



wwPDB X-ray Structure Validation Summary Report

Sep 17, 2014 – 08:14 PM EDT

PDB ID : 1VVJ
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 bound to Codon CCC-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-05-24
Resolution : 3.44 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

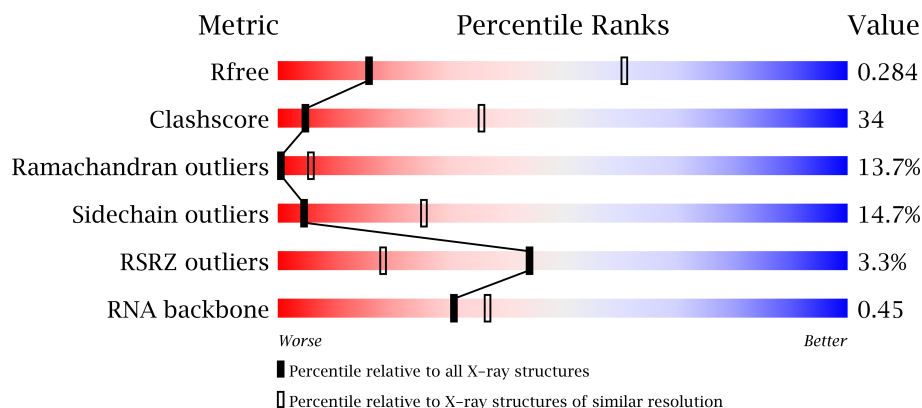
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.44 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	1032 (3.58-3.30)
Clashscore	79885	1296 (3.58-3.30)
Ramachandran outliers	78287	1256 (3.58-3.30)
Sidechain outliers	78261	1256 (3.58-3.30)
RSRZ outliers	66119	1032 (3.58-3.30)
RNA backbone	1838	1004 (4.10-2.76)

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 ≥ 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	

Continued on next page...

Continued from previous page...

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	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	Z6	3	
55	Z8	3	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 291123 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	1501	Total	C	N	O	P	0	0	0
			32269	14363	5986	10420	1500			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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 A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			
23	XX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			
24	XY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	3			
45	YZ	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	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 L32.

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 L33.

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 L34.

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 L35.

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 tRNA acceptor end mimic.

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 RNA chain called RNA (5'-R(*CP*CP*(PPU))-3').

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

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

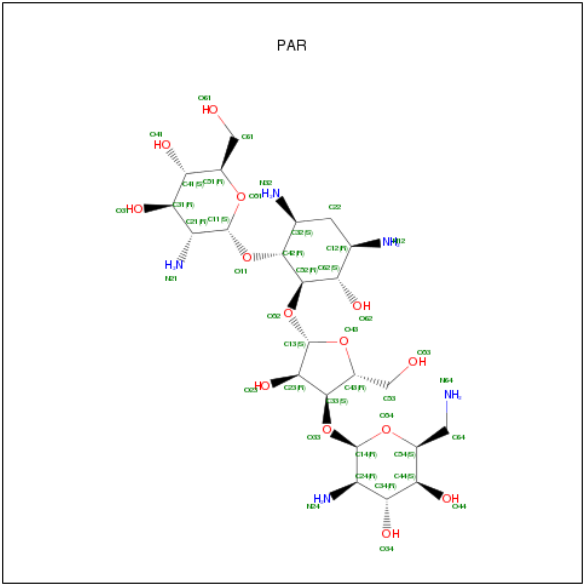
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RE	2	Total	Mg	0	0
			2	2		
56	YX	1	Total	Mg	0	0
			1	1		
56	XA	63	Total	Mg	0	0
			63	63		
56	QA	60	Total	Mg	0	0
			60	60		
56	Y5	1	Total	Mg	0	0
			1	1		
56	RP	1	Total	Mg	0	0
			1	1		
56	QX	2	Total	Mg	0	0
			2	2		
56	YA	242	Total	Mg	0	0
			242	242		
56	YB	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QF	1	Total	Mg	0	0
			1	1		
56	QM	1	Total	Mg	0	0
			1	1		
56	R5	1	Total	Mg	0	0
			1	1		
56	RB	2	Total	Mg	0	0
			2	2		
56	RA	212	Total	Mg	0	0
			212	212		
56	XM	2	Total	Mg	0	0
			2	2		
56	QH	1	Total	Mg	0	0
			1	1		
56	XV	2	Total	Mg	0	0
			2	2		
56	RF	1	Total	Mg	0	0
			1	1		
56	QV	2	Total	Mg	0	0
			2	2		
56	YE	2	Total	Mg	0	0
			2	2		

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

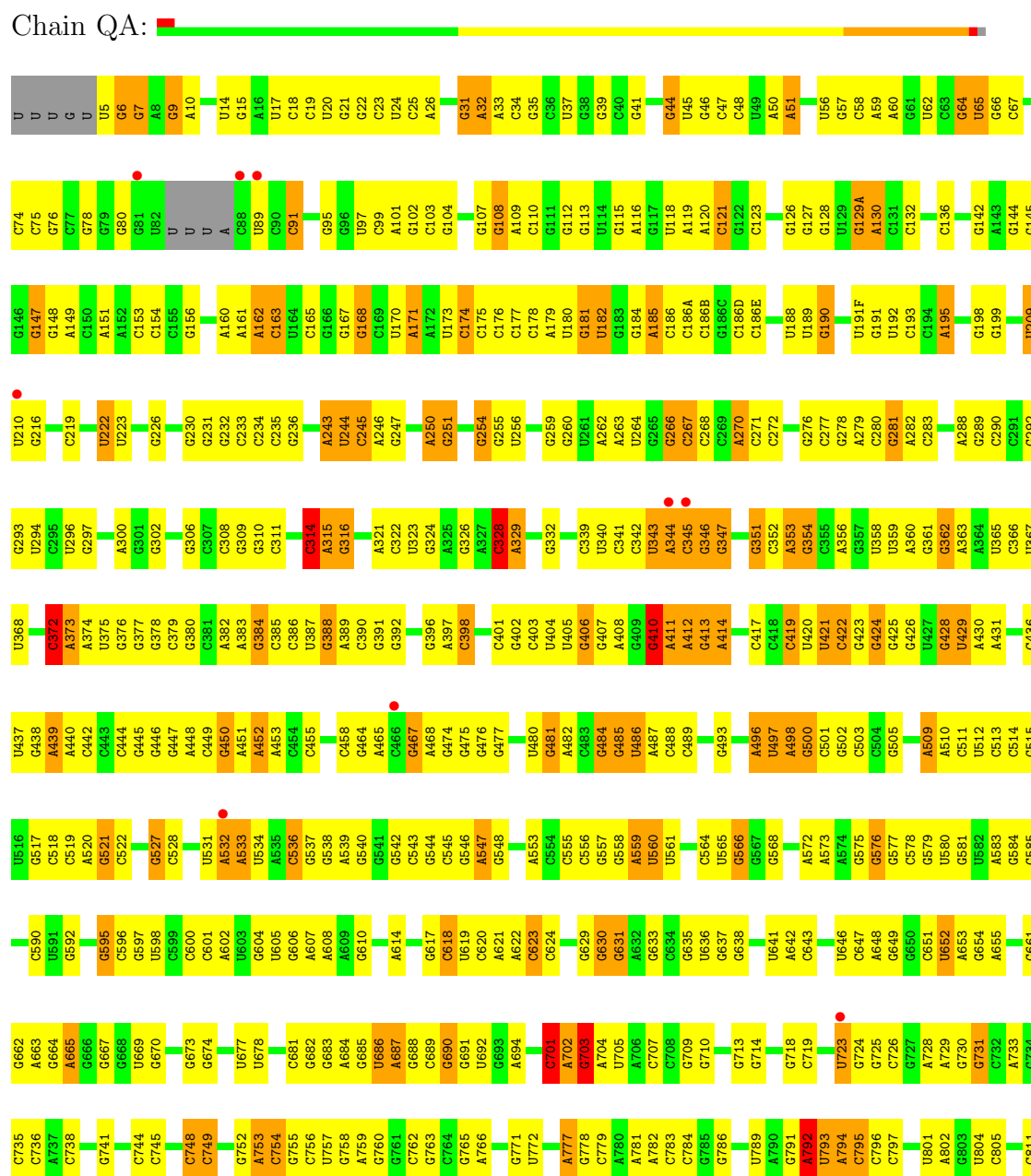
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

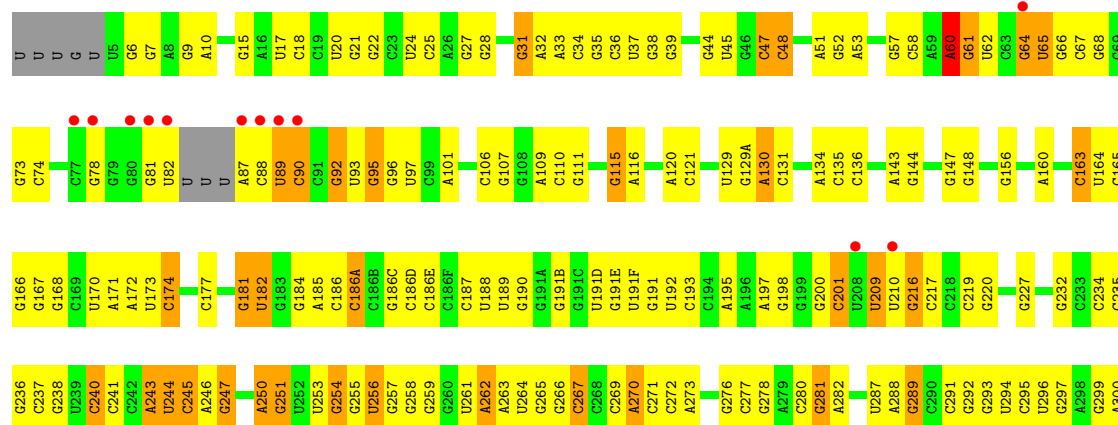
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	XD	1	Total	Zn	0	0
			1	1		
58	QD	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

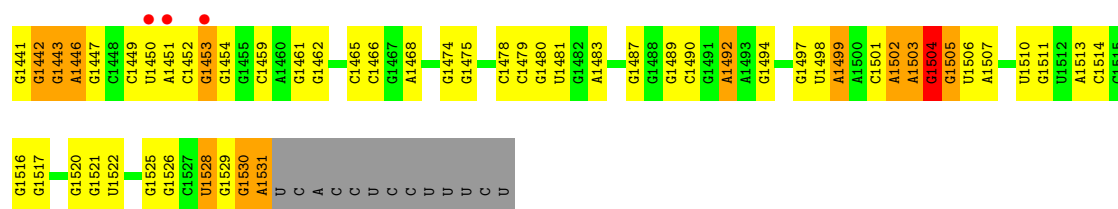
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA



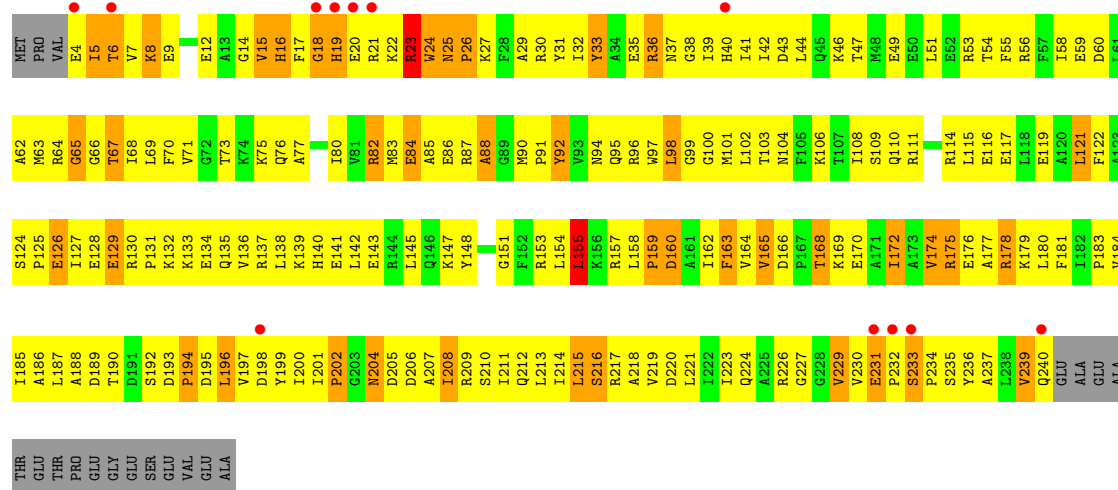


C1359	C1362	C1362A	A1363	A1364	G1365	C1366	C1367	C1368	C1369	G1370	G1371	U1372	G1373	A1374	U1381	C1388	C1389	U1390	U1391	G1392	U1393	A1394	C1397	A1398	C1399	C1400	G1401	C1402	C1403	C1411	C1412	A1413	U1414	G1415	A1418	G1419	C1420	G1421	G1422	U1427	A1428	C1429	C1430	C1431	C1432	A1433	A1434	G1435	U1436	C1439	C1440								
G1295	C1296	C1297	C1298	A1299	G1300	U1301	C1302	C1303	G1304	G1305	A1306	U1307	U1308	C1309	G1310	G1311	G1312	U1313	C1314	U1315	G1316	U1391	A1318	C1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	C1335	C1336	G1337	G1338	A1339	U1340	U1341	C1342	G1343	C1344	U1345	A1346	G1347	U1348	G1353	G1356	A1357	U1358		
G1224	A1225	C1226	A1227	C1228	G1229	C1230	G1231	U1232	C1233	C1234	U1235	A1236	C1237	A1238	C1239	G1240	G1241	U1242	C1243	C1244	C1245	C1246	A1252	G1253	A1256	U1257	C1258	C1262	C1263	G1266	C1267	A1268	C1269	C1270	G1271	C1272	G1273	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	C1287	A1288	G1291	U1292	C1293	G1294						
U1159	G1160	C1161	C1162	C1163	C1164	C1165	G1166	A1167	G1171	C1172	G1175	A1176	C1177	G1178	A1179	C1180	G1181	C1182	A1183	G1184	G1185	C1186	G1187	A1188	C1189	G1190	A1191	C1192	G1193	U1194	C1195	U1196	U1199	C1200	A1201	G1202	U1205	C1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	C1216	C1217	C1218	U1219	G1220	G1221	C1222	C1223				
U1091	U1020	G1021	C1022	G1023	C1024	U1025	G1026	C1027	U1028	C1029	G1030	G1031	U1032	C1033	G1034	A1035	C1036	C1037	C1038	G1039	U1040	G1048	G1049	A1050	C1051	G1052	C1053	A1054	C1055	U1056	G1057	C1058	C1059	U1062	C1063	G1064	U1065	C1066	C1069	U1070	C1071	G1072	U1073	G1074	G1077	A1078	C1079	A1080	U1085	U1086									
C940	G941	G942	A946	A947	C948	A949	U950	G951	U952	C953	G954	U955	U960	G961	C962	G963	A964	A965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	C978	A979	C980	G981	A982	C983	G984	C985	A986	G987	A988	A989	U990	C991	A992	G993	A994	G1001	U1002	G1003	A1004	C1005	C1006	C1007	G1008	C1009	G1010	A1014	A1015
C866	G867	U871	A872	A873	C874	C875	G876	C879	C880	C881	C882	C883	U884	C885	C886	C887	C888	A889	C890	U891	C892	C893	G894	C895	C896	A900	A901	G902	C903	C904	U905	C906	A907	A908	A909	A913	A914	A918	A919	U920	U921	C922	A923	C924	G925	G926	C927	C934	A935	C936	A937	U938	G939						
A1016	U1020	G1021	G1022	G1023	C1024	U1025	G1026	C1027	U1028	C1029	G1030	G1031	A1032	C1033	G1034	A1035	C1036	C1037	C1038	G1039	U1040	G1048	G1049	A1050	C1051	G1052	C1053	A1054	C1055	U1056	G1057	C1058	C1059	U1062	C1063	G1064	U1065	C1066	C1069	U1070	C1071	G1072	U1073	G1074	G1077	A1078	C1079	A1080	U1085	U1086									
U1091	U1020	G1021	C1022	G1023	C1024	U1025	G1026	C1027	U1028	C1029	G1030	G1031	A1032	C1033	G1034	A1035	C1036	C1037	C1038	G1039	U1040	G1048	G1049	A1050	C1051	G1052	C1053	A1054	C1055	U1056	G1057	C1058	C1059	U1062	C1063	G1064	U1065	C1066	C1069	U1070	C1071	G1072	U1073	G1074	G1077	A1078	C1079	A1080	U1085	U1086									
U1159	G1160	C1161	C1162	C1163	C1164	C1165	G1166	A1167	G1171	C1172	G1175	A1176	C1177	G1178	A1179	C1180	G1181	C1182	A1183	G1184	G1185	C1186	G1187	A1188	C1189	G1190	A1191	C1192	G1193	U1194	C1195	U1196	U1199	C1200	A1201	G1202	U1205	C1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	C1216	C1217	C1218	U1219	G1220	G1221	C1222	C1223				
G1224	A1225	C1226	A1227	C1228	G1229	C1230	G1231	U1232	C1233	C1234	U1235	A1236	C1237	A1238	C1239	G1240	G1241	U1242	C1243	C1244	C1245	C1246	A1252	G1253	A1256	U1257	C1258	C1262	C1263	G1266	C1267	A1268	C1269	C1270	G1271	C1272	G1273	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	C1287	A1288	G1291	U1292	C1293	G1294						
G1295	C1296	C1297	C1298	A1299	G1300	U1301	C1302	C1303	G1304	G1305	A1306	U1307	U1308	C1309	G1310	G1311	G1312	U1313	C1314	U1315	G1316	U1391	A1318	C1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	C1335	C1336	G1337	G1338	A1339	U1340	U1341	C1342	G1343	C1344	U1345	A1346	G1347	U1348	G1353	G1356	A1357	U1358		
C372	A373	A374	U375	C376	G377	C384	G388	A389	C390	G391	C392	A397	C398	C401	C402	C406	G407	G410	A411	A412	A413	A414	A418	A419	C420	G421	C422	G423	C424	U427	C428	U429	A430	U434	C435	C436	U437	C438	A439	A440	C442	C443	A448	C449	C450	A451	C369	C370	G371										
C454	C458	C464	A465	C466	C467	A468	C474	C475	U480	C481	A482	C483	C484	C485	C486	A487	C488	C489	C490	G491	C492	C493	U494	A495	C496	U497	A498	A500	C501	G502	C507	C508	A509	A510	C511	C518	C519	A520	C521	C522	A523	C524	C525	C526	C527	C528	C529	G530	U531	A532	A533	U534	A535	C536	G537				
G538	A539	G540	G541	G542	C545	A546	A547	C548	C549	G550	C554	C555	C556	G557	C558	A559	U560	C561	C562	A563	C564	U565	C566	G569	G570	C571	C572	C573	C574	C575	C576	C577	C578	C579	U580	G581	G584	C585	G588	C589	U590	C592	G593	C594	G595	C596	C597	U598	C599	G606	A607	A608	G630						
G630	G631	A632	G633	C634	G637	G638	G639	A640	A641	A642	C643	C644	C645	C646	C647	A648	G649	G650	C651	U652	A653	C654	U659	G660	G661	C662	A663	G664	A665	C666	G667	G668	G673	C674	A675	A676	U677	U678	C679	C680	U686	A687	G688	C689	G690	G691	U692	G693	A694	A695	A696	C701	A702	G703					
A704	C707	C708	G711	A712	G713	C714	A715	U719	C720	G721	A722	U723	G724	C725	C726	G727	A728	C729	C730	U731	C732	A816	C817	C818	A819	U820	A821	G825	C826	U827	C828	A829	C830	U831	C832	U833	C834	U835	C836	U841	C842	U843	C848	G851	G852	G853	C854	G855	A859	A864	A865								
G774	A777	C778	C779	A780	C784	G785	U789	C790	A791	C792	U793	C794	C795	C796	C797	C798	C811	C812	U813	A816	C817	C818	A819	U820	A821	G825	C826	U827	C828	A829	C830	U831	C832	U833	C834	U835	C836	U841	C842	U843	C848	G851	G852	G853	C854	G855	A859	A864	A865										
C866	G867	U871	A872	A873	C874	C875	G876	C879	C880	C881	C882	C883	U884	C885	C886	C887	C888	A889	C890	U891	C892	C893	G894	C895	C896	A900	A901	G902	C903	C904	U905	C906	A907	A908	A909	A913	A914	A918	A919	U920	U921	C922	A923	C924	G925	G926	C927	C934	A935	C936	A937	U938	G939						
C940	G941	G942	A946	A947	C948	A949	U950	G951	U952	C953	G954	U955	U960	G961	C962	G963	A964	A965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	C978	A979	C980	G981	A982	C983	G984	C985	A986	G987	A988	A989	U990	C991	A992	G993	A994	G1001	U1002	G1003	A1004	C1005	C1006	C1007	G1008	C1009	G1010	A1014	A1015
A1016	U1020	G1021	G1022	G1023	C1024	U1025	G1026	C1027	U1028	C1029	G1030	G1031	A1032	C1033	G1034	A1035	C1036	C1037	C1038	G1039	U1040	G1048	G1049	A1050	C1051	G1052	C1053	A1054	C1055	U1056	G1057	C1058	C1059	U1062	C1063	G1064	U1065	C1066	C1069	U1070	C1071	G1072	U1073	G1074	G1077	A1078	C1079	A1080	U1085	U1086									
U1091	U1020	G1021	C1022	G1023	C1024	U1025	G1026	C1027	U1028	C1029	G1030	G1031	A1032	C1033	G1034	A1035	C1036	C1037	C1038	G1039	U1040	G1048	G1049	A1050	C1051	G1052	C1053	A1054	C1055	U1056	G1057	C1058	C1059	U1062	C1063	G1064	U1065	C1066	C1069	U1070	C1071	G1072	U1073	G1074	G1077	A1078	C1079	A1080	U1085	U1086									
U1159	G1160	C1161	C1162	C1163	C1164	C1165	G1166	A1167	G1171	C1172	G1175	A1176	C1177	G1178	A1179	C1180	G1181	C1182	A1183	G1184	G1185	C1186	G1187	A1188	C1189	G1190	A1191	C1192	G1193	U1194	C1195	U1196	U1199	C1200	A1201	G1202	U1205	C1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	C1216	C1217	C1218	U1219	G1220	G1221	C1222	C1223				
G1224	A1225	C1226	A1227	C1228	G1229	C1230	G1231	U1232	C1233	C1234	U1235	A1236	C1237	A1238	C1239	G1240	G1241	U1242	C1243	C1244	C1245	C1246	A1252	G1253	A1256	U1257	C1258	C1262	C1263	G1266	C1267	A1268	C1269	C1270	G1271	C1272	G1273	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	C1287	A1288	G1291	U1292	C1293	G1294						
G1295	C1296	C1297	C1298	A1299	G1300	U1301	C1302	C1303	G1304	G1305	A1306	U1307	U1308	C1309	G1310	G1311	G1312	U1313	C1314	U1315	G1316	U1391	A1318	C1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	C1335	C1336	G1337	G1338	A1339	U1340	U1341	C1342	G1343	C1344	U1345	A1346	G1347	U1348	G1353	G1356	A1357	U1358		
C1359	C1362	C1362A	A1363	A1364	G1365	C1366	C1367	C1368	C1369	G1370	G1371	U1372	G1373	A1374	U1381	C1388	C1389	U1390	U1391	G1392	U1393	A1394	C1397	A1398	C1399	C1400	G1																																



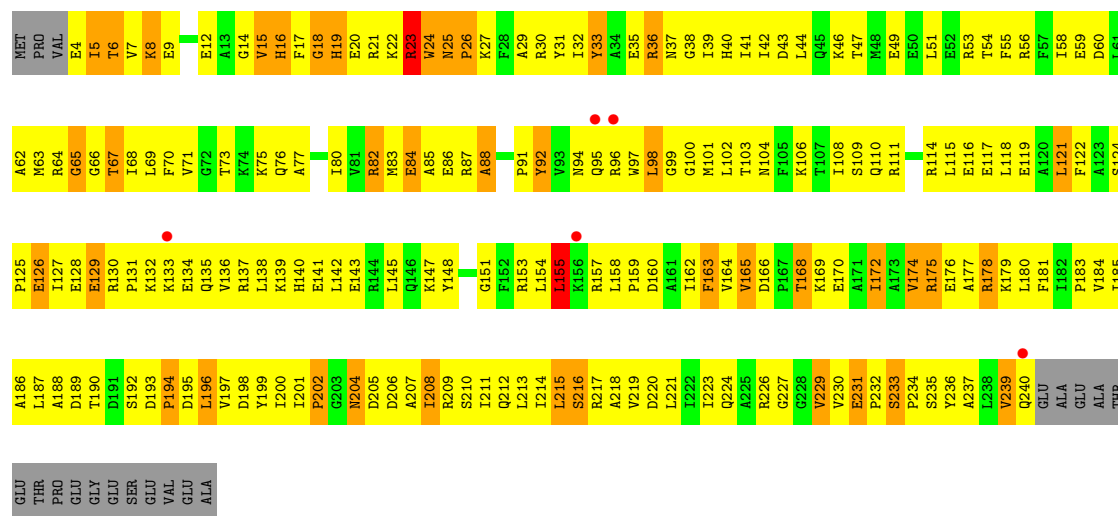
• Molecule 2: 30S ribosomal protein S2

Chain QB:



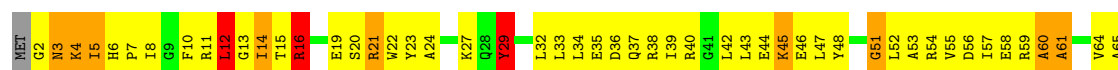
• Molecule 2: 30S ribosomal protein S2

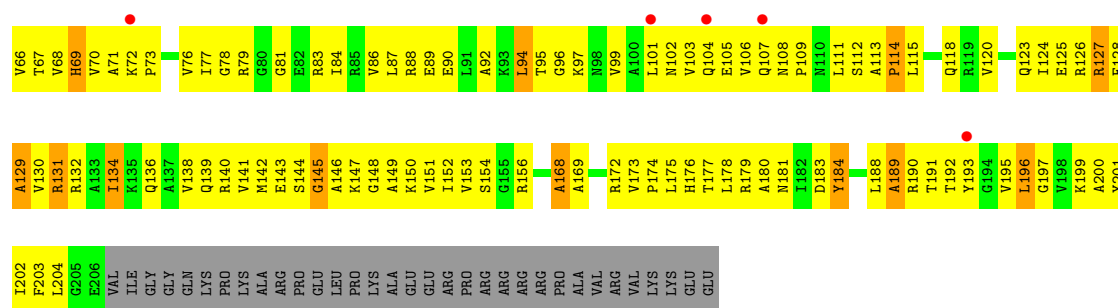
Chain XB:



• Molecule 3: 30S ribosomal protein S3

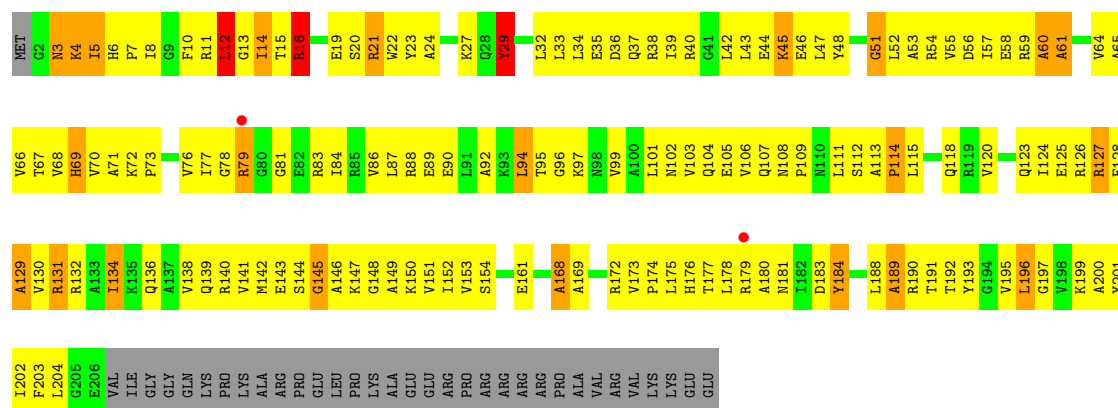
Chain QC:





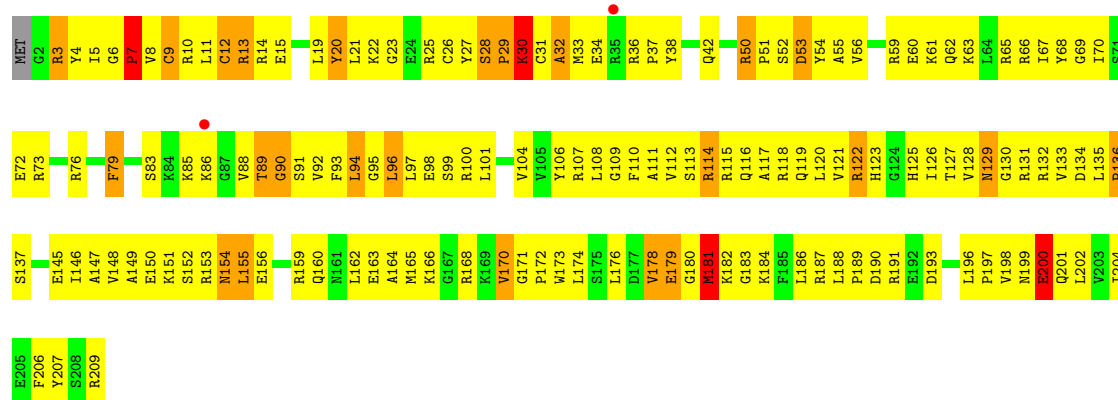
• Molecule 3: 30S ribosomal protein S3

Chain XC:



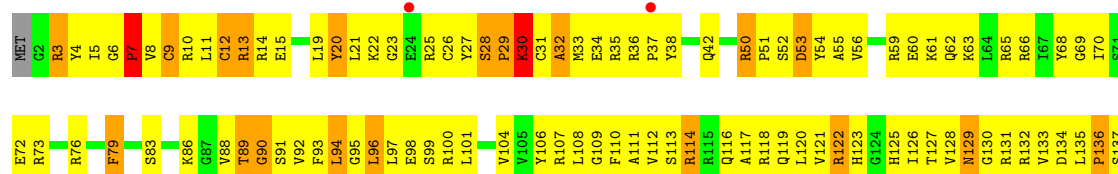
• Molecule 4: 30S ribosomal protein S4

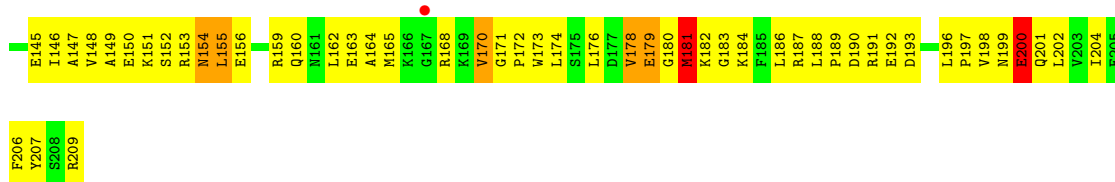
Chain QD:



• Molecule 4: 30S ribosomal protein S4

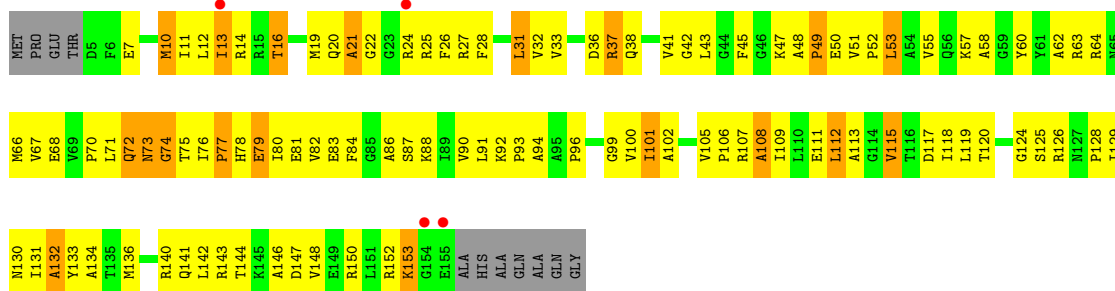
Chain XD:





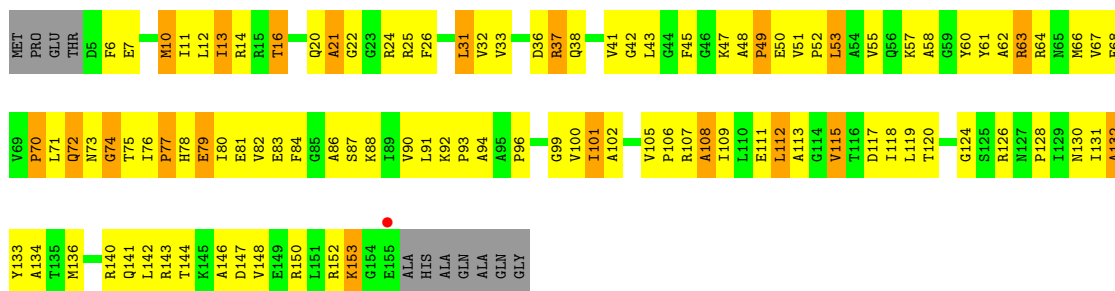
• Molecule 5: 30S ribosomal protein S5

Chain QE:



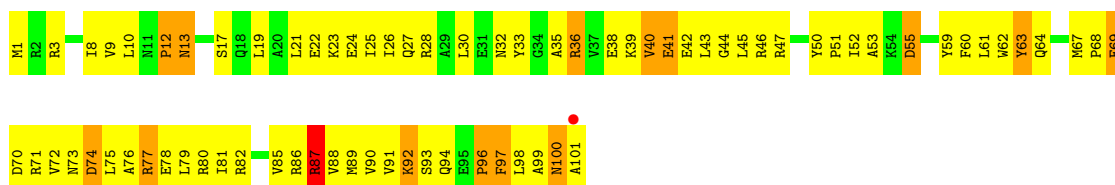
• Molecule 5: 30S ribosomal protein S5

Chain XE:



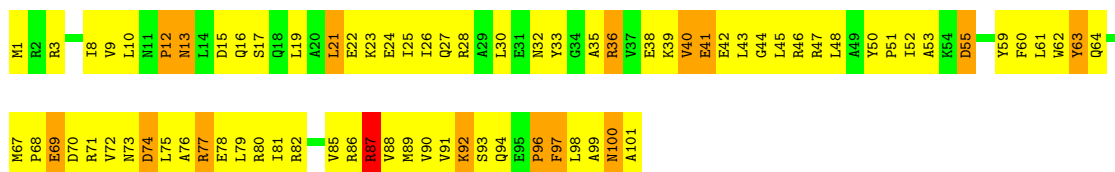
• Molecule 6: 30S ribosomal protein S6

Chain QF:

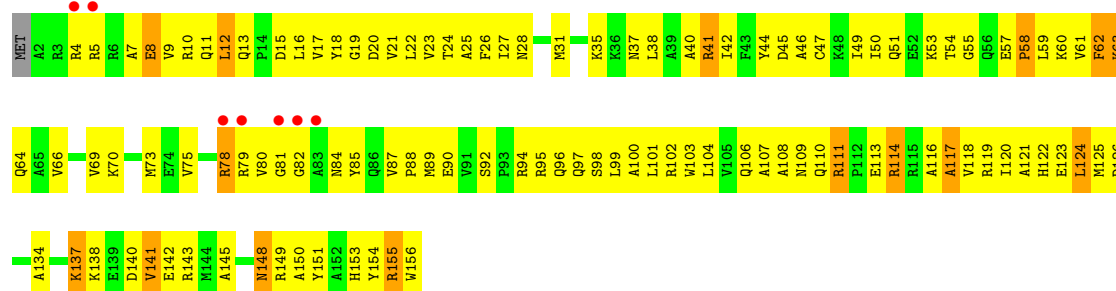


• Molecule 6: 30S ribosomal protein S6

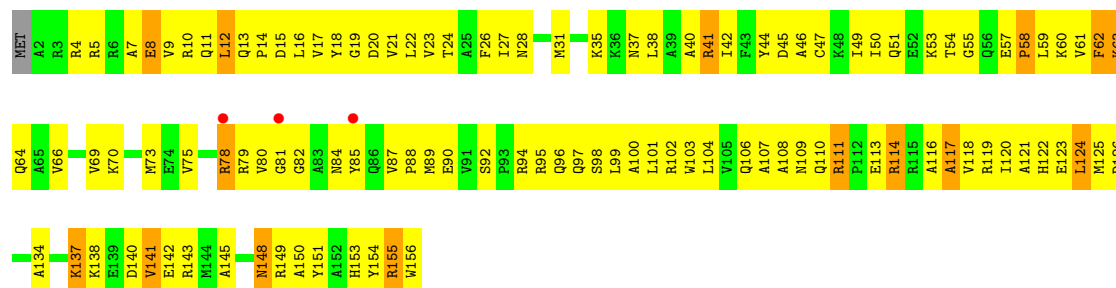
Chain XF:



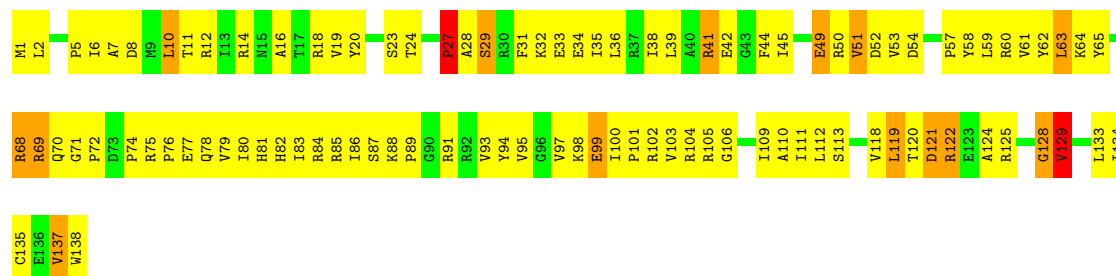
- Molecule 7: 30S ribosomal protein S7

Chain QG: 

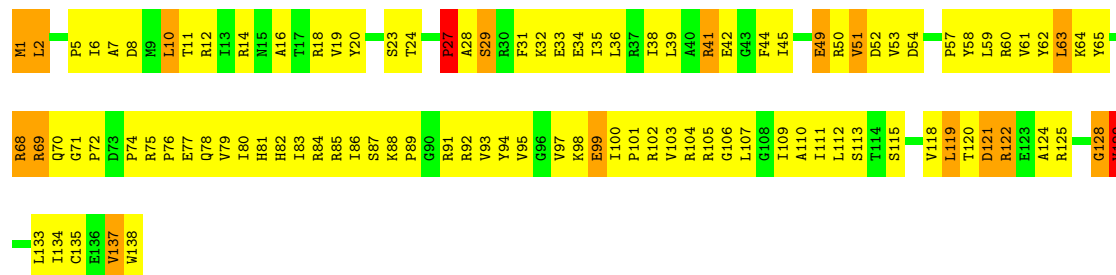
- Molecule 7: 30S ribosomal protein S7

Chain XG: 

- Molecule 8: 30S ribosomal protein S8

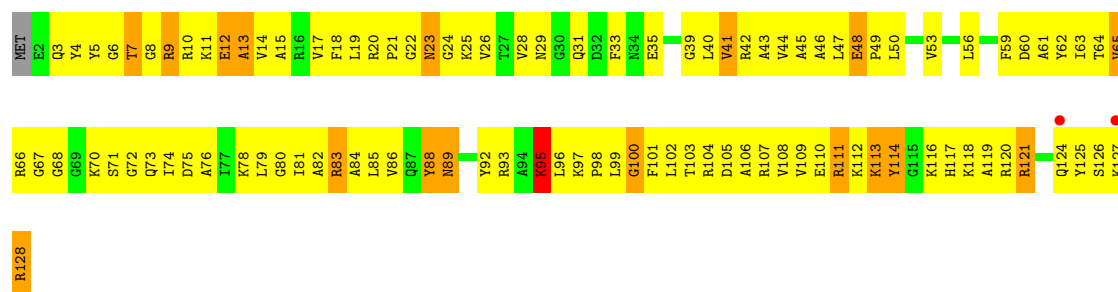
Chain QH: 

- Molecule 8: 30S ribosomal protein S8

Chain XH: 

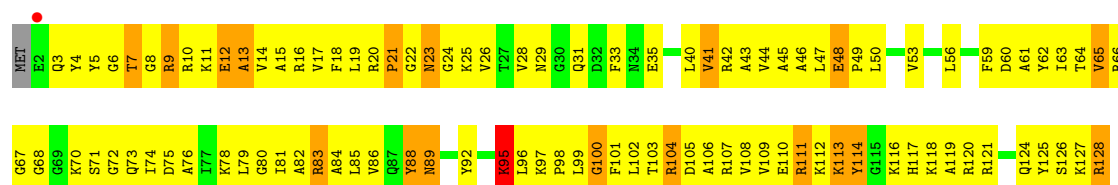
- Molecule 9: 30S ribosomal protein S9

Chain QI:



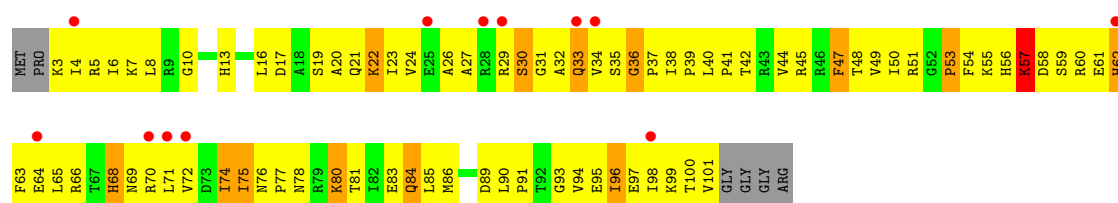
- Molecule 9: 30S ribosomal protein S9

Chain XI:



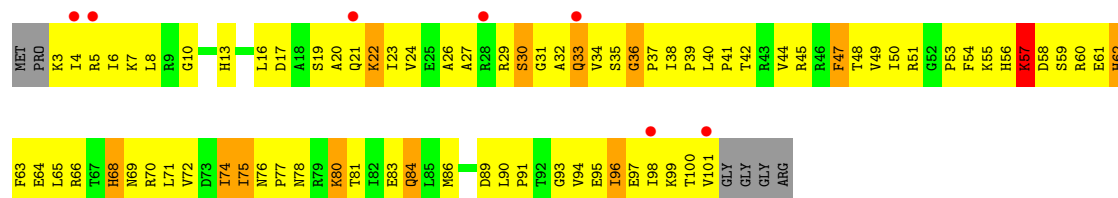
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



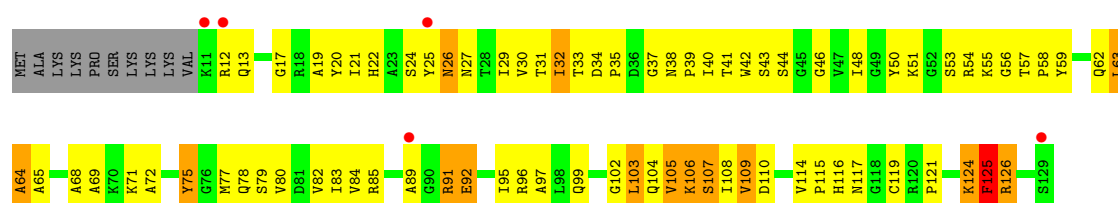
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



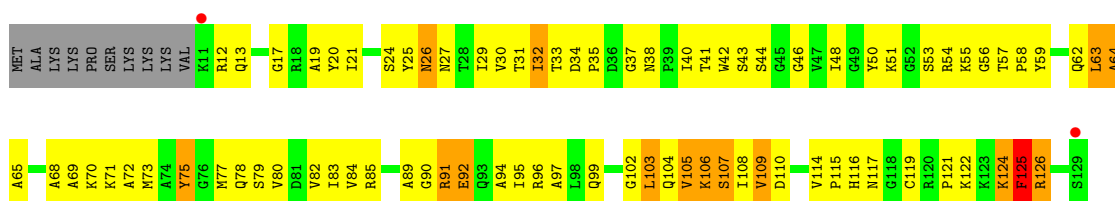
- Molecule 11: 30S ribosomal protein S11

Chain QK:



- Molecule 11: 30S ribosomal protein S11

Chain XK:



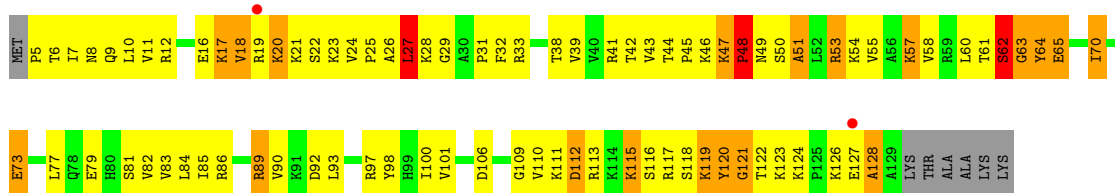
- Molecule 12: 30S ribosomal protein S12

Chain QL:



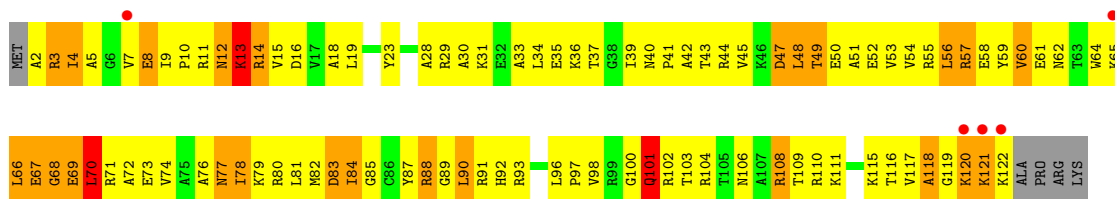
- Molecule 12: 30S ribosomal protein S12

Chain XL:



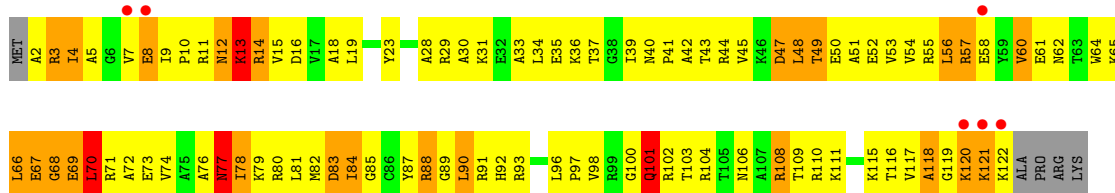
- Molecule 13: 30S ribosomal protein S13

Chain QM:



- Molecule 13: 30S ribosomal protein S13

Chain XM:



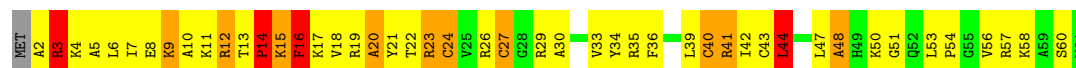
- Molecule 14: 30S ribosomal protein S14

Chain QN:



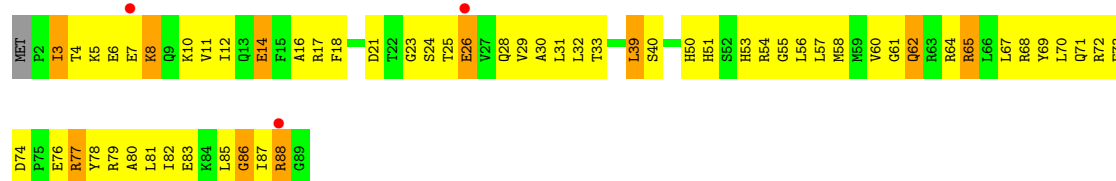
- Molecule 14: 30S ribosomal protein S14

Chain XN:



- Molecule 15: 30S ribosomal protein S15

Chain QO:



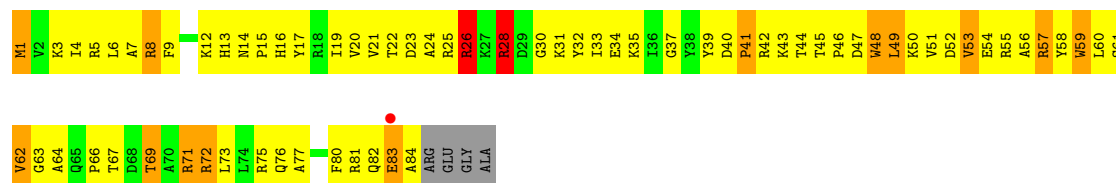
- Molecule 15: 30S ribosomal protein S15

Chain XO:



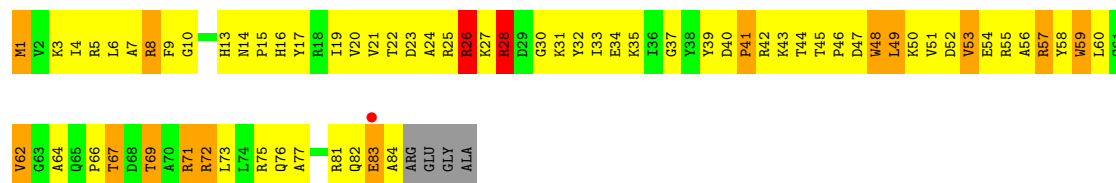
- Molecule 16: 30S ribosomal protein S16

Chain QP:



- Molecule 16: 30S ribosomal protein S16

Chain XP:



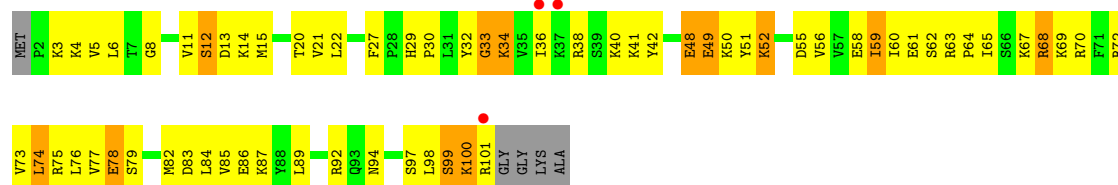
- Molecule 17: 30S ribosomal protein S17

Chain QQ: 



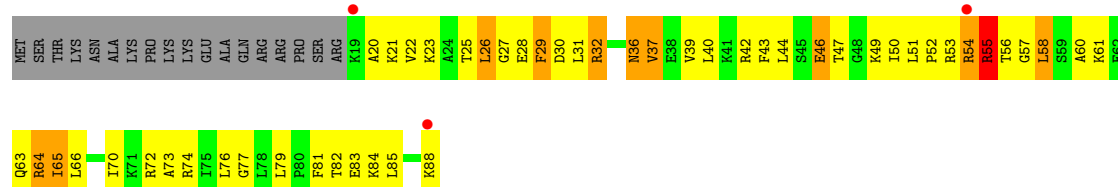
- Molecule 17: 30S ribosomal protein S17

Chain XQ: 



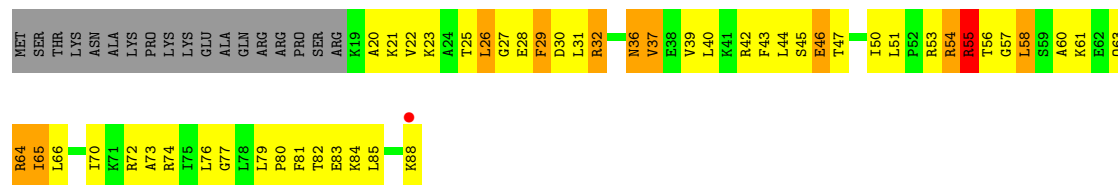
- Molecule 18: 30S ribosomal protein S18

Chain QR: 



- Molecule 18: 30S ribosomal protein S18

Chain XR: 



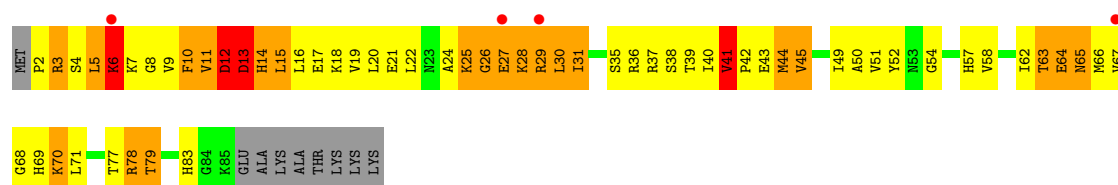
- Molecule 19: 30S ribosomal protein S19

Chain QS: 



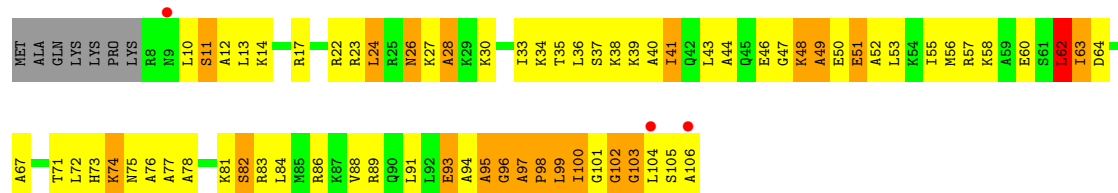
- Molecule 19: 30S ribosomal protein S19

Chain XS: 



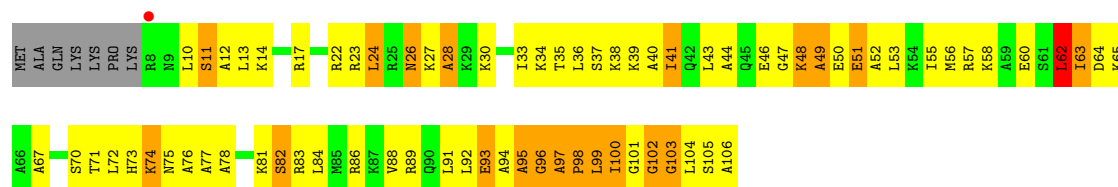
- Molecule 20: 30S ribosomal protein S20

Chain QT:



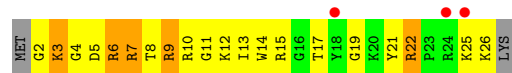
- Molecule 20: 30S ribosomal protein S20

Chain XT:



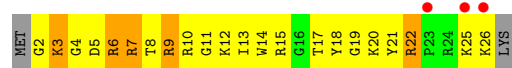
- Molecule 21: 30S ribosomal protein S21

Chain QU:



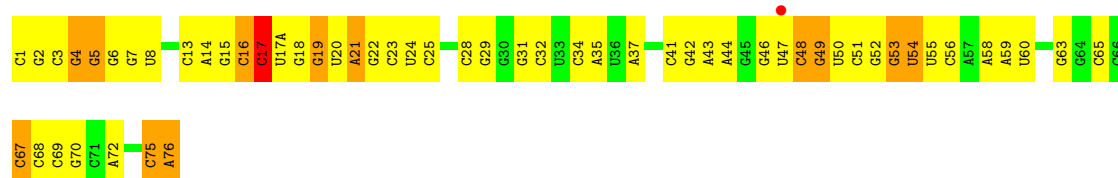
- Molecule 21: 30S ribosomal protein S21

Chain XU:



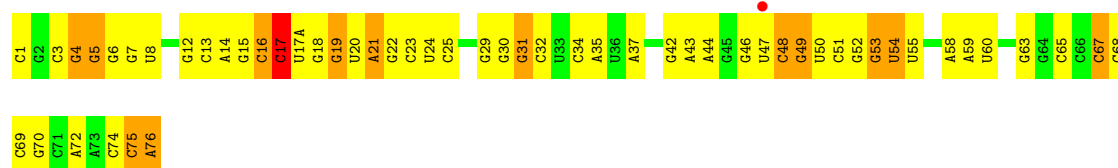
- Molecule 22: P-site tRNA fMet

Chain QV:



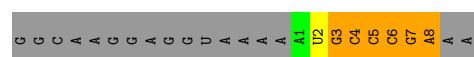
- Molecule 22: P-site tRNA fMet

Chain XV:



- Molecule 23: A-site ASL SufA6

Chain QX:



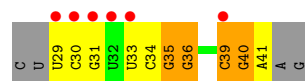
- Molecule 23: A-site ASL SufA6

Chain XX:



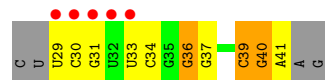
- Molecule 24: messenger RNA

Chain QY:



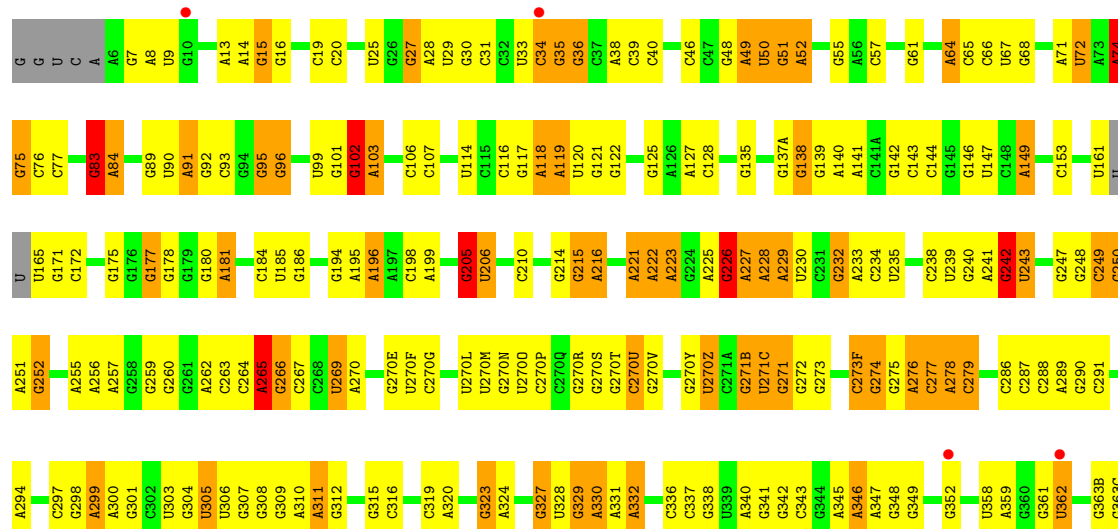
- Molecule 24: messenger RNA

Chain XY:



- Molecule 25: 23S rRNA

Chain RA:



A1373	C1297	G1212	C1135	U1066	A1000	U922	G853	G775	U639	C574	U504	A428	G363D
A1379	C1298	A1213	G1136	A1067	A1001	C923	G854	G776	C640	A575	A505	A429	U363E
G1380	G1299	G1216	G1137	G1068	G1002	C924	G855	A782	C641	U576	G506	A430	A363F
G1381	G1300	G1216	G1138	A1069	G1003	C925	C856	A783	G642	A577	G507	U431	C364
G1382	A1301	A1220	G1140	G1071	G1004	A926	C857	A784	C645	A578	G508	A432	C365
G1383	A1302	C1221	U1141	A1072	C1005	G928	U858	G785	A646	G579	C509	C433	C366
A1384	G1303	C1222	U1142	G1073	C1006	G929	G859	C786	G647	C580	C512	U434	G370
G1385	C1304	G1226	A1142A	C1075	C1007	U930	U860	U787	G649	C581	A513	C435	A371
C1386	A1143	G1227	U1143	C1076	G1011	G931	A861	A788	C650	G582	C516	A442	G372
C1387	G1143	G1228	A1148	A1077	G1012	G932	A862	A789	G651	C583	A443	A374	U373
G1388	A1148	G1228	A1148	U1078	U1012	G940	A863	C790	C652	G585	G517	C444	C375
G1389	G1151	G1232	G1151	C1079	C1013	A941	C864	C791	A653	A586	G518	C447	C376
G1310	G1233	G1232	G1151	C1080	U1014	G942	C865	G792	A654	C587	U519	A447	C377
G1311	C1233	G1233	G1157	U1081	G1015	A945	U868	C796	C654A	U588	G520	U448	U380
G1312	C1234	G1234	G1157	U1082	G1015	G946	G869	C797	G654B	C589	G521	A449	U381
G1313	G1238	G1238	U1159	U1083	U1019	G947	A870	A716	G	G522	G523	G450	G382
C1314	G1239	G1239	G1160	A1084	A1020	G948	U871	G717	G	C524	C525	C451	G383
A1317	U1240	U1240	G1161	A1085	A1021	C949	A872	A718	C	U524	U525	C452	U384
C1318	A1241	A1241	G1162	A1086	G1022	C949	A872	C719	C	U526	A526	C453	U385
G1319	A1242	A1242	U1165	A1087	U1023	A953	G881	C720	C	C527	C528	C454	G386
C1320	A1242	A1242	U1165	A1088	G1024	G954	G880	A722	C	A527	A528	C455	G386
A1321	G1245	G1245	U1167	U1090	U1026	G956	G882	A723	C	A529	A530	A457	G389
G1327	G1250	G1250	G1173	G1093	A1027	A957	G883	G724	C	G530	G531	U458	C392
G1328	C1251	C1251	G1173	U1094	G1030	U958	G884	G725	G	G532	C531	U459	C392
U1329	G1252	G1252	A1174	A1095	U1033	A959	C885	G726	C	G533	A532	U464	U395
C1330	G1256	G1256	U1175	A1096	U1033	A960	C886	A727	C	G534	G535	G465	G396
A1331	G1256	G1256	G1176	U1097	G1034	C961	A887	G728	C	U607	G537	G468	G397
G1332	A1262	A1262	A1177	U1098	U1035	G962	C888	G729	C	G609A	G539	G468	G398
U1335	U1263	U1263	C1178	G1099	U1036	U963	C889	C730	C	G612	G540	G468	G399
A1336	G1264	G1264	C1179	C1100	G1037	G968	A890	A734	C	U613	C541	A470	G400
G1337	G1265	G1265	C1180	U1094	G1038	U969	G892	G738	C	U614	C542	A471	A401
G1338	G1266	G1266	G1181	A1103	G1039	G972	C893	U740	C	G544	G545	A472	A402
G1339	U1267	U1267	A1182	U1105	G1040	A973	A896	U740	C	A616	G546	U475	U403
U1340	A1268	A1268	G1183	G1106	C1041	A974	C897	C658	C	G617	C547	G476	U405
A1341	U1269	U1269	G1186	U1077	C1042	G974	C898	C659	C	G618	A548	A479	G406
U1420	G1270	G1270	G1187	U1108	C1043	C974A	A899	U747	C	G618A	G549	A480	G407
G1417	G1271	G1271	U1188	C1109	A1045	G975	A900	G748	C	G619	G620	A481	G408
A1418	G1272	G1272	A1189	G1110	A1046	G975	A901	G748	C	G620	U553	G482	C409
A1419	U1273	U1273	G1190	A1111	G1047	G978	C902	A751	C	A621	U554	A483	G410
G1424	A1274	A1274	G1190	U1112	A1048	G979	C903	A752	C	G622	G554	A483	G411
G1425	G1277	G1277	G1195	U1113	C1049	A983	C904	C753	C	G623	G555	C484	A412
G1426	A1278	A1278	C1196	G1114	A1050	A984	U905	C754	C	G624	U557	C485	C413
A1427	G1279	G1279	G1197	G1115	G1051	C985	G906	C755	C	G625	G558	C486	C414
G1428	U1282	U1282	U1198	C1118	A1054	C986	U907	C756	C	U626	U562	A492	A415
G1429	G1283	G1283	C1200	G1118	G1055	G987	A910	G760	C	A627	G563	C493	C416
C1430	U1284	U1284	C1201	C1124	G1056	A988	A911	A761	C	G628	C564	G494	C417
U1431	G1285	G1285	C1202	G1125	A1057	G989	C912	A677	C	G629	C565	G495	C418
G1432	A1286	A1286	G1203	U1126	G1058	A990	U913	C678	C	A631	U566	C496	C419
A1434	G1287	G1287	A1204	A1127	G1059	C991	C914	C679	C	A632	U567	A497	C420
G1435	U1288	U1288	U1205	U1128	U1060	C992	A917	G680	C	A633	U568	C498	U421
G1436	G1288	G1288	G1206	A1129	U1061	G993	A918	G681	C	C634	U569	U499	A423
C1437	U1291	U1291	G1209	U1130	G1062	G994	A919	G770	C	C635	G570	G500	G424
U1438	C1370	C1370	G1209	U1131	G1063	C995	G920	G771	C	C636	A571	A501	U438
A1439	U1292	U1292	A1210	A1132	C1064	A996	G921	A774	C	G638	A572	A502	G425
G1440	C1293	C1293	U1211	U1133	U1065	G997	G921	A774	C	G638	A573	A503	C426

A2531	U2457	G2388	G2315	G2235	G2159	C2095	A2013	U1931	A1854	A1780	G1678	A1587	A1510	G1442
G2532	G2458	A2388	G2318	G2236	G2160	U2096	A2014	A1932	G1857	C1781	C1684	C1588	A1511	G1443
A2533	A2459	G2391	G2319	G2237	C2161	U2102	G1933	G1858	A1784	A1784	C1684	C1589	C1512	G1444
G2535	A2460	A2320	A2320	G2238	G2162	G2103	C1934	C1858	A1785	A1785	A1689	G1593	C1513	A1444A
G2536	C2466	A2321	A2321	G2239	C2163	C2104	A1935	G1859	A1786	A1786	U1689	G1594	U1514	C1445
U2537	C2467	A2322	A2322	U2243	G2165	C2105	A2020	G1860	A1787	A1787	U1693	G1595	G1515	
C2538	G2468	G2323	G2323	U2244	G2166	C2106	U2022	G1861			U1693	G1596	U1520	G1448
A2539	A2469	G2324	G2324	U2245	G2167	G2107	A1938	U1864	C1790	C1790	C1694	A1597	G1521	A1449
G2540	G2470	G2325	G2325	G2246	G2168	C2108	U1939	G1869	A1791	A1791	G1695	A1598	G1522	G1449A
A2541	C2471	G2326	G2326	A2247	U2169	U2109	C1940	C1870	G1792	G1792	G1696	C1599	U1523	C1451
A2542	G2472	G2248	G2248	G2248	A2170	G2110	C1942	A1871	G1793	G1793	G1697	G1600	G1524	C1453
G2543	G2400	A2328	A2328		A2171	G2111	U1943	A1872	U1794	U1794	A1698	G1601	U1454	A1454
G2544	U2401	G2329	G2329	G2251	U2172	G2112	U1944	G1878	C1795	C1795	G1699	U1602	G1455	G1455
A2545	A2476	G2330	G2330	G2252	C2173	U2113	G1949	C1879	U1796	U1796	A1700	A1603	A1529	G1459
G2548	G2481	G2331	G2331	G2253	C2174	U2114	U1950	C1881	U1798	U1798	G1704	A1608	G1530	A1460
G2549	C2482	G2334	G2334	G2254	C2175	G2115	G1951	G1889	G1799	G1799	G1705	A1609	A1461	G1461
G2550	C2483	A2335	A2335	G2255	A2176	A2117	A1952	A1884	C1800	C1800	U1706	A1610	G1533	G1465
G2551	G2484	G2336	G2336	G2256	C2179	U2118	A1953	A1885	G1801	G1801	C1711	A1614	U1535	C1484
G2552	G2485	G2337	G2337		U2180	U2119	G1954		A1902	A1902	C1712	A1617	U1536	G1466
G2553	G2486	G2340	G2340	G2257	G2181	G2120	U1955	G1888	A1803	A1803	G1725	C1617	G1538	C1467
G2554	G2487	G2341	G2341	G2276	G2182	U2122	U1956	A1890	A1804	A1804	G1726	A1618	G1539	G1468
G2555	A2488	A2342	A2342	G2275	G2183	G2123	U1963	A1893	A1810	A1810	U1727	G1622	G1540	G1469
G2556	G2489	G2343	G2343	G2276	G2184	G2124	G1964	C1894	G1811	G1811	G1728	G1623	U1541	G1470
G2557	G2490	G2344	G2344	G2277	G2190	G2125	C1965	C1895	A1812	A1812	A1729	A1542	A1543	A1471
G2558	G2491	G2345	G2345	G2277	U2191	A2126	A1966	C1896	G1813	G1813	G1730	A1632	A1544	A1472
C2559	G2492	G2346	G2346	G2278	G2192	G2127	C1967	G1897	G1814	G1814	G1731	C1544	G1473	G1473
A2560	G2493	G2347	G2347	G2280	G2193	C2128	G1968	U1898	A1815	A1815	A1732	C1636	A1545	C1474
A2561	G2494	G2350	G2350	G2283	C2196	U2130	A1970	G1899	G1816	G1816	G1733	C1637	C1475	G1475
G2562	A2497	G2351	G2351		U2197	A2054	A1971		G1817	G1817	C1742	C1638	C1476	C1476
G2563	C2498	G2352	G2352	G2286	U2198	A2055	A1972	C1902	U1818	U1818	G1743	U1639	A1477	A1477
G2564	G2499	G2353	G2353	G2287	A2199	G2056	A1976	G1903	U1820	U1820	C1743	G1640	G1478	G1478
G2565	A2503	G2354	G2354	G2288	A2205	A2134	G1904	G1906	A1821	A1821	G1751	A1641	G1479	G1479
G2566	U2504	G2355	G2355	G2289	C2206	C2135	C1905	G1907			C1752	G1642	A1554	A1482
G2567	G2505	G2356	G2356	G2290	C2207	C2136	G1906	G1908	G1824	G1824	C1753	C1646	G1559	G1483
G2568	U2506	G2357	G2357	U2291	U2208	C2137	A1981	G1907	G1825	G1825	G1754	G1647	G1560	G1484
G2569	C2507	G2358	G2358	C2292	C2209	C2138	C1982	G1908	G1826	G1826	A1755	G1648	G1561	G1485
G2570	G2508	A2432	A2432	C2293	G2210	C2139	G1986	G1910	C1827	C1827	G1756	G1649	A1562	A1486
G2571	U2511	G2435	G2435	C2294	G2211	C2140	U1986	G1913	G1828	G1828	U1757	G1650	A1566	A1490
G2572	C2512	G2436	G2436	C2295	A2212	G2141	G1987	C1913	A1829	A1829	G1758	G1651	A1567	A1491
G2573	G2513	G2437	G2437	A2298	U2213	C2142	C1988	C1914	U1833	U1833	C1771	A1652	G1568	G1492
G2574	G2514	U2437	U2437	G2299	G2216	U2144	G1989	G1915	U1834	U1834	A1762	G1653	A1569	C1493
G2575	G2515	G2438	G2438	G2300	G2217	C2145	C1990	A1916	G1835	G1835	G1763	A1654	A1570	A1494
G2576	C2517	A2439	A2439	G2301	G2218	C2146	U1991	G1916	G1836	G1836	G1764	A1655	A1571	A1495
G2577	A2518	G2372	G2372	G2302	G2219	G2147	U1993	A1919	G1839	G1839	U1766	C1656	A1572	A1496
G2578	U2519	G2373	G2373	G2303	G2224	G2148	U1993	C1920	G1839	G1839	U1766	C1657	G1573	U1497
G2579	C2520	C2374	C2374	G2304	G2225	G2149	G1988	G1921				C1658	C1488	C1488
U2580	G2521	A2377	A2377	A2305	G2226	U2150	C1998	G1922	C1844	C1844	C1771	C1577	C1499	C1499
G2581	G2512	G2378	G2378	G2306	G2227	G2151	C1999	U1923	G1845	G1845	G1772	U1578	G1500	G1500
G2582	G2513	G2379	G2379	G2307	G2228	G2152	C2006	U1923	G1846	G1846	A1773	A1579		
G2583	G2514	G2380	G2380	G2308	G2229	U2086	C2007	C1925	A1847	A1847	C1774	A1668	A1580	C1504
G2584	G2515	C2381	C2381	G2309	G2230	G2088	C2008	U1926	A1848	A1848	U1775	A1669	G1581	G1505
U2585	C2516	G2382	G2382	G2310	G2231	U2089	G2009	A1927	G1849	G1849	G1776	G1674	C1582	C1506
G2586	G2517	U2332	U2332	G2311	G2232	U2092	G2010	A1928	G1850	G1850	U1777	C1675	A1583	A1507
G2587	G2518	G2313	G2313	G2312	G2233	G2156	U2011	U1928			U1778	A1676	C1585	A1508
G2588	A2530	G2314	G2314	G2314	G2234	A2158	G2012	G1930	A1853	A1853	U1779	A1677	A1586	C1509

