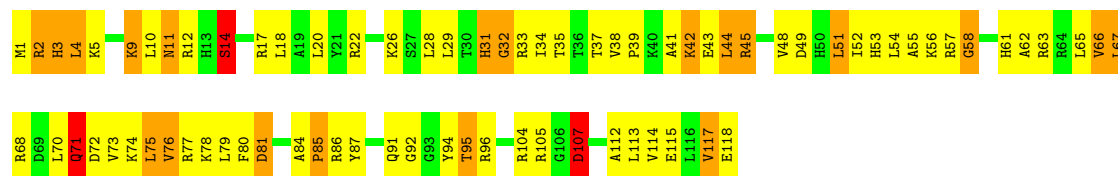
Chain RR:



- Molecule 37: 50S ribosomal protein L17

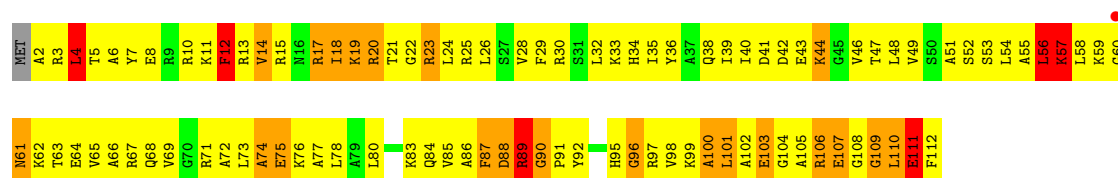


Chain YR:



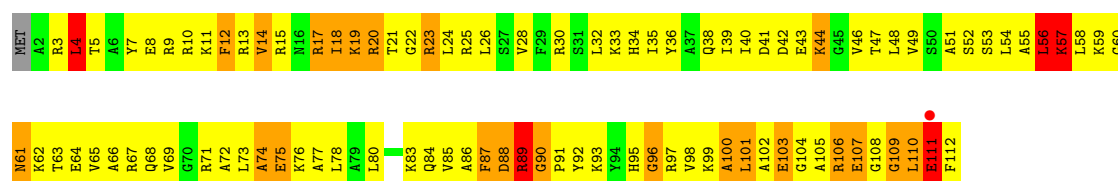
- Molecule 38: 50S ribosomal protein L18

Chain RS:



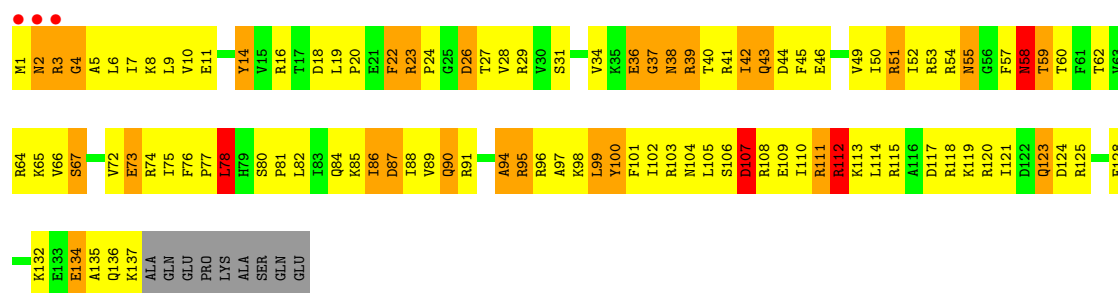
- Molecule 38: 50S ribosomal protein L18

Chain YS:



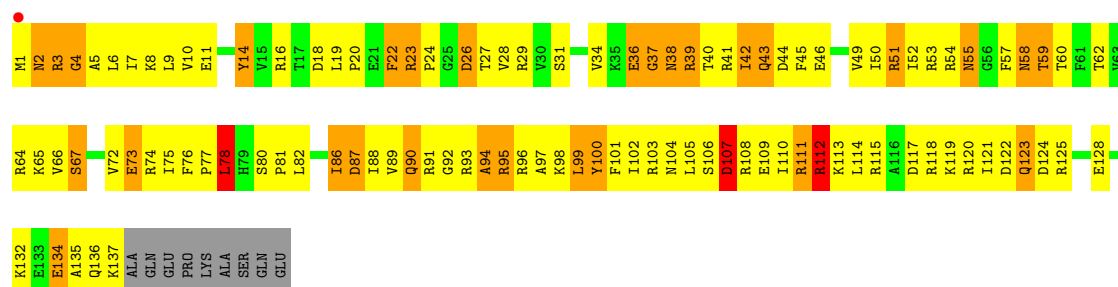
- Molecule 39: 50S ribosomal protein L19

Chain RT:

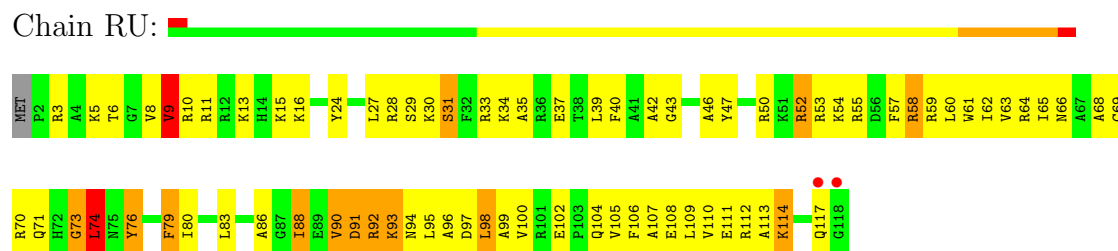


- Molecule 39: 50S ribosomal protein L19

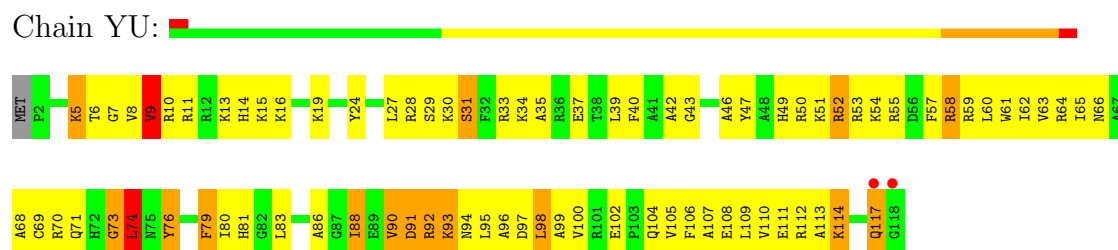
Chain YT:



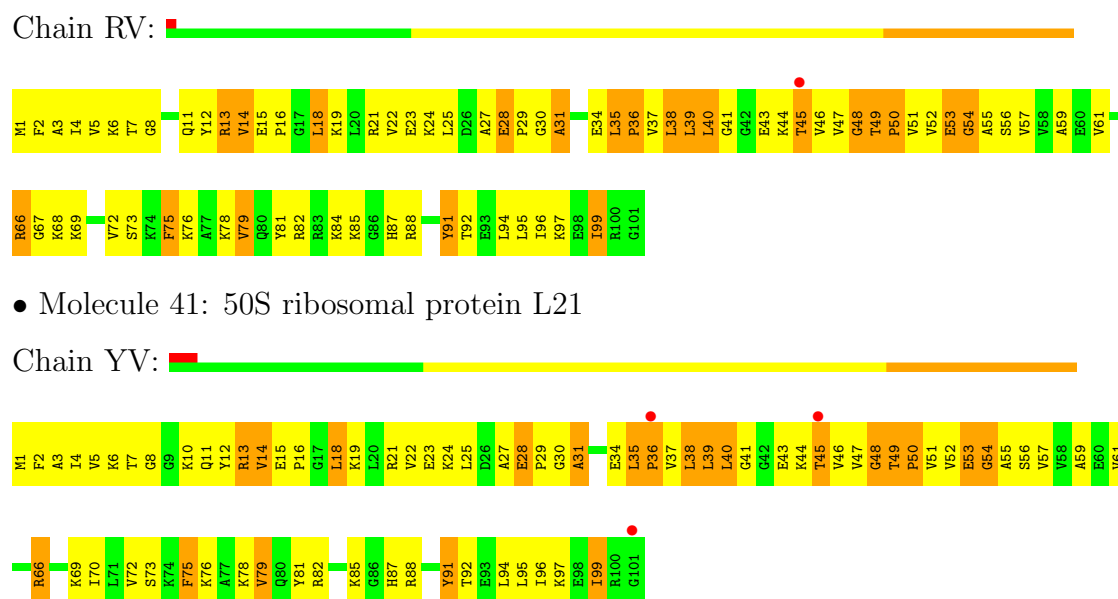
- Molecule 40: 50S ribosomal protein L20



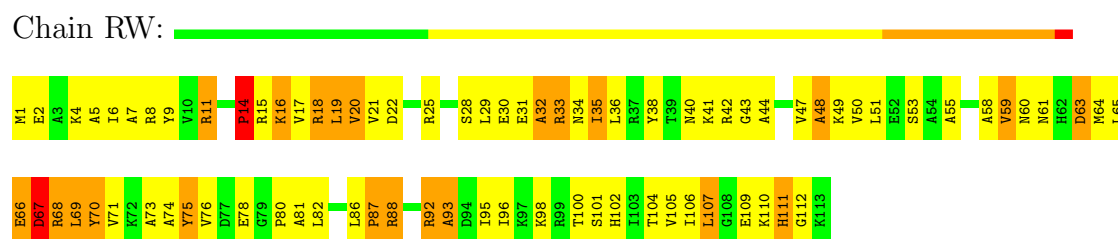
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21

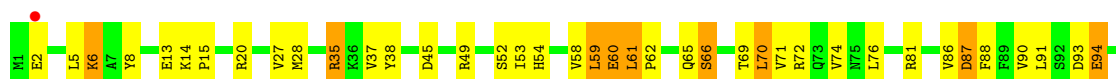


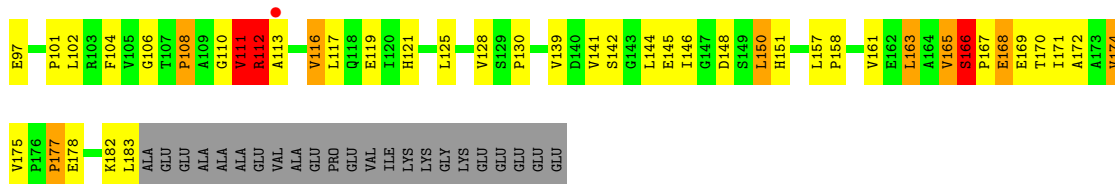
- Molecule 42: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L22

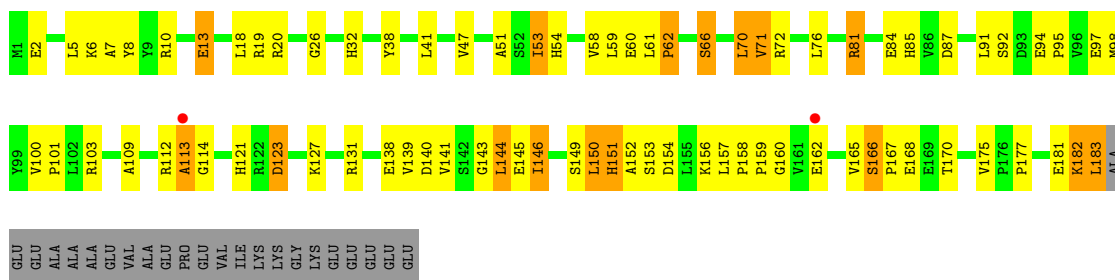






- Molecule 45: 50S ribosomal protein L25

Chain YZ:



- Molecule 46: 50S ribosomal protein L27

Chain R0:



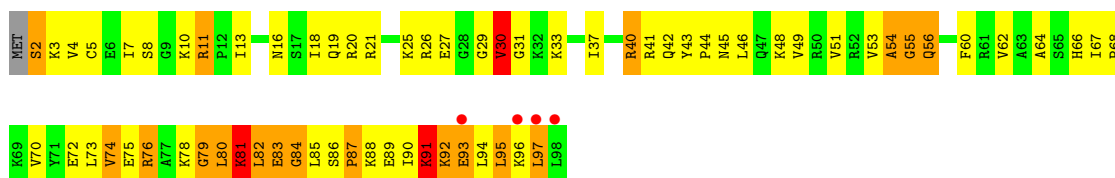
- Molecule 46: 50S ribosomal protein L27

Chain Y0:



