



wwPDB X-ray Structure Validation Summary Report

Sep 18, 2014 – 04:21 AM EDT

PDB ID : 4LFZ
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U in the Absence of Paromomycin
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-27
Resolution : 3.92 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>

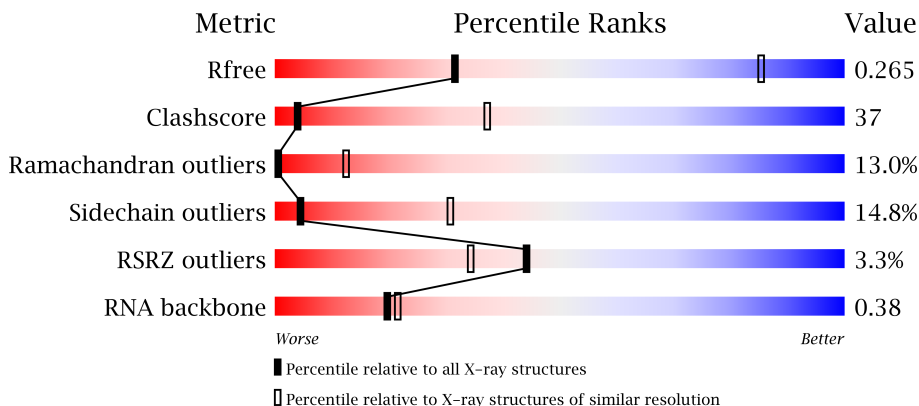
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.92 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	1008 (4.40-3.44)
Clashscore	79885	1180 (4.34-3.50)
Ramachandran outliers	78287	1124 (4.34-3.50)
Sidechain outliers	78261	1112 (4.34-3.50)
RSRZ outliers	66119	1008 (4.40-3.44)
RNA backbone	1838	1018 (5.00-2.80)

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	

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Mol	Chain	Length	Quality of chain
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	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	

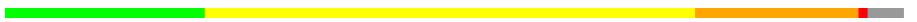
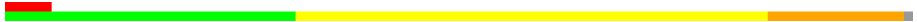



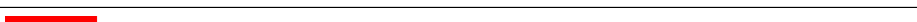

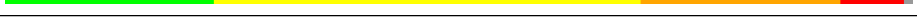


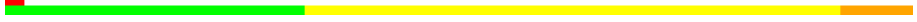
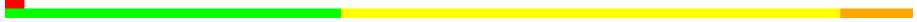




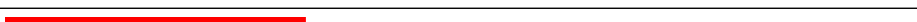
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Mol	Chain	Length	Quality of chain
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	

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

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291868 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
23	XX	7	Total	C	N	O	P	0	0	0
			145	65	23	50	7			

- 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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
25	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	64	Total	Mg	0	0
			64	64		
57	RP	1	Total	Mg	0	0
			1	1		
57	QX	1	Total	Mg	0	0
			1	1		
57	YA	269	Total	Mg	0	0
			269	269		
57	QM	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XX	1	Total 1	Mg 1	0	0
57	QV	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	R0	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	XB	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	239	Total 239	Mg 239	0	0
57	YP	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	YB	3	Total 3	Mg 3	0	0
57	XV	2	Total 2	Mg 2	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0

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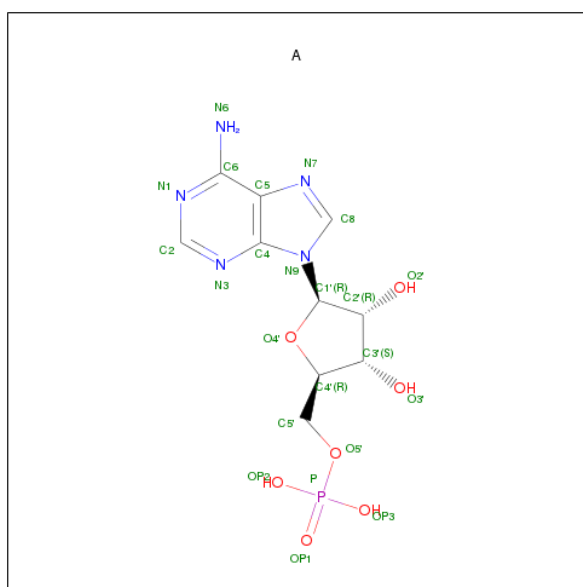
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XM	1	Total	Mg	0	0
			1	1		
57	YE	1	Total	Mg	0	0
			1	1		

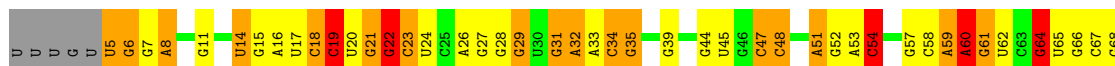
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

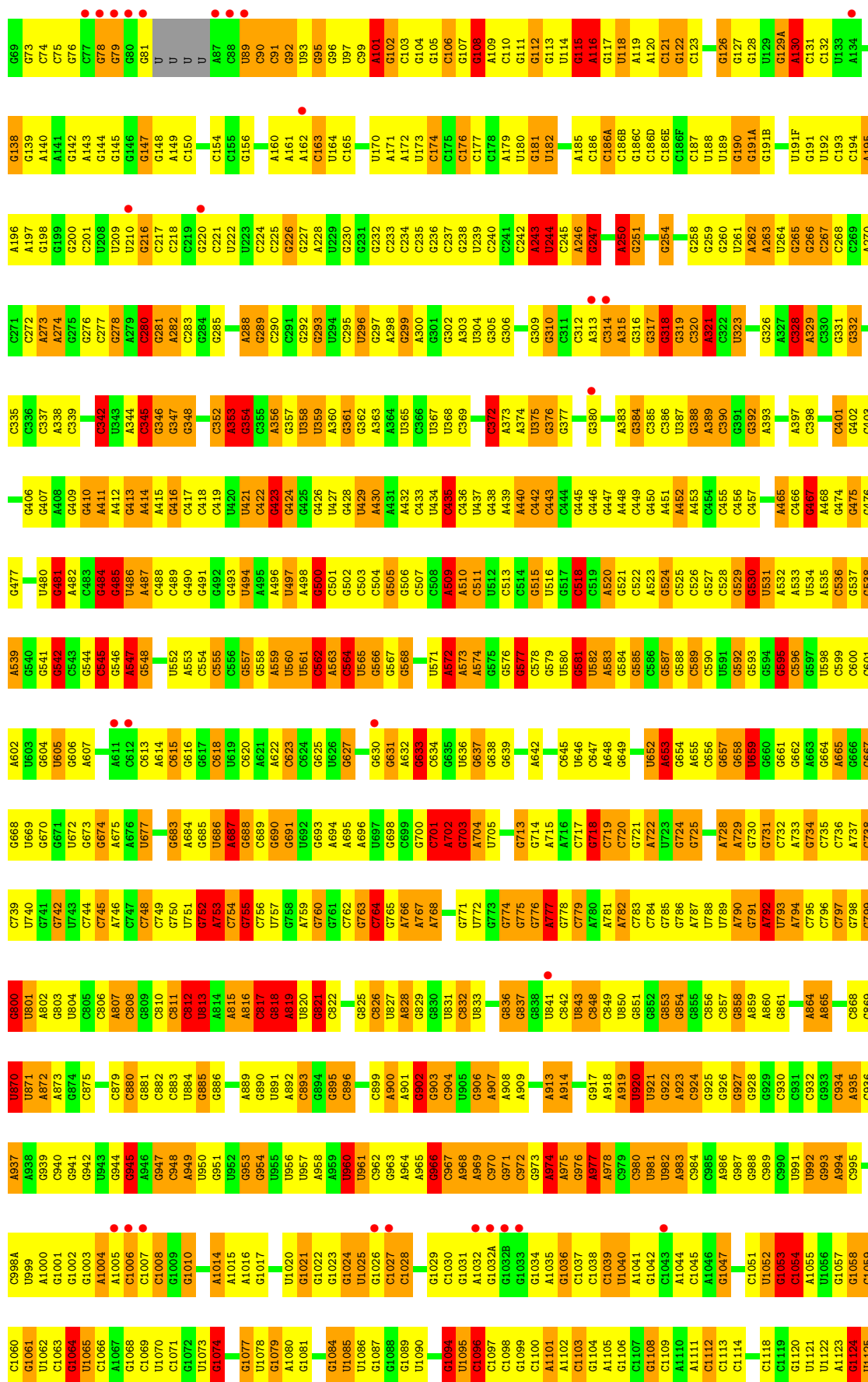
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y9	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		
58	QD	1	Total	Zn	0	0
			1	1		
58	XD	1	Total	Zn	0	0
			1	1		
58	R9	1	Total	Zn	0	0
			1	1		

- Molecule 59 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: C₁₀H₁₄N₅O₇P).

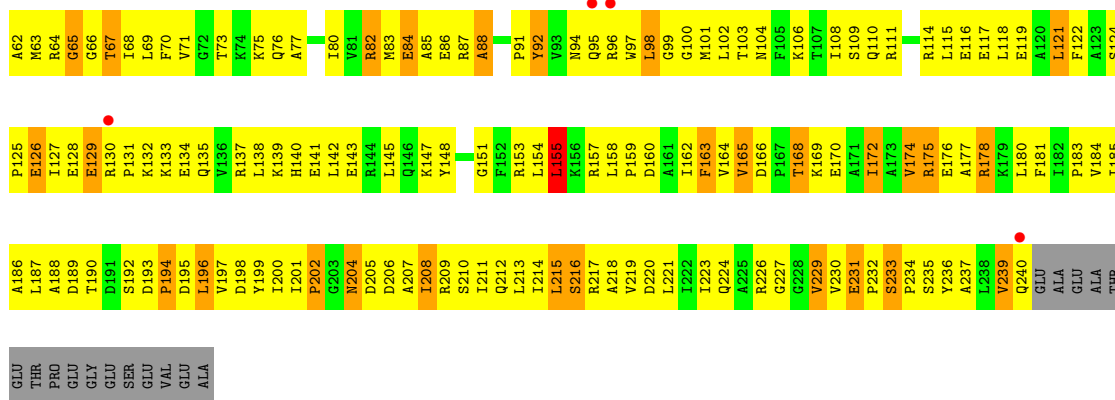


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	XX	1	Total	C	N	O P	0	0
			22	10	5	6 1		