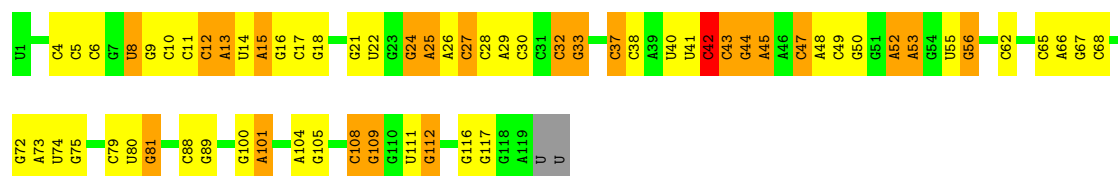


U1775	U1688	C1537	G1466	A1395	A1317	G1245	U1175	U1101	G956	G881	C806	U724
G1776	A1689	G1538	G1466	U1396	C1318	A1246	G1176	C1102	A957	G882	U807	G725
U1779	A1690	G1542	G1467	U1397	G1319	A1247	A1177	A1103	U958	G883	C812	G726
G1780	C1692	A1543	C1398	C1399	C1320	G1248	C1178	C1104	A959	G884	C813	A727
G1782	U1694	A1544	A1469	G1400	A1321	U1249	C1179	U1105	A960	C885	U813	G728
G1695	C1694	A1545	G1470	G1401	A1322	C1251	C1180	U1108	C961	C886	C814	G729
A1783	G1695	A1546	A1471	C1402	G1328	G1252	C1181	U1109	C971	A887	C817	C730
U1784	A1618	C1547	A1472	C1403	U1329	A1253	A1182	G1110	G972	C888	G818	C731
A1785	G1697	C1548	G1473	U1405	A1331	U1256	G1183	A1048	A973	C889	A819	G738
A1786	A1698	C1549	C1474	U1406	G1332	U1257	A1184	G1111	G974	A890	A820	G739
G1699	G1699	C1550	A1477	G1407	A1333	C1258	G1187	G1112	C974A	G982	A821	U740
A1700	C1550	C1408	G1478	C1408	C1333	G1258	U1188	U1113	G975	C993	U822	G741
A1701	G1553	G1479	G1479	C1409	G1338	G1264	A1189	G1114	C976	A896	G823	G742
G1705	A1554	G1480	G1482	G1410	U1340	A1265	G1190	G1115	G977	C997	A824	G743
U1706	G1555	U1482	G1483	C1411	A1344	G1266	G1193	G1120	G978	C998	A825	
U1709	C1556	A1486		A1412	G1344	A1269	A1194	C1121	G979	A899	U826	A746
C1710	C1557	A1490		G1416	C1345	G1270	G1195	G1122	A983	A900	U827	U747
G1717	A1558	A1494		G1417	A1349	A1271	G1196	G1123	A984	A901	U828	G748
G1718	G1561	A1495		G1418	A1352	A1272	G1197	C1124	U985	C904	A829	A752
G1725	A1562	A1496		A1419	U1353	A1273	U1198	G1125	U905	U905	G830	C753
G1726	G1563	A1497		U1420	A1354	A1274	U1199	A1126	C986	G906		
G1800	A1564	A1498		G1421	G1355		C1200	A1127	G987	G907	A835	U757
G1801	C1566	A1499		A1427	A1356	G1279	C1201	A1128	A988	U907	G836	C758
A1802	A1567	A1500		C1428	A1357	U1282	C1202	U1130	A990	C908	G837	G759
A1804	G1568	G1501		G1429	G1358	U1283	A1203	G1131	C991	A910	C838	A761
U1805	A1569	C1505		A1431	A1359	A1284	A1204	C1135	C992	C912	C844	A764
C1806	G1575	C1506		G1432	A1364	G1285	G1205	G1136	C993	G915	C845	G765
G1807	U1576	C1507		A1433	A1365	U1286	G1206	G1137	C994	A917	C846	
	C1577	A1508		G1434	A1366	A1287	A1210	G1138	C995	A918	U847	G768
C1741	U1578	A1509		G1435	A1367	U1288	U1211	U1141	G1002	A919	G848	G769
G1742	A1579	C1510		G1436	A1368	C1289	U1212	U1142	A926	C925	A849	
G1743	U1580	A1511		C1437	G1368	A1290	A1213	A1143	G1003	A928	G852	A774
G1760	G1581	C1512		U1438	A1369	C1291	G1214	G1144	C1004	G929	G853	G775
	C1585	G1513		A1439	C1370	U1292	G1215	U1077	C1005	U930	G854	G776
G1763	A1586	U1514		G1440	G1371	C1293	C1217	U1078	C1006	G931	G855	
C1754	A1587	C1515		G1441	U1372	U1294	C1218	C1080	A1009	G932	C856	G780
G1756	C1588	U1519		C1445	A1373	C1295	G1219	U1081	G933	A933	U858	A781
U1820	U1590	U1520		G1446	G1374	G1296	A1220	G1149	G934	G934	G859	A782
A1821	G1591	G1522		G1447	C1375	C1297	A1221	C1150	U1011	G935	U860	A783
G1759	G1594	G1525		A1448	C1376	C1298	G1224	C1153	U1012	C935	A861	A784
	G1595	G1526		G1449	G1377	U1300	C1225	G1154	U1013	G938	A862	G785
G1762	C1598	U1527		G1449A	A1379	A1301	G1228	A1084	U1014		A863	
G1764	U1599	G1528		C1450	G1380	A1302	U1307	A1085	G1015	A941	C864	C790
U1677	C1599	A1529		C1451	A1384	G1303	G1230	A1087	C1018	G942	C865	C791
U1679	G1600	U1530		A1453	G1385	A1307	G1231	U1089	U1019	U943	A866	A793
G1681	U1601	C1531		C1387	A1386	G1309	G1236	G1091	A1020	G944	G869	G794
G1682	U1602	C1532		G1388	A1387	G1309	A1237	C1092	G1022	A945	U870	C795
C1683	A1603	C1533		G1389	C1388	U1312	G1238	G1093	U1023	G947	U871	C796
C1684	G1604	C1534		U1390	G1389	U1313	A1241	A1095	G1024	G950	A872	G798
C1685	G1605	U1535		U1391	U1390	C1314	A1242	A1096	G1025	C951	G873	
C1686	U1536	A1536		A1392	C1458	C1315	G1243	U1097	U1026	G953	A878	G801
C1687	C1607			G1461	G1459	G1460	A1243	C1100	A1028	A953	G879	A802
							G1244		A1029		G880	G805

C2875	C2876	C2877	C2878	C2879	C2880	C2881	C2882	A2883	U2884	C2889	C2891	A2892	C2893	C2894	U2897	U	G	A	C	C	C	C	U	C																																						
G2805	G2807	U2808	A2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	A2820	A2821	G2822	A2826	C2827	C2828	G2831	G2832	G2833	G2834	A2835	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	U2849	A2850	A2851	G2852	G2853	G2854	G2855	A2860	G2861	G2864	U2865	U2866	G2867	A2868	G2869	G2870	G2871	G2872	G2873	G2874								
U2728	G2729	C2730	A2731	A2732	A2733	A2734	G2735	A2741	G2744	A2748	A2749	A2750	A2751	C2752	A2753	U2756	A2757	A2758	G2759	G2760	G2761	A2764	A2765	G2766	C2767	C2771	C2774	A2775	A2776	G2777	A2778	U2779	G2780	A2781	C2784	C2787	C2788	G2789	A2790	G2791	G2792	G2793	G2794	G2795	U2797	G2798	G2799	A2801	G2802	G2803	C2804											
A2654	G2655	U2656	A2657	G2658	G2659	A2660	G2661	A2662	A2665	C2666	G2673	G2677	G2678	A2679	C2680	G2681	U2682	C2683	U2687	U2688	C2689	C2690	C2691	G2692	A2693	G2694	C2695	U2696	U2697	U2698	C2699	C2700	C2701	U2702	C2703	C2710	A2711	U2712	A2713	A2714	C2715	U2716	G2717	G2718	G2719	U2720	A2721	G2722	C2723	C2724	A2725	U2726	G2727									
U2580	G2581	G2582	G2583	U2584	U2585	G2586	G2587	C2591	G2592	U2593	C2594	G2597	U2598	G2599	A2602	G2607	G2608	U2609	G2610	G2611	C2612	U2613	G2617	G2618	G2619	C2620	A2621	G2622	G2623	G2624	G2625	U2626	A2629	G2630	G2631	A2632	G2633	U2636	U2637	G2638	A2639	G2640	G2641	G2642	G2645	G2646	U2647	C2648	U2649	U2653												
U2506	C2507	G2508	G2509	G2510	C2512	G2513	G2516	C2517	A2518	U2519	C2520	G2524	G2525	U2528	G2529	A2530	A2531	G2535	C2538	G2539	C2540	A2541	A2542	G2543	G2544	G2545	G2550	G2551	U2552	G2553	U2554	U2555	C2556	G2557	C2558	C2559	G2560	A2561	U2562	U2563	A2564	A2565	U2566	U2567	G2569	A2572	C2573	G2576	C2579													
G2429	A2430	A2433	A2434	A2435	U2438	A2439	C2440	C2441	C2442	G2445	G2446	G2447	A2448	U2449	A2450	A2451	A2452	G2455	U2460	C2463	A2464	C2465	C2466	C2467	C2468	A2469	G2470	C2474	C2475	A2476	G2477	A2478	G2481	G2482	C2483	G2484	G2485	G2489	G2494	G2495	C2496	A2497	C2498	C2499	G2502	A2503	U2504	G2505														
A2360	A2361	C2364	C2365	A2366	G2367	G2370	G2371	G2372	C2373	C2374	G2375	A2376	A2377	A2378	G2379	C2380	C2381	G2382	G2383	G2384	C2385	C2386	U2387	G2388	U2389	U2390	C2391	A2392	A2393	C2394	G2395	G2396	G2397	U2398	U2401	C2402	C2403	C2404	G2405	U2406	G2407	U2408	A2411	G2415	U2419	A2422	U2423	C2424	A2425	A2426	G2427	G2428										
U2290	U2291	C2292	C2293	C2294	C2295	U2296	G2297	A2298	G2302	G2303	G2304	A2305	C2306	G2307	G2308	A2309	A2310	U2311	U2312	C2313	C2314	G2315	C2316	C2317	G2318	G2319	A2320	G2325	C2326	A2327	A2328	G2329	G2330	G2331	G2334	A2335	A2336	G2341	C2342	C2343	U2344	G2345	A2346	C2347	U2348	G2349	C2350	G2351	G2354	G2355	C2356	U2357	G2358	C2359								
G2215	G2216	G2217	G2218	G2219	G2220	A2221	G2222	C2223	U2232	U2233	G2234	G2238	G2239	C2240	U2243	U2244	U2245	U2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	U2257	G2258	C2259	C2260	G2261	U2262	C2263	A2268	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2279	G2280	C2281	G2282	C2283	C2284	C2285	A2286	A2287	G2288	G2289											
C2145	C2146	G2147	G2148	G2149	U2150	G2151	G2152	G2153	G2154	G2157	A2158	G2159	G2160	C2161	G2162	C2163	G2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	C2175	A2176	G2177	G2178	G2181	G2182	G2185	G2186	G2187	C2188	U2189	G2190	G2191	G2192	G2193	G2194	U2197	A2198	A2199	C2205	C2206	C2207	U2208	C2209	G2210	G2211	A2212	U2213							
G2069	G2070	A2071	U2074	G2083	G2084	C2085	G2086	G2087	G2093	C2097	U2098	U2099	A2013	A2014	A2015	U2016	U2017	A2020	C2021	C2022	G2023	A2030	A2031	G2032	A2033	U2034	G2037	G2038	C2039	C2040	U2041	G2042	C2043	C2044	G2048	G2049	C2050	A2051	G2052	C2055	G2056	A2059	A2060	C2061	A2062	C2063	G2067	U2068														
A1916	U1917	A1918	A1919	C1920	U1924	C1925	G1929	G1930	U1931	A1932	G1933	A1936	A1937	A1938	U1939	U1940	C1941	C1942	U1943	U1944	G1945	U1946	C1947	G1950	U1951	A1952	A1953	G1954	U1955	U1956	C1957	A1958	U1963	G1964	C1965	A1966	G1967	G1968	A1969	A1970	A1971	A1972	G1979	G1980	A1981	C1982	G1985	G1988	G1989	C1990	U1991											
C1843	C1844	A1847	A1848	G1849	G1850	U1851	C1852	A1853	A1854	G1855	A1856	G1857	G1858	G1860	G1861	G1862	G1863	U1864	G1865	C1866	G1867	G1868	A1869	A1870	A1871	A1872	G1873	C1874	C1875	C1876	C1877	G1878	C1879	C1880	C1881	A1882	G1883	A1884	A1885	G1886	G1887	G1888	A1889	A1890	G1891	C1892	C1895	G1896	G1897	U1898	A1900	A1901	G1902	G1903	G1906	G1907	C1908	G1909	G1910	A1913	C1914	U1915

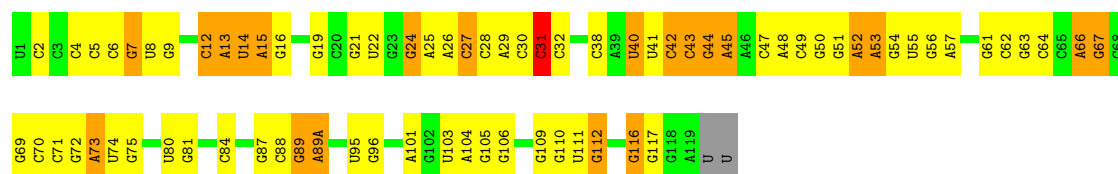
• Molecule 26: 5S rRNA

Chain RB:



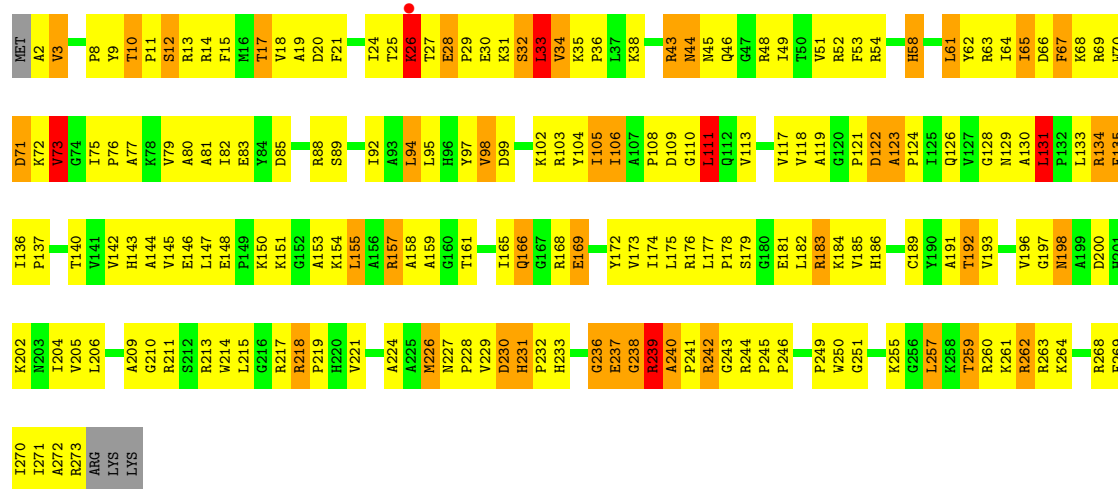
• Molecule 26: 5S rRNA

Chain YB:



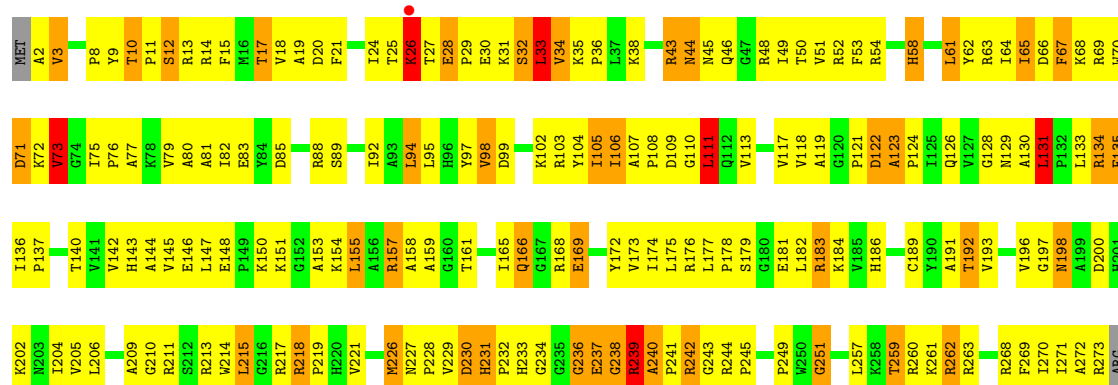
• Molecule 27: 50S ribosomal protein L2

Chain RD:



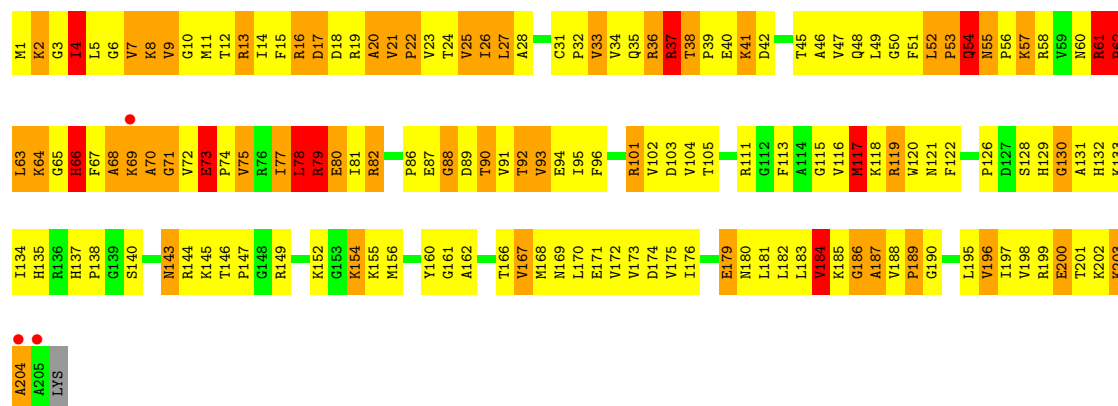
• Molecule 27: 50S ribosomal protein L2

Chain YD:

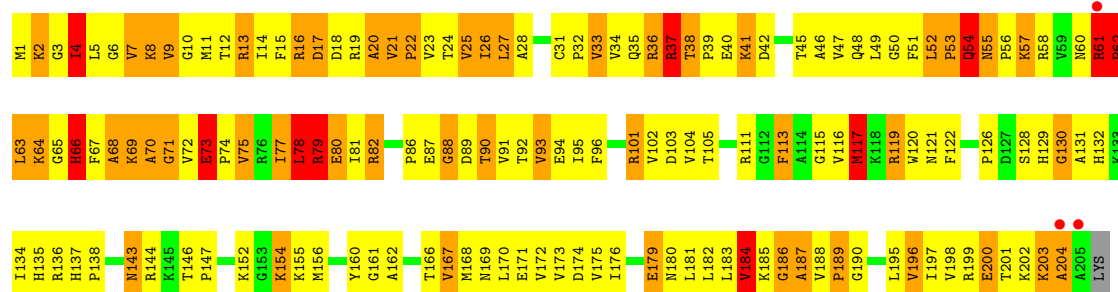


LYS
LYS

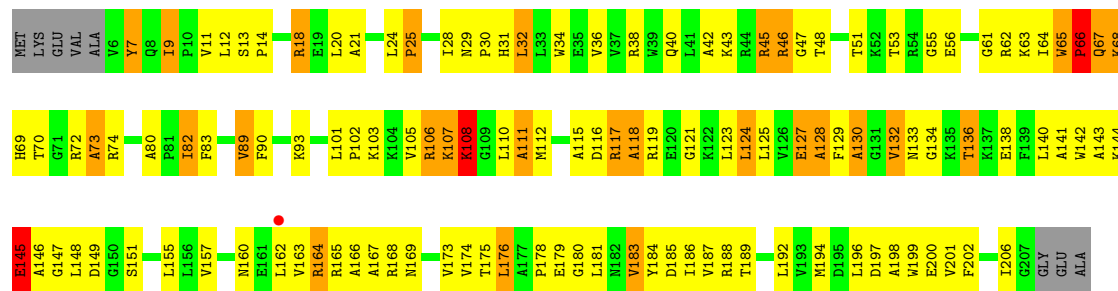
- Molecule 28: 50S ribosomal protein L3

Chain RE: 

- Molecule 28: 50S ribosomal protein L3

Chain YE: 

- Molecule 29: 50S ribosomal protein L4

Chain RF: 

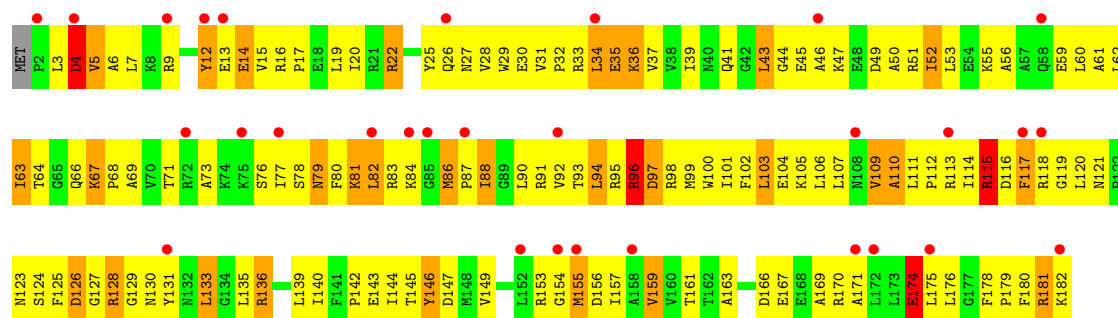
- Molecule 29: 50S ribosomal protein L4

Chain YF: 



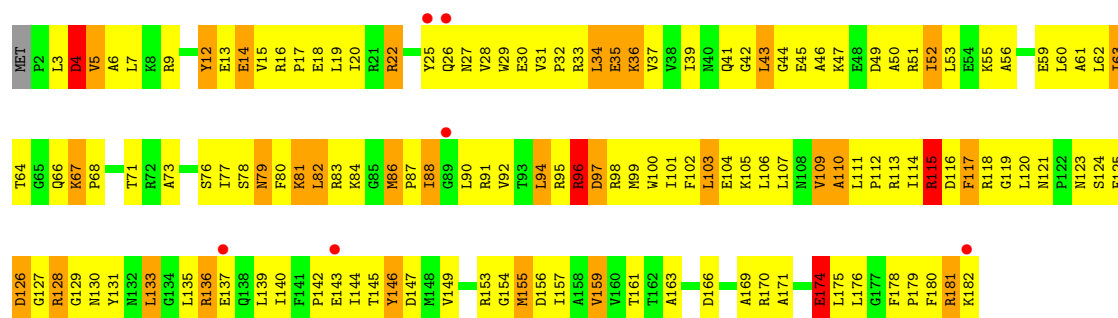
- Molecule 30: 50S ribosomal protein L5

Chain RG:



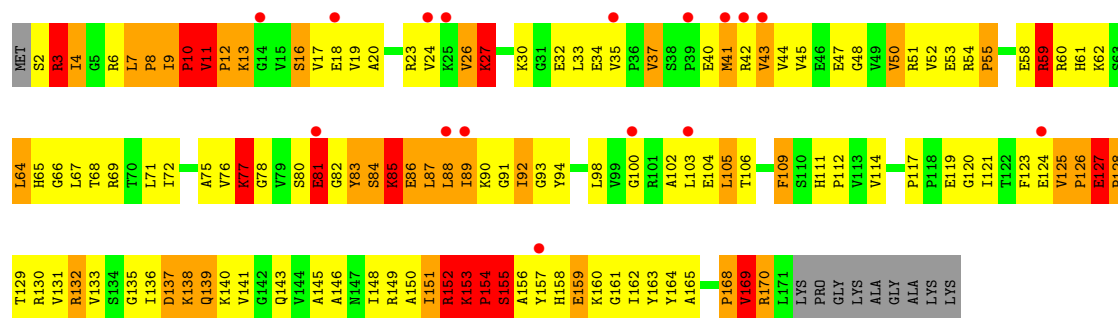
- Molecule 30: 50S ribosomal protein L5

Chain YG:



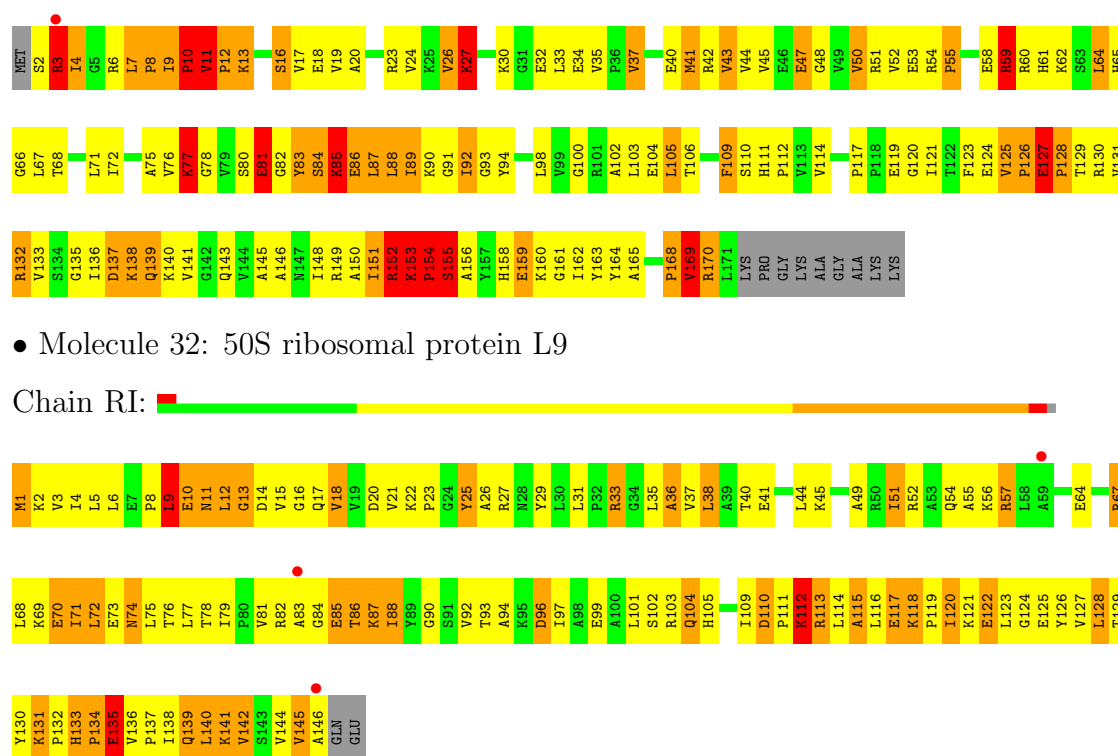
- Molecule 31: 50S ribosomal protein L6

Chain RH:

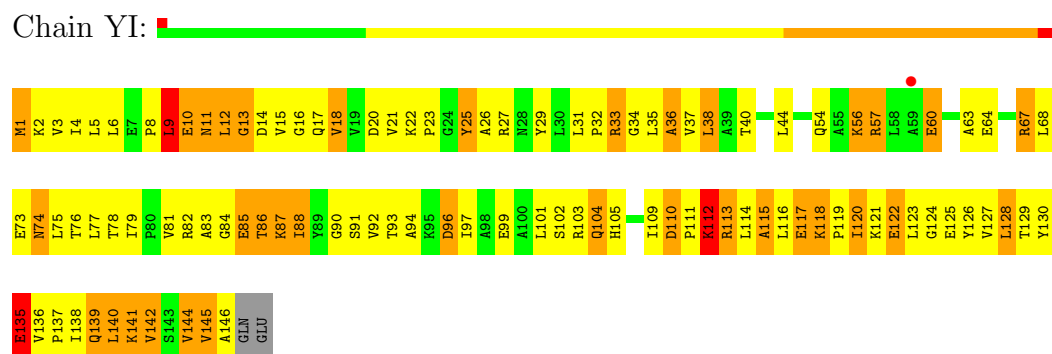


- Molecule 31: 50S ribosomal protein L6

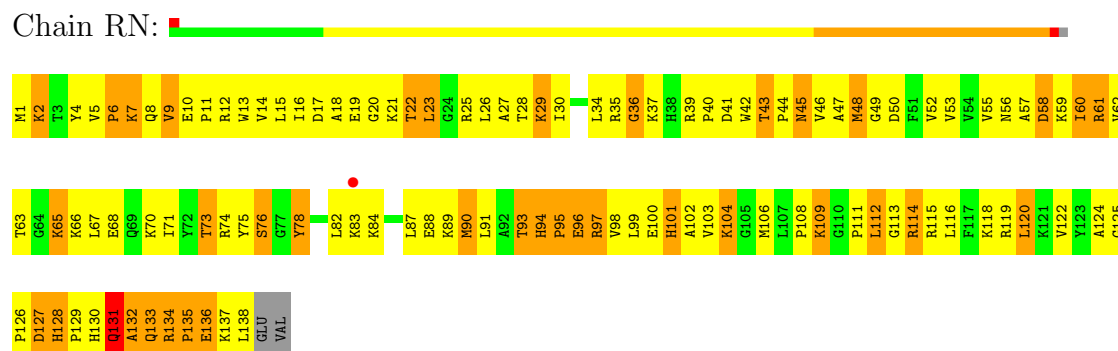
Chain YH:



• Molecule 32: 50S ribosomal protein L9

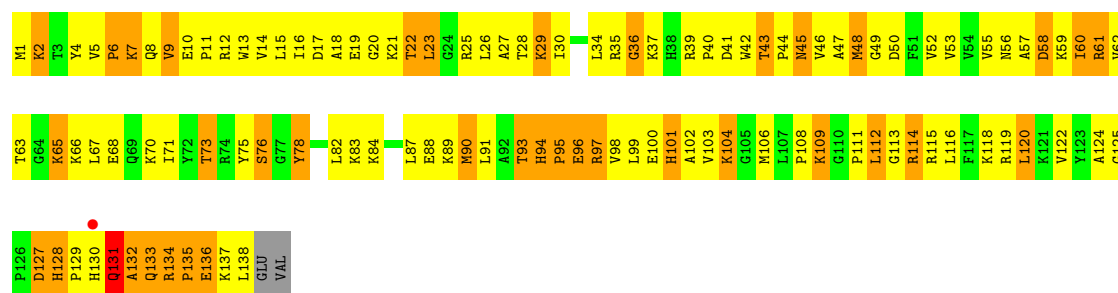


• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13





• Molecule 34: 50S ribosomal protein L14

Chain RO:

• Molecule 34: 50S ribosomal protein L14

Chain YO:

• Molecule 35: 50S ribosomal protein L15

Chain RP:

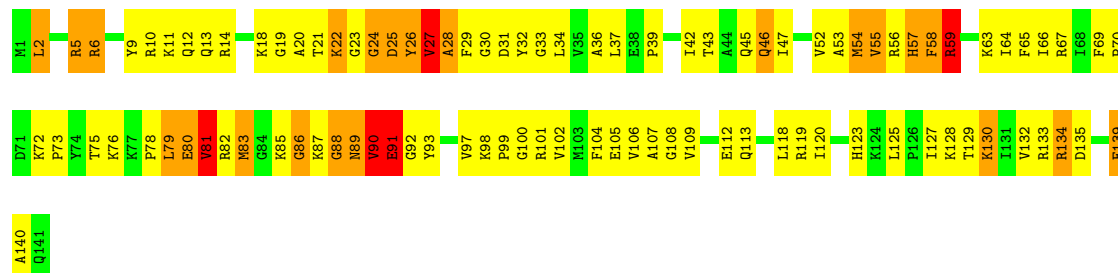
• Molecule 35: 50S ribosomal protein L15

Chain YP:



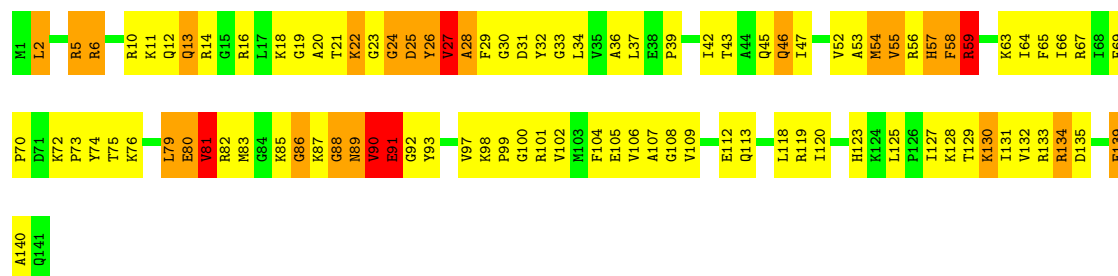
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



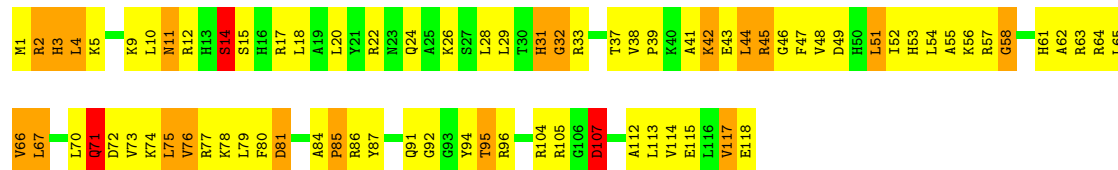
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



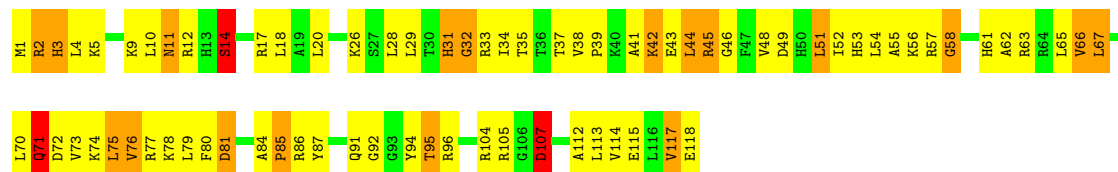
- Molecule 37: 50S ribosomal protein L17

Chain RR:



- Molecule 37: 50S ribosomal protein L17

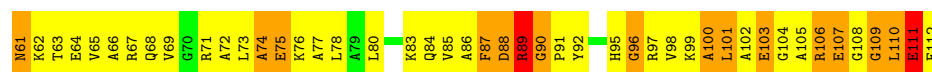
Chain YR:



- Molecule 38: 50S ribosomal protein L18

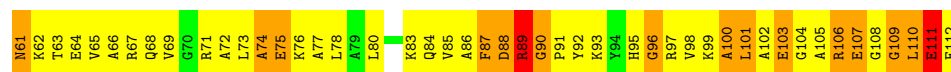
Chain RS:





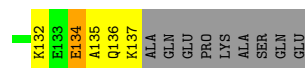
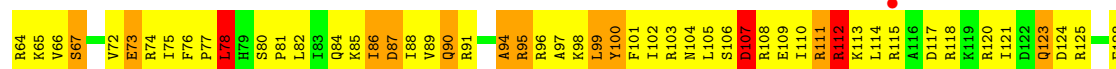
- Molecule 38: 50S ribosomal protein L18

Chain YS:



- Molecule 39: 50S ribosomal protein L19

Chain RT:



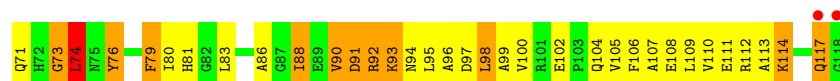
- Molecule 39: 50S ribosomal protein L19

Chain YT:



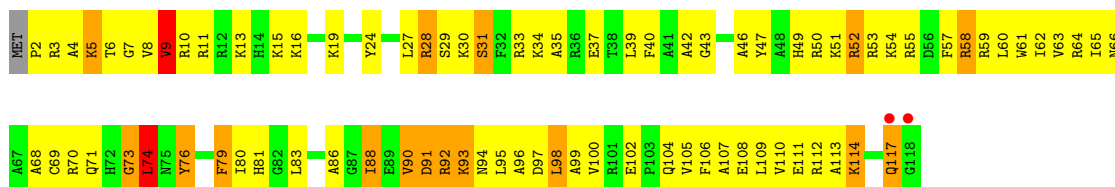
- Molecule 40: 50S ribosomal protein L20

Chain RU:



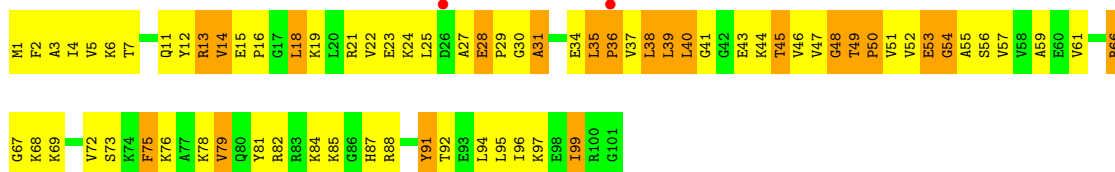
- Molecule 40: 50S ribosomal protein L20

Chain YU:



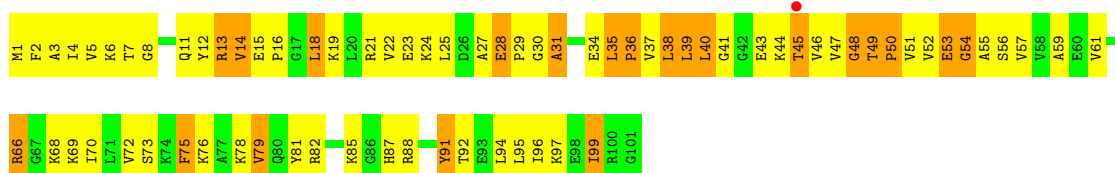
• Molecule 41: 50S ribosomal protein L21

Chain RV:



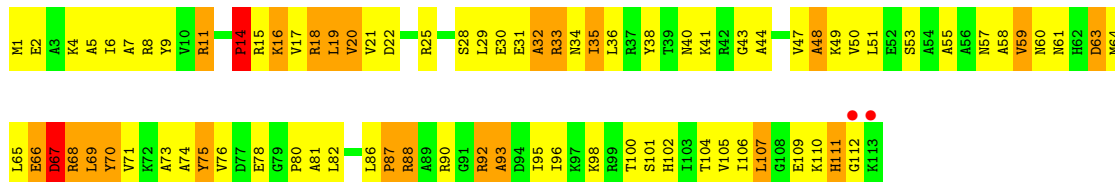
• Molecule 41: 50S ribosomal protein L21

Chain YV:



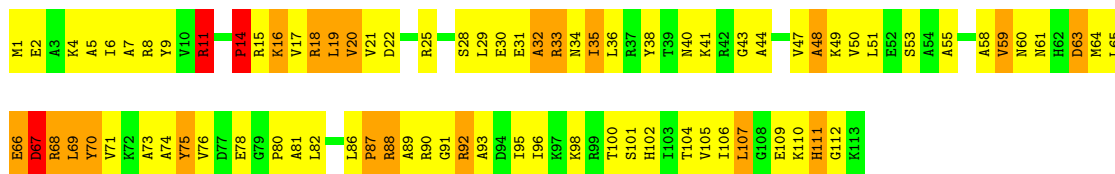
• Molecule 42: 50S ribosomal protein L22

Chain RW:



• Molecule 42: 50S ribosomal protein L22

Chain YW:



• Molecule 43: 50S ribosomal protein L23

Chain RX:





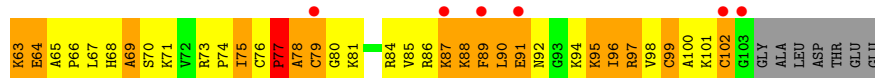
• Molecule 43: 50S ribosomal protein L23

Chain YX:



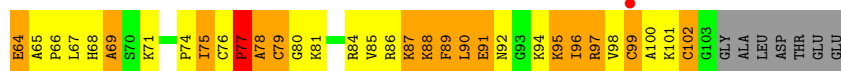
• Molecule 44: 50S ribosomal protein L24

Chain RY:



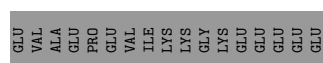
• Molecule 44: 50S ribosomal protein L24

Chain YY:



• Molecule 45: 50S ribosomal protein L25

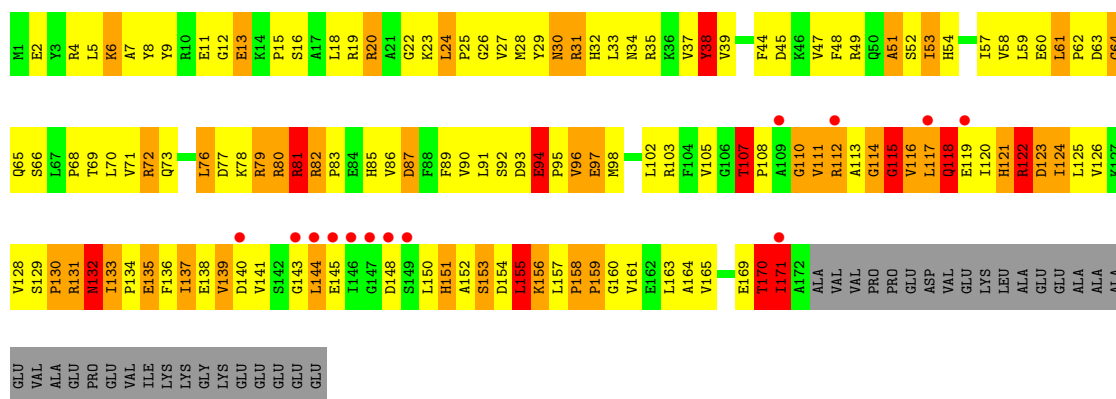
Chain RZ:



• Molecule 45: 50S ribosomal protein L25

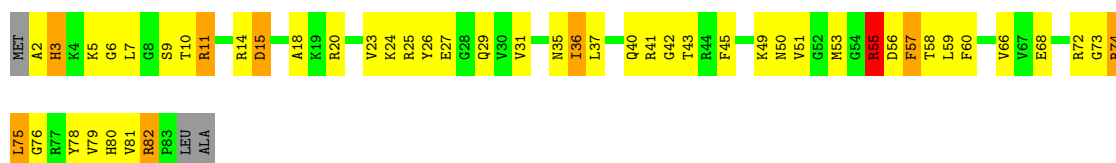
Chain YZ:





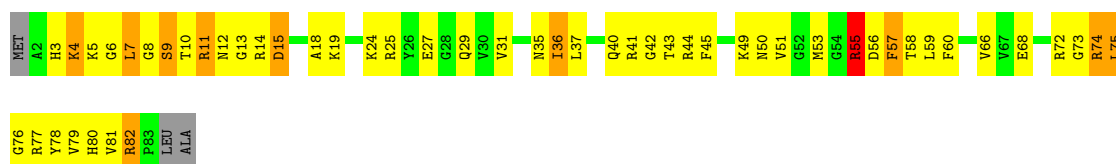
• Molecule 46: 50S ribosomal protein L27

Chain R0:



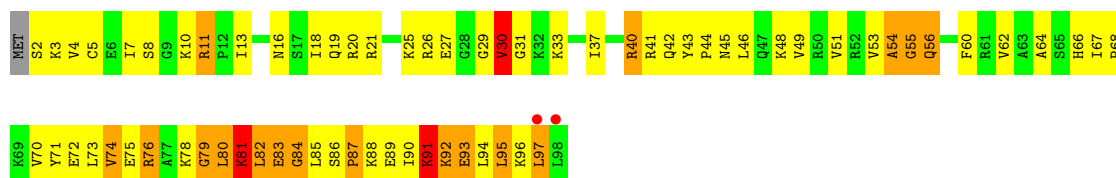
• Molecule 46: 50S ribosomal protein L27

Chain Y0:



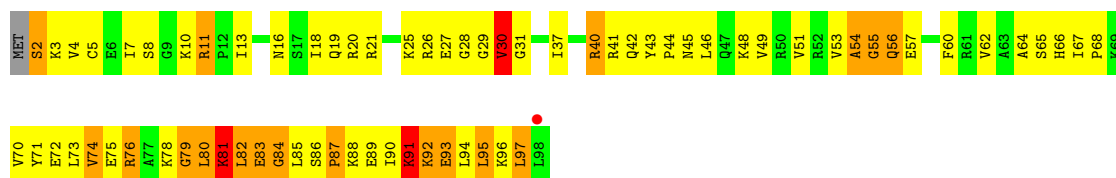
• Molecule 47: 50S ribosomal protein L28

Chain R1:



• Molecule 47: 50S ribosomal protein L28

Chain Y1:



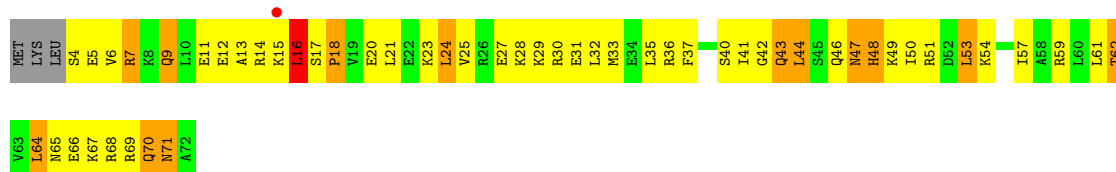
• Molecule 48: 50S ribosomal protein L29

Chain R2:



- Molecule 48: 50S ribosomal protein L29

Chain Y2:



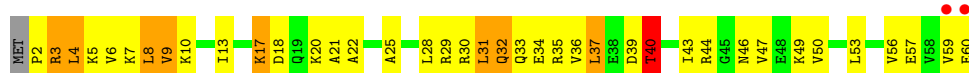
- Molecule 49: 50S ribosomal protein L30

Chain R3:



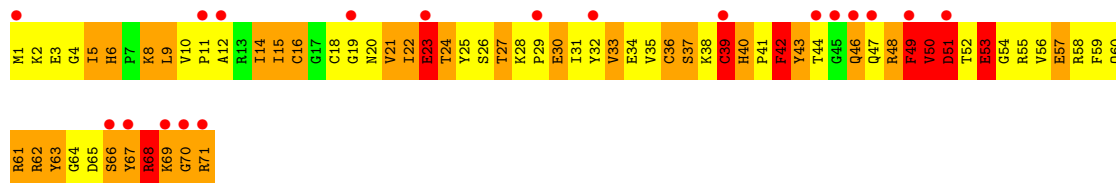
- Molecule 49: 50S ribosomal protein L30

Chain Y3:



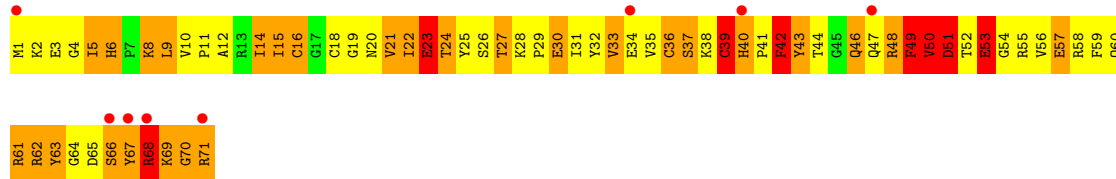
- Molecule 50: 50S ribosomal protein L32

Chain R4:



- Molecule 50: 50S ribosomal protein L32

Chain Y4:



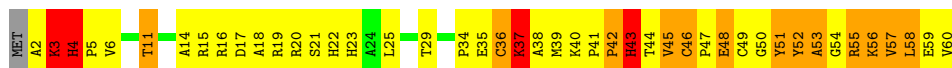
- Molecule 51: 50S ribosomal protein L33

Chain R5:



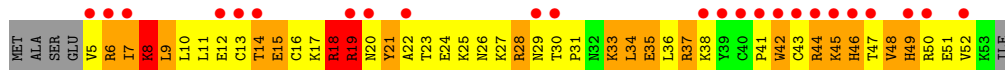
- Molecule 51: 50S ribosomal protein L33

Chain Y5:



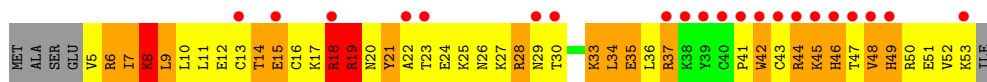
- Molecule 52: 50S ribosomal protein L34

Chain R6:



- Molecule 52: 50S ribosomal protein L34

Chain Y6:



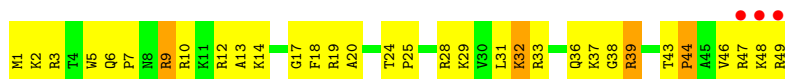
- Molecule 53: 50S ribosomal protein L35

Chain R7:



- Molecule 53: 50S ribosomal protein L35

Chain Y7:



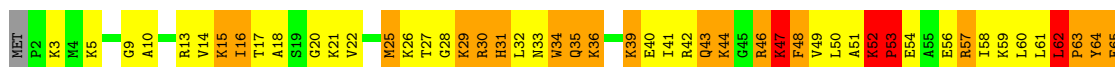
- Molecule 54: tRNA acceptor end mimic

Chain R8:



- Molecule 54: tRNA acceptor end mimic

Chain Y8:



- Molecule 55: RNA (5'-R(*CP*CP*(PPU))-3')

Chain Z6:



- Molecule 55: RNA (5'-R(*CP*CP*(PPU))-3')