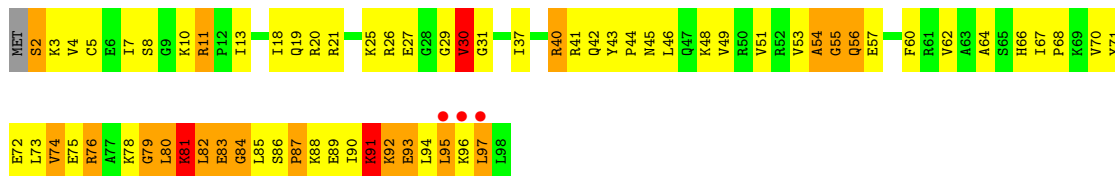
- Molecule 47: 50S ribosomal protein L28

Chain R1:



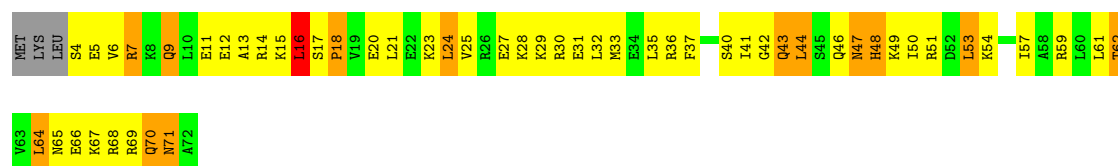
- Molecule 47: 50S ribosomal protein L28

Chain Y1:



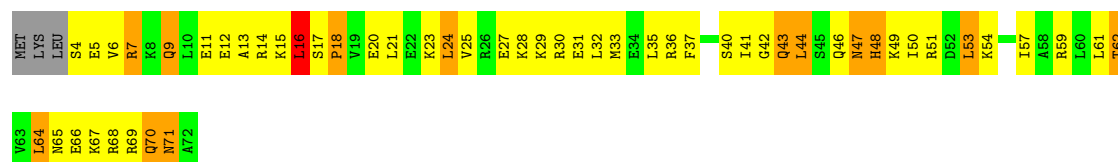
- Molecule 48: 50S ribosomal protein L29

Chain R2: 



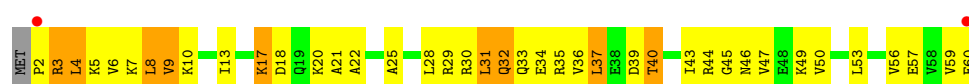
- Molecule 48: 50S ribosomal protein L29

Chain Y2: 



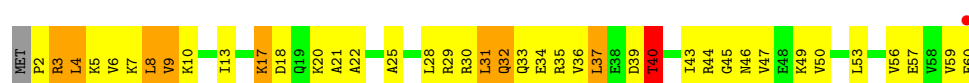
- Molecule 49: 50S ribosomal protein L30

Chain R3: 



- Molecule 49: 50S ribosomal protein L30

Chain Y3: 



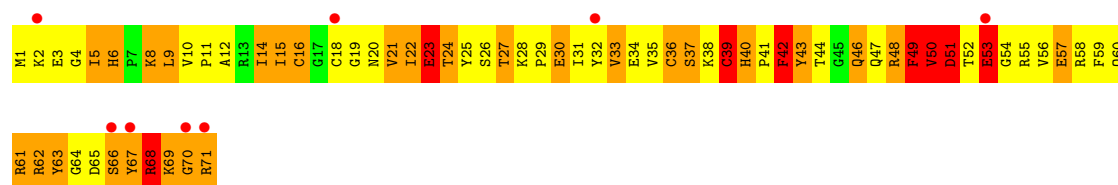
- Molecule 50: 50S ribosomal protein L31

Chain R4: 



- Molecule 50: 50S ribosomal protein L31

Chain Y4: 



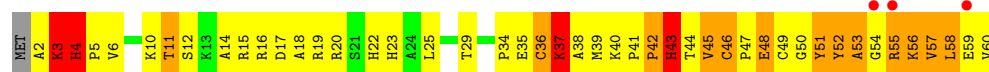
- Molecule 51: 50S ribosomal protein L32

Chain R5: 



- Molecule 51: 50S ribosomal protein L32

Chain Y5:



- Molecule 52: 50S ribosomal protein L33

Chain R6:



- Molecule 52: 50S ribosomal protein L33

Chain Y6:



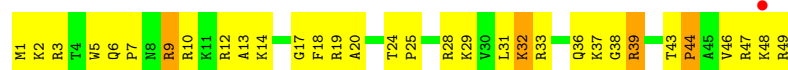
- Molecule 53: 50S ribosomal protein L34

Chain R7:



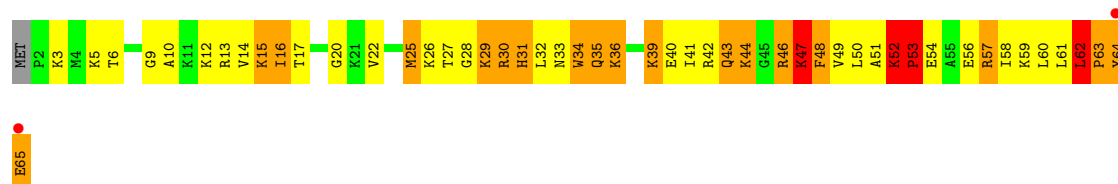
- Molecule 53: 50S ribosomal protein L34

Chain Y7:



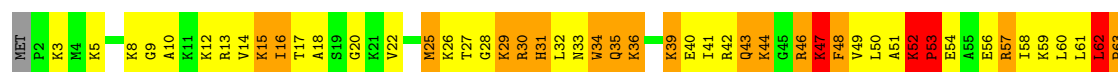
- Molecule 54: 50S ribosomal protein L35

Chain R8:



- Molecule 54: 50S ribosomal protein L35

Chain Y8:



Y64  
E85

- Molecule 55: 50S ribosomal protein L36

Chain R9:

- Molecule 55: 50S ribosomal protein L36

Chain Y9:

- Molecule 56: tRNA acceptor end mimic

Chain Z6:

C74  
G75  
A76

- Molecule 56: tRNA acceptor end mimic

Chain Z8:

C74  
G75  
A76

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.25Å 448.40Å 624.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.97 – 3.48 34.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.97-3.48) 99.2 (34.97-3.30)	Depositor EDS
$R_{merge}$	0.32	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.230 , 0.270 0.230 , 0.270	Depositor DCC
$R_{free}$ test set	33692 reflections (4.57%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 32.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 860144 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	292002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 1MG, PPU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	QA	0.31	0/36098	0.83	43/56341 (0.1%)
1	XA	0.35	0/36101	0.86	41/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.36	0/1959	0.65	0/2642
3	QC	0.37	0/1629	0.60	0/2195
3	XC	0.37	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.39	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.36	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.53	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.38	0/221	0.63	0/288
22	QV	0.53	0/1836	0.99	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QY	0.28	0/333	1.11	1/517 (0.2%)
23	XY	0.30	0/333	1.11	1/517 (0.2%)
24	QX	0.96	3/193 (1.6%)	1.43	3/299 (1.0%)
24	XX	0.96	3/193 (1.6%)	1.44	3/299 (1.0%)
25	RA	0.38	4/69521 (0.0%)	0.89	62/108529 (0.1%)
25	YA	0.44	4/69543 (0.0%)	0.95	91/108563 (0.1%)
26	RB	0.31	0/2878	0.82	1/4490 (0.0%)
26	YB	0.38	0/2878	0.89	0/4490
27	RD	0.59	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	3/1802 (0.2%)
32	RI	0.32	0/1151	0.58	0/1558
32	YI	0.32	0/1151	0.60	0/1558
33	RN	0.46	0/1131	0.77	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.50	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.90	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YS	0.45	0/892	0.83	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.47	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.78	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.81	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.29	0/1493	0.53	0/2026
45	YZ	0.33	0/1493	0.56	0/2026
46	R0	0.30	0/657	0.54	1/874 (0.1%)
46	Y0	0.38	0/657	0.54	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.83	1/771 (0.1%)
48	Y2	0.51	0/583	0.84	1/771 (0.1%)
49	R3	0.47	0/474	0.72	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.43	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.60	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.80	0/40	1.78	1/60 (1.7%)
56	Z8	0.80	0/40	1.80	1/60 (1.7%)
All	All	0.41	16/316383 (0.0%)	0.86	323/473007 (0.1%)

The worst 5 of 16 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	RA	1472	A	N9-C8	-11.04	1.28	1.37
27	RD	236	GLY	C-N	8.56	1.53	1.34
25	RA	1472	A	C8-N7	-8.20	1.25	1.31
25	RA	1413	G	N9-C4	-7.25	1.32	1.38
25	YA	1473	G	C8-N7	-6.84	1.26	1.30

The worst 5 of 323 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	QL	47	LYS	C-N-CD	-20.49	75.52	120.60
12	XL	47	LYS	C-N-CD	-20.45	75.61	120.60
23	QY	40	G	P-O3'-C3'	-16.23	100.23	119.70
23	XY	40	G	P-O3'-C3'	-16.18	100.28	119.70
25	RA	1472	A	N7-C8-N9	12.07	119.84	113.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	536	0
1	XA	32249	0	16279	560	0
2	QB	1924	0	1975	284	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	205	0
3	XC	1605	0	1668	207	0
4	QD	1703	0	1764	254	0
4	XD	1703	0	1765	212	1
5	QE	1155	0	1213	143	0
5	XE	1155	0	1213	136	0
6	QF	843	0	857	93	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	XF	843	0	857	98	0
7	QG	1257	0	1296	146	0
7	XG	1257	0	1294	143	0
8	QH	1116	0	1175	149	0
8	XH	1116	0	1177	148	0
9	QI	1010	0	1037	146	0
9	XI	1010	0	1037	158	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	135	0
11	QK	885	0	904	100	0
11	XK	885	0	904	109	0
12	QL	975	0	1062	107	0
12	XL	975	0	1062	103	0
13	QM	964	0	1034	151	0
13	XM	964	0	1034	160	0
14	QN	492	0	529	95	0
14	XN	492	0	529	96	0
15	QO	734	0	771	74	0
15	XO	734	0	771	73	0
16	QP	705	0	725	111	0
16	XP	705	0	725	107	0
17	QQ	834	0	904	81	0
17	XQ	834	0	904	73	0
18	QR	574	0	644	65	0
18	XR	574	0	644	68	0
19	QS	674	0	699	110	0
19	XS	674	0	699	133	0
20	QT	763	0	860	105	0
20	XT	763	0	861	100	0
21	QU	217	0	234	27	0
21	XU	217	0	234	24	0
22	QV	1644	0	836	35	0
22	XV	1644	0	836	35	0
23	QY	323	0	165	4	0
23	XY	323	0	165	7	0
24	QX	173	0	88	7	0
24	XX	173	0	88	6	0
25	RA	62071	0	31288	884	1
25	YA	62091	0	31294	903	1
26	RB	2573	0	1306	66	0
26	YB	2573	0	1306	33	0
27	RD	2115	0	2195	306	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	YD	2115	0	2195	331	0
28	RE	1568	0	1634	272	0
28	YE	1568	0	1634	263	0
29	RF	1585	0	1632	173	0
29	YF	1585	0	1632	171	0
30	RG	1474	0	1535	207	1
30	YG	1474	0	1535	201	1
31	RH	1307	0	1382	225	0
31	YH	1307	0	1382	226	0
32	RI	1136	0	1223	40	0
32	YI	1136	0	1223	50	0
33	RN	1104	0	1180	197	0
33	YN	1104	0	1180	186	0
34	RO	933	0	996	120	0
34	YO	933	0	996	127	0
35	RP	1145	0	1228	246	0
35	YP	1145	0	1228	239	1
36	RQ	1122	0	1179	153	0
36	YQ	1122	0	1179	150	0
37	RR	968	0	1033	113	0
37	YR	968	0	1033	105	0
38	RS	882	0	943	162	0
38	YS	882	0	943	162	0
39	RT	1141	0	1202	151	0
39	YT	1141	0	1202	154	0
40	RU	964	0	1022	128	0
40	YU	964	0	1022	136	0
41	RV	779	0	852	130	0
41	YV	779	0	852	131	13
42	RW	900	0	964	101	0
42	YW	900	0	964	102	0
43	RX	725	0	778	67	0
43	YX	725	0	778	67	0
44	RY	785	0	878	161	0
44	YY	785	0	878	153	0
45	RZ	1461	0	1493	52	0
45	YZ	1461	0	1493	40	0
46	R0	648	0	672	21	0
46	Y0	648	0	672	23	0
47	R1	763	0	848	143	0
47	Y1	763	0	848	136	0
48	R2	581	0	629	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Y2	581	0	629	76	0
49	R3	469	0	518	39	1
49	Y3	469	0	518	42	0
50	R4	581	0	574	148	0
50	Y4	581	0	574	165	0
51	R5	459	0	480	73	0
51	Y5	459	0	480	76	13
52	R6	424	0	450	94	0
52	Y6	424	0	450	92	0
53	R7	430	0	480	39	0
53	Y7	430	0	480	44	0
54	R8	517	0	582	105	0
54	Y8	517	0	582	99	0
55	R9	307	0	335	20	0
55	Y9	307	0	335	18	0
56	Z6	74	0	51	7	0
56	Z8	74	0	51	6	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	241	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	74	0	0	0	0
57	Y0	1	0	0	0	0
57	Y5	1	0	0	0	0
57	YA	268	0	0	0	0
57	YB	4	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0
58	QA	42	0	45	0	0
58	XA	42	0	45	1	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	R9	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	292002	0	198357	14284	17