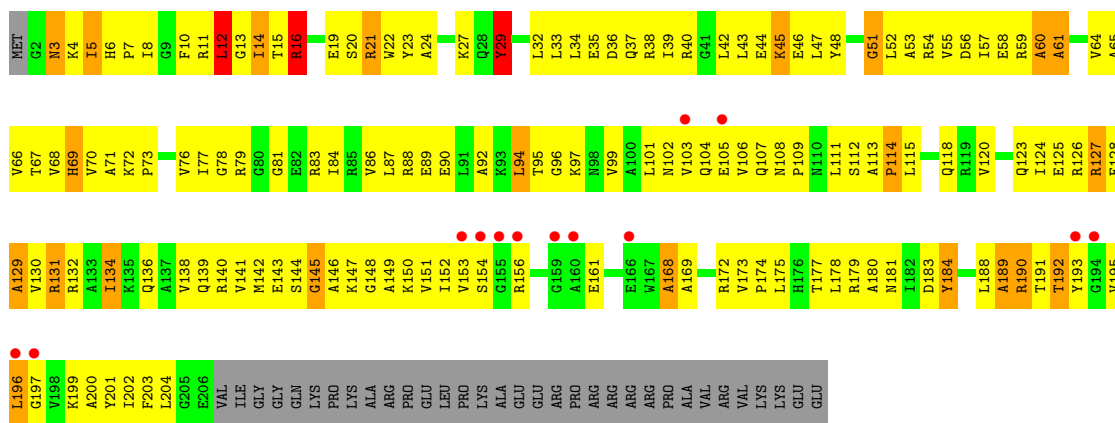






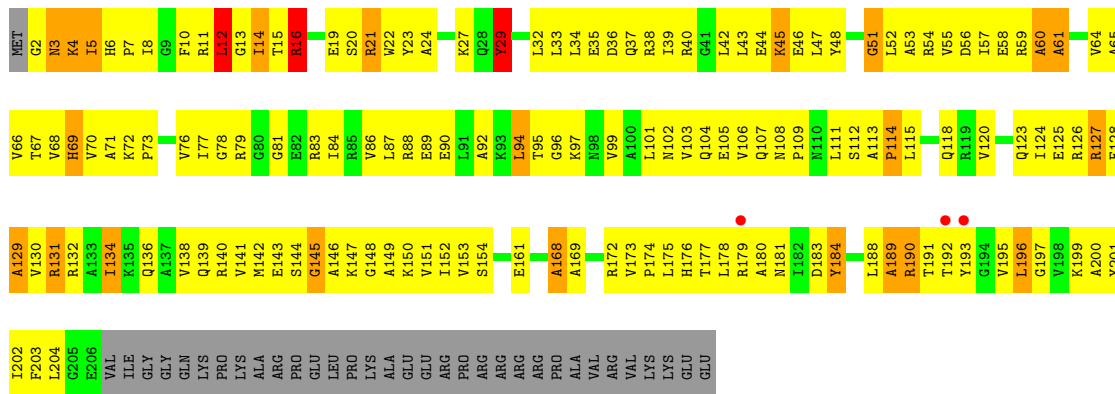
• Molecule 3: 30S ribosomal protein S3

Chain QC: ■ ■ ■ ■



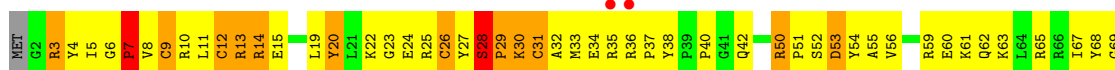
• Molecule 3: 30S ribosomal protein S3

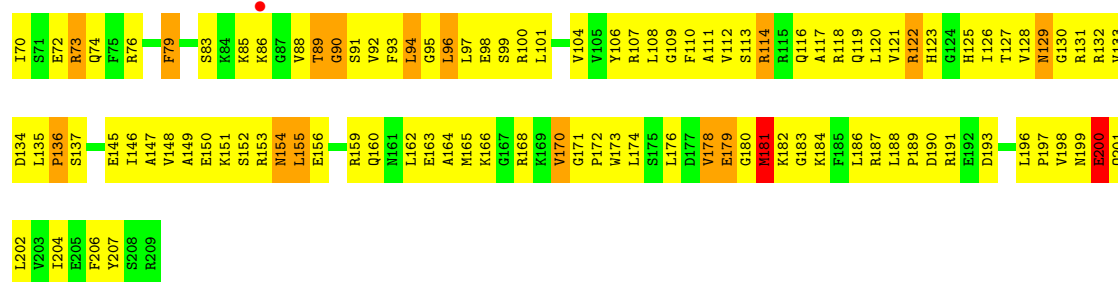
Chain XC: ■ ■ ■ ■



• Molecule 4: 30S ribosomal protein S4

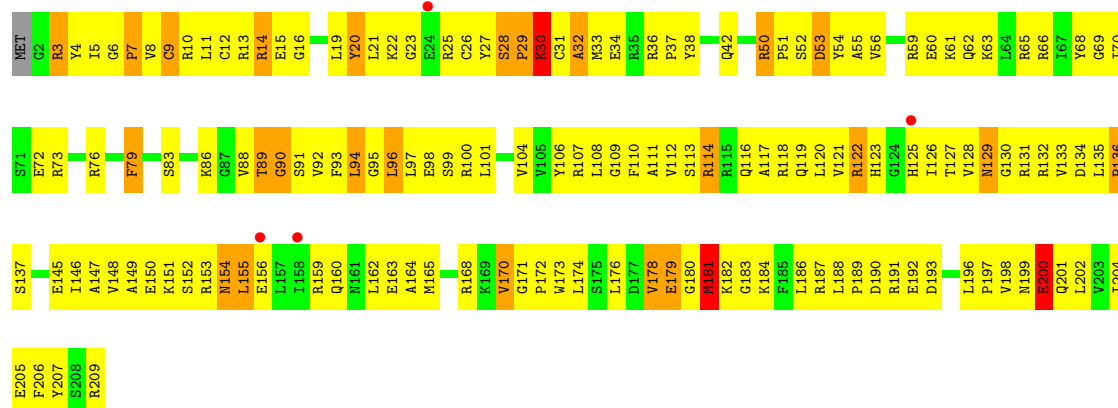
Chain QD: ■ ■ ■ ■





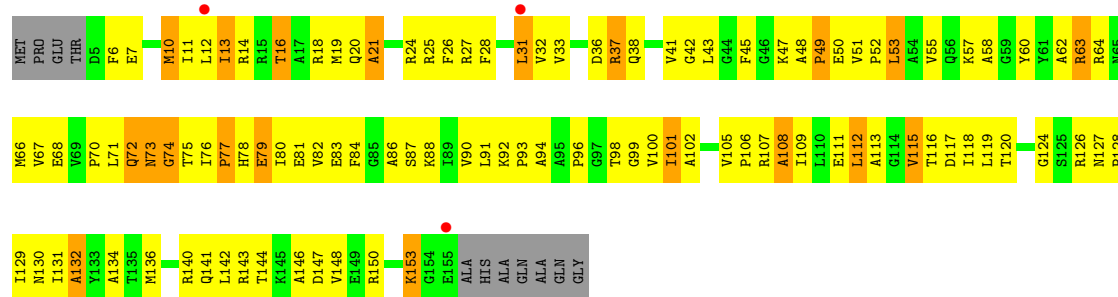
• Molecule 4: 30S ribosomal protein S4

Chain XD:



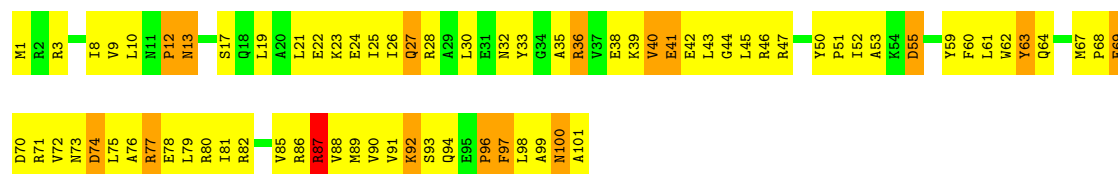
• Molecule 5: 30S ribosomal protein S5

Chain QE:



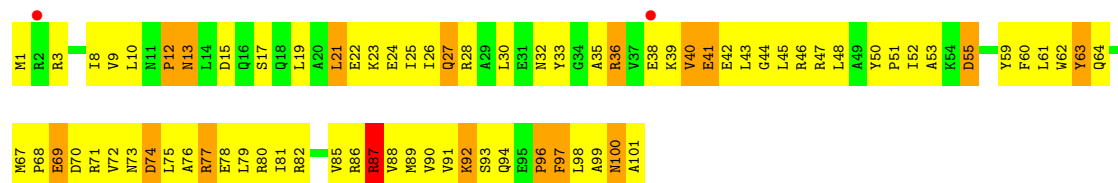
- Molecule 6: 30S ribosomal protein S6

Chain QF:



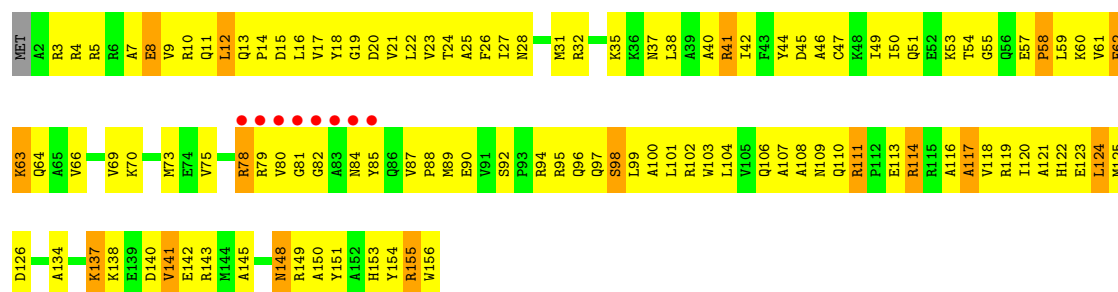
- Molecule 6: 30S ribosomal protein S6

Chain XF:



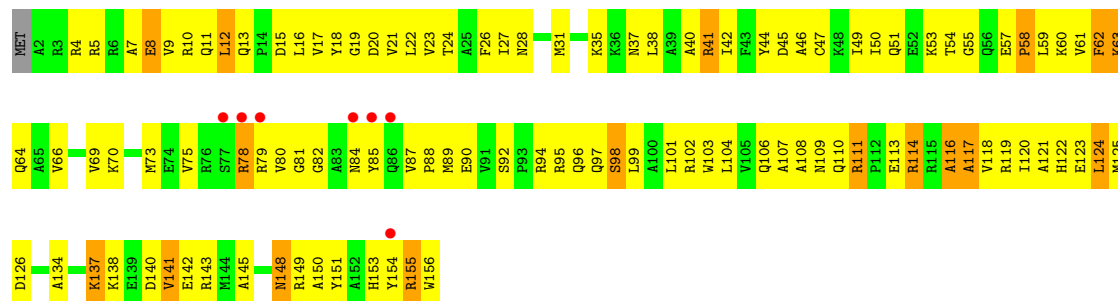
- Molecule 7: 30S ribosomal protein S7

Chain QG:



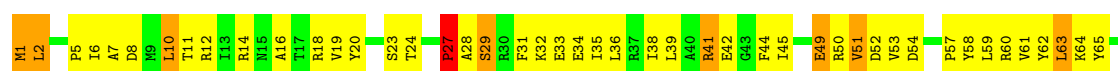
- Molecule 7: 30S ribosomal protein S7

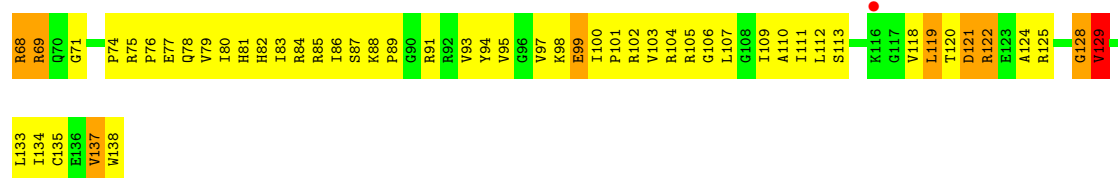
Chain XG:



- Molecule 8: 30S ribosomal protein S8

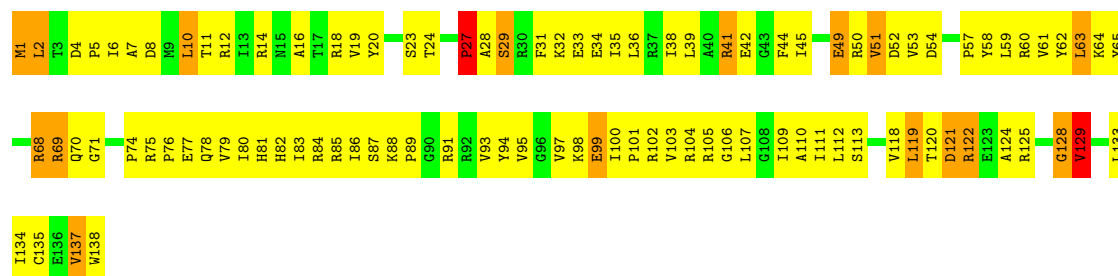
Chain QH:





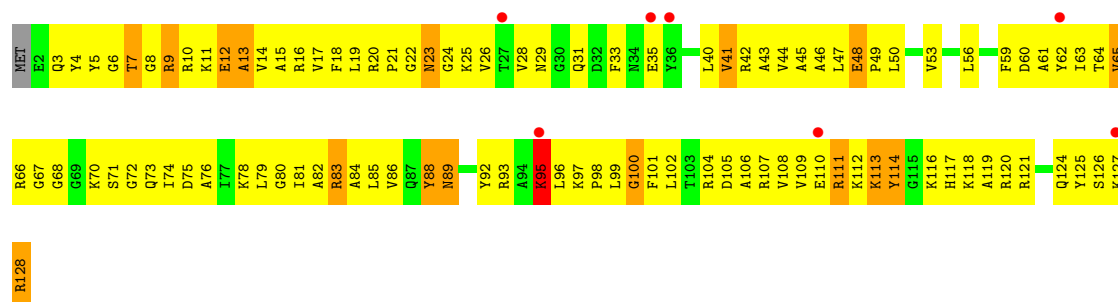
• Molecule 8: 30S ribosomal protein S8

Chain XH:



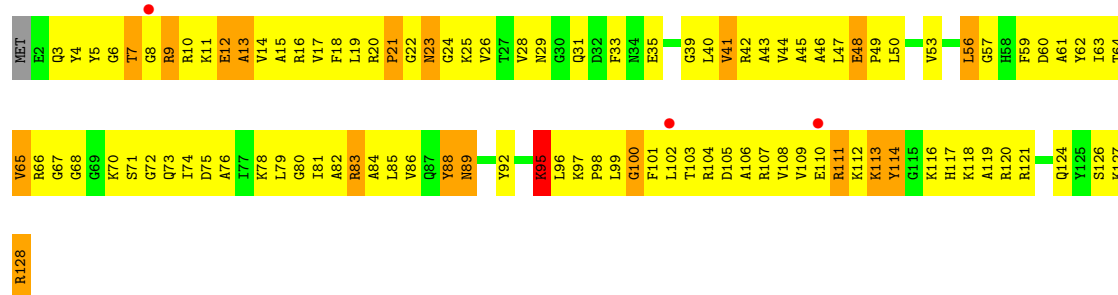
• Molecule 9: 30S ribosomal protein S9

Chain QI:



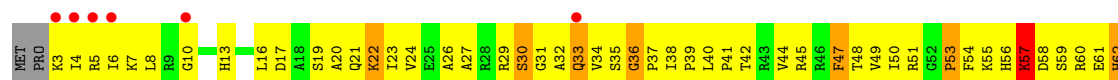
• Molecule 9: 30S ribosomal protein S9

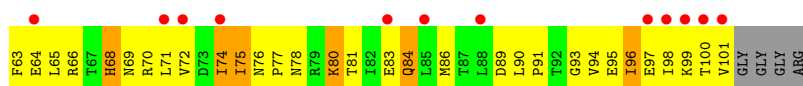
Chain XI:



• Molecule 10: 30S ribosomal protein S10

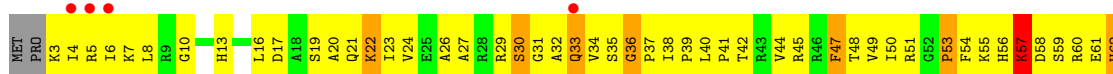
Chain QJ:





- 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:



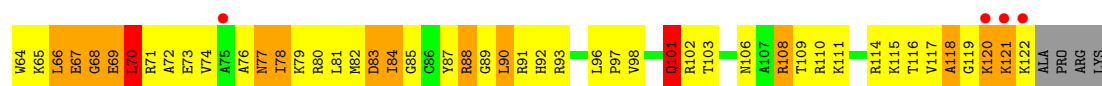
- Molecule 12: 30S ribosomal protein S12

Chain XL:

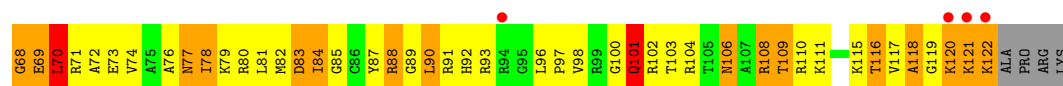
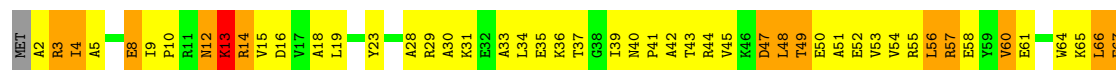




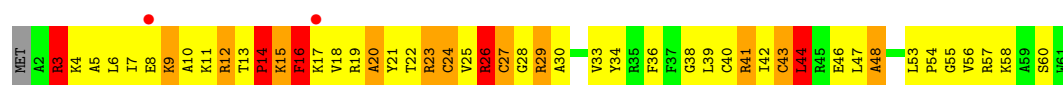
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13



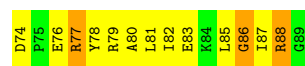
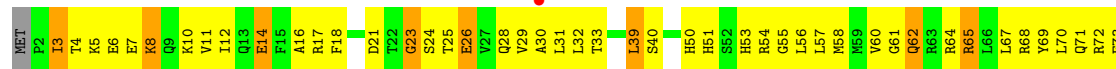
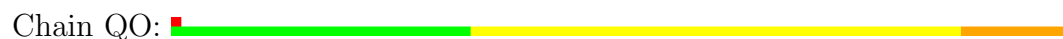
• Molecule 14: 30S ribosomal protein S14



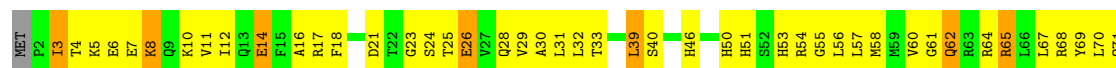
• Molecule 14: 30S ribosomal protein S14

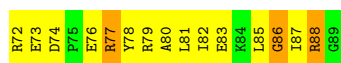


• Molecule 15: 30S ribosomal protein S15



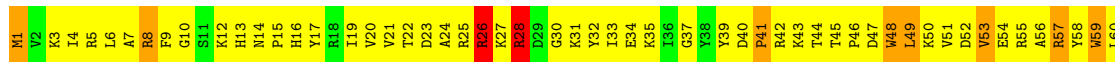
• Molecule 15: 30S ribosomal protein S15





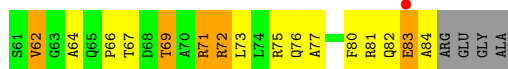
- Molecule 16: 30S ribosomal protein S16

Chain QP:



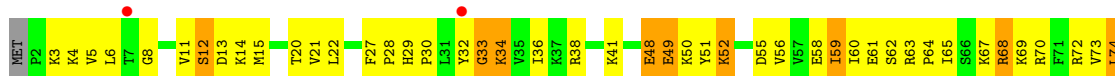
- Molecule 16: 30S ribosomal protein S16

Chain XP:



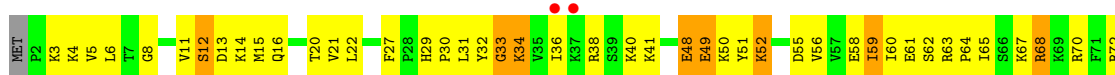
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



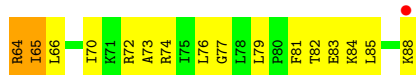
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



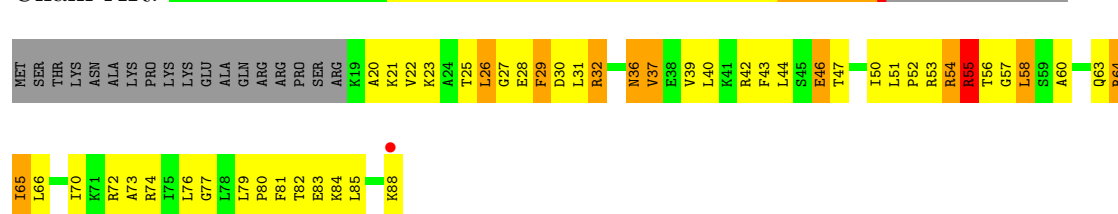
- Molecule 18: 30S ribosomal protein S18

Chain QR:



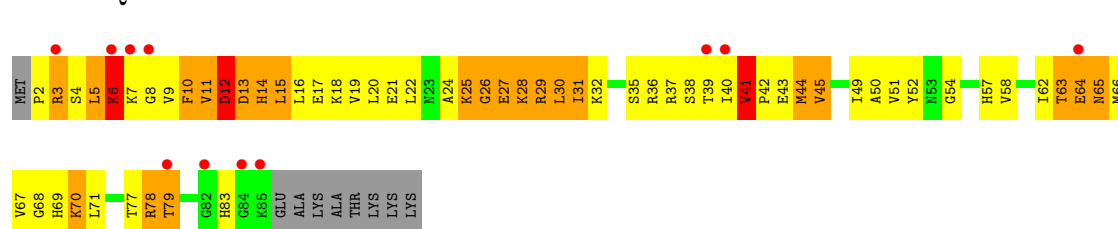
- Molecule 18: 30S ribosomal protein S18

Chain XR:



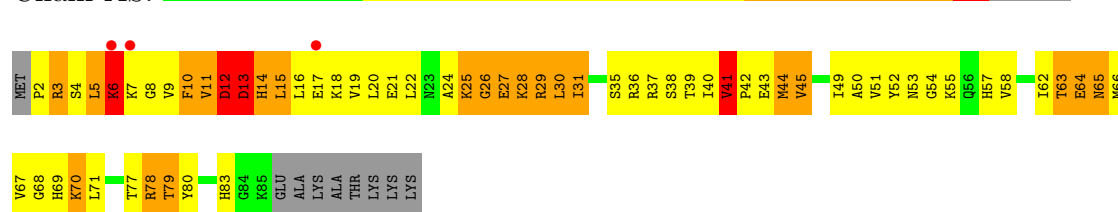
- Molecule 19: 30S ribosomal protein S19

Chain QS:



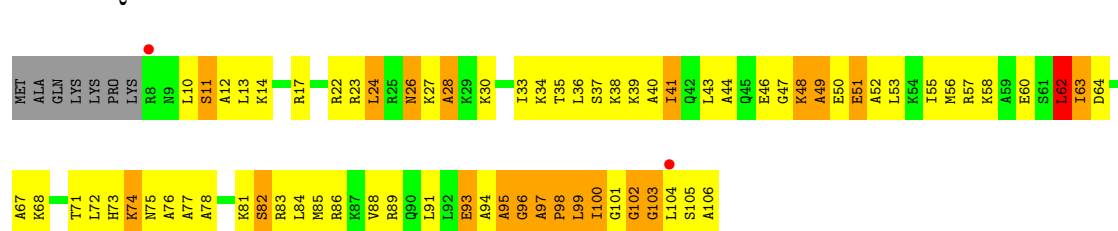
- Molecule 19: 30S ribosomal protein S19

Chain XS:



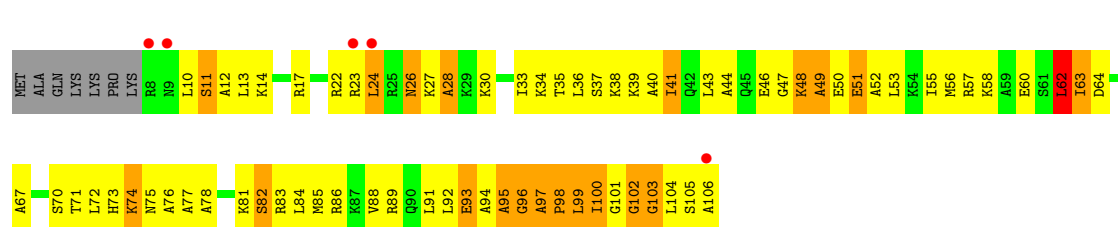
- Molecule 20: 30S ribosomal protein S20

Chain QT:



- Molecule 20: 30S ribosomal protein S20

Chain XT:



- Molecule 21: 30S ribosomal protein S21

MET	G2	K3	G4	D5	R6	R7	T8	R9	R10	G11	K12	I13	W14	R15	G16	T17	Y18	G19	K20	Y21	R22	P23	R24	K25	K26	LYS
-----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain XU:

Relative abundance of amino acids in the protein. The chart shows the relative abundance of various amino acids, with red dots indicating specific modifications. The x-axis lists amino acids: MET, G2, K3, G4, D5, R6, R7, T8, R9, R10, G11, K12, I13, W14, R15, G16, T17, Y18, G19, K20, Y21, R22, K25, K26, and LYS. The y-axis represents relative abundance from 0 to 1.0. Bars are colored by group: MET (grey), G2 (yellow), K3 (orange), G4 (yellow), D5 (yellow), R6 (orange), R7 (orange), T8 (yellow), R9 (yellow), R10 (yellow), G11 (yellow), K12 (green), I13 (yellow), W14 (yellow), R15 (yellow), G16 (green), T17 (yellow), Y18 (green), G19 (yellow), K20 (yellow), Y21 (yellow), R22 (orange), K25 (yellow), K26 (yellow), and LYS (grey). Red dots above the bars indicate specific modifications: G16, T17, Y18, R22, K25, and K26.

- Chain QV:

Category	Value
C1	1
C2	1
C3	1
C4	1
C5	1
C6	1
C7	1
C8	1
C9	1
C10	1
C11	1
C12	1
C13	1
C14	1
C15	1
C16	1
C17	1
C18	1
C19	1
C20	1
C21	1
C22	1
C23	1
C24	1
C25	1
C26	1
C27	1
C28	1
C29	1
C30	1
C31	1
C32	1
C33	1
C34	1
C35	1
C36	1
C37	1
C38	1
C39	1
C40	1
C41	1
C42	1
C43	1
C44	1
C45	1
C46	1
C47	1
C48	1
C49	1
C50	1
C51	1
C52	1
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C54	1
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C57	1
C58	1
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C61	1
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C67	1
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C69	1
C70	1
C71	1
C72	1
C73	1
C74	1
C75	1
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C77	1
C78	1
C79	1
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C81	1
C82	1
C83	1
C84	1
C85	1
C86	1
C87	1
C88	1
C89	1
C90	1
C91	1
C92	1
C93	1
C94	1
C95	1
C96	1
C97	1
C98	1
C99	1
C100	1

- Chain XV:

Age Group	Number of Cases (approx.)
C1	2
C2	1
C3	1
C4	1
C5	1
C6	1
C7	1
C8	1
C9	1
C10	1
C11	1
C12	1
C13	1
C14	1
C15	1
C16	1
C17	1
C18	1
C19	1
C20	1
C21	1
C22	1
C23	1
C24	1
C25	1
C26	1
C27	1
C28	1
C29	1
C30	1
C31	1
C32	1
C33	1
C34	1
C35	1
C36	1
C37	1
C38	1
C39	1
C40	1
C41	1
C42	1
C43	1
C44	1
C45	1
C46	1
C47	165
C48	1
C49	1
C50	1
C51	1
C52	1
C53	1
C54	1
C55	1
C56	1
C57	1
C58	1
C59	1
C60	1
C61	1
C62	1
C63	15
C64	1
C65	1
C66	1
C67	1
C68	1
C69	1
C70	1

- Chain QX: 