Chain Z8: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.55Å 449.21Å 619.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.44 34.81 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.81-3.44) 98.2 (34.81-3.26)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.243 , 0.285 0.243 , 0.284	Depositor DCC
R_{free} test set	34671 reflections (4.59%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 24.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 881904 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	291123	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.42	0/36098	0.97	58/56341 (0.1%)
1	XA	0.45	0/36123	1.00	71/56380 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.42	0/1733	0.69	1/2318 (0.0%)
4	XD	0.42	0/1733	0.70	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	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	0.37	0/1276	0.61	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	0.35	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	0.45	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	0.43	0/501	0.70	1/664 (0.2%)
14	XN	0.43	0/501	0.70	1/664 (0.2%)
15	QO	0.39	0/745	0.66	0/992
15	XO	0.39	0/745	0.66	0/992
16	QP	0.37	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	0.38	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	0.73	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	0.34	0/765	0.69	0/1007
20	XT	0.33	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.62	0/288
22	QV	0.52	0/1836	0.99	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.40	0/189	0.75	0/292
23	XX	0.66	0/189	1.09	2/292 (0.7%)
24	QY	0.51	0/311	0.88	0/483
24	XY	0.52	0/311	0.89	0/483
25	RA	0.52	2/69543 (0.0%)	1.06	149/108563 (0.1%)
25	YA	0.59	2/69521 (0.0%)	1.10	200/108529 (0.2%)
26	RB	0.44	0/2878	1.04	7/4490 (0.2%)
26	YB	0.46	0/2878	1.03	2/4490 (0.0%)
27	RD	0.62	2/2165 (0.1%)	0.90	3/2919 (0.1%)
27	YD	0.62	2/2165 (0.1%)	0.90	3/2919 (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	4/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.40	0/1151	0.80	1/1558 (0.1%)
32	YI	0.40	0/1151	0.79	1/1558 (0.1%)
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.53	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.94	3/1544 (0.2%)
35	YP	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.53	0/1143	0.89	3/1527 (0.2%)
36	YQ	0.53	0/1143	0.89	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	0.82	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	0.82	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	0.78	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	0.47	0/1408	0.77	1/1908 (0.1%)
45	YZ	0.47	0/1408	0.77	1/1908 (0.1%)
46	R0	0.57	0/657	0.80	0/874
46	Y0	0.60	0/657	0.85	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	0.50	0/583	0.83	1/771 (0.1%)
48	Y2	0.50	0/583	0.84	1/771 (0.1%)
49	R3	0.43	0/474	0.71	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	0.42	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	Z6	0.82	0/40	1.81	1/60 (1.7%)
55	Z8	0.80	0/40	1.80	1/60 (1.7%)
All	All	0.50	8/315563 (0.0%)	0.98	571/471909 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	236	GLY	C-N	8.59	1.53	1.34
27	RD	236	GLY	C-N	8.55	1.53	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	239	ARG	CA-C	-6.77	1.35	1.52
27	RD	239	ARG	CA-C	-6.76	1.35	1.52
25	YA	783	A	N7-C5	-5.95	1.35	1.39

The worst 5 of 571 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	QL	47	LYS	C-N-CD	-20.50	75.51	120.60
12	XL	47	LYS	C-N-CD	-20.46	75.58	120.60
25	YA	761	A	N1-C6-N6	12.76	126.25	118.60
25	YA	945	A	N9-C1'-C2'	12.75	130.58	114.00
22	QV	17	C	C2-N1-C1'	11.85	131.84	118.80

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	16275	828	0
1	XA	32269	0	16289	816	0
2	QB	1924	0	1975	291	0
2	XB	1924	0	1975	301	0
3	QC	1605	0	1668	208	0
3	XC	1605	0	1668	209	1
4	QD	1703	0	1762	240	0
4	XD	1703	0	1763	215	0
5	QE	1155	0	1213	147	0
5	XE	1155	0	1213	142	0
6	QF	843	0	857	93	0
6	XF	843	0	857	99	0
7	QG	1257	0	1296	149	0
7	XG	1257	0	1296	147	0
8	QH	1116	0	1176	155	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	XH	1116	0	1177	164	0
9	QI	1010	0	1037	151	0
9	XI	1010	0	1037	160	0
10	QJ	801	0	849	138	0
10	XJ	801	0	849	136	0
11	QK	885	0	904	108	1
11	XK	885	0	904	118	0
12	QL	975	0	1062	109	0
12	XL	975	0	1062	113	0
13	QM	964	0	1034	171	0
13	XM	964	0	1034	180	0
14	QN	492	0	531	89	0
14	XN	492	0	529	87	0
15	QO	734	0	771	75	0
15	XO	734	0	771	74	0
16	QP	705	0	725	114	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	84	0
17	XQ	834	0	904	82	0
18	QR	574	0	644	68	0
18	XR	574	0	644	67	0
19	QS	674	0	699	104	0
19	XS	674	0	699	143	0
20	QT	763	0	860	108	0
20	XT	763	0	861	102	0
21	QU	217	0	234	30	0
21	XU	217	0	234	29	0
22	QV	1644	0	836	41	0
22	XV	1644	0	836	40	0
23	QX	170	0	87	16	0
23	XX	170	0	88	10	0
24	QY	303	0	154	13	0
24	XY	303	0	154	17	0
25	RA	62091	0	31301	1401	0
25	YA	62071	0	31286	1351	0
26	RB	2573	0	1306	70	0
26	YB	2573	0	1306	61	0
27	RD	2115	0	2195	324	0
27	YD	2115	0	2195	350	0
28	RE	1568	0	1634	277	0
28	YE	1568	0	1634	266	0
29	RF	1585	0	1632	174	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	YF	1585	0	1632	182	0
30	RG	1474	0	1535	212	0
30	YG	1474	0	1535	206	0
31	RH	1307	0	1382	217	0
31	YH	1307	0	1382	219	1
32	RI	1136	0	1223	179	0
32	YI	1136	0	1223	176	0
33	RN	1104	0	1180	194	0
33	YN	1104	0	1180	186	0
34	RO	933	0	996	123	0
34	YO	933	0	996	124	0
35	RP	1145	0	1228	248	0
35	YP	1145	0	1228	247	0
36	RQ	1122	0	1179	168	0
36	YQ	1122	0	1179	168	0
37	RR	968	0	1033	115	0
37	YR	968	0	1033	112	0
38	RS	882	0	943	158	0
38	YS	882	0	943	163	0
39	RT	1141	0	1202	152	0
39	YT	1141	0	1202	156	0
40	RU	964	0	1022	130	0
40	YU	964	0	1022	138	0
41	RV	779	0	852	132	0
41	YV	779	0	852	130	1
42	RW	900	0	964	101	0
42	YW	900	0	964	108	0
43	RX	725	0	778	68	0
43	YX	725	0	778	82	0
44	RY	785	0	878	163	0
44	YY	785	0	878	154	1
45	RZ	1378	0	1407	227	0
45	YZ	1378	0	1407	227	0
46	R0	648	0	672	88	0
46	Y0	648	0	672	85	0
47	R1	763	0	848	141	0
47	Y1	763	0	848	145	0
48	R2	581	0	629	80	0
48	Y2	581	0	629	75	0
49	R3	469	0	518	40	0
49	Y3	469	0	518	41	0
50	R4	581	0	574	159	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	Y4	581	0	574	180	0
51	R5	459	0	480	77	0
51	Y5	459	0	480	75	1
52	R6	424	0	450	93	0
52	Y6	424	0	450	90	0
53	R7	430	0	480	47	0
53	Y7	430	0	480	42	0
54	R8	517	0	582	106	0
54	Y8	517	0	582	100	0
55	Z6	74	0	51	10	0
55	Z8	74	0	51	4	0
56	QA	60	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	2	0	0	0	0
56	QX	2	0	0	0	0
56	R5	1	0	0	0	0
56	RA	212	0	0	0	0
56	RB	2	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RP	1	0	0	0	0
56	XA	63	0	0	0	0
56	XM	2	0	0	0	0
56	XV	2	0	0	0	0
56	Y5	1	0	0	0	0
56	YA	242	0	0	0	0
56	YB	2	0	0	0	0
56	YE	2	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	4	0
57	XA	42	0	45	1	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
All	All	291123	0	197505	16608	3

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 34.

The worst 5 of 16608 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:QN:39:LEU:HD22	14:QN:43:CYS:SG	1.33	1.63
36:YQ:81:VAL:HG23	46:Y0:7:LEU:CD2	1.21	1.60
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.54
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
19:QS:5:LEU:HD22	50:R4:67:TYR:CE2	1.45	1.51

All (3) 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:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.98	0.22
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.04	0.16
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.06	0.14

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	7
2	XB	235/256 (92%)	152 (65%)	53 (23%)	30 (13%)	0	7
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	14
3	XC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	14
4	QD	206/209 (99%)	133 (65%)	51 (25%)	22 (11%)	1	10
4	XD	206/209 (99%)	133 (65%)	50 (24%)	23 (11%)	1	9
5	QE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	1	10
5	XE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	12
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	15
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	15
7	QG	153/156 (98%)	102 (67%)	37 (24%)	14 (9%)	1	15
7	XG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	10
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	10
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	7
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	7
10	QJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	11
10	XJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	14
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	20
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	20
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	9
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	9
13	QM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	3
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	3
14	QN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	3
14	XN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	3
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	23
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	23
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	6
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	6
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	18
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	18
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	9
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	9
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	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	3
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	3
27	RD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	2	22
27	YD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	2	22
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	12
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	12
30	RG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	1	9
30	YG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	1	9
31	RH	168/180 (93%)	94 (56%)	35 (21%)	39 (23%)	0	1
31	YH	168/180 (93%)	95 (56%)	35 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	83 (58%)	33 (23%)	28 (19%)	0	2
32	YI	144/148 (97%)	85 (59%)	32 (22%)	27 (19%)	0	2
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	4
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	4
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	21
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	21
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%)	94 (68%)	30 (22%)	15 (11%)	1	10
36	YQ	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	1	10
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	8
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	8
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	3
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	19
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	19
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	12
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	12
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	7
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	7
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	30
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	RY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	1
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	1
45	RZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
45	YZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
46	R0	80/85 (94%)	61 (76%)	14 (18%)	5 (6%)	2	27
46	Y0	80/85 (94%)	62 (78%)	12 (15%)	6 (8%)	2	21
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	9
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	9
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	6
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	6
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	32
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	32
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	26
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	26
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3
All	All	11378/12054 (94%)	7461 (66%)	2359 (21%)	1558 (14%)	0	6

5 of 1558 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	46
3	XC	159/188 (85%)	143 (90%)	16 (10%)	11	46
4	QD	180/181 (99%)	164 (91%)	16 (9%)	14	54
4	XD	180/181 (99%)	164 (91%)	16 (9%)	14	54
5	QE	116/123 (94%)	107 (92%)	9 (8%)	18	61
5	XE	116/123 (94%)	108 (93%)	8 (7%)	22	68
6	QF	90/90 (100%)	77 (86%)	13 (14%)	5	26
6	XF	90/90 (100%)	77 (86%)	13 (14%)	5	26
7	QG	126/127 (99%)	115 (91%)	11 (9%)	15	56
7	XG	126/127 (99%)	115 (91%)	11 (9%)	15	56
8	QH	119/119 (100%)	106 (89%)	13 (11%)	9	41
8	XH	119/119 (100%)	106 (89%)	13 (11%)	9	41
9	QI	98/99 (99%)	87 (89%)	11 (11%)	9	39
9	XI	98/99 (99%)	87 (89%)	11 (11%)	9	39
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	14	53
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	14	53
11	QK	90/99 (91%)	81 (90%)	9 (10%)	11	46
11	XK	90/99 (91%)	81 (90%)	9 (10%)	11	46
12	QL	104/109 (95%)	90 (86%)	14 (14%)	6	29
12	XL	104/109 (95%)	90 (86%)	14 (14%)	6	29
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	20
13	XM	97/101 (96%)	80 (82%)	17 (18%)	3	16
14	QN	49/50 (98%)	45 (92%)	4 (8%)	17	59
14	XN	49/50 (98%)	42 (86%)	7 (14%)	5	27
15	QO	79/80 (99%)	73 (92%)	6 (8%)	19	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	XO	79/80 (99%)	73 (92%)	6 (8%)	19	63
16	QP	72/74 (97%)	63 (88%)	9 (12%)	7	33
16	XP	72/74 (97%)	63 (88%)	9 (12%)	7	33
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	37
18	XR	61/77 (79%)	54 (88%)	7 (12%)	8	37
19	QS	73/80 (91%)	62 (85%)	11 (15%)	4	24
19	XS	73/80 (91%)	62 (85%)	11 (15%)	4	24
20	QT	76/82 (93%)	68 (90%)	8 (10%)	10	43
20	XT	76/82 (93%)	68 (90%)	8 (10%)	10	43
21	QU	20/22 (91%)	19 (95%)	1 (5%)	34	78
21	XU	20/22 (91%)	19 (95%)	1 (5%)	34	78
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%)	127 (77%)	38 (23%)	1	6
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	6
29	RF	161/166 (97%)	140 (87%)	21 (13%)	6	31
29	YF	161/166 (97%)	139 (86%)	22 (14%)	5	28
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	21
30	YG	155/156 (99%)	131 (84%)	24 (16%)	4	23
31	RH	142/148 (96%)	115 (81%)	27 (19%)	2	11
31	YH	142/148 (96%)	115 (81%)	27 (19%)	2	11
32	RI	122/124 (98%)	98 (80%)	24 (20%)	2	10
32	YI	122/124 (98%)	97 (80%)	25 (20%)	2	9
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	46
34	YO	100/100 (100%)	90 (90%)	10 (10%)	11	46
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	6
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	RQ	111/111 (100%)	92 (83%)	19 (17%)	3	17
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	3	17
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%)	97 (81%)	23 (19%)	2	11
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
45	RZ	152/179 (85%)	124 (82%)	28 (18%)	2	13
45	YZ	152/179 (85%)	124 (82%)	28 (18%)	2	13
46	R0	65/67 (97%)	55 (85%)	10 (15%)	4	23
46	Y0	65/67 (97%)	56 (86%)	9 (14%)	5	28
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	41
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	9	41
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	7
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	7
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	3
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	3
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	6
52	R6	48/52 (92%)	38 (79%)	10 (21%)	2	8
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	2	8
53	R7	42/42 (100%)	39 (93%)	3 (7%)	21	66
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	21	66
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	3
All	All	9614/9998 (96%)	8197 (85%)	1417 (15%)	4	25

5 of 1417 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	17	LYS
7	XG	148	ASN
45	YZ	132	ASN
50	R4	53	GLU
2	XB	94	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
47	R1	56	GLN
5	XE	78	HIS
43	YX	87	GLN
48	R2	9	GLN
2	XB	135	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	343 (22%)	51 (3%)
1	XA	1499/1522 (98%)	333 (22%)	55 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	6 (85%)	1 (14%)
23	XX	7/25 (28%)	2 (28%)	0
24	QY	13/18 (72%)	6 (46%)	1 (7%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2880/2916 (98%)	734 (25%)	76 (2%)
25	YA	2879/2916 (98%)	747 (25%)	75 (2%)
26	RB	119/122 (97%)	30 (25%)	2 (1%)
26	YB	119/122 (97%)	38 (31%)	1 (0%)
55	Z6	1/3 (33%)	0	0
55	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	2304 (25%)	265 (2%)

5 of 2304 RNA backbone outliers are listed below:

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

5 of 265 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2566	A
1	XA	481	G
25	YA	2198	A
25	RA	2689	U
1	XA	64	G

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$
24	1MG	QY	37	24	24,26,27	3.02	6 (25%)	34,39,42	3.83	12 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	1MG	XY	37	24	24,26,27	3.03	6 (25%)	34,39,42	3.38	12 (35%)
55	PPU	Z6	76	55,25	38,40,41	2.42	9 (23%)	54,57,60	2.60	14 (25%)
55	PPU	Z8	76	55,25	38,40,41	2.41	9 (23%)	54,57,60	2.60	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
24	1MG	QY	37	24	-	0/8/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/8/25/26	0/3/3/3
55	PPU	Z6	76	55,25	-	0/26/43/44	0/4/4/4
55	PPU	Z8	76	55,25	-	0/26/43/44	0/4/4/4

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Z6	76	PPU	O-C	9.16	1.41	1.23
55	Z8	76	PPU	O-C	9.15	1.41	1.23
24	QY	37	1MG	C4-N3	8.30	1.49	1.35
24	XY	37	1MG	C4-N3	8.15	1.49	1.35
24	XY	37	1MG	C2-N1	7.52	1.47	1.37

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	QY	37	1MG	C6-C5-N7	-16.25	133.37	134.24
24	XY	37	1MG	C6-N1-C2	12.33	124.09	120.71
24	QY	37	1MG	C6-N1-C2	11.68	123.91	120.71
24	XY	37	1MG	C6-C5-N7	-11.65	133.62	134.24
55	Z6	76	PPU	N3-C2-N1	-8.57	121.35	128.89

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 607 ligands modelled in this entry, 605 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	$\# Z > 2$
57	PAR	QA	1661	-	45,45,45	1.28	6 (13%)	67,67,67	1.37	7 (10%)
57	PAR	XA	1664	-	45,45,45	1.32	6 (13%)	67,67,67	1.32	6 (8%)

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
57	PAR	QA	1661	-	-	0/18/94/94	0/4/4/4
57	PAR	XA	1664	-	-	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)
57	XA	1664	PAR	C52-C42	3.13	1.58	1.52
57	QA	1661	PAR	C52-C42	3.08	1.58	1.52
57	XA	1664	PAR	C11-C21	2.91	1.58	1.52
57	QA	1661	PAR	O54-C14	2.89	1.49	1.41
57	QA	1661	PAR	C64-C54	2.73	1.58	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1661	PAR	O52-C13-C23	4.66	115.81	107.50
57	QA	1661	PAR	C14-O54-C54	4.24	121.94	113.73
57	XA	1664	PAR	O52-C13-C23	4.12	114.86	107.50
57	XA	1664	PAR	C14-O54-C54	4.09	121.65	113.73
57	XA	1664	PAR	O33-C14-C24	3.84	115.67	108.08

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	-0.11	35 (2%) 57 25	30, 83, 175, 356	0
1	XA	1501/1522 (98%)	-0.22	31 (2%) 60 27	30, 76, 171, 324	0
2	QB	237/256 (92%)	0.43	12 (5%) 27 10	56, 138, 222, 266	0
2	XB	237/256 (92%)	0.27	5 (2%) 60 27	55, 126, 194, 238	0
3	QC	205/239 (85%)	0.26	5 (2%) 56 24	54, 122, 199, 216	0
3	XC	205/239 (85%)	0.08	2 (0%) 79 44	39, 95, 158, 217	0
4	QD	208/209 (99%)	0.08	2 (0%) 79 44	44, 92, 154, 184	0
4	XD	208/209 (99%)	0.18	3 (1%) 72 35	39, 95, 161, 234	0
5	QE	151/162 (93%)	0.28	4 (2%) 53 22	29, 104, 175, 237	0
5	XE	151/162 (93%)	0.01	1 (0%) 84 52	34, 79, 149, 229	0
6	QF	101/101 (100%)	0.03	1 (0%) 79 44	44, 86, 125, 222	0
6	XF	101/101 (100%)	0.03	0 100 100	36, 86, 144, 209	0
7	QG	155/156 (99%)	0.19	7 (4%) 32 13	51, 106, 181, 215	0
7	XG	155/156 (99%)	0.12	3 (1%) 64 29	46, 103, 177, 230	0
8	QH	138/138 (100%)	0.07	0 100 100	48, 108, 167, 204	0
8	XH	138/138 (100%)	0.04	0 100 100	48, 96, 158, 208	0
9	QI	127/128 (99%)	0.35	2 (1%) 68 32	53, 124, 188, 214	0
9	XI	127/128 (99%)	0.31	1 (0%) 83 49	43, 116, 194, 219	0
10	QJ	99/105 (94%)	0.85	12 (12%) 5 3	67, 145, 212, 246	0
10	XJ	99/105 (94%)	0.54	7 (7%) 16 7	37, 119, 193, 210	0
11	QK	119/129 (92%)	0.36	5 (4%) 35 14	42, 92, 152, 199	0
11	XK	119/129 (92%)	0.21	2 (1%) 67 31	39, 89, 165, 204	0
12	QL	125/132 (94%)	0.31	5 (4%) 36 14	42, 84, 176, 269	0
12	XL	125/132 (94%)	0.05	2 (1%) 68 32	30, 66, 131, 242	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.35	5 (4%) 35 14	43, 124, 197, 254	0
13	XM	121/126 (96%)	0.18	6 (4%) 28 11	44, 98, 183, 264	0
14	QN	60/61 (98%)	0.74	3 (5%) 28 11	61, 128, 195, 227	0
14	XN	60/61 (98%)	0.07	0 100 100	47, 87, 134, 161	0
15	QO	88/89 (98%)	0.23	3 (3%) 43 18	42, 97, 165, 235	0
15	XO	88/89 (98%)	0.02	1 (1%) 77 41	39, 79, 130, 178	0
16	QP	84/88 (95%)	0.11	1 (1%) 75 39	41, 79, 136, 206	0
16	XP	84/88 (95%)	0.20	1 (1%) 75 39	54, 92, 151, 203	0
17	QQ	100/105 (95%)	0.19	2 (2%) 62 28	53, 102, 165, 210	0
17	XQ	100/105 (95%)	0.31	3 (3%) 48 20	38, 101, 159, 213	0
18	QR	70/88 (79%)	0.11	3 (4%) 34 13	34, 90, 156, 213	0
18	XR	70/88 (79%)	0.07	1 (1%) 72 35	30, 88, 138, 206	0
19	QS	84/93 (90%)	0.82	10 (11%) 5 3	87, 149, 204, 237	0
19	XS	84/93 (90%)	0.42	4 (4%) 29 12	55, 105, 176, 244	0
20	QT	99/106 (93%)	0.30	3 (3%) 48 20	48, 101, 192, 233	0
20	XT	99/106 (93%)	0.15	1 (1%) 79 44	50, 107, 163, 197	0
21	QU	25/27 (92%)	1.21	3 (12%) 5 3	41, 100, 139, 189	0
21	XU	25/27 (92%)	1.04	3 (12%) 5 3	52, 96, 135, 165	0
22	QV	77/77 (100%)	0.12	1 (1%) 74 37	40, 91, 151, 170	0
22	XV	77/77 (100%)	-0.05	1 (1%) 74 37	34, 77, 126, 180	0
23	QX	8/25 (32%)	0.54	0 100 100	61, 82, 137, 169	0
23	XX	8/25 (32%)	0.46	1 (12%) 5 3	39, 67, 104, 175	0
24	QY	14/18 (77%)	3.01	6 (42%) 1 1	93, 213, 294, 312	0
24	XY	14/18 (77%)	2.49	5 (35%) 1 1	69, 188, 276, 278	0
25	RA	2883/2916 (98%)	-0.15	138 (4%) 29 12	24, 57, 221, 389	0
25	YA	2882/2916 (98%)	-0.26	115 (3%) 36 14	17, 48, 215, 377	0
26	RB	120/122 (98%)	-0.15	0 100 100	52, 91, 141, 150	0
26	YB	120/122 (98%)	-0.33	0 100 100	44, 74, 109, 158	0
27	RD	272/276 (98%)	0.02	1 (0%) 90 68	19, 60, 98, 243	0
27	YD	272/276 (98%)	-0.08	1 (0%) 90 68	13, 50, 85, 221	0
28	RE	205/206 (99%)	0.02	3 (1%) 70 33	24, 78, 165, 260	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.06	3 (1%) 70 33	22, 76, 161, 238	0
29	RF	202/210 (96%)	0.09	1 (0%) 88 61	21, 82, 158, 250	0
29	YF	202/210 (96%)	-0.04	1 (0%) 88 61	13, 64, 130, 197	0
30	RG	181/182 (99%)	1.12	30 (16%) 2 2	58, 164, 258, 303	0
30	YG	181/182 (99%)	0.53	6 (3%) 44 18	59, 108, 186, 248	0
31	RH	170/180 (94%)	0.87	16 (9%) 9 5	78, 171, 239, 267	0
31	YH	170/180 (94%)	0.22	1 (0%) 86 56	39, 100, 156, 260	0
32	RI	146/148 (98%)	0.30	3 (2%) 60 27	56, 118, 204, 240	0
32	YI	146/148 (98%)	0.11	1 (0%) 84 52	40, 104, 169, 214	0
33	RN	138/140 (98%)	0.08	1 (0%) 84 52	32, 84, 153, 194	0
33	YN	138/140 (98%)	-0.06	1 (0%) 84 52	31, 78, 128, 166	0
34	RO	122/122 (100%)	-0.05	0 100 100	24, 71, 133, 170	0
34	YO	122/122 (100%)	-0.02	0 100 100	23, 66, 114, 153	0
35	RP	150/150 (100%)	0.22	5 (3%) 44 18	15, 79, 185, 232	0
35	YP	150/150 (100%)	0.10	2 (1%) 74 37	5, 68, 135, 230	0
36	RQ	141/141 (100%)	0.19	0 100 100	38, 85, 149, 219	0
36	YQ	141/141 (100%)	-0.02	0 100 100	27, 66, 118, 196	0
37	RR	118/118 (100%)	-0.08	0 100 100	28, 68, 107, 171	0
37	YR	118/118 (100%)	-0.04	0 100 100	20, 64, 114, 153	0
38	RS	111/112 (99%)	0.10	0 100 100	40, 90, 146, 203	0
38	YS	111/112 (99%)	-0.05	0 100 100	36, 77, 134, 207	0
39	RT	137/146 (93%)	0.15	1 (0%) 84 52	39, 90, 189, 221	0
39	YT	137/146 (93%)	0.11	1 (0%) 84 52	41, 78, 176, 220	0
40	RU	117/118 (99%)	0.12	2 (1%) 67 31	27, 73, 155, 249	0
40	YU	117/118 (99%)	-0.03	2 (1%) 67 31	20, 59, 129, 212	0
41	RV	101/101 (100%)	0.13	2 (1%) 62 28	28, 88, 167, 278	0
41	YV	101/101 (100%)	0.06	1 (0%) 79 44	25, 82, 143, 255	0
42	RW	113/113 (100%)	0.02	2 (1%) 65 30	28, 63, 127, 241	0
42	YW	113/113 (100%)	-0.03	0 100 100	22, 60, 109, 204	0
43	RX	92/96 (95%)	0.00	0 100 100	31, 65, 108, 137	0
43	YX	92/96 (95%)	0.03	0 100 100	21, 50, 92, 134	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.64	13 (12%) 4 3	46, 106, 214, 270	0
44	YY	102/110 (92%)	0.17	2 (1%) 62 28	25, 85, 144, 243	0
45	RZ	172/206 (83%)	0.76	22 (12%) 4 3	62, 130, 264, 332	0
45	YZ	172/206 (83%)	0.52	13 (7%) 14 6	33, 111, 243, 361	0
46	R0	82/85 (96%)	0.13	0 100 100	35, 72, 105, 143	0
46	Y0	82/85 (96%)	-0.05	0 100 100	28, 63, 99, 116	0
47	R1	97/98 (98%)	0.33	2 (2%) 60 27	24, 67, 167, 259	0
47	Y1	97/98 (98%)	0.18	1 (1%) 79 44	20, 65, 161, 211	0
48	R2	69/72 (95%)	0.03	0 100 100	34, 82, 149, 217	0
48	Y2	69/72 (95%)	0.04	1 (1%) 72 35	22, 72, 138, 203	0
49	R3	59/60 (98%)	0.19	1 (1%) 67 31	35, 81, 147, 173	0
49	Y3	59/60 (98%)	0.11	2 (3%) 43 18	33, 67, 108, 178	0
50	R4	71/71 (100%)	1.53	19 (26%) 1 1	102, 207, 283, 352	0
50	Y4	71/71 (100%)	0.85	8 (11%) 6 4	88, 160, 251, 277	0
51	R5	59/60 (98%)	0.48	5 (8%) 11 5	12, 64, 224, 264	0
51	Y5	59/60 (98%)	0.01	0 100 100	20, 71, 220, 229	0
52	R6	49/54 (90%)	2.64	24 (48%) 1 1	119, 196, 290, 297	0
52	Y6	49/54 (90%)	2.10	21 (42%) 1 1	120, 182, 235, 265	0
53	R7	49/49 (100%)	-0.06	0 100 100	19, 44, 100, 216	0
53	Y7	49/49 (100%)	0.03	3 (6%) 21 8	15, 37, 100, 216	0
54	R8	64/65 (98%)	0.20	2 (3%) 47 20	18, 62, 156, 228	0
54	Y8	64/65 (98%)	0.11	0 100 100	20, 61, 116, 173	0
55	Z6	3/3 (100%)	2.84	1 (33%) 1 1	49, 49, 51, 53	0
55	Z8	3/3 (100%)	2.14	1 (33%) 1 1	36, 36, 37, 41	0
All	All	20780/21420 (97%)	0.05	695 (3%) 44 18	5, 78, 195, 389	0