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

The worst 5 of 14284 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.55
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

The worst 5 of 17 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
41:YV:50:PRO:C	51:Y5:60:VAL:O[4_445]	1.47	0.73
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.50	0.70
41:YV:51:VAL:N	51:Y5:60:VAL:C[4_445]	1.60	0.60
41:YV:50:PRO:CG	51:Y5:60:VAL:CA[4_445]	1.78	0.42
41:YV:50:PRO:CA	51:Y5:60:VAL:O[4_445]	1.83	0.37

## 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	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0 9
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	16
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	1	16
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	1	15
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	1	13
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	14
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	1	13
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	17
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	17
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	15
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	17
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	12
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	12
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	9
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	9
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	17
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	14
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	2	26
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	22
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	11
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	11
13	QM	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	4
13	XM	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	4
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	2
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	25
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	25
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	8
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	8
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	20
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	20
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	XR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	1	11
19	QS	82/93 (88%)	47 (57%)	17 (21%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	4
21	XU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	4
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	2	25
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	2	25
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	14
29	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	1	14
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	11
30	YG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	1	11
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	102 (71%)	29 (20%)	13 (9%)	1	17
32	YI	144/148 (97%)	101 (70%)	26 (18%)	17 (12%)	1	11
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	5
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	5
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	23
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	23
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	14
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	14
37	RR	116/118 (98%)	83 (72%)	19 (16%)	14 (12%)	1	10
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	10
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	4
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	6
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	6
40	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	21
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	21
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	14
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	14
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	10
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	10
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	33
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	33
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	1
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	1
45	RZ	181/206 (88%)	126 (70%)	40 (22%)	15 (8%)	1	20
45	YZ	181/206 (88%)	125 (69%)	38 (21%)	18 (10%)	1	15
46	R0	80/85 (94%)	68 (85%)	9 (11%)	3 (4%)	5	46
46	Y0	80/85 (94%)	71 (89%)	9 (11%)	0	100	100
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	11
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	11
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	8
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	8
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	34
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	34
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	28
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	28
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7650 (67%)	2346 (20%)	1474 (13%)	0	9

5 of 1474 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	8	37
2	XB	205/220 (93%)	181 (88%)	24 (12%)	8	37
3	QC	159/188 (85%)	143 (90%)	16 (10%)	11	47
3	XC	159/188 (85%)	143 (90%)	16 (10%)	11	47
4	QD	180/181 (99%)	160 (89%)	20 (11%)	9	41
4	XD	180/181 (99%)	165 (92%)	15 (8%)	16	58
5	QE	116/123 (94%)	108 (93%)	8 (7%)	22	68
5	XE	116/123 (94%)	108 (93%)	8 (7%)	22	68
6	QF	90/90 (100%)	76 (84%)	14 (16%)	4	23
6	XF	90/90 (100%)	76 (84%)	14 (16%)	4	23
7	QG	126/127 (99%)	114 (90%)	12 (10%)	12	50
7	XG	126/127 (99%)	115 (91%)	11 (9%)	15	56
8	QH	119/119 (100%)	106 (89%)	13 (11%)	9	42
8	XH	119/119 (100%)	106 (89%)	13 (11%)	9	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	QI	98/99 (99%)	87 (89%)	11 (11%)	9	40
9	XI	98/99 (99%)	87 (89%)	11 (11%)	9	40
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	14	54
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	14	54
11	QK	90/99 (91%)	81 (90%)	9 (10%)	11	48
11	XK	90/99 (91%)	81 (90%)	9 (10%)	11	48
12	QL	104/109 (95%)	90 (86%)	14 (14%)	6	30
12	XL	104/109 (95%)	90 (86%)	14 (14%)	6	30
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	19
13	XM	97/101 (96%)	81 (84%)	16 (16%)	3	19
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	13
14	XN	49/50 (98%)	44 (90%)	5 (10%)	11	47
15	QO	79/80 (99%)	73 (92%)	6 (8%)	19	64
15	XO	79/80 (99%)	73 (92%)	6 (8%)	19	64
16	QP	72/74 (97%)	63 (88%)	9 (12%)	7	34
16	XP	72/74 (97%)	63 (88%)	9 (12%)	7	34
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	25	72
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	25	72
18	QR	61/77 (79%)	54 (88%)	7 (12%)	8	38
18	XR	61/77 (79%)	54 (88%)	7 (12%)	8	38
19	QS	73/80 (91%)	62 (85%)	11 (15%)	4	25
19	XS	73/80 (91%)	62 (85%)	11 (15%)	4	25
20	QT	76/82 (93%)	68 (90%)	8 (10%)	10	45
20	XT	76/82 (93%)	68 (90%)	8 (10%)	10	45
21	QU	20/22 (91%)	19 (95%)	1 (5%)	34	79
21	XU	20/22 (91%)	19 (95%)	1 (5%)	34	79
27	RD	214/218 (98%)	177 (83%)	37 (17%)	3	16
27	YD	214/218 (98%)	177 (83%)	37 (17%)	3	16
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	7
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	7
29	RF	161/166 (97%)	140 (87%)	21 (13%)	6	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	YF	161/166 (97%)	140 (87%)	21 (13%)	6	32
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	21
30	YG	155/156 (99%)	130 (84%)	25 (16%)	3	21
31	RH	142/148 (96%)	114 (80%)	28 (20%)	2	11
31	YH	142/148 (96%)	114 (80%)	28 (20%)	2	11
32	RI	122/124 (98%)	98 (80%)	24 (20%)	2	11
32	YI	122/124 (98%)	98 (80%)	24 (20%)	2	11
33	RN	117/119 (98%)	98 (84%)	19 (16%)	3	20
33	YN	117/119 (98%)	98 (84%)	19 (16%)	3	20
34	RO	100/100 (100%)	90 (90%)	10 (10%)	11	48
34	YO	100/100 (100%)	90 (90%)	10 (10%)	11	48
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	6
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	6
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	20
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	3	20
37	RR	101/101 (100%)	84 (83%)	17 (17%)	3	18
37	YR	101/101 (100%)	84 (83%)	17 (17%)	3	18
38	RS	87/88 (99%)	74 (85%)	13 (15%)	4	25
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	25
39	RT	120/127 (94%)	97 (81%)	23 (19%)	2	11
39	YT	120/127 (94%)	98 (82%)	22 (18%)	2	13
40	RU	93/94 (99%)	80 (86%)	13 (14%)	5	28
40	YU	93/94 (99%)	80 (86%)	13 (14%)	5	28
41	RV	82/82 (100%)	71 (87%)	11 (13%)	6	30
41	YV	82/82 (100%)	71 (87%)	11 (13%)	6	30
42	RW	92/92 (100%)	77 (84%)	15 (16%)	3	20
42	YW	92/92 (100%)	77 (84%)	15 (16%)	3	20
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	25
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	25
44	RY	85/91 (93%)	70 (82%)	15 (18%)	3	15
44	YY	85/91 (93%)	70 (82%)	15 (18%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	RZ	162/179 (90%)	139 (86%)	23 (14%)	5	27
45	YZ	162/179 (90%)	139 (86%)	23 (14%)	5	27
46	R0	65/67 (97%)	61 (94%)	4 (6%)	26	72
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	13	52
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	13
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	13
48	R2	64/67 (96%)	57 (89%)	7 (11%)	9	42
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	9	42
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	8
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	8
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	4
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	4
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	6
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	6
52	R6	48/52 (92%)	38 (79%)	10 (21%)	2	9
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	2	9
53	R7	42/42 (100%)	39 (93%)	3 (7%)	21	67
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	21	67
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	4
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	4
55	R9	34/34 (100%)	32 (94%)	2 (6%)	28	74
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	28	74
All	All	9702/10066 (96%)	8296 (86%)	1406 (14%)	5	26

5 of 1406 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	8	LEU
7	XG	84	ASN
45	YZ	144	LEU
50	R4	49	PHE
2	XB	63	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
48	R2	9	GLN
6	XF	64	GLN
44	YY	57	GLN
49	R3	19	GLN
2	XB	204	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	269 (17%)	42 (2%)
1	XA	1499/1522 (98%)	289 (19%)	46 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QY	14/17 (82%)	7 (50%)	1 (7%)
23	XY	14/17 (82%)	7 (50%)	1 (7%)
24	QX	7/25 (28%)	4 (57%)	1 (14%)
24	XX	7/25 (28%)	4 (57%)	1 (14%)
25	RA	2879/2916 (98%)	620 (21%)	66 (2%)
25	YA	2880/2916 (98%)	623 (21%)	60 (2%)
26	RB	119/122 (97%)	24 (20%)	2 (1%)
26	YB	119/122 (97%)	24 (20%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9364 (98%)	1931 (21%)	223 (2%)

5 of 1931 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	51	A

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2481	G
1	XA	266	G
25	YA	1929	G
25	RA	2610	C
1	XA	5	U



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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
23	1MG	QY	37	23	24,26,27	2.76	5 (20%)	34,39,42	2.82	7 (20%)
23	1MG	XY	37	23	24,26,27	2.76	5 (20%)	34,39,42	2.76	7 (20%)
56	PPU	Z6	76	25,56	38,40,41	2.43	9 (23%)	54,57,60	2.62	14 (25%)
56	PPU	Z8	76	57,56	38,40,41	2.42	9 (23%)	54,57,60	2.61	14 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	1MG	QY	37	23	-	0/8/25/26	0/3/3/3
23	1MG	XY	37	23	-	0/8/25/26	0/3/3/3
56	PPU	Z6	76	25,56	-	0/26/43/44	0/4/4/4
56	PPU	Z8	76	57,56	-	0/26/43/44	0/4/4/4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.24	1.41	1.23
56	Z6	76	PPU	O-C	9.22	1.41	1.23
23	XY	37	1MG	C4-N3	8.18	1.49	1.35
23	QY	37	1MG	C4-N3	8.09	1.49	1.35
23	QY	37	1MG	C2-N2	6.32	1.47	1.33