G G C A A G G G A G G U A A A A
 A1 U2 G3 C4 C5 C6 U7 U8 A A

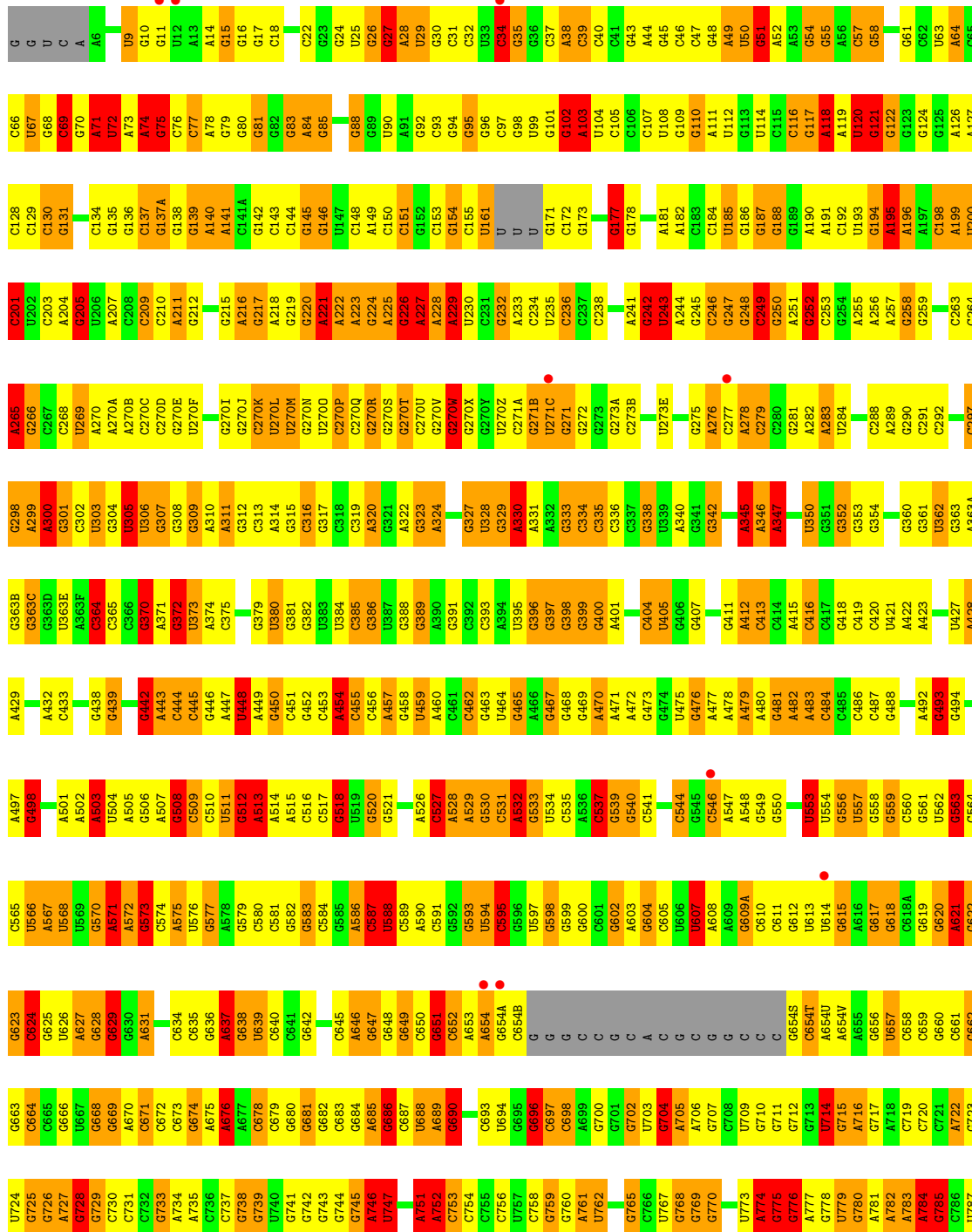
- Chain XX: 

G	G	C	A	A	G	G	A	G	G	U	A	A	A	A	A1	U2	G3	C4	C5	C6	U7	A	A	A
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	---	---	---

- Chain QY:

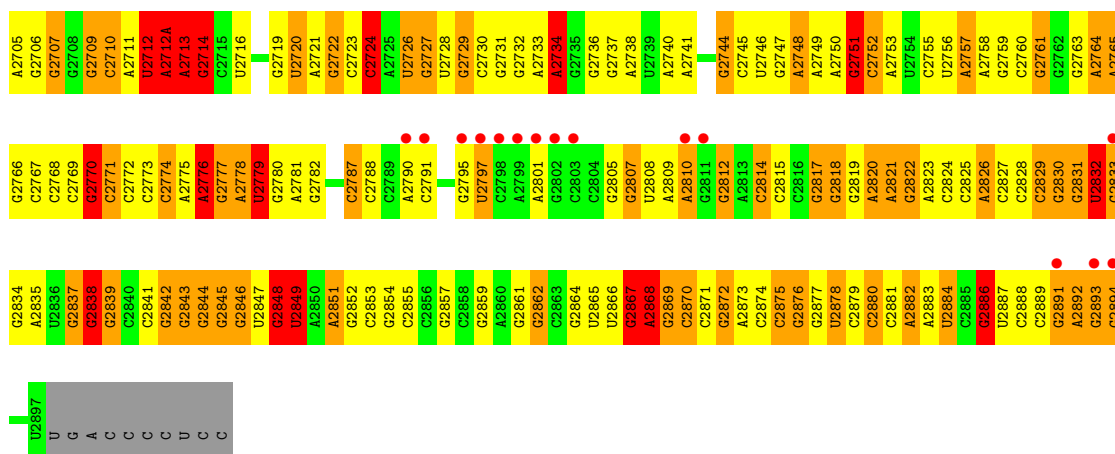
- Molecule 24: messenger RNA

Chain RA:



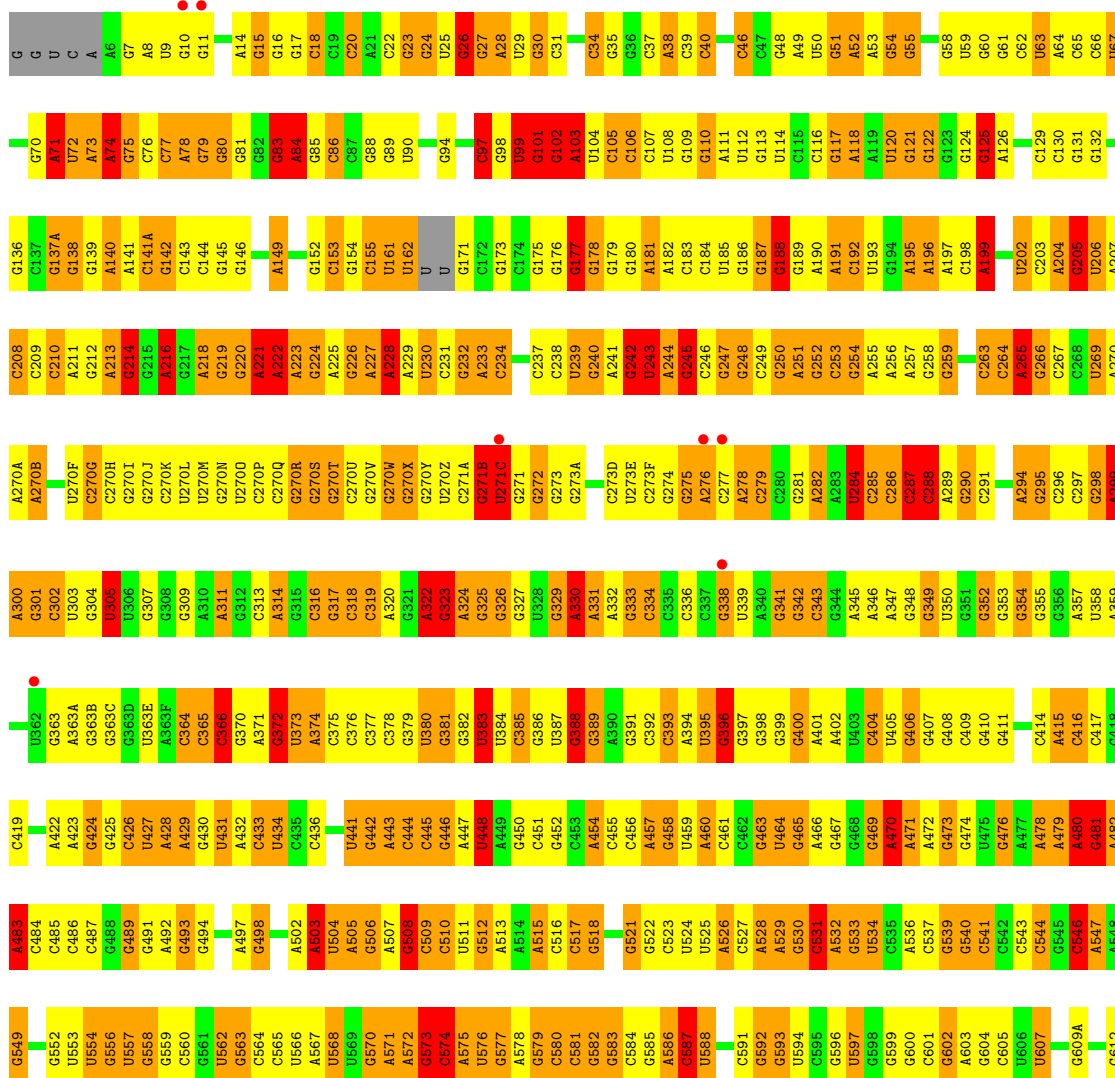


G2638	G2639	G2576	G2513	G2452	G2391	G2330	A2267	G2194	G2127	C2065	A2005	G1945	G1878	U1805	G1735
G2640	G2641	G2577	G2514	A2453	A2392	G2331	A2268	G2195	C2128	C2066	C2006	U1946	G1879	G1806	C1741
G2642	G2643	G2578	G2515	G2454	A2393	U2332	A2269	C2196	U2130	G2067	C2007	G1947	G1882	G1807	G1742
G2644	G2645	U2580	G2516	G2455	A2394	A2332	G2270	U2197	U2131	U2068	C2008	G1948	G1883	U1808	G1743
G2646	G2647	G2581	G2517	G2456	G2395	G2334	G2271	A2198	G2132	G2069	G2009	G1949	A1884	A1809	G1746
G2648	G2649	G2582	A2518	U2457	A2396	A2335	U2272	A2199	U2133	G2070	G2010	G1950	A1885	A1810	G1747
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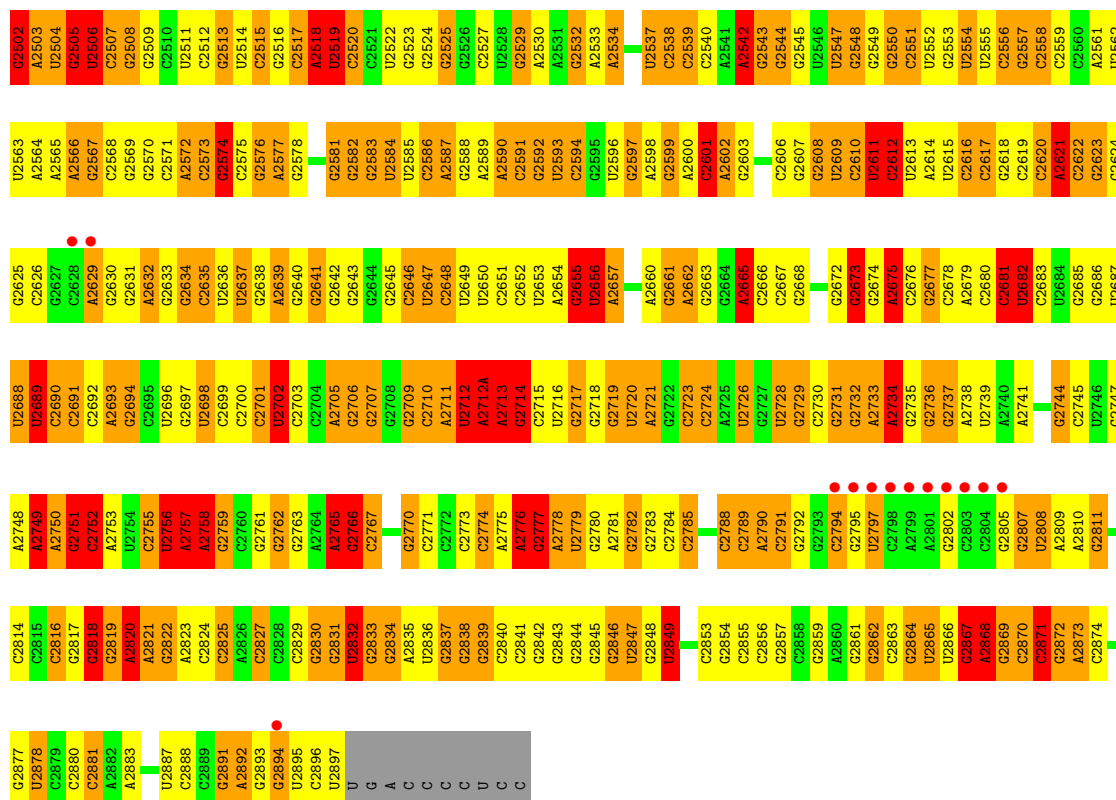
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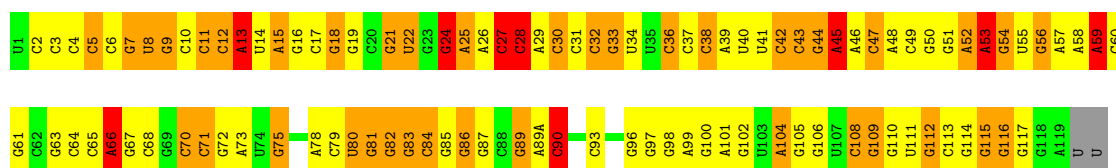
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G2489	G2490	G2406	G2345	G2284	G2224	G2141	C2076	A2015	G1954	A1890	A1819	A1755	G1674	C1546	C1546
G2491	G2492	C2407	A2346	C2285	C2225	C2142	C2077	A2016	U1955	G1891	G1820	C1756	C1675	C1547	C1547
G2493	G2494	C2408	G2347	A2286	C2226	C2143	G2078	U2017	C1956	G1892	A1821	U1757	A1676	G1548	C1548
G2495	G2496	G2409	U2348	G2287	G2227	G2144	U2079	U2018	C1957	C1893	G1822	G1758	C1677	C1549	C1549
G2497	G2498	C2410	G2349	A2288	G2228	C2145	C2080	G2019	G1958	C1894	G1823	C1759	C1678	C1550	C1550
G2499	G2500	G2411	C2350	G2289	C2229	G2146	C2081	G2018	C1959	C1895	G1824	C1761	U1679	G1551	G1551
G2501	G2502	C2412	G2351	G2290	G2230	C2147	C2082	G2019	C1960	G1896	G1825	C1762	U1680	C1552	C1552
G2503	G2504	G2413	A2352	U2291	C2231	G2148	C2083	A2020	A1960	C1897	A1826	C1763	C1681	G1553	G1553
G2505	G2506	C2414	G2353	C2292	U2232	G2149	C2084	C2021	C1961	C1898	G1827	C1764	C1682	C1554	C1554
G2507	G2508	G2415	G2354	G2293	U2233	C2150	C2085	G2022	C1962	C1899	G1828	C1765	C1683	G1557	G1557
G2509	G2510	C2416	C2355	C2294	G2234	G2151	C2086	C2023	C1963	C1900	A1829	C1766	C1684	A1558	A1558
G2511	G2512	G2417	G2356	G2295	G2235	A2158	U2089	G2025	G1964	A1901	G1830	C1767	C1685	G1559	G1559
G2513	G2514	C2418	C2357	U2296	C2236	G2159	C2090	G2026	C1965	C1902	C1831	U1768	C1686	G1560	G1560
G2515	G2516	G2419	G2358	G2297	G2237	G2160	U2091	G2027	A1966	C1903	G1832	U1769	C1687	G1561	G1561
G2517	G2518	C2420	C2359	A2298	G2238	G2161	U2092	U2028	C1967	C1904	G1833	U1770	C1688	G1562	G1562
G2519	G2520	G2421	A2360	G2299	G2239	C2162	G2093	G2029	G1968	C1905	U1833	C1771	U1688	G1563	G1563
G2521	G2522	C2422	A2361	G2300	C2240	C2163	G2094	A2030	A1969	G1906	U1834	G1772	G1626	C1564	C1564
G2523	G2524	G2423	C2362	C2301	A2241	C2164	C2095	A2031	A1970	C1907	G1835	A1773	A1590	C1565	C1565
G2525	G2526	C2424	C2363	G2302	G2242	C2165	U2096	G2032	A1971	C1908	C1836	C1774	C1627	G1566	G1566
G2527	G2528	G2425	C2364	G2303	U2243	G2166	C2097	A2033	A1972	C1913	C1837	C1775	U1692	A1566	A1566
G2529	G2530	C2426	G2365	C2304	U2244	U2167	U2098	U2034	G1973	C1914	C1838	U1776	U1693	A1567	A1567
G2531	G2532	G2427	A2366	A2307	G2245	G2168	U2099	G2035	C1974	C1915	G1839	U1777	C1694	G1568	G1568
G2533	G2534	C2428	G2367	G2308	G2246	A2169	G2100	G2036	G1975	U1915	G1840	U1778	C1695	A1569	A1569
G2535	G2536	G2429	C2368	A2309	A2247	A2170	G2101	G2037	U1976	A1916	G1841	U1779	G1696	A1570	A1570
G2537	G2538	C2430	G2369	A2310	C2248	A2171	U2102	G2038	A1977	U1917	G1842	A1780	G1697	A1571	A1571
G2539	G2540	U2431	G2370	A2311	U2249	U2172	G2103	C2039	A1978	U1918	C1843	C1781	C1698	A1572	A1572
G2541	G2542	C2432	A2371	A2312	G2250	C2174	G2104	C2040	C1979	A1919	C1844	C1782	C1699	G1573	G1573
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G2547	G2548	G2435	G2374	C2314	G2253	C2177	U2107	C2043	C1983	G1922	A1847	A1784	C1638	G1576	G1576
G2549	G2550	C2436	G2375	G2315	C2254	G2178	C2108	C2044	G1984	U1923	A1848	A1786	U1639	C1577	C1577
G2551	G2552	A2377	A2376	G2316	G2255	C2179	C2109	G2045	G1985	C1924	G1849	A1787	C1640	U1578	U1578
G2553	G2554	G2437	G2378	C2317	U2256	G2182	U2113	G2046	A1986	G1926	G1850	C1788	A1641	C1579	C1579
G2555	G2556	C2438	A2379	G2318	U2257	C2183	A2114	C2050	G1987	U1926	U1851	A1789	G1705	A1580	A1580