The worst 5 of 695 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	2173	A	16.7
25	YA	2174	C	15.5
24	QY	32	U	14.1
25	YA	2175	C	13.3
52	R6	43	CYS	13.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	PPU	Z6	76	37/38	0.29	-	53,53,53,53	0
24	1MG	QY	37	24/25	0.23	-	124,124,124,124	0
24	1MG	XY	37	24/25	0.14	-	89,89,89,89	0
55	PPU	Z8	76	37/38	0.26	-	40,40,40,40	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	YA	3041	1/1	0.27	-	6,6,6,6	0
56	MG	XA	1635	1/1	0.10	-	36,36,36,36	0
56	MG	YA	3040	1/1	0.10	-	1,1,1,1	0
56	MG	XA	1647	1/1	0.57	-	58,58,58,58	0
56	MG	YA	3158	1/1	0.12	-	20,20,20,20	0
56	MG	QA	1626	1/1	0.38	-	77,77,77,77	0
56	MG	RA	3160	1/1	0.23	-	25,25,25,25	0
56	MG	YA	3164	1/1	0.28	-	25,25,25,25	0
56	MG	YA	3037	1/1	0.20	-	3,3,3,3	0
56	MG	XA	1614	1/1	0.11	-	14,14,14,14	0
56	MG	RA	3107	1/1	0.30	-	21,21,21,21	0
56	MG	RA	3030	1/1	0.29	-	15,15,15,15	0
56	MG	YA	3137	1/1	0.07	-	15,15,15,15	0
56	MG	YA	3207	1/1	0.28	-	66,66,66,66	0
56	MG	RA	3027	1/1	0.73	-	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3060	1/1	0.21	-	25,25,25,25	0
56	MG	YA	3088	1/1	0.25	-	20,20,20,20	0
56	MG	YA	3193	1/1	0.20	-	39,39,39,39	0
56	MG	YA	3161	1/1	0.07	-	30,30,30,30	0
56	MG	YA	3027	1/1	0.12	-	5,5,5,5	0
56	MG	RA	3123	1/1	0.14	-	32,32,32,32	0
56	MG	QX	101	1/1	0.09	-	24,24,24,24	0
56	MG	YA	3070	1/1	0.17	-	22,22,22,22	0
56	MG	YA	3124	1/1	0.20	-	22,22,22,22	0
56	MG	YA	3006	1/1	0.19	-	0,0,0,0	0
56	MG	RA	3151	1/1	0.21	-	23,23,23,23	0
56	MG	RA	3131	1/1	0.22	-	77,77,77,77	0
56	MG	YB	202	1/1	0.13	-	42,42,42,42	0
56	MG	XA	1623	1/1	0.33	-	31,31,31,31	0
56	MG	RA	3078	1/1	0.17	-	15,15,15,15	0
56	MG	YA	3162	1/1	0.23	-	34,34,34,34	0
56	MG	RA	3044	1/1	0.29	-	21,21,21,21	0
56	MG	RA	3084	1/1	0.30	-	17,17,17,17	0
56	MG	YA	3007	1/1	0.14	-	6,6,6,6	0
56	MG	YA	3145	1/1	0.14	-	42,42,42,42	0
56	MG	RA	3176	1/1	0.55	-	71,71,71,71	0
56	MG	RA	3165	1/1	0.09	-	5,5,5,5	0
56	MG	YA	3238	1/1	0.19	-	34,34,34,34	0
56	MG	XA	1607	1/1	0.11	-	5,5,5,5	0
56	MG	YA	3123	1/1	0.11	-	15,15,15,15	0
56	MG	YA	3220	1/1	0.15	-	18,18,18,18	0
56	MG	YA	3205	1/1	0.12	-	28,28,28,28	0
56	MG	RA	3099	1/1	0.12	-	21,21,21,21	0
56	MG	YA	3016	1/1	0.15	-	19,19,19,19	0
56	MG	RA	3145	1/1	0.19	-	37,37,37,37	0
56	MG	YA	3011	1/1	0.30	-	13,13,13,13	0
56	MG	YA	3206	1/1	0.14	-	24,24,24,24	0
56	MG	YA	3103	1/1	0.08	-	12,12,12,12	0
56	MG	YA	3224	1/1	0.22	-	18,18,18,18	0
56	MG	RA	3016	1/1	0.23	-	2,2,2,2	0
56	MG	QA	1601	1/1	0.20	-	27,27,27,27	0
56	MG	XA	1662	1/1	0.21	-	27,27,27,27	0
56	MG	QA	1630	1/1	0.14	-	66,66,66,66	0
56	MG	RA	3055	1/1	0.14	-	12,12,12,12	0
56	MG	RA	3036	1/1	0.31	-	10,10,10,10	0
56	MG	YA	3021	1/1	0.21	-	12,12,12,12	0
56	MG	RA	3057	1/1	0.05	-	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3059	1/1	0.29	-	21,21,21,21	0
56	MG	YA	3076	1/1	0.37	-	7,7,7,7	0
56	MG	RA	3031	1/1	0.31	-	26,26,26,26	0
56	MG	QA	1614	1/1	0.16	-	38,38,38,38	0
56	MG	RA	3134	1/1	0.19	-	18,18,18,18	0
56	MG	XA	1648	1/1	0.33	-	25,25,25,25	0
56	MG	QA	1651	1/1	0.23	-	70,70,70,70	0
56	MG	YA	3064	1/1	0.13	-	23,23,23,23	0
56	MG	YA	3156	1/1	0.18	-	33,33,33,33	0
56	MG	YA	3004	1/1	0.21	-	13,13,13,13	0
56	MG	YA	3098	1/1	0.14	-	49,49,49,49	0
56	MG	YA	3176	1/1	0.11	-	54,54,54,54	0
56	MG	YA	3117	1/1	0.34	-	60,60,60,60	0
56	MG	XA	1654	1/1	0.10	-	50,50,50,50	0
56	MG	YA	3010	1/1	0.14	-	3,3,3,3	0
56	MG	RA	3038	1/1	0.18	-	14,14,14,14	0
56	MG	YA	3147	1/1	0.09	-	11,11,11,11	0
56	MG	XA	1636	1/1	0.20	-	58,58,58,58	0
56	MG	RA	3047	1/1	0.20	-	7,7,7,7	0
56	MG	YA	3108	1/1	0.14	-	5,5,5,5	0
56	MG	QA	1627	1/1	0.36	-	57,57,57,57	0
58	ZN	XN	101	1/1	0.11	-	107,107,107,107	0
56	MG	YA	3150	1/1	0.16	-	54,54,54,54	0
56	MG	YA	3171	1/1	0.28	-	72,72,72,72	0
56	MG	YA	3175	1/1	0.09	-	12,12,12,12	0
56	MG	RA	3002	1/1	0.28	-	8,8,8,8	0
56	MG	YA	3172	1/1	0.16	-	55,55,55,55	0
56	MG	XA	1606	1/1	0.24	-	17,17,17,17	0
56	MG	YX	101	1/1	0.08	-	28,28,28,28	0
56	MG	YA	3104	1/1	0.28	-	6,6,6,6	0
56	MG	RA	3140	1/1	0.18	-	45,45,45,45	0
56	MG	YA	3215	1/1	0.15	-	51,51,51,51	0
56	MG	QA	1607	1/1	0.16	-	22,22,22,22	0
56	MG	RA	3124	1/1	0.27	-	21,21,21,21	0
56	MG	QA	1640	1/1	0.18	-	54,54,54,54	0
56	MG	Y5	101	1/1	0.19	-	25,25,25,25	0
56	MG	QA	1636	1/1	0.07	-	15,15,15,15	0
56	MG	RP	201	1/1	0.31	-	37,37,37,37	0
56	MG	YA	3242	1/1	0.30	-	34,34,34,34	0
56	MG	RA	3132	1/1	0.15	-	12,12,12,12	0
56	MG	YA	3058	1/1	0.32	-	16,16,16,16	0
56	MG	RA	3074	1/1	0.27	-	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3164	1/1	0.24	-	52,52,52,52	0
56	MG	RA	3017	1/1	0.16	-	13,13,13,13	0
56	MG	YA	3126	1/1	0.16	-	27,27,27,27	0
56	MG	RA	3081	1/1	0.40	-	28,28,28,28	0
56	MG	YA	3179	1/1	0.37	-	31,31,31,31	0
56	MG	XA	1651	1/1	0.12	-	18,18,18,18	0
56	MG	RA	3152	1/1	0.20	-	26,26,26,26	0
56	MG	YA	3198	1/1	0.39	-	32,32,32,32	0
56	MG	QH	201	1/1	0.30	-	124,124,124,124	0
56	MG	YA	3203	1/1	0.11	-	24,24,24,24	0
56	MG	YA	3062	1/1	0.12	-	6,6,6,6	0
56	MG	YA	3034	1/1	0.22	-	3,3,3,3	0
56	MG	RA	3061	1/1	0.19	-	28,28,28,28	0
56	MG	RA	3042	1/1	0.18	-	11,11,11,11	0
56	MG	RA	3088	1/1	0.14	-	24,24,24,24	0
56	MG	YA	3029	1/1	0.36	-	17,17,17,17	0
56	MG	R5	101	1/1	0.16	-	27,27,27,27	0
56	MG	RA	3167	1/1	0.17	-	35,35,35,35	0
56	MG	QA	1631	1/1	0.13	-	55,55,55,55	0
56	MG	YA	3148	1/1	0.11	-	25,25,25,25	0
56	MG	XA	1618	1/1	0.16	-	24,24,24,24	0
56	MG	XA	1611	1/1	0.16	-	29,29,29,29	0
56	MG	RA	3101	1/1	0.16	-	50,50,50,50	0
56	MG	YA	3199	1/1	0.25	-	42,42,42,42	0
56	MG	YA	3113	1/1	0.19	-	21,21,21,21	0
56	MG	RA	3066	1/1	0.23	-	12,12,12,12	0
56	MG	RA	3019	1/1	0.12	-	10,10,10,10	0
56	MG	YA	3114	1/1	0.28	-	6,6,6,6	0
56	MG	YA	3186	1/1	0.30	-	50,50,50,50	0
56	MG	RA	3095	1/1	0.14	-	31,31,31,31	0
56	MG	RA	3122	1/1	0.24	-	70,70,70,70	0
56	MG	YA	3055	1/1	0.23	-	16,16,16,16	0
56	MG	YA	3192	1/1	0.27	-	40,40,40,40	0
56	MG	XA	1620	1/1	0.10	-	55,55,55,55	0
56	MG	RB	201	1/1	0.04	-	13,13,13,13	0
56	MG	RA	3192	1/1	0.25	-	56,56,56,56	0
56	MG	YA	3102	1/1	0.21	-	5,5,5,5	0
56	MG	YA	3013	1/1	0.28	-	3,3,3,3	0
56	MG	XA	1643	1/1	0.08	-	47,47,47,47	0
56	MG	YA	3173	1/1	0.23	-	43,43,43,43	0
56	MG	RA	3069	1/1	0.27	-	43,43,43,43	0
56	MG	YA	3023	1/1	0.20	-	4,4,4,4	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3200	1/1	0.09	-	15,15,15,15	0
56	MG	XA	1645	1/1	0.20	-	31,31,31,31	0
56	MG	RA	3178	1/1	0.19	-	62,62,62,62	0
56	MG	RA	3146	1/1	0.18	-	44,44,44,44	0
56	MG	RA	3183	1/1	0.41	-	49,49,49,49	0
56	MG	RA	3186	1/1	0.17	-	90,90,90,90	0
56	MG	QA	1616	1/1	0.10	-	42,42,42,42	0
56	MG	XA	1657	1/1	0.19	-	28,28,28,28	0
56	MG	QA	1605	1/1	0.17	-	51,51,51,51	0
56	MG	YA	3144	1/1	0.17	-	13,13,13,13	0
56	MG	YA	3154	1/1	0.25	-	15,15,15,15	0
56	MG	YA	3047	1/1	0.23	-	6,6,6,6	0
56	MG	YA	3129	1/1	0.07	-	22,22,22,22	0
56	MG	RA	3045	1/1	0.29	-	12,12,12,12	0
56	MG	YA	3049	1/1	0.28	-	15,15,15,15	0
56	MG	RA	3120	1/1	0.10	-	10,10,10,10	0
56	MG	YA	3073	1/1	0.31	-	24,24,24,24	0
56	MG	XA	1663	1/1	0.30	-	85,85,85,85	0
56	MG	RA	3039	1/1	0.29	-	18,18,18,18	0
56	MG	QA	1653	1/1	0.22	-	39,39,39,39	0
56	MG	YA	3209	1/1	0.14	-	41,41,41,41	0
56	MG	XA	1630	1/1	0.14	-	39,39,39,39	0
56	MG	YA	3188	1/1	0.20	-	38,38,38,38	0
56	MG	YA	3139	1/1	0.24	-	32,32,32,32	0
56	MG	YA	3181	1/1	0.28	-	51,51,51,51	0
56	MG	YA	3096	1/1	0.22	-	15,15,15,15	0
56	MG	QV	102	1/1	0.15	-	8,8,8,8	0
56	MG	QA	1602	1/1	0.25	-	19,19,19,19	0
56	MG	XV	102	1/1	0.10	-	22,22,22,22	0
56	MG	RA	3205	1/1	0.25	-	54,54,54,54	0
56	MG	YA	3204	1/1	0.16	-	43,43,43,43	0
56	MG	RA	3210	1/1	0.33	-	38,38,38,38	0
56	MG	RA	3115	1/1	0.22	-	59,59,59,59	0
56	MG	QA	1648	1/1	0.03	-	100,100,100,100	0
56	MG	XA	1626	1/1	0.32	-	27,27,27,27	0
56	MG	RA	3077	1/1	0.31	-	14,14,14,14	0
56	MG	YA	3127	1/1	0.48	-	44,44,44,44	0
56	MG	RA	3194	1/1	0.14	-	14,14,14,14	0
56	MG	YA	3054	1/1	0.13	-	14,14,14,14	0
56	MG	YA	3130	1/1	0.19	-	16,16,16,16	0
56	MG	YA	3185	1/1	0.10	-	10,10,10,10	0
56	MG	YA	3153	1/1	0.21	-	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3118	1/1	0.20	-	12,12,12,12	0
56	MG	RA	3085	1/1	0.07	-	15,15,15,15	0
56	MG	YA	3043	1/1	0.35	-	9,9,9,9	0
56	MG	YA	3045	1/1	0.36	-	22,22,22,22	0
56	MG	YA	3222	1/1	0.05	-	9,9,9,9	0
56	MG	RA	3168	1/1	0.09	-	31,31,31,31	0
56	MG	YA	3002	1/1	0.36	-	15,15,15,15	0
56	MG	RA	3073	1/1	0.40	-	5,5,5,5	0
56	MG	YA	3152	1/1	0.37	-	38,38,38,38	0
56	MG	RA	3135	1/1	0.22	-	32,32,32,32	0
56	MG	RA	3118	1/1	0.14	-	14,14,14,14	0
56	MG	YB	201	1/1	0.15	-	21,21,21,21	0
56	MG	YA	3227	1/1	0.13	-	22,22,22,22	0
56	MG	YA	3014	1/1	0.39	-	12,12,12,12	0
56	MG	RA	3094	1/1	0.13	-	19,19,19,19	0
56	MG	YA	3170	1/1	0.40	-	10,10,10,10	0
56	MG	XA	1621	1/1	0.15	-	22,22,22,22	0
56	MG	RA	3142	1/1	0.08	-	15,15,15,15	0
56	MG	YA	3187	1/1	0.25	-	58,58,58,58	0
56	MG	YA	3149	1/1	0.26	-	26,26,26,26	0
56	MG	QA	1618	1/1	0.14	-	41,41,41,41	0
56	MG	RA	3201	1/1	0.36	-	22,22,22,22	0
56	MG	QA	1641	1/1	0.28	-	25,25,25,25	0
56	MG	QA	1646	1/1	0.18	-	14,14,14,14	0
56	MG	QA	1656	1/1	0.19	-	53,53,53,53	0
56	MG	YA	3169	1/1	0.19	-	84,84,84,84	0
56	MG	RA	3125	1/1	0.28	-	24,24,24,24	0
56	MG	RA	3053	1/1	0.20	-	5,5,5,5	0
56	MG	RA	3207	1/1	0.13	-	51,51,51,51	0
56	MG	YA	3044	1/1	0.24	-	9,9,9,9	0
56	MG	RA	3161	1/1	0.13	-	32,32,32,32	0
56	MG	RA	3049	1/1	0.15	-	10,10,10,10	0
56	MG	RA	3028	1/1	0.16	-	12,12,12,12	0
56	MG	RA	3097	1/1	0.20	-	24,24,24,24	0
56	MG	RA	3171	1/1	0.26	-	49,49,49,49	0
56	MG	RA	3102	1/1	0.27	-	32,32,32,32	0
56	MG	YA	3106	1/1	0.29	-	32,32,32,32	0
56	MG	YA	3202	1/1	0.07	-	21,21,21,21	0
56	MG	YE	302	1/1	0.19	-	13,13,13,13	0
56	MG	YA	3060	1/1	0.21	-	13,13,13,13	0
56	MG	YA	3116	1/1	0.20	-	28,28,28,28	0
56	MG	YA	3090	1/1	0.37	-	11,11,11,11	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1660	1/1	0.18	-	45,45,45,45	0
56	MG	XA	1650	1/1	0.25	-	39,39,39,39	0
56	MG	XA	1642	1/1	0.17	-	49,49,49,49	0
56	MG	RA	3015	1/1	0.15	-	15,15,15,15	0
56	MG	YA	3033	1/1	0.23	-	6,6,6,6	0
56	MG	RA	3065	1/1	0.28	-	21,21,21,21	0
56	MG	RA	3100	1/1	0.14	-	44,44,44,44	0
56	MG	RA	3117	1/1	0.26	-	42,42,42,42	0
56	MG	QA	1649	1/1	0.36	-	45,45,45,45	0
56	MG	YA	3191	1/1	0.19	-	24,24,24,24	0
56	MG	RA	3153	1/1	0.15	-	36,36,36,36	0
56	MG	YA	3217	1/1	0.09	-	35,35,35,35	0
56	MG	RA	3035	1/1	0.09	-	21,21,21,21	0
56	MG	YA	3063	1/1	0.11	-	6,6,6,6	0
56	MG	RA	3185	1/1	0.27	-	44,44,44,44	0
56	MG	YA	3036	1/1	0.18	-	3,3,3,3	0
56	MG	QA	1625	1/1	0.14	-	66,66,66,66	0
56	MG	YA	3136	1/1	0.14	-	4,4,4,4	0
56	MG	YA	3026	1/1	0.38	-	9,9,9,9	0
56	MG	RA	3144	1/1	0.18	-	36,36,36,36	0
56	MG	RA	3082	1/1	0.14	-	13,13,13,13	0
56	MG	RE	301	1/1	0.10	-	22,22,22,22	0
56	MG	YA	3066	1/1	0.44	-	18,18,18,18	0
56	MG	RA	3048	1/1	0.25	-	13,13,13,13	0
56	MG	YA	3125	1/1	0.14	-	18,18,18,18	0
56	MG	RA	3138	1/1	0.14	-	21,21,21,21	0
56	MG	YA	3239	1/1	0.46	-	48,48,48,48	0
56	MG	RA	3143	1/1	0.47	-	16,16,16,16	0
56	MG	QA	1658	1/1	0.09	-	68,68,68,68	0
56	MG	RA	3087	1/1	0.12	-	9,9,9,9	0
56	MG	YA	3074	1/1	0.19	-	28,28,28,28	0
56	MG	RA	3010	1/1	0.33	-	4,4,4,4	0
56	MG	YA	3146	1/1	0.09	-	50,50,50,50	0
56	MG	YA	3095	1/1	0.24	-	5,5,5,5	0
56	MG	YA	3080	1/1	0.26	-	3,3,3,3	0
56	MG	RA	3091	1/1	0.14	-	21,21,21,21	0
56	MG	XA	1624	1/1	0.14	-	35,35,35,35	0
56	MG	XA	1612	1/1	0.28	-	21,21,21,21	0
56	MG	RA	3156	1/1	0.18	-	22,22,22,22	0
56	MG	YA	3008	1/1	0.27	-	17,17,17,17	0
56	MG	QA	1617	1/1	0.22	-	41,41,41,41	0
56	MG	YA	3085	1/1	0.16	-	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1638	1/1	0.38	-	53,53,53,53	0
56	MG	RA	3034	1/1	0.33	-	16,16,16,16	0
56	MG	YA	3142	1/1	0.15	-	30,30,30,30	0
56	MG	XA	1633	1/1	0.14	-	32,32,32,32	0
56	MG	RA	3070	1/1	0.29	-	37,37,37,37	0
56	MG	RA	3013	1/1	0.20	-	10,10,10,10	0
56	MG	YA	3232	1/1	0.28	-	43,43,43,43	0
56	MG	RA	3148	1/1	0.18	-	21,21,21,21	0
56	MG	XA	1604	1/1	0.04	-	31,31,31,31	0
56	MG	QA	1647	1/1	0.10	-	41,41,41,41	0
56	MG	YA	3109	1/1	0.27	-	25,25,25,25	0
56	MG	YA	3223	1/1	0.08	-	30,30,30,30	0
58	ZN	QN	101	1/1	0.14	-	155,155,155,155	0
56	MG	RA	3001	1/1	0.15	-	36,36,36,36	0
56	MG	YA	3229	1/1	0.10	-	52,52,52,52	0
56	MG	YA	3028	1/1	0.18	-	23,23,23,23	0
56	MG	YA	3018	1/1	0.35	-	24,24,24,24	0
56	MG	YA	3053	1/1	0.20	-	4,4,4,4	0
56	MG	RA	3141	1/1	0.27	-	43,43,43,43	0
56	MG	YA	3020	1/1	0.34	-	8,8,8,8	0
56	MG	RA	3058	1/1	0.22	-	13,13,13,13	0
56	MG	YA	3052	1/1	0.23	-	17,17,17,17	0
56	MG	YA	3182	1/1	0.27	-	30,30,30,30	0
56	MG	YA	3210	1/1	0.11	-	35,35,35,35	0
56	MG	RA	3158	1/1	0.16	-	14,14,14,14	0
56	MG	YA	3219	1/1	0.23	-	29,29,29,29	0
56	MG	XA	1641	1/1	0.12	-	24,24,24,24	0
56	MG	YA	3235	1/1	0.12	-	26,26,26,26	0
56	MG	YA	3084	1/1	0.20	-	23,23,23,23	0
56	MG	QA	1644	1/1	0.18	-	23,23,23,23	0
56	MG	RA	3177	1/1	0.14	-	59,59,59,59	0
56	MG	YA	3093	1/1	0.11	-	18,18,18,18	0