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QY	37	1MG	C6-N1-C2	11.45	123.85	120.71
23	XY	37	1MG	C6-N1-C2	11.07	123.75	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z8	76	PPU	N3-C2-N1	-8.62	121.31	128.89
56	Z6	76	PPU	N3-C2-N1	-8.56	121.36	128.89
56	Z8	76	PPU	C3'-N3'-C	-8.14	110.23	123.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 680 ligands modelled in this entry, 678 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PAR	QA	1666	-	45,45,45	1.31	6 (13%)	67,67,67	1.40	8 (11%)
58	PAR	XA	1675	-	45,45,45	1.35	6 (13%)	67,67,67	1.33	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	QA	1666	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1675	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C52-C42	3.24	1.58	1.52
58	XA	1675	PAR	C52-C42	3.07	1.58	1.52
58	QA	1666	PAR	C64-C54	2.94	1.59	1.51
58	XA	1675	PAR	O54-C14	2.86	1.49	1.41
58	QA	1666	PAR	O54-C14	2.84	1.49	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1666	PAR	O52-C13-C23	4.71	115.91	107.50
58	XA	1675	PAR	C14-O54-C54	4.38	122.20	113.73
58	XA	1675	PAR	O52-C13-C23	4.24	115.06	107.50
58	XA	1675	PAR	O33-C14-C24	4.14	116.27	108.08
58	QA	1666	PAR	C14-O54-C54	3.85	121.18	113.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	QA	1500/1522 (98%)	0.06	32 (2%) 60 28	43, 89, 165, 301	0
1	XA	1500/1522 (98%)	-0.04	26 (1%) 67 33	33, 76, 161, 285	0
2	QB	237/256 (92%)	0.33	7 (2%) 48 21	74, 140, 206, 264	0
2	XB	237/256 (92%)	0.25	3 (1%) 74 39	68, 121, 186, 246	0
3	QC	205/239 (85%)	0.27	0 100 100	66, 125, 179, 210	0
3	XC	205/239 (85%)	0.06	0 100 100	46, 95, 150, 198	0
4	QD	208/209 (99%)	0.11	0 100 100	47, 92, 146, 223	0
4	XD	208/209 (99%)	0.16	1 (0%) 88 63	45, 96, 162, 182	0
5	QE	151/162 (93%)	0.18	2 (1%) 74 39	42, 101, 170, 220	0
5	XE	151/162 (93%)	0.08	0 100 100	35, 84, 142, 186	0
6	QF	101/101 (100%)	0.14	0 100 100	40, 90, 127, 156	0
6	XF	101/101 (100%)	0.17	1 (0%) 79 46	38, 84, 127, 150	0
7	QG	155/156 (99%)	0.31	7 (4%) 32 13	56, 121, 175, 232	0
7	XG	155/156 (99%)	0.22	9 (5%) 22 9	51, 93, 148, 196	0
8	QH	138/138 (100%)	0.12	0 100 100	51, 100, 142, 160	0
8	XH	138/138 (100%)	0.03	0 100 100	51, 89, 134, 187	0
9	QI	127/128 (99%)	0.55	7 (5%) 24 10	71, 131, 189, 204	0
9	XI	127/128 (99%)	0.23	1 (0%) 83 51	46, 112, 165, 221	0
10	QJ	99/105 (94%)	0.79	5 (5%) 27 11	80, 153, 212, 237	0
10	XJ	99/105 (94%)	0.54	5 (5%) 27 11	42, 120, 186, 217	0
11	QK	119/129 (92%)	0.41	6 (5%) 28 11	42, 89, 165, 231	0
11	XK	119/129 (92%)	0.18	3 (2%) 54 24	49, 81, 135, 193	0
12	QL	125/132 (94%)	0.29	5 (4%) 36 15	40, 83, 150, 208	0
12	XL	125/132 (94%)	0.13	3 (2%) 56 25	29, 68, 134, 239	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	0.48	4 (3%) 44 19	52, 130, 190, 269	0
13	XM	121/126 (96%)	0.23	1 (0%) 83 51	43, 98, 161, 256	0
14	QN	60/61 (98%)	0.64	1 (1%) 67 33	72, 121, 165, 182	0
14	XN	60/61 (98%)	0.25	1 (1%) 67 33	38, 87, 148, 182	0
15	QO	88/89 (98%)	0.20	0 100 100	48, 95, 154, 187	0
15	XO	88/89 (98%)	0.09	1 (1%) 77 42	43, 82, 128, 167	0
16	QP	84/88 (95%)	0.15	1 (1%) 75 41	44, 86, 146, 195	0
16	XP	84/88 (95%)	0.15	0 100 100	46, 92, 133, 208	0
17	QQ	100/105 (95%)	0.21	1 (1%) 79 46	63, 94, 151, 215	0
17	XQ	100/105 (95%)	0.15	0 100 100	45, 95, 148, 188	0
18	QR	70/88 (79%)	0.17	1 (1%) 72 37	45, 85, 146, 166	0
18	XR	70/88 (79%)	0.11	1 (1%) 72 37	35, 81, 137, 153	0
19	QS	84/93 (90%)	0.62	5 (5%) 21 9	82, 137, 196, 229	0
19	XS	84/93 (90%)	0.20	0 100 100	53, 96, 156, 198	0
20	QT	99/106 (93%)	0.25	1 (1%) 79 46	55, 103, 165, 201	0
20	XT	99/106 (93%)	0.20	1 (1%) 79 46	50, 101, 158, 190	0
21	QU	25/27 (92%)	1.42	5 (20%) 2 2	66, 117, 146, 190	0
21	XU	25/27 (92%)	1.00	2 (8%) 12 6	61, 89, 133, 169	0
22	QV	77/77 (100%)	0.28	3 (3%) 37 16	49, 99, 152, 188	0
22	XV	77/77 (100%)	0.29	3 (3%) 37 16	43, 82, 137, 198	0
23	QY	15/17 (88%)	0.55	2 (13%) 4 3	85, 102, 178, 179	0
23	XY	15/17 (88%)	0.69	2 (13%) 4 3	63, 81, 141, 145	0
24	QX	8/25 (32%)	1.30	2 (25%) 1 2	68, 91, 144, 227	0
24	XX	8/25 (32%)	0.92	2 (25%) 1 2	51, 69, 129, 197	0
25	RA	2882/2916 (98%)	0.06	135 (4%) 30 12	32, 68, 203, 342	0
25	YA	2883/2916 (98%)	-0.14	90 (3%) 47 21	21, 52, 190, 313	0
26	RB	120/122 (98%)	0.21	1 (0%) 83 51	62, 105, 144, 172	0
26	YB	120/122 (98%)	-0.25	0 100 100	43, 68, 101, 139	0
27	RD	272/276 (98%)	-0.05	0 100 100	32, 60, 102, 187	0
27	YD	272/276 (98%)	-0.00	1 (0%) 90 70	11, 55, 94, 228	0
28	RE	205/206 (99%)	0.09	3 (1%) 70 35	30, 74, 135, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YE	205/206 (99%)	-0.04	2 (0%) 79 46	20, 58, 130, 245	0
29	RF	202/210 (96%)	0.03	0 100 100	27, 82, 150, 199	0
29	YF	202/210 (96%)	-0.12	0 100 100	17, 58, 119, 164	0
30	RG	181/182 (99%)	1.22	28 (15%) 3 2	58, 182, 252, 270	0
30	YG	181/182 (99%)	0.70	4 (2%) 59 27	52, 114, 185, 251	0
31	RH	170/180 (94%)	0.65	7 (4%) 35 15	71, 144, 203, 244	0
31	YH	170/180 (94%)	0.19	1 (0%) 86 58	41, 86, 147, 171	0
32	RI	146/148 (98%)	0.21	0 100 100	47, 100, 170, 202	0
32	YI	146/148 (98%)	0.08	0 100 100	43, 98, 153, 180	0
33	RN	138/140 (98%)	0.09	0 100 100	43, 83, 138, 196	0
33	YN	138/140 (98%)	-0.05	0 100 100	29, 60, 118, 171	0
34	RO	122/122 (100%)	0.05	0 100 100	21, 75, 123, 179	0
34	YO	122/122 (100%)	-0.17	0 100 100	18, 59, 94, 134	0
35	RP	150/150 (100%)	0.31	4 (2%) 52 23	21, 86, 180, 219	0
35	YP	150/150 (100%)	0.07	3 (2%) 62 29	14, 67, 136, 235	0
36	RQ	141/141 (100%)	0.21	1 (0%) 84 55	45, 88, 145, 231	0
36	YQ	141/141 (100%)	-0.03	0 100 100	24, 65, 135, 196	0
37	RR	118/118 (100%)	-0.06	0 100 100	38, 69, 130, 147	0
37	YR	118/118 (100%)	-0.16	0 100 100	26, 55, 91, 142	0
38	RS	111/112 (99%)	0.19	1 (0%) 81 49	49, 104, 167, 222	0
38	YS	111/112 (99%)	-0.07	1 (0%) 81 49	39, 71, 123, 181	0
39	RT	137/146 (93%)	0.21	3 (2%) 59 27	42, 86, 185, 226	0
39	YT	137/146 (93%)	-0.03	1 (0%) 84 55	25, 70, 160, 220	0
40	RU	117/118 (99%)	0.07	2 (1%) 67 33	31, 69, 130, 222	0
40	YU	117/118 (99%)	-0.05	2 (1%) 67 33	21, 50, 107, 201	0
41	RV	101/101 (100%)	0.04	1 (0%) 79 46	44, 92, 155, 249	0
41	YV	101/101 (100%)	0.12	3 (2%) 48 21	26, 71, 136, 264	0
42	RW	113/113 (100%)	-0.03	0 100 100	31, 63, 128, 188	0
42	YW	113/113 (100%)	-0.12	0 100 100	17, 54, 114, 186	0
43	RX	92/96 (95%)	0.05	1 (1%) 77 42	41, 78, 122, 150	0
43	YX	92/96 (95%)	-0.08	0 100 100	28, 56, 92, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RY	102/110 (92%)	0.64	9 (8%) 10 6	50, 106, 193, 237	0
44	YY	102/110 (92%)	0.22	2 (1%) 62 29	39, 82, 158, 234	0
45	RZ	183/206 (88%)	0.40	2 (1%) 77 42	56, 124, 189, 247	0
45	YZ	183/206 (88%)	0.11	2 (1%) 77 42	41, 86, 169, 257	0
46	R0	82/85 (96%)	-0.05	0 100 100	42, 72, 103, 131	0
46	Y0	82/85 (96%)	-0.25	0 100 100	26, 49, 80, 99	0
47	R1	97/98 (98%)	0.43	4 (4%) 35 15	34, 75, 194, 262	0
47	Y1	97/98 (98%)	0.26	3 (3%) 47 21	27, 61, 143, 210	0
48	R2	69/72 (95%)	0.09	0 100 100	48, 94, 168, 184	0
48	Y2	69/72 (95%)	-0.02	0 100 100	22, 66, 131, 195	0
49	R3	59/60 (98%)	0.43	2 (3%) 43 18	42, 90, 161, 183	0
49	Y3	59/60 (98%)	-0.03	1 (1%) 67 33	33, 61, 113, 179	0
50	R4	71/71 (100%)	1.22	12 (16%) 2 2	129, 204, 273, 302	0
50	Y4	71/71 (100%)	0.85	8 (11%) 6 4	84, 166, 258, 313	0
51	R5	59/60 (98%)	0.42	4 (6%) 17 7	25, 73, 191, 257	0
51	Y5	59/60 (98%)	0.29	3 (5%) 27 11	29, 62, 189, 319	0
52	R6	49/54 (90%)	1.17	7 (14%) 3 3	66, 147, 198, 224	0
52	Y6	49/54 (90%)	0.93	3 (6%) 21 9	59, 116, 196, 225	0
53	R7	49/49 (100%)	0.08	1 (2%) 62 29	27, 55, 129, 235	0
53	Y7	49/49 (100%)	-0.07	1 (2%) 62 29	23, 42, 102, 186	0
54	R8	64/65 (98%)	0.25	2 (3%) 47 21	34, 73, 129, 210	0
54	Y8	64/65 (98%)	0.05	0 100 100	24, 56, 101, 237	0
55	R9	37/37 (100%)	1.02	6 (16%) 2 2	64, 96, 157, 235	0
55	Y9	37/37 (100%)	0.74	2 (5%) 25 10	48, 83, 136, 176	0
56	Z6	3/3 (100%)	4.41	1 (33%) 1 1	74, 74, 77, 77	0
56	Z8	3/3 (100%)	3.91	1 (33%) 1 1	51, 51, 60, 70	0
All	All	20877/21492 (97%)	0.11	534 (2%) 53 23	11, 79, 179, 342	0

The worst 5 of 534 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	1058	G	15.6
25	RA	1060	U	12.8