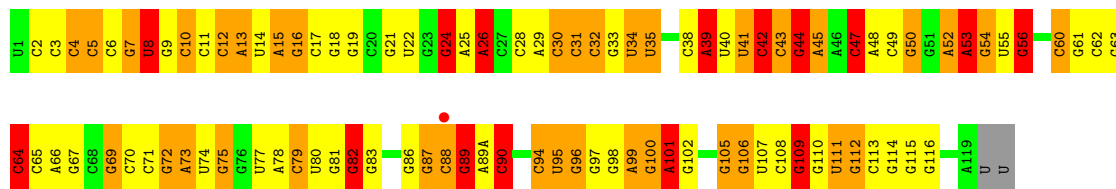
• Molecule 26: 5S rRNA

Chain RB:



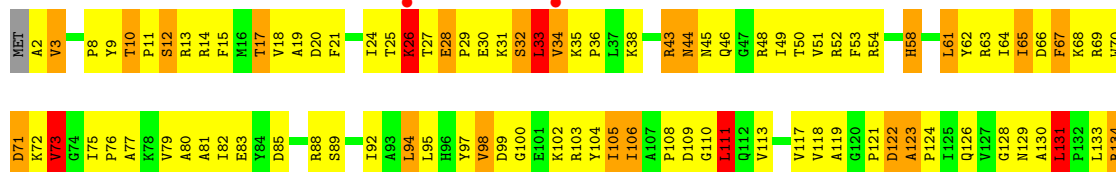
• Molecule 26: 5S rRNA

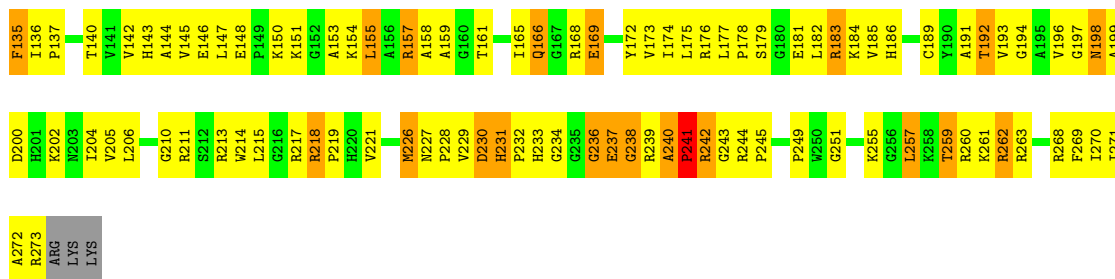
Chain YB:



• Molecule 27: 50S ribosomal protein L2

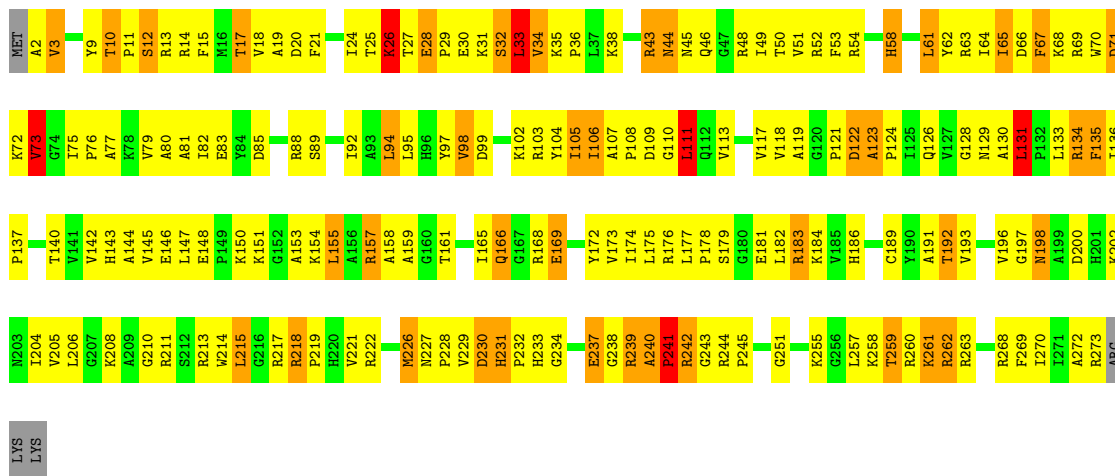
Chain RD:





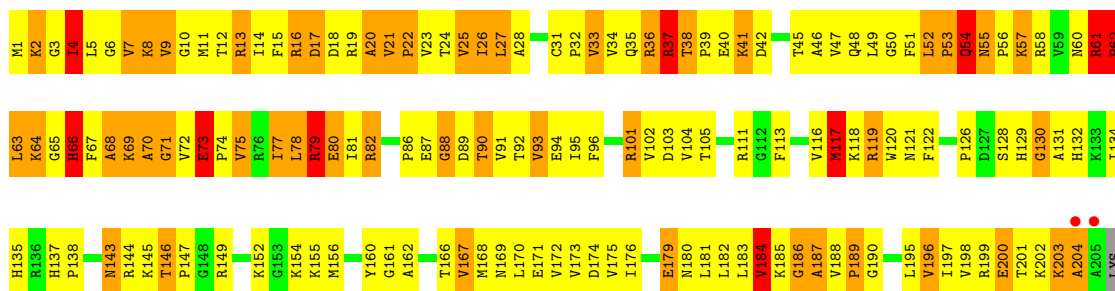
• Molecule 27: 50S ribosomal protein L2

Chain YD:



• Molecule 28: 50S ribosomal protein L3

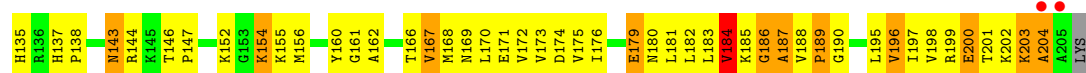
Chain RE:



• Molecule 28: 50S ribosomal protein L3

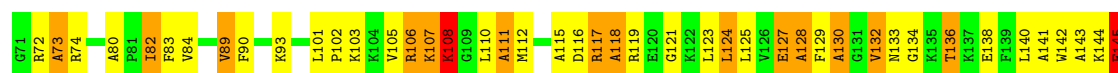
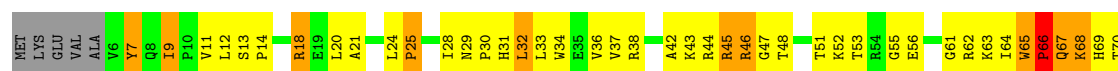
Chain YE:





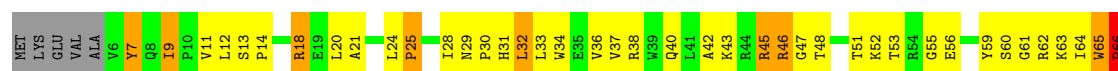
- Molecule 29: 50S ribosomal protein L4

Chain RF:



- Molecule 29: 50S ribosomal protein L4

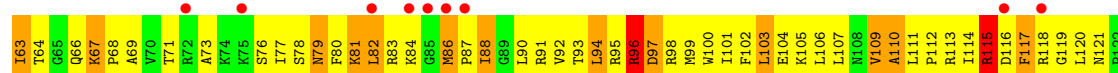
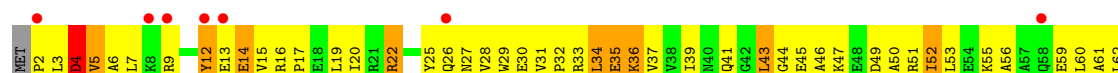
Chain YF:



ALA

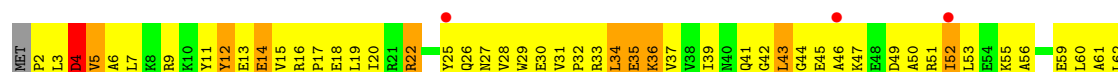
- Molecule 30: 50S ribosomal protein L5

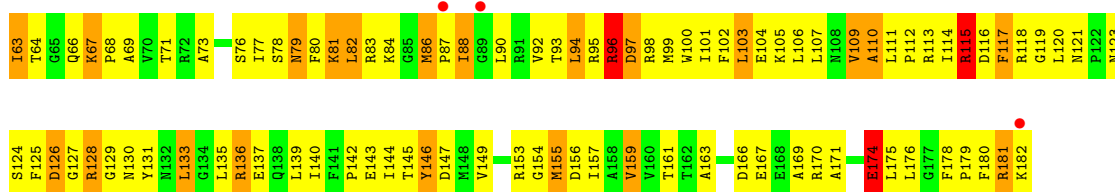
Chain RG:



- Molecule 30: 50S ribosomal protein L5

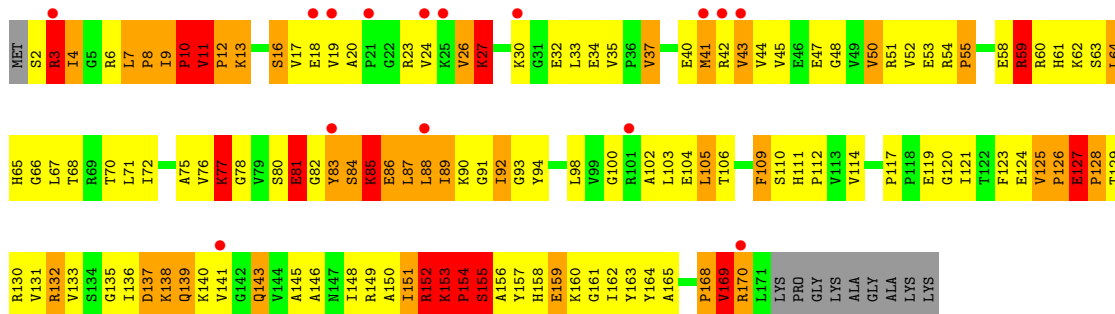
Chain YG:





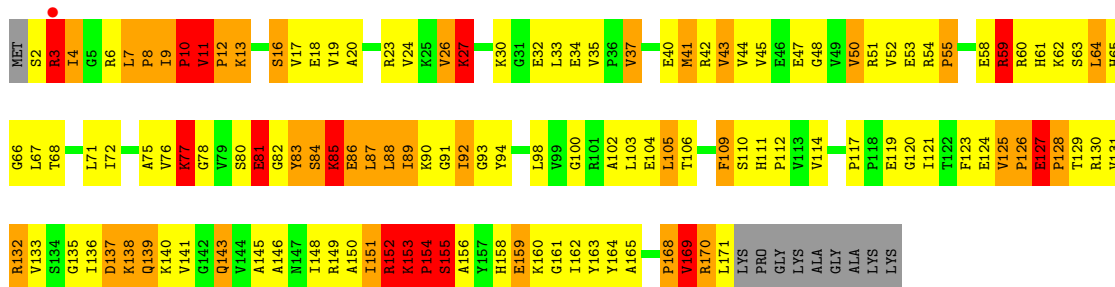
• Molecule 31: 50S ribosomal protein L6

Chain RH:



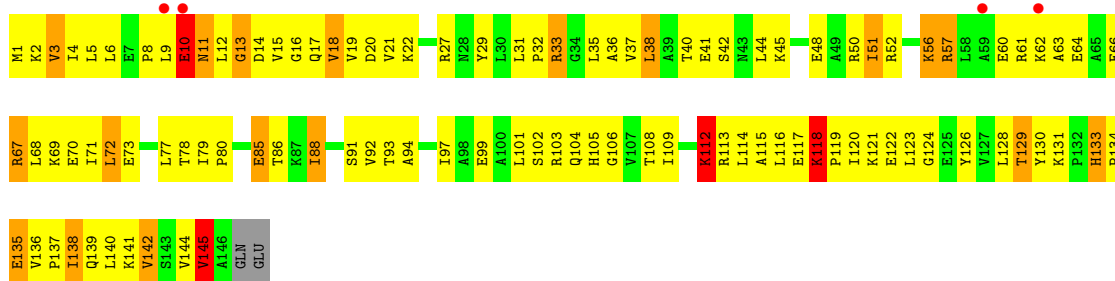
• Molecule 31: 50S ribosomal protein L6

Chain YH:



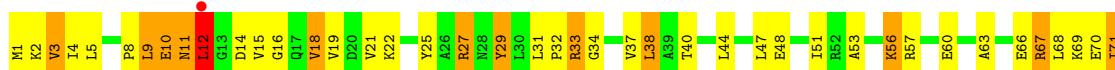
• Molecule 32: 50S ribosomal protein L9

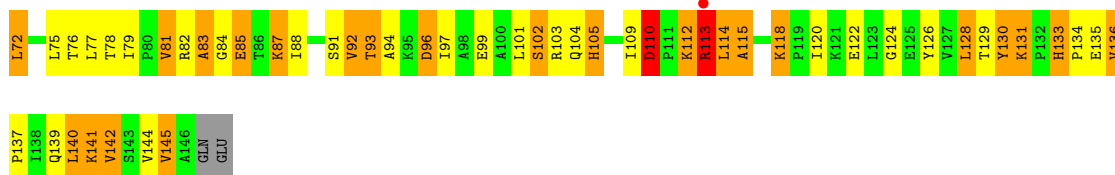
Chain RI:



• Molecule 32: 50S ribosomal protein L9

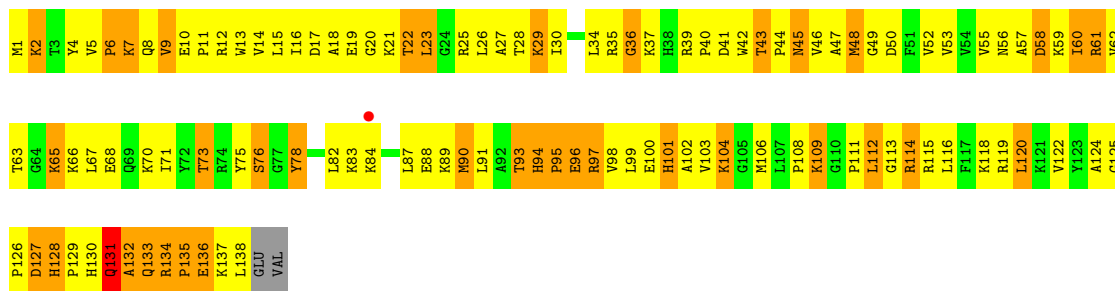
Chain YI:





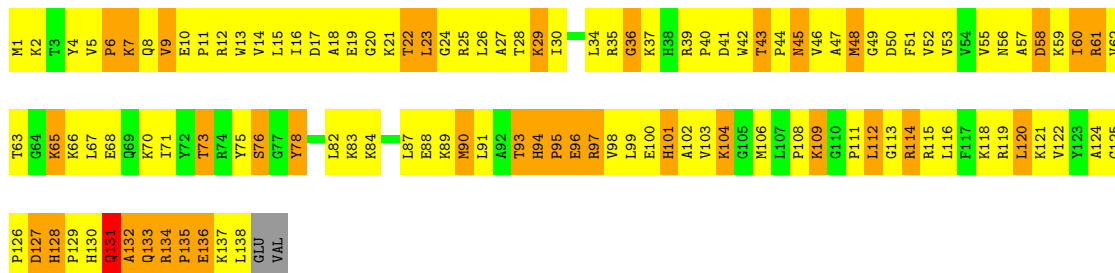
- Molecule 33: 50S ribosomal protein L13

Chain RN:



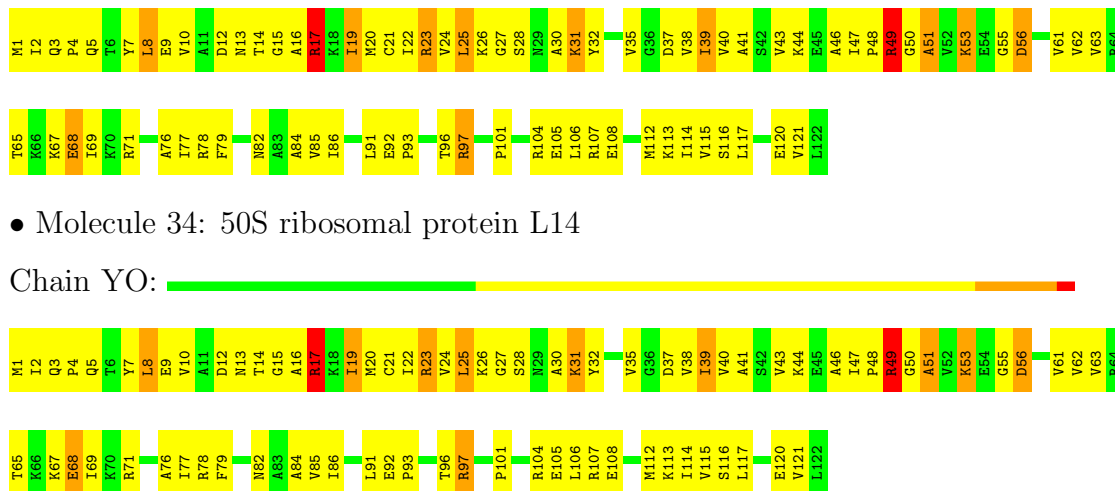
- Molecule 33: 50S ribosomal protein L13

Chain YN:



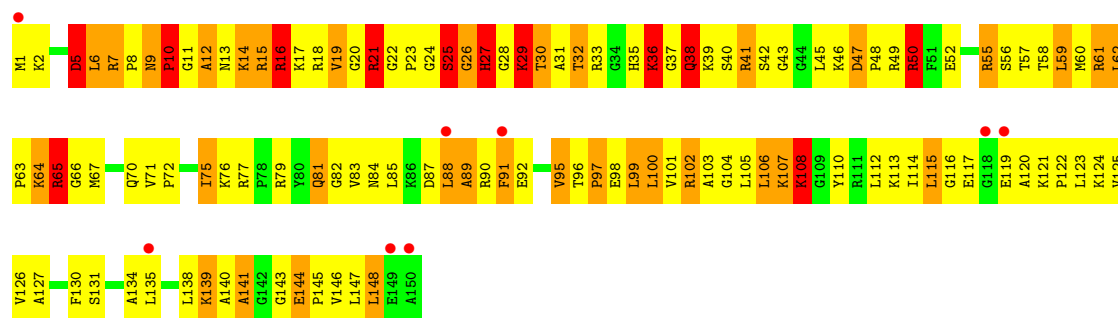
- Molecule 34: 50S ribosomal protein L14

Chain RO:



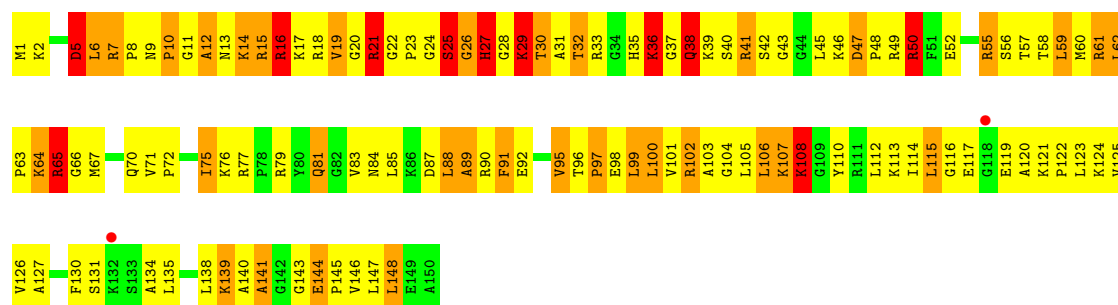
- Molecule 35: 50S ribosomal protein L15

Chain RP:



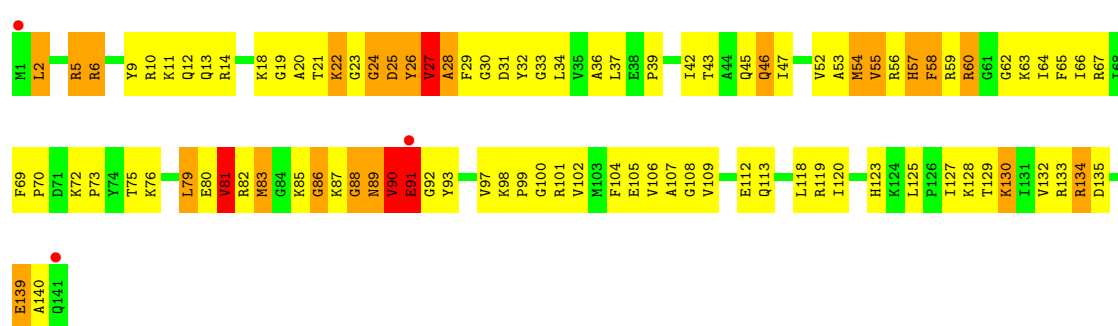
- Molecule 35: 50S ribosomal protein L15

Chain YP:



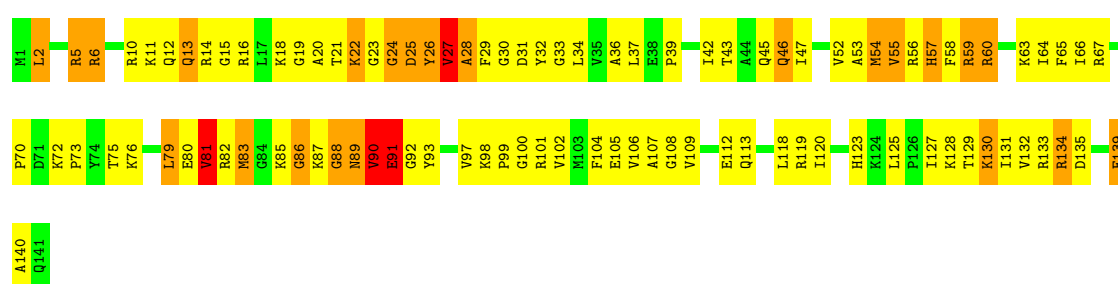
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