56	MG	RA	3075	1/1	0.34	-	4,4,4,4	0
56	MG	YA	3159	1/1	0.34	-	43,43,43,43	0
56	MG	XA	1629	1/1	0.20	-	49,49,49,49	0
56	MG	RA	3012	1/1	0.33	-	26,26,26,26	0
56	MG	RA	3150	1/1	0.19	-	26,26,26,26	0
56	MG	RA	3089	1/1	0.27	-	26,26,26,26	0
56	MG	YA	3012	1/1	1.48	-	80,80,80,80	0
56	MG	RA	3200	1/1	0.28	-	58,58,58,58	0
56	MG	YA	3212	1/1	0.09	-	21,21,21,21	0
56	MG	RA	3209	1/1	0.26	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XV	101	1/1	0.18	-	14,14,14,14	0
56	MG	YA	3105	1/1	0.25	-	16,16,16,16	0
56	MG	QA	1650	1/1	0.18	-	36,36,36,36	0
56	MG	RA	3067	1/1	0.06	-	7,7,7,7	0
56	MG	RA	3173	1/1	0.18	-	71,71,71,71	0
56	MG	RA	3127	1/1	0.22	-	47,47,47,47	0
56	MG	RA	3184	1/1	0.29	-	33,33,33,33	0
56	MG	YA	3177	1/1	0.14	-	35,35,35,35	0
56	MG	YA	3030	1/1	0.28	-	24,24,24,24	0
56	MG	QA	1629	1/1	0.25	-	68,68,68,68	0
56	MG	YA	3138	1/1	0.15	-	15,15,15,15	0
56	MG	YA	3240	1/1	0.15	-	45,45,45,45	0
56	MG	YA	3163	1/1	0.19	-	40,40,40,40	0
56	MG	QA	1637	1/1	0.18	-	49,49,49,49	0
56	MG	RA	3174	1/1	0.27	-	68,68,68,68	0
56	MG	QA	1612	1/1	0.07	-	37,37,37,37	0
56	MG	RA	3193	1/1	0.16	-	49,49,49,49	0
56	MG	YA	3087	1/1	0.22	-	7,7,7,7	0
56	MG	QA	1657	1/1	0.09	-	76,76,76,76	0
56	MG	YA	3233	1/1	0.18	-	44,44,44,44	0
56	MG	RA	3052	1/1	0.45	-	24,24,24,24	0
56	MG	YA	3178	1/1	0.37	-	68,68,68,68	0
56	MG	RE	302	1/1	0.29	-	22,22,22,22	0
56	MG	YA	3131	1/1	0.14	-	20,20,20,20	0
56	MG	RA	3189	1/1	0.19	-	34,34,34,34	0
56	MG	RA	3163	1/1	0.18	-	38,38,38,38	0
56	MG	XA	1625	1/1	0.19	-	20,20,20,20	0
56	MG	RA	3050	1/1	0.13	-	0,0,0,0	0
56	MG	YA	3197	1/1	0.11	-	33,33,33,33	0
56	MG	RA	3112	1/1	0.30	-	50,50,50,50	0
56	MG	RA	3086	1/1	0.22	-	33,33,33,33	0
56	MG	YA	3236	1/1	0.30	-	57,57,57,57	0
56	MG	XA	1603	1/1	0.12	-	23,23,23,23	0
56	MG	RA	3033	1/1	0.18	-	62,62,62,62	0
56	MG	YA	3155	1/1	0.20	-	22,22,22,22	0
56	MG	YA	3234	1/1	0.24	-	34,34,34,34	0
56	MG	XA	1628	1/1	0.22	-	24,24,24,24	0
56	MG	YA	3165	1/1	0.22	-	42,42,42,42	0
56	MG	YA	3038	1/1	0.13	-	12,12,12,12	0
56	MG	YA	3157	1/1	0.22	-	29,29,29,29	0
56	MG	XA	1601	1/1	0.15	-	15,15,15,15	0
56	MG	YA	3214	1/1	0.18	-	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	PAR	XA	1664	42/42	0.27	-	57,57,57,57	0
56	MG	QA	1643	1/1	0.22	-	24,24,24,24	0
56	MG	YA	3042	1/1	0.29	-	28,28,28,28	0
56	MG	YA	3112	1/1	0.10	-	41,41,41,41	0
56	MG	RA	3187	1/1	0.39	-	68,68,68,68	0
56	MG	YA	3069	1/1	0.17	-	16,16,16,16	0
56	MG	QA	1603	1/1	0.09	-	28,28,28,28	0
56	MG	XM	201	1/1	0.13	-	28,28,28,28	0
56	MG	RA	3062	1/1	0.33	-	21,21,21,21	0
56	MG	QA	1619	1/1	0.31	-	48,48,48,48	0
56	MG	RA	3121	1/1	0.56	-	35,35,35,35	0
56	MG	XA	1652	1/1	0.14	-	64,64,64,64	0
56	MG	RA	3190	1/1	0.15	-	50,50,50,50	0
56	MG	YA	3059	1/1	0.15	-	74,74,74,74	0
56	MG	RA	3179	1/1	0.23	-	22,22,22,22	0
56	MG	YA	3071	1/1	0.12	-	18,18,18,18	0
56	MG	RA	3139	1/1	0.13	-	31,31,31,31	0
56	MG	YA	3231	1/1	0.23	-	32,32,32,32	0
56	MG	RA	3196	1/1	0.20	-	53,53,53,53	0
56	MG	YA	3166	1/1	0.31	-	51,51,51,51	0
56	MG	RA	3072	1/1	0.29	-	24,24,24,24	0
56	MG	YA	3022	1/1	0.21	-	6,6,6,6	0
56	MG	RA	3157	1/1	0.42	-	20,20,20,20	0
56	MG	YA	3196	1/1	0.11	-	33,33,33,33	0
56	MG	YA	3024	1/1	0.11	-	10,10,10,10	0
56	MG	QM	201	1/1	0.18	-	34,34,34,34	0
56	MG	XA	1634	1/1	0.16	-	28,28,28,28	0
56	MG	YA	3061	1/1	0.11	-	35,35,35,35	0
56	MG	QA	1609	1/1	0.23	-	34,34,34,34	0
56	MG	RA	3009	1/1	0.16	-	21,21,21,21	0
56	MG	RA	3032	1/1	0.17	-	17,17,17,17	0
56	MG	XA	1631	1/1	0.28	-	45,45,45,45	0
56	MG	QA	1611	1/1	0.08	-	32,32,32,32	0
56	MG	RA	3147	1/1	0.32	-	49,49,49,49	0
56	MG	RA	3007	1/1	0.14	-	8,8,8,8	0
56	MG	RA	3202	1/1	0.25	-	84,84,84,84	0
56	MG	YA	3003	1/1	0.14	-	13,13,13,13	0
56	MG	YA	3237	1/1	0.08	-	15,15,15,15	0
56	MG	RA	3119	1/1	0.31	-	34,34,34,34	0
56	MG	XA	1639	1/1	0.18	-	32,32,32,32	0
56	MG	YA	3213	1/1	0.12	-	41,41,41,41	0
56	MG	QA	1620	1/1	0.51	-	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1627	1/1	0.29	-	31,31,31,31	0
56	MG	RA	3024	1/1	0.44	-	4,4,4,4	0
56	MG	RA	3096	1/1	0.16	-	8,8,8,8	0
56	MG	XA	1646	1/1	0.18	-	23,23,23,23	0
56	MG	YA	3019	1/1	0.41	-	21,21,21,21	0
56	MG	XA	1658	1/1	0.24	-	50,50,50,50	0
56	MG	YA	3135	1/1	0.05	-	33,33,33,33	0
56	MG	RA	3056	1/1	0.16	-	26,26,26,26	0
56	MG	YA	3119	1/1	0.36	-	35,35,35,35	0
56	MG	YA	3120	1/1	0.24	-	36,36,36,36	0
56	MG	QA	1604	1/1	0.09	-	33,33,33,33	0
56	MG	YA	3035	1/1	0.22	-	10,10,10,10	0
56	MG	YA	3075	1/1	0.09	-	14,14,14,14	0
56	MG	YA	3160	1/1	0.19	-	37,37,37,37	0
56	MG	RA	3029	1/1	0.17	-	2,2,2,2	0
56	MG	YA	3128	1/1	0.25	-	23,23,23,23	0
56	MG	YA	3015	1/1	0.42	-	10,10,10,10	0
56	MG	YA	3009	1/1	0.52	-	27,27,27,27	0
56	MG	YA	3046	1/1	0.08	-	4,4,4,4	0
56	MG	RA	3136	1/1	0.25	-	49,49,49,49	0
56	MG	YA	3051	1/1	0.23	-	4,4,4,4	0
56	MG	RA	3128	1/1	0.24	-	27,27,27,27	0
56	MG	RA	3106	1/1	0.50	-	24,24,24,24	0
56	MG	RA	3191	1/1	0.15	-	62,62,62,62	0
56	MG	RA	3169	1/1	0.14	-	23,23,23,23	0
56	MG	QA	1655	1/1	0.44	-	50,50,50,50	0
56	MG	XA	1610	1/1	0.25	-	37,37,37,37	0
56	MG	RA	3159	1/1	0.41	-	26,26,26,26	0
56	MG	YA	3221	1/1	0.17	-	26,26,26,26	0
56	MG	XA	1617	1/1	0.15	-	26,26,26,26	0
56	MG	XA	1649	1/1	0.31	-	28,28,28,28	0
56	MG	YA	3226	1/1	0.15	-	14,14,14,14	0
56	MG	RA	3079	1/1	0.20	-	32,32,32,32	0
56	MG	YA	3091	1/1	0.11	-	23,23,23,23	0
56	MG	YA	3225	1/1	0.14	-	32,32,32,32	0
56	MG	RA	3195	1/1	0.25	-	28,28,28,28	0
56	MG	XA	1615	1/1	0.13	-	19,19,19,19	0
56	MG	YA	3081	1/1	0.20	-	18,18,18,18	0
56	MG	YA	3134	1/1	0.09	-	29,29,29,29	0
56	MG	YA	3180	1/1	0.11	-	53,53,53,53	0
56	MG	RA	3005	1/1	0.25	-	8,8,8,8	0
56	MG	QA	1628	1/1	0.22	-	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3105	1/1	0.18	-	50,50,50,50	0
56	MG	RA	3175	1/1	0.24	-	99,99,99,99	0
56	MG	RA	3018	1/1	0.23	-	6,6,6,6	0
56	MG	RA	3093	1/1	0.11	-	24,24,24,24	0
56	MG	YA	3025	1/1	0.15	-	6,6,6,6	0
56	MG	YA	3039	1/1	0.20	-	30,30,30,30	0
56	MG	XA	1640	1/1	0.21	-	47,47,47,47	0
56	MG	RA	3162	1/1	0.24	-	56,56,56,56	0
56	MG	XA	1653	1/1	0.31	-	44,44,44,44	0
56	MG	RA	3109	1/1	0.06	-	26,26,26,26	0
56	MG	YA	3101	1/1	0.28	-	5,5,5,5	0
56	MG	YA	3133	1/1	0.63	-	43,43,43,43	0
56	MG	YA	3107	1/1	0.20	-	25,25,25,25	0
56	MG	RA	3110	1/1	0.12	-	51,51,51,51	0
56	MG	YA	3082	1/1	0.17	-	13,13,13,13	0
58	ZN	XD	301	1/1	0.23	-	49,49,49,49	0
56	MG	QA	1645	1/1	0.18	-	22,22,22,22	0
56	MG	YA	3097	1/1	0.24	-	19,19,19,19	0
56	MG	RA	3166	1/1	0.27	-	56,56,56,56	0
56	MG	YA	3067	1/1	0.11	-	15,15,15,15	0
56	MG	YA	3218	1/1	0.11	-	19,19,19,19	0
56	MG	YA	3056	1/1	0.18	-	9,9,9,9	0
56	MG	YA	3032	1/1	0.19	-	9,9,9,9	0
56	MG	RA	3064	1/1	0.38	-	25,25,25,25	0
56	MG	YA	3216	1/1	0.08	-	42,42,42,42	0
56	MG	XA	1637	1/1	0.12	-	39,39,39,39	0
56	MG	YA	3092	1/1	0.14	-	11,11,11,11	0
56	MG	RA	3204	1/1	0.26	-	30,30,30,30	0
56	MG	RA	3004	1/1	0.10	-	5,5,5,5	0
56	MG	RA	3103	1/1	0.57	-	48,48,48,48	0
58	ZN	QD	301	1/1	0.19	-	59,59,59,59	0
56	MG	RA	3133	1/1	0.15	-	32,32,32,32	0
56	MG	YA	3077	1/1	0.12	-	8,8,8,8	0
56	MG	QA	1654	1/1	0.14	-	14,14,14,14	0
56	MG	RA	3063	1/1	0.21	-	27,27,27,27	0
56	MG	RA	3172	1/1	0.21	-	29,29,29,29	0
56	MG	RB	202	1/1	0.07	-	31,31,31,31	0
56	MG	XA	1613	1/1	0.11	-	45,45,45,45	0
56	MG	YA	3230	1/1	0.20	-	43,43,43,43	0
56	MG	QA	1632	1/1	0.25	-	41,41,41,41	0
56	MG	YA	3168	1/1	0.27	-	65,65,65,65	0
56	MG	RF	301	1/1	0.20	-	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3170	1/1	0.10	-	41,41,41,41	0
56	MG	QA	1622	1/1	0.28	-	60,60,60,60	0
56	MG	XA	1656	1/1	0.15	-	37,37,37,37	0
56	MG	YA	3086	1/1	0.15	-	3,3,3,3	0
56	MG	YA	3083	1/1	0.34	-	21,21,21,21	0
56	MG	YA	3099	1/1	0.31	-	11,11,11,11	0
56	MG	RA	3043	1/1	0.09	-	30,30,30,30	0
56	MG	QA	1634	1/1	0.10	-	48,48,48,48	0
56	MG	YA	3167	1/1	0.07	-	12,12,12,12	0
56	MG	QA	1606	1/1	0.17	-	7,7,7,7	0
56	MG	RA	3003	1/1	0.24	-	17,17,17,17	0
56	MG	RA	3129	1/1	0.19	-	26,26,26,26	0
56	MG	YA	3121	1/1	0.14	-	23,23,23,23	0
56	MG	YA	3110	1/1	0.07	-	10,10,10,10	0
56	MG	YA	3190	1/1	0.20	-	51,51,51,51	0
56	MG	RA	3180	1/1	0.18	-	28,28,28,28	0
56	MG	QA	1623	1/1	0.16	-	28,28,28,28	0
56	MG	RA	3116	1/1	0.21	-	69,69,69,69	0
56	MG	YA	3005	1/1	0.12	-	19,19,19,19	0
56	MG	QA	1610	1/1	0.14	-	33,33,33,33	0
56	MG	RA	3111	1/1	0.19	-	52,52,52,52	0
56	MG	YA	3115	1/1	0.17	-	21,21,21,21	0
56	MG	RA	3025	1/1	0.18	-	9,9,9,9	0
56	MG	RA	3040	1/1	0.16	-	9,9,9,9	0
56	MG	RA	3080	1/1	0.30	-	44,44,44,44	0
56	MG	QA	1659	1/1	0.26	-	79,79,79,79	0
56	MG	RA	3054	1/1	0.19	-	5,5,5,5	0
56	MG	RA	3022	1/1	0.28	-	3,3,3,3	0
56	MG	YA	3050	1/1	0.20	-	2,2,2,2	0
56	MG	YA	3141	1/1	0.37	-	43,43,43,43	0
56	MG	XA	1605	1/1	0.34	-	126,126,126,126	0
56	MG	YA	3143	1/1	0.12	-	33,33,33,33	0
56	MG	RA	3155	1/1	0.19	-	12,12,12,12	0
56	MG	RA	3090	1/1	0.14	-	14,14,14,14	0
56	MG	YA	3195	1/1	0.07	-	55,55,55,55	0
56	MG	RA	3199	1/1	0.27	-	47,47,47,47	0
56	MG	YA	3189	1/1	0.10	-	31,31,31,31	0
56	MG	XA	1661	1/1	0.15	-	38,38,38,38	0
56	MG	XA	1638	1/1	0.26	-	55,55,55,55	0
56	MG	RA	3026	1/1	0.25	-	6,6,6,6	0
56	MG	YA	3201	1/1	0.10	-	122,122,122,122	0
56	MG	RA	3108	1/1	0.17	-	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1644	1/1	0.24	-	59,59,59,59	0
56	MG	QA	1608	1/1	0.15	-	27,27,27,27	0
56	MG	YE	301	1/1	0.12	-	1,1,1,1	0
57	PAR	QA	1661	42/42	0.23	-	75,75,75,75	0
56	MG	RA	3206	1/1	0.22	-	38,38,38,38	0
56	MG	RA	3197	1/1	0.13	-	50,50,50,50	0
56	MG	YA	3100	1/1	0.33	-	1,1,1,1	0
56	MG	RA	3130	1/1	0.40	-	44,44,44,44	0
56	MG	XA	1609	1/1	0.18	-	15,15,15,15	0
56	MG	QA	1639	1/1	0.13	-	44,44,44,44	0
56	MG	RA	3114	1/1	0.09	-	30,30,30,30	0
56	MG	XA	1602	1/1	0.17	-	15,15,15,15	0
56	MG	YA	3094	1/1	0.27	-	10,10,10,10	0
56	MG	YA	3068	1/1	0.32	-	12,12,12,12	0
56	MG	RA	3051	1/1	0.39	-	1,1,1,1	0
56	MG	RA	3068	1/1	0.14	-	16,16,16,16	0
56	MG	RA	3041	1/1	0.14	-	5,5,5,5	0
56	MG	YA	3241	1/1	0.28	-	33,33,33,33	0
56	MG	YA	3211	1/1	0.19	-	42,42,42,42	0
56	MG	RA	3149	1/1	0.24	-	48,48,48,48	0
56	MG	YA	3031	1/1	0.33	-	6,6,6,6	0
56	MG	YA	3079	1/1	0.28	-	18,18,18,18	0
56	MG	YA	3174	1/1	0.14	-	29,29,29,29	0
56	MG	XA	1660	1/1	0.08	-	61,61,61,61	0
56	MG	RA	3020	1/1	0.19	-	29,29,29,29	0
56	MG	YA	3151	1/1	0.36	-	26,26,26,26	0
56	MG	RA	3076	1/1	0.33	-	22,22,22,22	0
56	MG	YA	3072	1/1	0.13	-	10,10,10,10	0
56	MG	YA	3132	1/1	0.05	-	13,13,13,13	0
56	MG	RA	3104	1/1	0.29	-	44,44,44,44	0
56	MG	XM	202	1/1	0.27	-	43,43,43,43	0
56	MG	YA	3183	1/1	0.12	-	36,36,36,36	0
56	MG	XA	1616	1/1	0.21	-	20,20,20,20	0
56	MG	YA	3184	1/1	0.15	-	33,33,33,33	0
56	MG	RA	3071	1/1	0.14	-	32,32,32,32	0
56	MG	QX	102	1/1	0.09	-	42,42,42,42	0
56	MG	XA	1622	1/1	0.09	-	40,40,40,40	0
56	MG	YA	3208	1/1	0.20	-	53,53,53,53	0
56	MG	XA	1632	1/1	0.14	-	11,11,11,11	0
56	MG	RA	3211	1/1	0.26	-	13,13,13,13	0
56	MG	QA	1635	1/1	0.25	-	31,31,31,31	0
56	MG	RA	3198	1/1	0.04	-	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1633	1/1	0.36	-	50,50,50,50	0
56	MG	XA	1655	1/1	0.20	-	33,33,33,33	0
56	MG	RA	3208	1/1	0.18	-	47,47,47,47	0
56	MG	QA	1642	1/1	0.09	-	49,49,49,49	0
56	MG	RA	3008	1/1	0.21	-	13,13,13,13	0
56	MG	RA	3037	1/1	0.19	-	10,10,10,10	0
56	MG	QV	101	1/1	0.17	-	17,17,17,17	0
56	MG	RA	3126	1/1	0.22	-	27,27,27,27	0
56	MG	RA	3083	1/1	0.19	-	26,26,26,26	0
56	MG	RA	3098	1/1	0.15	-	11,11,11,11	0
56	MG	QA	1615	1/1	0.65	-	46,46,46,46	0
56	MG	RA	3014	1/1	0.21	-	10,10,10,10	0
56	MG	YA	3001	1/1	0.37	-	13,13,13,13	0
56	MG	XA	1619	1/1	0.17	-	46,46,46,46	0
56	MG	YA	3078	1/1	0.28	-	25,25,25,25	0
56	MG	QA	1613	1/1	0.31	-	56,56,56,56	0
56	MG	YA	3111	1/1	0.18	-	30,30,30,30	0
56	MG	YA	3089	1/1	0.24	-	2,2,2,2	0
56	MG	QF	201	1/1	0.17	-	56,56,56,56	0
56	MG	YA	3017	1/1	0.10	-	16,16,16,16	0
56	MG	YA	3065	1/1	0.12	-	12,12,12,12	0
56	MG	YA	3228	1/1	0.18	-	45,45,45,45	0
56	MG	YA	3048	1/1	0.17	-	4,4,4,4	0
56	MG	YA	3057	1/1	0.45	-	22,22,22,22	0
56	MG	QA	1652	1/1	0.17	-	36,36,36,36	0
56	MG	XA	1659	1/1	0.09	-	60,60,60,60	0
56	MG	RA	3113	1/1	0.30	-	24,24,24,24	0
56	MG	RA	3006	1/1	0.12	-	3,3,3,3	0
56	MG	RA	3046	1/1	0.35	-	31,31,31,31	0
56	MG	YA	3122	1/1	0.17	-	35,35,35,35	0
56	MG	RA	3021	1/1	0.37	-	27,27,27,27	0
56	MG	XA	1608	1/1	0.13	-	7,7,7,7	0
56	MG	RA	3182	1/1	0.35	-	25,25,25,25	0
56	MG	RA	3154	1/1	0.13	-	12,12,12,12	0
56	MG	RA	3137	1/1	0.17	-	36,36,36,36	0
56	MG	RA	3092	1/1	0.14	-	18,18,18,18	0
56	MG	RA	3212	1/1	0.27	-	18,18,18,18	0
56	MG	RA	3188	1/1	0.31	-	58,58,58,58	0
56	MG	YA	3140	1/1	0.25	-	2,2,2,2	0
56	MG	YA	3194	1/1	0.43	-	42,42,42,42	0
56	MG	QA	1624	1/1	0.40	-	24,24,24,24	0
56	MG	RA	3011	1/1	0.22	-	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3023	1/1	0.28	-	24,24,24,24	0
56	MG	RA	3181	1/1	0.29	-	34,34,34,34	0
56	MG	RA	3203	1/1	0.27	-	73,73,73,73	0
56	MG	QA	1621	1/1	0.17	-	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.