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Mol	Chain	Res	Type	RSRZ
25	RA	1070	A	12.2
25	RA	1096	A	11.0
25	RA	1061	U	11.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	1MG	QY	37	24/25	0.21	-	86,86,86,86	0
56	PPU	Z6	76	37/38	0.35	-	73,73,73,73	0
56	PPU	Z8	76	37/38	0.34	-	70,70,70,70	0
23	1MG	XY	37	24/25	0.17	-	62,62,62,62	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	QA	1660	1/1	0.43	-	35,35,35,35	0
57	MG	RA	3020	1/1	0.15	-	7,7,7,7	0
57	MG	YA	3134	1/1	0.09	-	37,37,37,37	0
57	MG	RA	3057	1/1	0.38	-	34,34,34,34	0
57	MG	QA	1642	1/1	0.13	-	25,25,25,25	0
57	MG	YA	3072	1/1	0.29	-	15,15,15,15	0
57	MG	YA	3251	1/1	0.31	-	60,60,60,60	0
57	MG	RA	3097	1/1	0.17	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3041	1/1	0.26	-	2,2,2,2	0
57	MG	XA	1619	1/1	0.26	-	33,33,33,33	0
57	MG	QA	1650	1/1	0.11	-	27,27,27,27	0
57	MG	RA	3240	1/1	0.25	-	23,23,23,23	0
57	MG	YA	3005	1/1	0.08	-	7,7,7,7	0
57	MG	RA	3090	1/1	0.22	-	7,7,7,7	0
57	MG	QA	1639	1/1	0.13	-	45,45,45,45	0
57	MG	RA	3155	1/1	0.25	-	41,41,41,41	0
57	MG	YA	3176	1/1	0.11	-	32,32,32,32	0
57	MG	RA	3152	1/1	0.16	-	33,33,33,33	0
57	MG	YA	3068	1/1	0.14	-	26,26,26,26	0
57	MG	YA	3208	1/1	0.14	-	30,30,30,30	0
57	MG	YA	3123	1/1	0.12	-	28,28,28,28	0
57	MG	RA	3139	1/1	0.54	-	51,51,51,51	0
57	MG	RA	3179	1/1	0.25	-	29,29,29,29	0
57	MG	XA	1670	1/1	0.20	-	79,79,79,79	0
57	MG	YA	3241	1/1	0.17	-	39,39,39,39	0
57	MG	XA	1668	1/1	0.20	-	30,30,30,30	0
57	MG	RA	3060	1/1	0.18	-	3,3,3,3	0
57	MG	XA	1634	1/1	0.20	-	43,43,43,43	0
59	ZN	Y9	101	1/1	0.10	-	87,87,87,87	0
57	MG	RA	3186	1/1	0.15	-	52,52,52,52	0
57	MG	QA	1632	1/1	0.24	-	40,40,40,40	0
57	MG	YA	3170	1/1	0.09	-	26,26,26,26	0
57	MG	RA	3146	1/1	0.17	-	37,37,37,37	0
57	MG	YA	3210	1/1	0.19	-	47,47,47,47	0
57	MG	RA	3130	1/1	0.27	-	94,94,94,94	0
57	MG	YA	3122	1/1	0.49	-	95,95,95,95	0
57	MG	RA	3198	1/1	0.21	-	22,22,22,22	0
59	ZN	QD	301	1/1	0.25	-	53,53,53,53	0
57	MG	YA	3091	1/1	0.28	-	7,7,7,7	0
57	MG	RA	3069	1/1	0.05	-	28,28,28,28	0
57	MG	YA	3096	1/1	0.34	-	7,7,7,7	0
57	MG	RA	3125	1/1	0.20	-	29,29,29,29	0
57	MG	RA	3038	1/1	0.16	-	8,8,8,8	0
57	MG	YA	3221	1/1	1.05	-	42,42,42,42	0
57	MG	QA	1655	1/1	0.24	-	48,48,48,48	0
57	MG	YA	3173	1/1	0.50	-	32,32,32,32	0
57	MG	YA	3172	1/1	0.19	-	48,48,48,48	0
57	MG	XA	1608	1/1	0.26	-	60,60,60,60	0
57	MG	RA	3087	1/1	0.10	-	27,27,27,27	0
57	MG	QA	1622	1/1	0.16	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3177	1/1	0.45	-	71,71,71,71	0
57	MG	YA	3063	1/1	0.17	-	17,17,17,17	0
57	MG	YA	3117	1/1	0.25	-	46,46,46,46	0
57	MG	YA	3051	1/1	0.18	-	4,4,4,4	0
57	MG	QH	201	1/1	0.24	-	74,74,74,74	0
57	MG	RA	3021	1/1	0.33	-	8,8,8,8	0
57	MG	YA	3189	1/1	0.08	-	33,33,33,33	0
57	MG	QA	1623	1/1	0.21	-	29,29,29,29	0
57	MG	YA	3222	1/1	0.37	-	40,40,40,40	0
57	MG	RA	3221	1/1	0.48	-	55,55,55,55	0
57	MG	YA	3213	1/1	0.09	-	31,31,31,31	0
57	MG	RA	3110	1/1	0.08	-	12,12,12,12	0
57	MG	XA	1624	1/1	0.42	-	39,39,39,39	0
57	MG	RA	3204	1/1	0.30	-	63,63,63,63	0
57	MG	RA	3196	1/1	0.25	-	46,46,46,46	0
57	MG	YA	3039	1/1	0.10	-	14,14,14,14	0
57	MG	RA	3088	1/1	0.23	-	25,25,25,25	0
57	MG	YA	3010	1/1	0.17	-	0,0,0,0	0
57	MG	YA	3081	1/1	0.19	-	5,5,5,5	0
57	MG	RA	3212	1/1	0.18	-	37,37,37,37	0
57	MG	RA	3006	1/1	0.15	-	7,7,7,7	0
57	MG	YA	3125	1/1	0.17	-	65,65,65,65	0
57	MG	YA	3255	1/1	0.33	-	0,0,0,0	0
57	MG	RA	3107	1/1	0.13	-	27,27,27,27	0
57	MG	YA	3248	1/1	0.12	-	32,32,32,32	0
57	MG	YA	3087	1/1	0.29	-	6,6,6,6	0
57	MG	YA	3093	1/1	0.17	-	18,18,18,18	0
57	MG	YA	3104	1/1	0.08	-	22,22,22,22	0
57	MG	RA	3004	1/1	0.23	-	2,2,2,2	0
57	MG	YA	3207	1/1	0.29	-	52,52,52,52	0
57	MG	XA	1627	1/1	0.09	-	24,24,24,24	0
57	MG	YA	3024	1/1	0.19	-	1,1,1,1	0
57	MG	RA	3103	1/1	0.16	-	26,26,26,26	0
57	MG	YA	3247	1/1	0.19	-	26,26,26,26	0
57	MG	YA	3146	1/1	0.22	-	40,40,40,40	0
57	MG	YA	3137	1/1	0.11	-	21,21,21,21	0
57	MG	RA	3185	1/1	0.29	-	45,45,45,45	0
57	MG	XA	1622	1/1	0.09	-	33,33,33,33	0
57	MG	YA	3073	1/1	0.18	-	7,7,7,7	0
57	MG	RA	3012	1/1	0.12	-	14,14,14,14	0
57	MG	YA	3166	1/1	0.57	-	55,55,55,55	0
57	MG	RA	3195	1/1	0.34	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RF	301	1/1	0.18	-	65,65,65,65	0
57	MG	YA	3034	1/1	0.27	-	7,7,7,7	0
57	MG	YA	3203	1/1	0.12	-	18,18,18,18	0
57	MG	RA	3124	1/1	0.10	-	28,28,28,28	0
57	MG	RA	3172	1/1	0.25	-	31,31,31,31	0
57	MG	YA	3064	1/1	0.15	-	19,19,19,19	0
57	MG	RA	3082	1/1	0.35	-	26,26,26,26	0
57	MG	QA	1645	1/1	0.08	-	37,37,37,37	0
57	MG	YA	3057	1/1	0.13	-	1,1,1,1	0
57	MG	RA	3050	1/1	0.26	-	13,13,13,13	0
57	MG	RA	3009	1/1	0.17	-	26,26,26,26	0
57	MG	YA	3224	1/1	0.09	-	35,35,35,35	0
57	MG	QA	1620	1/1	0.09	-	29,29,29,29	0
57	MG	YA	3215	1/1	0.15	-	24,24,24,24	0
57	MG	RA	3143	1/1	0.17	-	30,30,30,30	0
57	MG	YA	3044	1/1	0.27	-	4,4,4,4	0
57	MG	QV	101	1/1	0.13	-	24,24,24,24	0
57	MG	YA	3217	1/1	0.23	-	38,38,38,38	0
57	MG	YA	3250	1/1	0.23	-	37,37,37,37	0
57	MG	RA	3238	1/1	0.18	-	31,31,31,31	0
57	MG	YA	3120	1/1	0.17	-	18,18,18,18	0
57	MG	YA	3102	1/1	0.40	-	11,11,11,11	0
57	MG	RA	3008	1/1	0.21	-	47,47,47,47	0
57	MG	RA	3180	1/1	0.28	-	33,33,33,33	0
57	MG	YA	3085	1/1	0.58	-	65,65,65,65	0
57	MG	YA	3257	1/1	0.12	-	12,12,12,12	0
57	MG	YA	3193	1/1	0.29	-	35,35,35,35	0
57	MG	QA	1659	1/1	0.10	-	24,24,24,24	0
57	MG	YA	3199	1/1	0.15	-	30,30,30,30	0
57	MG	XA	1664	1/1	0.34	-	84,84,84,84	0
57	MG	YA	3151	1/1	0.19	-	38,38,38,38	0
57	MG	RA	3162	1/1	0.15	-	39,39,39,39	0
57	MG	RA	3049	1/1	0.10	-	14,14,14,14	0
57	MG	R0	101	1/1	0.17	-	32,32,32,32	0
57	MG	YA	3252	1/1	0.33	-	41,41,41,41	0
57	MG	QA	1641	1/1	0.13	-	22,22,22,22	0
57	MG	QA	1661	1/1	0.11	-	41,41,41,41	0
57	MG	RA	3034	1/1	0.30	-	23,23,23,23	0
57	MG	RA	3077	1/1	0.26	-	24,24,24,24	0
57	MG	XA	1639	1/1	0.16	-	59,59,59,59	0
57	MG	YA	3140	1/1	0.15	-	3,3,3,3	0
57	MG	QA	1647	1/1	0.31	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3076	1/1	0.13	-	6,6,6,6	0
57	MG	YA	3094	1/1	0.10	-	5,5,5,5	0
57	MG	RA	3036	1/1	0.24	-	4,4,4,4	0
57	MG	YA	3229	1/1	0.18	-	20,20,20,20	0
57	MG	XA	1667	1/1	0.11	-	55,55,55,55	0
57	MG	RA	3091	1/1	0.42	-	65,65,65,65	0
57	MG	QA	1635	1/1	0.16	-	49,49,49,49	0
57	MG	YA	3162	1/1	0.19	-	19,19,19,19	0
57	MG	RA	3177	1/1	0.23	-	47,47,47,47	0
57	MG	YA	3062	1/1	0.10	-	18,18,18,18	0
57	MG	YP	201	1/1	0.18	-	153,153,153,153	0
57	MG	QA	1646	1/1	0.30	-	46,46,46,46	0
57	MG	YA	3202	1/1	0.15	-	33,33,33,33	0
57	MG	YA	3115	1/1	0.14	-	32,32,32,32	0
57	MG	RA	3122	1/1	0.24	-	29,29,29,29	0
57	MG	YA	3078	1/1	0.14	-	8,8,8,8	0
57	MG	RA	3070	1/1	0.14	-	11,11,11,11	0
57	MG	XA	1638	1/1	0.43	-	91,91,91,91	0
57	MG	RA	3228	1/1	0.35	-	91,91,91,91	0
57	MG	YA	3196	1/1	0.07	-	11,11,11,11	0
57	MG	RA	3084	1/1	0.21	-	27,27,27,27	0
57	MG	YA	3231	1/1	0.15	-	23,23,23,23	0
57	MG	RA	3041	1/1	0.22	-	20,20,20,20	0
57	MG	RA	3044	1/1	0.28	-	37,37,37,37	0
59	ZN	XD	301	1/1	0.26	-	45,45,45,45	0
57	MG	RA	3171	1/1	0.16	-	46,46,46,46	0
57	MG	YA	3055	1/1	0.14	-	37,37,37,37	0
57	MG	YA	3266	1/1	0.20	-	11,11,11,11	0
57	MG	YA	3259	1/1	0.24	-	14,14,14,14	0
57	MG	QA	1602	1/1	0.19	-	24,24,24,24	0
57	MG	RA	3187	1/1	0.09	-	25,25,25,25	0
57	MG	QM	201	1/1	0.13	-	66,66,66,66	0
57	MG	YA	3239	1/1	0.09	-	27,27,27,27	0
57	MG	YA	3118	1/1	0.28	-	33,33,33,33	0
57	MG	YA	3043	1/1	0.26	-	12,12,12,12	0
57	MG	QA	1654	1/1	0.21	-	69,69,69,69	0
57	MG	QA	1657	1/1	0.27	-	108,108,108,108	0
57	MG	YA	3025	1/1	0.11	-	4,4,4,4	0
57	MG	XA	1614	1/1	0.23	-	57,57,57,57	0
57	MG	RA	3150	1/1	0.15	-	32,32,32,32	0
57	MG	RA	3117	1/1	0.10	-	10,10,10,10	0
57	MG	RA	3154	1/1	0.10	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1608	1/1	0.31	-	68,68,68,68	0
57	MG	YA	3131	1/1	0.15	-	15,15,15,15	0
57	MG	RR	201	1/1	0.15	-	7,7,7,7	0
57	MG	XA	1661	1/1	0.19	-	28,28,28,28	0
57	MG	RA	3237	1/1	0.15	-	13,13,13,13	0
57	MG	YA	3031	1/1	0.37	-	26,26,26,26	0
57	MG	RA	3227	1/1	0.11	-	64,64,64,64	0
57	MG	QA	1652	1/1	0.12	-	31,31,31,31	0
57	MG	RA	3128	1/1	0.12	-	55,55,55,55	0
57	MG	RA	3096	1/1	0.28	-	22,22,22,22	0
57	MG	YA	3052	1/1	0.16	-	1,1,1,1	0
57	MG	XA	1659	1/1	0.21	-	41,41,41,41	0
57	MG	RA	3030	1/1	0.14	-	5,5,5,5	0
57	MG	YA	3240	1/1	0.14	-	31,31,31,31	0
57	MG	XA	1631	1/1	0.14	-	39,39,39,39	0
57	MG	YA	3028	1/1	0.10	-	3,3,3,3	0
57	MG	YA	3159	1/1	0.13	-	19,19,19,19	0
57	MG	RA	3094	1/1	0.31	-	23,23,23,23	0
59	ZN	QN	101	1/1	0.09	-	87,87,87,87	0
57	MG	YA	3228	1/1	0.18	-	4,4,4,4	0
57	MG	YA	3006	1/1	0.17	-	1,1,1,1	0
57	MG	YA	3212	1/1	0.18	-	67,67,67,67	0
57	MG	RA	3147	1/1	0.14	-	14,14,14,14	0
57	MG	YA	3084	1/1	0.35	-	6,6,6,6	0
57	MG	QA	1648	1/1	0.10	-	47,47,47,47	0
57	MG	XA	1650	1/1	0.20	-	31,31,31,31	0
57	MG	QA	1610	1/1	0.28	-	22,22,22,22	0
57	MG	QA	1603	1/1	0.36	-	22,22,22,22	0
57	MG	XA	1606	1/1	0.26	-	29,29,29,29	0
57	MG	RA	3014	1/1	0.21	-	3,3,3,3	0
57	MG	XA	1630	1/1	0.14	-	18,18,18,18	0
57	MG	XA	1674	1/1	0.18	-	35,35,35,35	0
57	MG	QA	1626	1/1	0.20	-	29,29,29,29	0
57	MG	XA	1673	1/1	0.46	-	56,56,56,56	0
57	MG	YA	3253	1/1	0.27	-	25,25,25,25	0
57	MG	QA	1625	1/1	0.32	-	94,94,94,94	0
57	MG	RA	3151	1/1	0.13	-	22,22,22,22	0
57	MG	RA	3080	1/1	0.25	-	15,15,15,15	0
57	MG	YA	3198	1/1	0.15	-	21,21,21,21	0
57	MG	RA	3200	1/1	0.24	-	36,36,36,36	0
57	MG	YA	3026	1/1	0.27	-	0,0,0,0	0
57	MG	YA	3150	1/1	0.14	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3136	1/1	0.19	-	26,26,26,26	0
57	MG	YA	3148	1/1	0.32	-	39,39,39,39	0
57	MG	YA	3018	1/1	0.19	-	6,6,6,6	0
57	MG	YA	3157	1/1	0.21	-	49,49,49,49	0
57	MG	RA	3226	1/1	0.28	-	38,38,38,38	0
57	MG	RA	3211	1/1	0.26	-	38,38,38,38	0
57	MG	YA	3019	1/1	0.22	-	0,0,0,0	0
57	MG	YA	3191	1/1	0.22	-	22,22,22,22	0
57	MG	RA	3174	1/1	0.16	-	26,26,26,26	0
57	MG	YA	3042	1/1	0.26	-	11,11,11,11	0
57	MG	RA	3055	1/1	0.22	-	21,21,21,21	0
57	MG	YA	3232	1/1	0.23	-	28,28,28,28	0
57	MG	RA	3013	1/1	0.35	-	26,26,26,26	0
57	MG	RA	3194	1/1	0.30	-	96,96,96,96	0
57	MG	YA	3066	1/1	0.07	-	20,20,20,20	0
57	MG	XA	1605	1/1	0.15	-	7,7,7,7	0
57	MG	R5	101	1/1	0.22	-	51,51,51,51	0
57	MG	YA	3100	1/1	0.28	-	7,7,7,7	0
57	MG	YA	3142	1/1	0.24	-	14,14,14,14	0
57	MG	YA	3234	1/1	0.15	-	28,28,28,28	0
57	MG	RA	3017	1/1	0.17	-	7,7,7,7	0
57	MG	YA	3144	1/1	0.14	-	13,13,13,13	0
57	MG	YA	3160	1/1	0.15	-	14,14,14,14	0
57	MG	XA	1616	1/1	0.27	-	14,14,14,14	0
57	MG	XA	1625	1/1	0.17	-	14,14,14,14	0
57	MG	RA	3163	1/1	0.39	-	79,79,79,79	0
57	MG	YA	3124	1/1	0.14	-	16,16,16,16	0
57	MG	QA	1629	1/1	0.13	-	47,47,47,47	0
57	MG	YB	203	1/1	0.19	-	43,43,43,43	0
57	MG	YA	3236	1/1	0.18	-	40,40,40,40	0
57	MG	YA	3158	1/1	0.18	-	16,16,16,16	0
57	MG	RA	3068	1/1	0.20	-	37,37,37,37	0
59	ZN	XN	101	1/1	0.21	-	103,103,103,103	0
57	MG	QA	1640	1/1	0.25	-	37,37,37,37	0
57	MG	YA	3103	1/1	0.27	-	26,26,26,26	0
57	MG	QA	1649	1/1	0.20	-	60,60,60,60	0
57	MG	RA	3047	1/1	0.30	-	13,13,13,13	0
57	MG	YA	3164	1/1	0.25	-	22,22,22,22	0
57	MG	YA	3071	1/1	0.11	-	18,18,18,18	0
58	PAR	XA	1675	42/42	0.33	-	74,74,74,74	0
57	MG	RA	3086	1/1	0.18	-	2,2,2,2	0
57	MG	RA	3140	1/1	0.15	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1611	1/1	0.12	-	20,20,20,20	0
57	MG	YA	3106	1/1	0.19	-	3,3,3,3	0
57	MG	YA	3260	1/1	0.26	-	11,11,11,11	0
57	MG	YA	3050	1/1	0.27	-	6,6,6,6	0
57	MG	YA	3258	1/1	0.35	-	9,9,9,9	0
57	MG	QA	1621	1/1	0.17	-	35,35,35,35	0
57	MG	YA	3185	1/1	0.24	-	34,34,34,34	0
57	MG	XA	1657	1/1	0.51	-	48,48,48,48	0
57	MG	XA	1666	1/1	0.09	-	61,61,61,61	0
57	MG	RA	3081	1/1	0.22	-	27,27,27,27	0
57	MG	YA	3223	1/1	0.33	-	42,42,42,42	0
57	MG	RA	3145	1/1	0.24	-	14,14,14,14	0
57	MG	RA	3216	1/1	0.10	-	31,31,31,31	0
57	MG	RA	3035	1/1	0.33	-	27,27,27,27	0
57	MG	RA	3159	1/1	0.21	-	40,40,40,40	0
57	MG	XA	1672	1/1	0.11	-	23,23,23,23	0
57	MG	YA	3083	1/1	0.09	-	0,0,0,0	0
57	MG	RA	3108	1/1	0.25	-	32,32,32,32	0
57	MG	XA	1642	1/1	0.16	-	37,37,37,37	0
57	MG	RA	3191	1/1	0.22	-	38,38,38,38	0
57	MG	RA	3019	1/1	0.28	-	21,21,21,21	0
57	MG	QA	1619	1/1	0.16	-	43,43,43,43	0
57	MG	YA	3007	1/1	0.11	-	2,2,2,2	0
57	MG	YA	3099	1/1	0.14	-	2,2,2,2	0
57	MG	YA	3190	1/1	0.12	-	13,13,13,13	0
57	MG	RA	3051	1/1	0.13	-	18,18,18,18	0
57	MG	XA	1603	1/1	0.19	-	24,24,24,24	0
57	MG	YA	3188	1/1	0.12	-	18,18,18,18	0
57	MG	RA	3029	1/1	0.21	-	6,6,6,6	0
57	MG	YA	3244	1/1	0.22	-	34,34,34,34	0
57	MG	YA	3237	1/1	0.18	-	9,9,9,9	0
57	MG	YA	3001	1/1	0.34	-	7,7,7,7	0
57	MG	QA	1604	1/1	0.21	-	10,10,10,10	0
57	MG	RA	3039	1/1	0.11	-	14,14,14,14	0
57	MG	XA	1601	1/1	0.22	-	7,7,7,7	0
57	MG	XA	1643	1/1	0.13	-	25,25,25,25	0
57	MG	RA	3223	1/1	0.47	-	88,88,88,88	0
57	MG	RA	3165	1/1	0.43	-	43,43,43,43	0
57	MG	RA	3075	1/1	0.12	-	39,39,39,39	0
57	MG	YA	3132	1/1	0.38	-	49,49,49,49	0
57	MG	RA	3126	1/1	0.52	-	39,39,39,39	0
57	MG	YA	3156	1/1	0.13	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3069	1/1	0.26	-	13,13,13,13	0
57	MG	YA	3235	1/1	0.14	-	37,37,37,37	0
57	MG	RA	3236	1/1	0.27	-	34,34,34,34	0
57	MG	YA	3119	1/1	0.11	-	22,22,22,22	0
57	MG	RA	3219	1/1	0.20	-	36,36,36,36	0
57	MG	YA	3126	1/1	0.14	-	17,17,17,17	0
57	MG	RA	3083	1/1	0.24	-	13,13,13,13	0
57	MG	QA	1617	1/1	0.60	-	50,50,50,50	0
57	MG	XA	1671	1/1	0.10	-	43,43,43,43	0
57	MG	YA	3112	1/1	0.25	-	23,23,23,23	0
57	MG	RA	3138	1/1	0.26	-	17,17,17,17	0
57	MG	QA	1663	1/1	0.12	-	85,85,85,85	0
57	MG	RA	3158	1/1	0.16	-	52,52,52,52	0
58	PAR	QA	1666	42/42	0.30	-	84,84,84,84	0
57	MG	RA	3116	1/1	0.16	-	2,2,2,2	0
57	MG	YA	3015	1/1	0.39	-	3,3,3,3	0
57	MG	RA	3190	1/1	0.16	-	33,33,33,33	0
57	MG	RA	3016	1/1	0.26	-	4,4,4,4	0
57	MG	YA	3226	1/1	0.17	-	20,20,20,20	0
57	MG	YA	3145	1/1	0.14	-	23,23,23,23	0
57	MG	QA	1601	1/1	0.22	-	58,58,58,58	0
57	MG	RA	3142	1/1	0.18	-	59,59,59,59	0
57	MG	RA	3015	1/1	0.16	-	19,19,19,19	0
57	MG	RA	3210	1/1	0.14	-	51,51,51,51	0
57	MG	YA	3155	1/1	0.29	-	48,48,48,48	0
57	MG	YA	3242	1/1	0.31	-	58,58,58,58	0
57	MG	QA	1606	1/1	0.16	-	44,44,44,44	0
57	MG	RA	3176	1/1	0.14	-	27,27,27,27	0
57	MG	RA	3001	1/1	0.15	-	2,2,2,2	0
57	MG	RA	3220	1/1	0.29	-	58,58,58,58	0
57	MG	RA	3169	1/1	0.17	-	44,44,44,44	0
57	MG	QA	1631	1/1	0.08	-	41,41,41,41	0
57	MG	RA	3024	1/1	0.15	-	17,17,17,17	0
57	MG	RA	3048	1/1	0.34	-	18,18,18,18	0
57	MG	RA	3209	1/1	0.13	-	23,23,23,23	0
57	MG	YA	3256	1/1	0.14	-	11,11,11,11	0
57	MG	RA	3156	1/1	0.27	-	22,22,22,22	0
57	MG	RA	3067	1/1	0.17	-	12,12,12,12	0
57	MG	RA	3026	1/1	0.11	-	3,3,3,3	0
57	MG	XA	1655	1/1	0.31	-	47,47,47,47	0
57	MG	XA	1623	1/1	0.07	-	27,27,27,27	0
57	MG	RA	3072	1/1	0.19	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3065	1/1	0.23	-	25,25,25,25	0
57	MG	XA	1647	1/1	0.10	-	25,25,25,25	0
57	MG	YA	3211	1/1	0.17	-	29,29,29,29	0
57	MG	RA	3046	1/1	0.11	-	19,19,19,19	0
57	MG	YA	3206	1/1	0.46	-	65,65,65,65	0
57	MG	YA	3174	1/1	0.13	-	27,27,27,27	0
57	MG	RE	301	1/1	0.21	-	30,30,30,30	0
57	MG	RA	3037	1/1	0.28	-	26,26,26,26	0
57	MG	XA	1665	1/1	0.26	-	46,46,46,46	0
57	MG	YA	3169	1/1	0.15	-	30,30,30,30	0
57	MG	RA	3053	1/1	0.17	-	13,13,13,13	0
57	MG	YA	3038	1/1	0.23	-	4,4,4,4	0
57	MG	YA	3214	1/1	0.19	-	28,28,28,28	0
57	MG	YA	3080	1/1	0.13	-	11,11,11,11	0
57	MG	Y5	101	1/1	0.19	-	18,18,18,18	0
57	MG	XA	1654	1/1	0.33	-	58,58,58,58	0
57	MG	QA	1612	1/1	0.25	-	18,18,18,18	0
57	MG	RA	3232	1/1	0.32	-	23,23,23,23	0
57	MG	YA	3092	1/1	0.18	-	25,25,25,25	0
57	MG	YA	3261	1/1	0.25	-	18,18,18,18	0
57	MG	YA	3048	1/1	0.30	-	6,6,6,6	0
57	MG	YA	3218	1/1	0.19	-	47,47,47,47	0
57	MG	XA	1636	1/1	0.35	-	23,23,23,23	0
57	MG	YA	3082	1/1	1.00	-	80,80,80,80	0
57	MG	RA	3028	1/1	0.21	-	37,37,37,37	0
57	MG	YA	3013	1/1	0.30	-	2,2,2,2	0
57	MG	QA	1662	1/1	0.11	-	63,63,63,63	0
57	MG	YA	3036	1/1	0.22	-	9,9,9,9	0
57	MG	RA	3144	1/1	0.18	-	11,11,11,11	0
57	MG	QA	1634	1/1	0.09	-	39,39,39,39	0
57	MG	RA	3234	1/1	0.26	-	44,44,44,44	0
57	MG	XA	1604	1/1	0.41	-	20,20,20,20	0
57	MG	RA	3104	1/1	0.10	-	6,6,6,6	0
57	MG	RA	3063	1/1	0.41	-	12,12,12,12	0
57	MG	YB	201	1/1	0.18	-	51,51,51,51	0
57	MG	RA	3121	1/1	0.26	-	45,45,45,45	0
57	MG	QA	1651	1/1	0.28	-	31,31,31,31	0
57	MG	RA	3202	1/1	0.12	-	31,31,31,31	0
57	MG	YA	3129	1/1	0.28	-	38,38,38,38	0
57	MG	YA	3219	1/1	0.19	-	33,33,33,33	0
57	MG	RA	3025	1/1	0.21	-	22,22,22,22	0
57	MG	YA	3127	1/1	0.16	-	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3021	1/1	0.27	-	17,17,17,17	0
57	MG	RA	3092	1/1	0.17	-	35,35,35,35	0
57	MG	RA	3123	1/1	0.18	-	19,19,19,19	0
57	MG	QX	101	1/1	0.23	-	67,67,67,67	0
57	MG	RA	3218	1/1	0.14	-	85,85,85,85	0
57	MG	RA	3207	1/1	0.36	-	105,105,105,105	0
57	MG	YA	3184	1/1	0.18	-	35,35,35,35	0
57	MG	YA	3152	1/1	0.14	-	43,43,43,43	0
57	MG	YA	3113	1/1	0.08	-	19,19,19,19	0
57	MG	RA	3045	1/1	0.25	-	23,23,23,23	0
57	MG	YA	3109	1/1	0.26	-	11,11,11,11	0
57	MG	YA	3183	1/1	0.10	-	21,21,21,21	0
57	MG	QA	1658	1/1	0.13	-	52,52,52,52	0
57	MG	RA	3074	1/1	0.13	-	7,7,7,7	0
57	MG	YA	3053	1/1	0.13	-	11,11,11,11	0
57	MG	YA	3249	1/1	0.18	-	34,34,34,34	0
57	MG	YA	3225	1/1	0.14	-	21,21,21,21	0
57	MG	QA	1614	1/1	0.25	-	31,31,31,31	0
57	MG	RA	3188	1/1	0.20	-	53,53,53,53	0
57	MG	RA	3134	1/1	0.16	-	42,42,42,42	0
57	MG	YA	3209	1/1	0.17	-	29,29,29,29	0
57	MG	XA	1628	1/1	0.10	-	19,19,19,19	0
57	MG	YA	3002	1/1	0.26	-	9,9,9,9	0
57	MG	YA	3187	1/1	0.12	-	19,19,19,19	0
57	MG	YA	3110	1/1	0.23	-	11,11,11,11	0
57	MG	RA	3113	1/1	0.13	-	22,22,22,22	0
57	MG	RA	3214	1/1	0.13	-	44,44,44,44	0
57	MG	RA	3222	1/1	0.26	-	50,50,50,50	0
57	MG	RA	3167	1/1	0.16	-	56,56,56,56	0
57	MG	YA	3245	1/1	0.22	-	28,28,28,28	0
57	MG	RA	3153	1/1	0.12	-	21,21,21,21	0
57	MG	RA	3239	1/1	0.32	-	24,24,24,24	0
57	MG	YA	3192	1/1	0.06	-	19,19,19,19	0
57	MG	YA	3135	1/1	0.40	-	40,40,40,40	0
57	MG	QF	201	1/1	0.47	-	62,62,62,62	0
57	MG	YA	3168	1/1	0.27	-	52,52,52,52	0
57	MG	YA	3101	1/1	0.44	-	24,24,24,24	0
57	MG	YA	3090	1/1	0.27	-	12,12,12,12	0
57	MG	YA	3059	1/1	0.19	-	15,15,15,15	0
57	MG	RA	3105	1/1	0.10	-	6,6,6,6	0
57	MG	RA	3164	1/1	0.09	-	27,27,27,27	0
57	MG	RA	3023	1/1	0.29	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3130	1/1	0.47	-	52,52,52,52	0
57	MG	QA	1616	1/1	0.14	-	18,18,18,18	0
57	MG	RA	3137	1/1	0.21	-	36,36,36,36	0
57	MG	RA	3229	1/1	0.25	-	41,41,41,41	0
57	MG	YA	3030	1/1	0.47	-	19,19,19,19	0
57	MG	RA	3129	1/1	0.15	-	38,38,38,38	0
57	MG	RA	3085	1/1	0.17	-	11,11,11,11	0
57	MG	RA	3192	1/1	0.12	-	19,19,19,19	0
57	MG	RA	3161	1/1	0.25	-	33,33,33,33	0
57	MG	QA	1627	1/1	0.14	-	92,92,92,92	0
57	MG	XA	1613	1/1	0.08	-	14,14,14,14	0
57	MG	YA	3138	1/1	0.11	-	15,15,15,15	0
57	MG	XA	1617	1/1	0.14	-	10,10,10,10	0
57	MG	QA	1644	1/1	0.13	-	36,36,36,36	0
57	MG	YA	3074	1/1	0.30	-	22,22,22,22	0
57	MG	YA	3181	1/1	0.15	-	36,36,36,36	0
57	MG	RA	3066	1/1	0.20	-	11,11,11,11	0
57	MG	YA	3098	1/1	0.12	-	19,19,19,19	0
57	MG	XA	1618	1/1	0.26	-	33,33,33,33	0
57	MG	YA	3243	1/1	0.25	-	32,32,32,32	0
57	MG	RA	3010	1/1	0.15	-	48,48,48,48	0
57	MG	XA	1637	1/1	0.25	-	39,39,39,39	0
57	MG	YA	3254	1/1	0.31	-	11,11,11,11	0
57	MG	YA	3089	1/1	0.15	-	5,5,5,5	0
57	MG	YA	3197	1/1	0.24	-	16,16,16,16	0
57	MG	RA	3007	1/1	0.23	-	11,11,11,11	0
57	MG	YA	3054	1/1	0.17	-	3,3,3,3	0
57	MG	YA	3004	1/1	0.13	-	5,5,5,5	0
57	MG	RA	3235	1/1	0.29	-	29,29,29,29	0
57	MG	YA	3116	1/1	0.26	-	12,12,12,12	0
57	MG	RA	3099	1/1	0.29	-	19,19,19,19	0
57	MG	RA	3135	1/1	0.29	-	55,55,55,55	0
57	MG	XA	1648	1/1	0.21	-	30,30,30,30	0
57	MG	RA	3064	1/1	0.30	-	3,3,3,3	0
57	MG	RA	3233	1/1	0.31	-	42,42,42,42	0
57	MG	YA	3268	1/1	0.27	-	21,21,21,21	0
57	MG	XA	1646	1/1	0.14	-	24,24,24,24	0
57	MG	RA	3106	1/1	0.21	-	28,28,28,28	0
57	MG	RA	3197	1/1	0.09	-	42,42,42,42	0
57	MG	YA	3194	1/1	0.12	-	34,34,34,34	0
57	MG	XA	1641	1/1	0.20	-	17,17,17,17	0
57	MG	XA	1609	1/1	0.14	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1638	1/1	0.23	-	54,54,54,54	0
57	MG	XA	1612	1/1	0.20	-	18,18,18,18	0
57	MG	RA	3203	1/1	0.29	-	61,61,61,61	0
57	MG	YA	3003	1/1	0.16	-	9,9,9,9	0
57	MG	YA	3263	1/1	0.08	-	15,15,15,15	0
57	MG	XA	1621	1/1	0.34	-	32,32,32,32	0
57	MG	XA	1663	1/1	0.24	-	35,35,35,35	0
57	MG	XA	1644	1/1	0.14	-	21,21,21,21	0
57	MG	RA	3131	1/1	0.23	-	31,31,31,31	0
57	MG	RA	3073	1/1	0.19	-	23,23,23,23	0
57	MG	QA	1665	1/1	0.20	-	29,29,29,29	0
57	MG	RA	3011	1/1	0.33	-	48,48,48,48	0
57	MG	QA	1613	1/1	0.14	-	22,22,22,22	0
57	MG	QA	1664	1/1	0.25	-	35,35,35,35	0
57	MG	RA	3078	1/1	0.26	-	34,34,34,34	0
57	MG	RA	3241	1/1	0.22	-	36,36,36,36	0
57	MG	RA	3102	1/1	0.18	-	5,5,5,5	0
57	MG	YA	3175	1/1	0.13	-	42,42,42,42	0
57	MG	XA	1669	1/1	0.16	-	17,17,17,17	0
57	MG	YA	3180	1/1	0.14	-	31,31,31,31	0
57	MG	YA	3023	1/1	0.26	-	14,14,14,14	0
57	MG	QA	1637	1/1	0.32	-	66,66,66,66	0
57	MG	YA	3061	1/1	0.18	-	16,16,16,16	0
57	MG	YA	3227	1/1	0.17	-	26,26,26,26	0
57	MG	YA	3233	1/1	0.23	-	32,32,32,32	0
57	MG	YA	3029	1/1	0.11	-	5,5,5,5	0
57	MG	YA	3230	1/1	0.12	-	35,35,35,35	0
57	MG	YA	3067	1/1	0.30	-	27,27,27,27	0
57	MG	YA	3047	1/1	0.24	-	13,13,13,13	0
57	MG	YA	3182	1/1	0.46	-	55,55,55,55	0
57	MG	YA	3195	1/1	0.22	-	44,44,44,44	0
57	MG	YA	3154	1/1	0.23	-	38,38,38,38	0
57	MG	RA	3089	1/1	0.25	-	6,6,6,6	0
57	MG	YA	3045	1/1	0.30	-	2,2,2,2	0
57	MG	XA	1652	1/1	0.22	-	64,64,64,64	0
57	MG	YA	3020	1/1	0.43	-	13,13,13,13	0
57	MG	RA	3100	1/1	0.20	-	43,43,43,43	0
57	MG	YA	3107	1/1	0.28	-	41,41,41,41	0
57	MG	RA	3217	1/1	0.11	-	49,49,49,49	0
57	MG	RA	3189	1/1	0.27	-	33,33,33,33	0
57	MG	RA	3071	1/1	0.28	-	18,18,18,18	0
57	MG	RA	3118	1/1	0.26	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3163	1/1	0.21	-	29,29,29,29	0
57	MG	YA	3086	1/1	0.29	-	58,58,58,58	0
57	MG	XA	1607	1/1	0.21	-	25,25,25,25	0
57	MG	YA	3136	1/1	0.08	-	29,29,29,29	0
57	MG	RA	3225	1/1	0.17	-	51,51,51,51	0
57	MG	RA	3022	1/1	0.39	-	23,23,23,23	0
57	MG	XA	1658	1/1	0.57	-	61,61,61,61	0
57	MG	RA	3109	1/1	0.15	-	21,21,21,21	0
57	MG	YA	3246	1/1	0.29	-	29,29,29,29	0
57	MG	RA	3115	1/1	0.29	-	47,47,47,47	0
57	MG	YA	3186	1/1	0.31	-	44,44,44,44	0
57	MG	YA	3014	1/1	0.22	-	3,3,3,3	0
57	MG	XA	1602	1/1	0.17	-	16,16,16,16	0
57	MG	YA	3147	1/1	0.25	-	28,28,28,28	0
57	MG	QA	1609	1/1	0.10	-	14,14,14,14	0
57	MG	RA	3054	1/1	0.08	-	14,14,14,14	0
57	MG	YA	3037	1/1	0.08	-	2,2,2,2	0
57	MG	QA	1618	1/1	0.28	-	42,42,42,42	0
57	MG	RA	3033	1/1	0.28	-	11,11,11,11	0
57	MG	YA	3076	1/1	0.11	-	25,25,25,25	0
57	MG	RB	202	1/1	0.09	-	46,46,46,46	0
57	MG	RA	3181	1/1	0.12	-	43,43,43,43	0
57	MG	YA	3095	1/1	0.28	-	5,5,5,5	0
57	MG	YP	202	1/1	0.18	-	31,31,31,31	0
57	MG	YA	3008	1/1	0.18	-	22,22,22,22	0
57	MG	YA	3056	1/1	0.17	-	7,7,7,7	0
57	MG	YA	3128	1/1	0.29	-	34,34,34,34	0
57	MG	YE	301	1/1	0.13	-	8,8,8,8	0
57	MG	YA	3046	1/1	0.32	-	11,11,11,11	0
57	MG	XA	1653	1/1	0.21	-	62,62,62,62	0
57	MG	QA	1656	1/1	0.21	-	100,100,100,100	0
57	MG	RA	3042	1/1	0.29	-	18,18,18,18	0
57	MG	YA	3077	1/1	0.24	-	11,11,11,11	0
57	MG	QA	1628	1/1	0.25	-	41,41,41,41	0
57	MG	XA	1645	1/1	0.27	-	30,30,30,30	0
57	MG	RA	3079	1/1	0.20	-	32,32,32,32	0
57	MG	RA	3182	1/1	0.27	-	55,55,55,55	0
57	MG	RA	3062	1/1	0.19	-	59,59,59,59	0
57	MG	RA	3005	1/1	0.29	-	11,11,11,11	0
57	MG	Y0	101	1/1	0.18	-	20,20,20,20	0
57	MG	YA	3262	1/1	0.35	-	24,24,24,24	0
57	MG	RA	3127	1/1	0.22	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3132	1/1	0.28	-	14,14,14,14	0
57	MG	YA	3265	1/1	0.22	-	36,36,36,36	0
57	MG	RA	3059	1/1	0.20	-	15,15,15,15	0
57	MG	RA	3114	1/1	0.15	-	35,35,35,35	0
57	MG	YA	3088	1/1	0.26	-	17,17,17,17	0
57	MG	RA	3133	1/1	0.12	-	51,51,51,51	0
57	MG	YA	3017	1/1	0.20	-	13,13,13,13	0
57	MG	RE	302	1/1	0.10	-	11,11,11,11	0
57	MG	RA	3230	1/1	0.16	-	15,15,15,15	0
57	MG	YA	3139	1/1	0.21	-	33,33,33,33	0
57	MG	RA	3173	1/1	0.10	-	90,90,90,90	0
57	MG	RA	3095	1/1	0.22	-	6,6,6,6	0
57	MG	YA	3079	1/1	0.24	-	18,18,18,18	0
57	MG	XA	1660	1/1	0.26	-	54,54,54,54	0
57	MG	YA	3011	1/1	0.25	-	25,25,25,25	0
57	MG	QA	1636	1/1	0.10	-	34,34,34,34	0
57	MG	RA	3061	1/1	0.25	-	32,32,32,32	0
57	MG	YA	3141	1/1	0.37	-	79,79,79,79	0
57	MG	YA	3058	1/1	0.30	-	11,11,11,11	0
57	MG	XA	1632	1/1	0.29	-	27,27,27,27	0
57	MG	RA	3052	1/1	0.10	-	9,9,9,9	0
57	MG	YA	3060	1/1	0.22	-	24,24,24,24	0
57	MG	RA	3199	1/1	0.38	-	72,72,72,72	0
57	MG	YA	3204	1/1	0.09	-	32,32,32,32	0
57	MG	YA	3171	1/1	0.20	-	22,22,22,22	0
57	MG	XA	1662	1/1	0.08	-	47,47,47,47	0
57	MG	RA	3166	1/1	0.15	-	53,53,53,53	0
57	MG	XA	1620	1/1	0.20	-	30,30,30,30	0
57	MG	RA	3120	1/1	0.39	-	89,89,89,89	0
57	MG	RA	3056	1/1	0.35	-	12,12,12,12	0
57	MG	YA	3108	1/1	0.39	-	20,20,20,20	0
57	MG	RA	3032	1/1	0.21	-	44,44,44,44	0
57	MG	YA	3121	1/1	0.14	-	31,31,31,31	0
57	MG	XA	1615	1/1	0.25	-	30,30,30,30	0
57	MG	RA	3205	1/1	0.21	-	54,54,54,54	0
57	MG	YA	3009	1/1	0.41	-	16,16,16,16	0
57	MG	QA	1630	1/1	0.12	-	26,26,26,26	0
57	MG	RA	3183	1/1	0.33	-	44,44,44,44	0
57	MG	YA	3040	1/1	0.14	-	9,9,9,9	0
57	MG	QA	1643	1/1	0.19	-	61,61,61,61	0
57	MG	YA	3143	1/1	0.25	-	66,66,66,66	0
57	MG	YA	3238	1/1	0.86	-	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3157	1/1	0.23	-	48,48,48,48	0
57	MG	RA	3119	1/1	0.22	-	28,28,28,28	0
57	MG	YA	3201	1/1	0.54	-	23,23,23,23	0
57	MG	RA	3101	1/1	0.30	-	43,43,43,43	0
57	MG	RA	3170	1/1	0.17	-	41,41,41,41	0
57	MG	YA	3205	1/1	0.13	-	37,37,37,37	0
59	ZN	R9	101	1/1	0.08	-	112,112,112,112	0
57	MG	RA	3002	1/1	0.27	-	41,41,41,41	0
57	MG	YA	3049	1/1	0.13	-	12,12,12,12	0
57	MG	RA	3058	1/1	0.21	-	27,27,27,27	0
57	MG	QA	1607	1/1	0.11	-	21,21,21,21	0
57	MG	XA	1611	1/1	0.20	-	8,8,8,8	0
57	MG	YA	3111	1/1	0.06	-	5,5,5,5	0
57	MG	RA	3193	1/1	0.23	-	114,114,114,114	0
57	MG	QA	1615	1/1	0.11	-	66,66,66,66	0
57	MG	YA	3033	1/1	0.19	-	10,10,10,10	0
57	MG	YA	3179	1/1	0.09	-	40,40,40,40	0
57	MG	RA	3208	1/1	0.17	-	69,69,69,69	0
57	MG	RD	301	1/1	0.31	-	38,38,38,38	0
57	MG	RA	3149	1/1	0.23	-	28,28,28,28	0
57	MG	YA	3133	1/1	0.17	-	12,12,12,12	0
57	MG	YB	202	1/1	0.21	-	52,52,52,52	0
57	MG	RA	3175	1/1	0.08	-	40,40,40,40	0
57	MG	QA	1653	1/1	0.11	-	82,82,82,82	0
57	MG	RA	3027	1/1	0.24	-	3,3,3,3	0
57	MG	RA	3031	1/1	0.21	-	7,7,7,7	0
57	MG	YA	3216	1/1	0.09	-	18,18,18,18	0
57	MG	RA	3003	1/1	0.35	-	15,15,15,15	0
57	MG	YA	3153	1/1	0.35	-	33,33,33,33	0
57	MG	RA	3065	1/1	0.18	-	23,23,23,23	0
57	MG	RA	3148	1/1	0.20	-	39,39,39,39	0
57	MG	YA	3161	1/1	0.17	-	29,29,29,29	0
57	MG	RA	3141	1/1	0.28	-	34,34,34,34	0
57	MG	RA	3111	1/1	0.16	-	20,20,20,20	0
57	MG	XA	1626	1/1	0.17	-	27,27,27,27	0
57	MG	RA	3018	1/1	0.14	-	9,9,9,9	0
57	MG	YA	3149	1/1	0.20	-	25,25,25,25	0
57	MG	YA	3264	1/1	0.18	-	3,3,3,3	0
57	MG	YA	3200	1/1	0.40	-	39,39,39,39	0
57	MG	YA	3016	1/1	0.20	-	20,20,20,20	0
57	MG	RA	3231	1/1	0.29	-	14,14,14,14	0
57	MG	QA	1624	1/1	0.24	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3105	1/1	0.18	-	7,7,7,7	0
57	MG	QA	1633	1/1	0.22	-	20,20,20,20	0
57	MG	RA	3201	1/1	0.10	-	22,22,22,22	0
57	MG	RR	202	1/1	0.17	-	20,20,20,20	0
57	MG	RA	3206	1/1	0.29	-	26,26,26,26	0
57	MG	YA	3220	1/1	0.19	-	53,53,53,53	0
57	MG	YA	3012	1/1	0.33	-	5,5,5,5	0
57	MG	RA	3178	1/1	0.14	-	30,30,30,30	0
57	MG	YA	3165	1/1	0.11	-	21,21,21,21	0
57	MG	YA	3032	1/1	0.26	-	3,3,3,3	0
57	MG	RA	3184	1/1	0.26	-	42,42,42,42	0
57	MG	XA	1635	1/1	0.25	-	26,26,26,26	0
57	MG	RA	3224	1/1	0.13	-	40,40,40,40	0
57	MG	YA	3114	1/1	0.26	-	9,9,9,9	0
57	MG	XA	1651	1/1	0.40	-	59,59,59,59	0
57	MG	XA	1649	1/1	0.35	-	48,48,48,48	0
57	MG	RA	3040	1/1	0.17	-	3,3,3,3	0
57	MG	YA	3267	1/1	0.18	-	40,40,40,40	0
57	MG	RA	3213	1/1	0.13	-	44,44,44,44	0
57	MG	YA	3035	1/1	0.33	-	12,12,12,12	0
57	MG	RA	3093	1/1	0.24	-	10,10,10,10	0
57	MG	YB	204	1/1	0.15	-	45,45,45,45	0
57	MG	XA	1610	1/1	0.20	-	19,19,19,19	0
57	MG	XA	1656	1/1	0.23	-	45,45,45,45	0
57	MG	XA	1629	1/1	0.15	-	44,44,44,44	0
57	MG	RB	201	1/1	0.10	-	54,54,54,54	0
57	MG	RA	3112	1/1	0.23	-	14,14,14,14	0
57	MG	RA	3098	1/1	0.22	-	11,11,11,11	0
57	MG	RA	3215	1/1	0.16	-	20,20,20,20	0
57	MG	YA	3097	1/1	0.23	-	30,30,30,30	0
57	MG	YA	3070	1/1	0.20	-	5,5,5,5	0
57	MG	RA	3168	1/1	0.23	-	43,43,43,43	0
57	MG	YA	3022	1/1	0.20	-	11,11,11,11	0
57	MG	YA	3027	1/1	0.20	-	9,9,9,9	0
57	MG	XA	1640	1/1	0.10	-	187,187,187,187	0
57	MG	XA	1633	1/1	0.22	-	30,30,30,30	0
57	MG	YA	3178	1/1	0.13	-	10,10,10,10	0
57	MG	RA	3043	1/1	0.11	-	14,14,14,14	0
57	MG	YA	3167	1/1	0.36	-	42,42,42,42	0
57	MG	QA	1605	1/1	0.35	-	15,15,15,15	0
57	MG	RA	3160	1/1	0.17	-	42,42,42,42	0
57	MG	YA	3075	1/1	0.12	-	23,23,23,23	0



## 6.5 Other polymers ⓘ

There are no such residues in this entry.