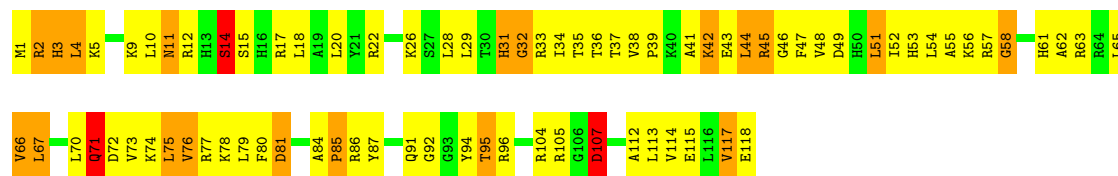
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



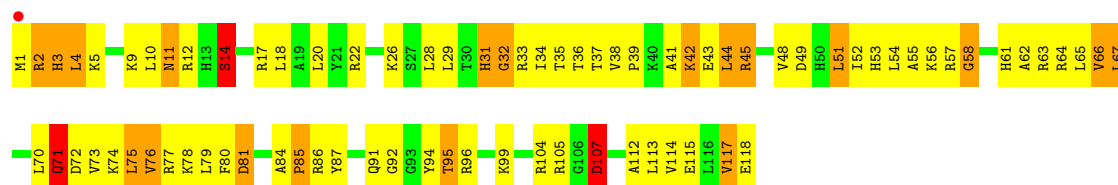
- Molecule 37: 50S ribosomal protein L17

Chain RR:



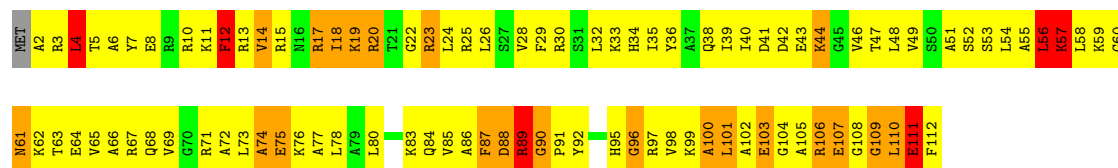
- Molecule 37: 50S ribosomal protein L17

Chain YR:



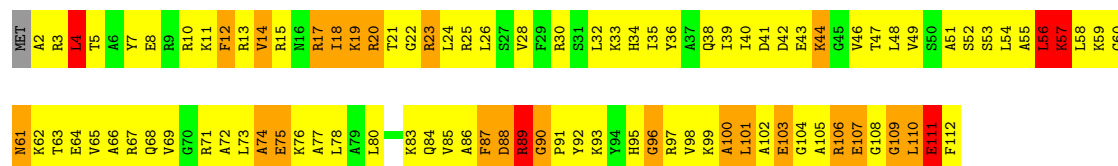
- Molecule 38: 50S ribosomal protein L18

Chain RS:



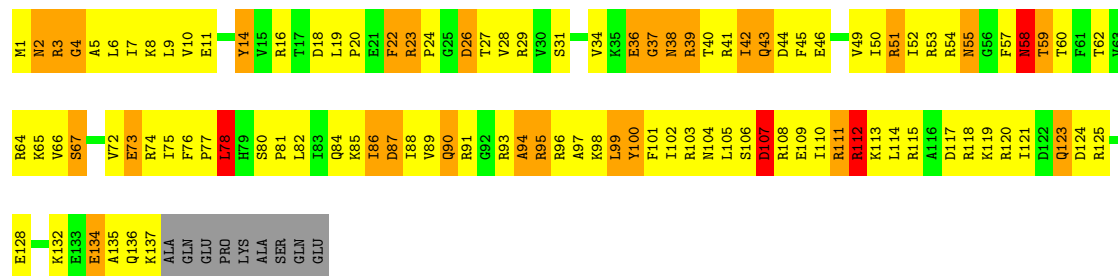
- Molecule 38: 50S ribosomal protein L18

Chain YS:



- Molecule 39: 50S ribosomal protein L19

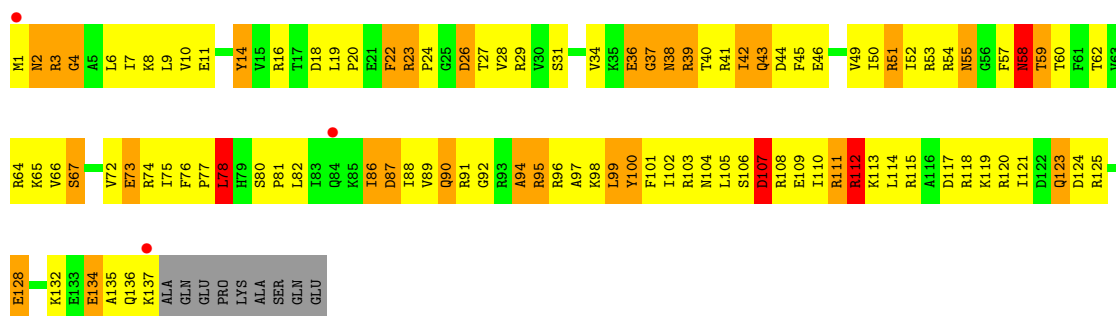
Chain RT:



- Molecule 39: 50S ribosomal protein L19

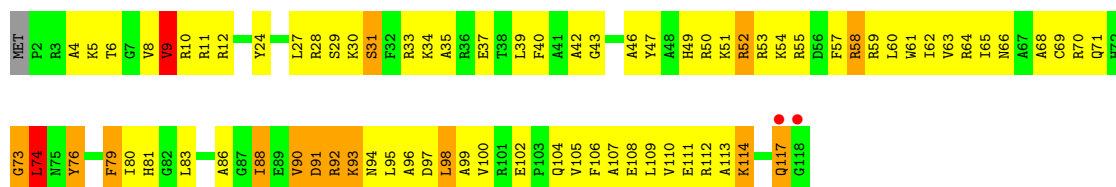
Chain YT:





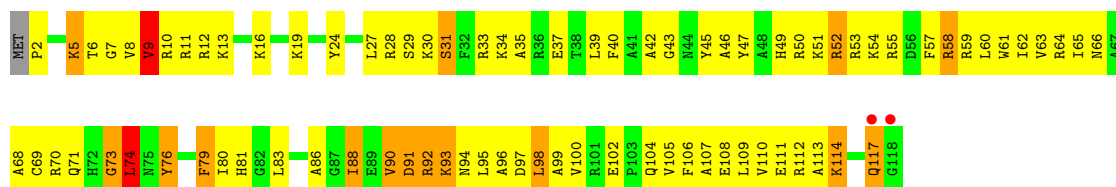
- Molecule 40: 50S ribosomal protein L20

Chain RU:



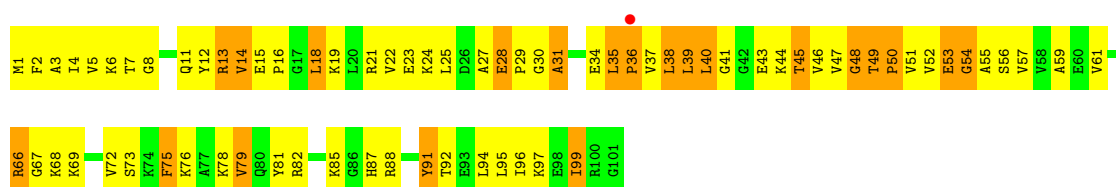
- Molecule 40: 50S ribosomal protein L20

Chain YU:



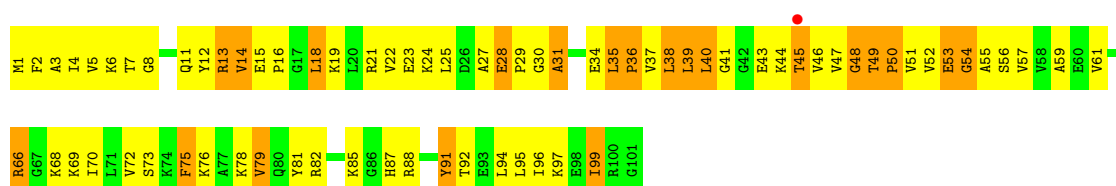
- Molecule 41: 50S ribosomal protein L21

Chain RV:



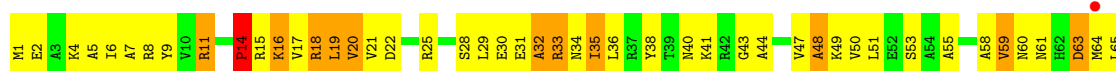
- Molecule 41: 50S ribosomal protein L21

Chain YV:



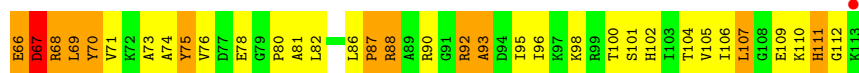
- Molecule 42: 50S ribosomal protein L22

Chain RW:



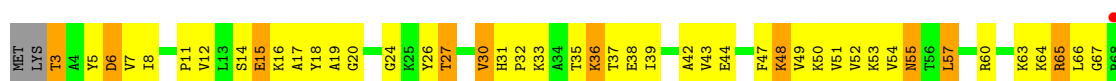
• Molecule 42: 50S ribosomal protein L22

Chain YW:



• Molecule 43: 50S ribosomal protein L23

Chain RX:



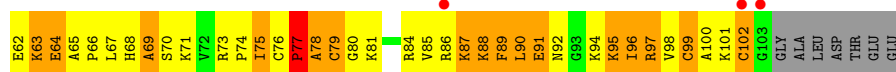
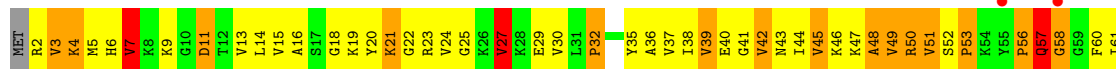
• Molecule 43: 50S ribosomal protein L23

Chain YX:



• Molecule 44: 50S ribosomal protein L24

Chain RY:

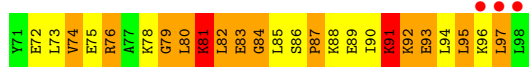


• Molecule 44: 50S ribosomal protein L24

Chain YY:

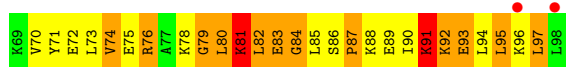






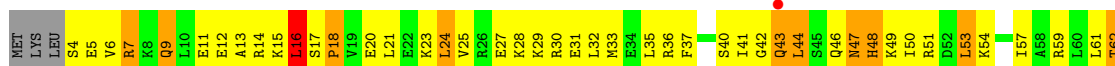
- Molecule 47: 50S ribosomal protein L28

Chain Y1:



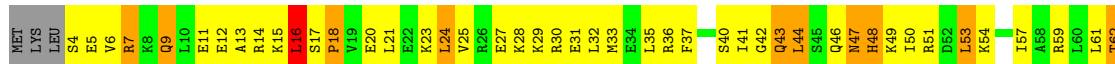
- Molecule 48: 50S ribosomal protein L29

Chain R2:



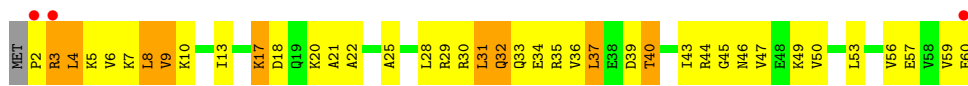
- Molecule 48: 50S ribosomal protein L29

Chain Y2:



- Molecule 49: 50S ribosomal protein L30

Chain R3:



- Molecule 49: 50S ribosomal protein L30

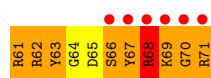
Chain Y3:



- Molecule 50: 50S ribosomal protein L31

Chain R4:





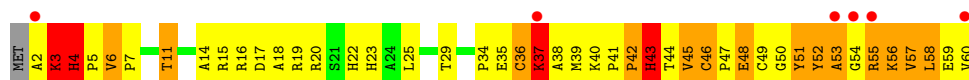
- Molecule 50: 50S ribosomal protein L31

Chain Y4:



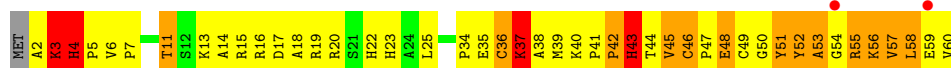
- Molecule 51: 50S ribosomal protein L32

Chain R5:



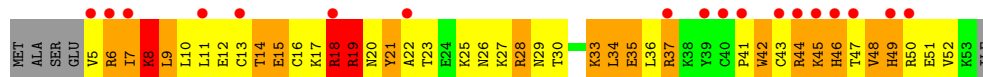
- Molecule 51: 50S ribosomal protein L32

Chain Y5:



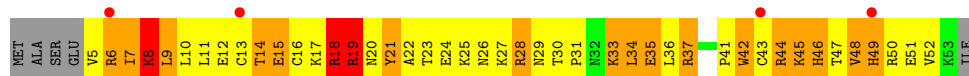
- Molecule 52: 50S ribosomal protein L33

Chain R6:



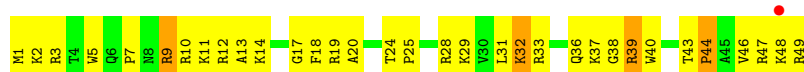
- Molecule 52: 50S ribosomal protein L33

Chain Y6:



- Molecule 53: 50S ribosomal protein L34

Chain R7:



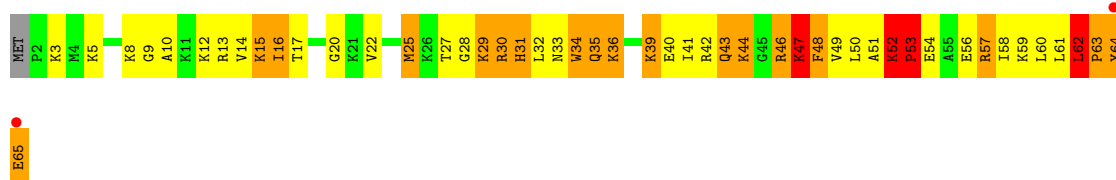
- Molecule 53: 50S ribosomal protein L34

Chain Y7:



- Molecule 54: 50S ribosomal protein L35

Chain R8:



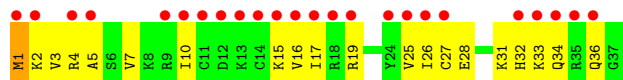
- Molecule 54: 50S ribosomal protein L35

Chain Y8:



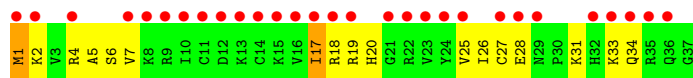
- Molecule 55: 50S ribosomal protein L36

Chain R9:



- Molecule 55: 50S ribosomal protein L36

Chain Y9:



- Molecule 56: tRNA acceptor end mimic

Chain Z6:



- Molecule 56: tRNA acceptor end mimic

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	210.38Å 451.02Å 621.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 3.92 34.83 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.77-3.92) 99.8 (34.83-3.80)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.265 0.207 , 0.265	Depositor DCC
R_{free} test set	23100 reflections (4.42%)	DCC
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , -1.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 573835 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	291868	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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, 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	0.84	19/36098 (0.1%)	1.59	747/56341 (1.3%)
1	XA	0.89	21/36101 (0.1%)	1.65	830/56346 (1.5%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.36	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	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	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	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	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	0.47	0/991	0.79	2/1327 (0.2%)
12	XL	0.52	1/991 (0.1%)	0.83	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.40	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.51	0/1836	1.00	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.39	0/185	0.71	0/285
23	XX	0.51	0/160	0.76	0/246
24	QY	0.52	0/311	0.87	0/483
24	XY	0.52	0/311	0.89	0/483
25	RA	1.03	104/69521 (0.1%)	1.85	2693/108529 (2.5%)
25	YA	1.19	254/69543 (0.4%)	1.98	3497/108563 (3.2%)
26	RB	0.82	1/2878 (0.0%)	1.59	60/4490 (1.3%)
26	YB	0.86	1/2878 (0.0%)	1.72	76/4490 (1.7%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.44	0/1151	0.77	1/1558 (0.1%)
32	YI	0.44	0/1151	0.76	0/1558
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	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.90	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.45	0/892	0.82	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	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.44	0/1493	0.70	0/2026
45	YZ	0.43	0/1493	0.70	0/2026
46	R0	0.52	0/657	0.73	0/874
46	Y0	0.55	0/657	0.80	1/874 (0.1%)
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.84	1/771 (0.1%)
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.47	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	R9	0.35	0/310	0.59	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.78	0/40	1.78	1/60 (1.7%)
56	Z8	0.79	0/40	1.81	1/60 (1.7%)
All	All	0.89	404/316298 (0.1%)	1.59	7980/472872 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
45	YZ	0	1

The worst 5 of 404 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	1201	A	C3'-C2'	12.06	1.66	1.52
1	XA	1054	C	C4'-C3'	11.40	1.65	1.53
25	YA	783	A	N7-C5	-11.18	1.32	1.39
25	YA	793	A	N7-C5	-10.74	1.32	1.39
25	YA	783	A	C5-C6	-10.48	1.31	1.41

The worst 5 of 7980 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	761	A	N1-C6-N6	19.13	130.07	118.60
25	RA	2490	G	C6-C5-N7	-18.87	119.08	130.40
25	RA	783	A	C6-C5-N7	-17.19	120.27	132.30
25	RA	783	A	N1-C6-N6	16.89	128.74	118.60
25	YA	783	A	N1-C6-N6	16.68	128.61	118.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	YZ	181	GLU	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	1130	0
1	XA	32249	0	16279	1064	1
2	QB	1924	0	1975	289	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	205	0
3	XC	1605	0	1668	211	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	QD	1703	0	1764	253	0
4	XD	1703	0	1765	214	0
5	QE	1155	0	1213	182	0
5	XE	1155	0	1213	147	0
6	QF	843	0	857	94	0
6	XF	843	0	857	99	0
7	QG	1257	0	1296	151	0
7	XG	1257	0	1294	142	0
8	QH	1116	0	1175	167	0
8	XH	1116	0	1177	150	0
9	QI	1010	0	1037	144	0
9	XI	1010	0	1037	152	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	132	0
11	QK	885	0	904	103	0
11	XK	885	0	904	107	0
12	QL	975	0	1062	100	0
12	XL	975	0	1062	111	0
13	QM	964	0	1034	169	0
13	XM	964	0	1034	163	0
14	QN	492	0	530	102	0
14	XN	492	0	530	99	0
15	QO	734	0	771	76	0
15	XO	734	0	771	78	0
16	QP	705	0	725	120	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	84	0
17	XQ	834	0	904	81	0
18	QR	574	0	644	66	0
18	XR	574	0	644	66	0
19	QS	674	0	699	109	0
19	XS	674	0	699	132	0
20	QT	763	0	860	108	0
20	XT	763	0	861	108	0
21	QU	217	0	234	30	0
21	XU	217	0	234	26	0
22	QV	1644	0	836	44	0
22	XV	1644	0	836	29	0
23	QX	167	0	87	13	0
23	XX	145	0	75	9	0
24	QY	303	0	154	11	0
24	XY	303	0	154	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	RA	62071	0	31285	1926	0
25	YA	62091	0	31293	1989	0
26	RB	2573	0	1306	121	0
26	YB	2573	0	1306	103	0
27	RD	2115	0	2195	324	0
27	YD	2115	0	2195	332	0
28	RE	1568	0	1634	270	0
28	YE	1568	0	1634	263	0
29	RF	1585	0	1632	178	0
29	YF	1585	0	1632	178	0
30	RG	1474	0	1535	201	0
30	YG	1474	0	1535	194	0
31	RH	1307	0	1382	226	0
31	YH	1307	0	1382	228	0
32	RI	1136	0	1223	79	1
32	YI	1136	0	1223	72	0
33	RN	1104	0	1180	200	0
33	YN	1104	0	1180	189	0
34	RO	933	0	996	126	0
34	YO	933	0	996	125	0
35	RP	1145	0	1228	256	0
35	YP	1145	0	1228	244	0
36	RQ	1122	0	1179	157	0
36	YQ	1122	0	1178	165	0
37	RR	968	0	1033	115	0
37	YR	968	0	1033	117	0
38	RS	882	0	943	166	0
38	YS	882	0	943	159	0
39	RT	1141	0	1202	151	0
39	YT	1141	0	1202	155	0
40	RU	964	0	1022	130	0
40	YU	964	0	1022	142	0
41	RV	779	0	852	130	0
41	YV	779	0	852	131	0
42	RW	900	0	964	100	0
42	YW	900	0	964	108	0
43	RX	725	0	778	70	0
43	YX	725	0	778	74	0
44	RY	785	0	878	167	0
44	YY	785	0	878	160	0
45	RZ	1461	0	1493	81	0
45	YZ	1461	0	1493	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	R0	648	0	671	55	0
46	Y0	648	0	672	51	0
47	R1	763	0	848	142	0
47	Y1	763	0	848	142	0
48	R2	581	0	629	83	0
48	Y2	581	0	629	78	0
49	R3	469	0	518	41	0
49	Y3	469	0	518	46	0
50	R4	581	0	574	159	0
50	Y4	581	0	574	167	0
51	R5	459	0	480	73	0
51	Y5	459	0	480	76	0
52	R6	424	0	450	90	0
52	Y6	424	0	450	97	0
53	R7	430	0	480	42	0
53	Y7	430	0	480	40	0
54	R8	517	0	582	104	0
54	Y8	517	0	582	105	0
55	R9	307	0	335	23	0
55	Y9	307	0	336	24	0
56	Z6	74	0	51	10	0
56	Z8	74	0	51	10	0
57	QA	64	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	239	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	72	0	0	1	0
57	XB	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XX	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	269	0	0	1	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	1	0	0	0	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	R9	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y9	1	0	0	0	0
59	XX	22	0	12	1	0
All	All	291868	0	198240	17856	1

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 37.

The worst 5 of 17856 close contacts within the same asymmetric unit are listed below.

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

All (1) 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)
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.02	0.18

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	13
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	13
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	23
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	1	23
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	1	21
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	1	17
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	20
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	1	17
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	24
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	24
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	21
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	24
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	16
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	16
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	13
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	13
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	23
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	19
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	29
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	2	34
12	QL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	1	14
12	XL	123/132 (93%)	83 (68%)	24 (20%)	16 (13%)	0	12
13	QM	119/126 (94%)	71 (60%)	29 (24%)	19 (16%)	0	7
13	XM	119/126 (94%)	72 (60%)	25 (21%)	22 (18%)	0	5
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	3
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	3
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	33
15	XO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	2	33
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	11
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	27
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	27
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	14
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	14
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	2
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	2
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	4
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	4
21	QU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	6
21	XU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	6
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	2	33
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	2	33
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	20
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	20
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	15
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	15
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
32	RI	144/148 (97%)	99 (69%)	32 (22%)	13 (9%)	1	24
32	YI	144/148 (97%)	93 (65%)	30 (21%)	21 (15%)	0	9
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	7
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	7
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	30
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	30
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	3
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	3
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	20
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	20
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	14
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	6
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	6
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	9
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	9
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	29
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	29
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	20
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	20
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	13
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	13
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	40
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	40
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	2
44	YY	100/110 (91%)	57 (57%)	16 (16%)	27 (27%)	0	1
45	RZ	181/206 (88%)	113 (62%)	46 (25%)	22 (12%)	1	14
45	YZ	181/206 (88%)	128 (71%)	36 (20%)	17 (9%)	1	23
46	R0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	3	43
46	Y0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	3	43
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
48	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	11
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	11
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	41
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	41
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	2
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	2
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	1
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	36
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	36
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	5
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	5
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7621 (66%)	2356 (20%)	1493 (13%)	0	12

5 of 1493 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	43
2	XB	205/220 (93%)	181 (88%)	24 (12%)	8	43
3	QC	159/188 (85%)	143 (90%)	16 (10%)	11	51
3	XC	159/188 (85%)	143 (90%)	16 (10%)	11	51
4	QD	180/181 (99%)	160 (89%)	20 (11%)	9	46
4	XD	180/181 (99%)	165 (92%)	15 (8%)	16	62
5	QE	116/123 (94%)	107 (92%)	9 (8%)	18	64
5	XE	116/123 (94%)	107 (92%)	9 (8%)	18	64
6	QF	90/90 (100%)	76 (84%)	14 (16%)	4	28
6	XF	90/90 (100%)	76 (84%)	14 (16%)	4	28
7	QG	126/127 (99%)	115 (91%)	11 (9%)	15	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	XG	126/127 (99%)	115 (91%)	11 (9%)	15	59
8	QH	119/119 (100%)	106 (89%)	13 (11%)	9	47
8	XH	119/119 (100%)	106 (89%)	13 (11%)	9	47
9	QI	98/99 (99%)	87 (89%)	11 (11%)	9	45
9	XI	98/99 (99%)	87 (89%)	11 (11%)	9	45
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	14	57
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	14	57
11	QK	90/99 (91%)	81 (90%)	9 (10%)	11	52
11	XK	90/99 (91%)	81 (90%)	9 (10%)	11	52
12	QL	104/109 (95%)	90 (86%)	14 (14%)	6	36
12	XL	104/109 (95%)	89 (86%)	15 (14%)	5	32
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	25
13	XM	97/101 (96%)	81 (84%)	16 (16%)	3	25
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	18
14	XN	49/50 (98%)	44 (90%)	5 (10%)	11	51
15	QO	79/80 (99%)	73 (92%)	6 (8%)	19	66
15	XO	79/80 (99%)	73 (92%)	6 (8%)	19	66
16	QP	72/74 (97%)	63 (88%)	9 (12%)	7	40
16	XP	72/74 (97%)	63 (88%)	9 (12%)	7	40
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	25	73
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	25	73
18	QR	61/77 (79%)	54 (88%)	7 (12%)	8	44
18	XR	61/77 (79%)	54 (88%)	7 (12%)	8	44
19	QS	73/80 (91%)	62 (85%)	11 (15%)	4	30
19	XS	73/80 (91%)	62 (85%)	11 (15%)	4	30
20	QT	76/82 (93%)	68 (90%)	8 (10%)	10	49
20	XT	76/82 (93%)	68 (90%)	8 (10%)	10	49
21	QU	20/22 (91%)	19 (95%)	1 (5%)	34	80
21	XU	20/22 (91%)	19 (95%)	1 (5%)	34	80
27	RD	214/218 (98%)	177 (83%)	37 (17%)	3	21
27	YD	214/218 (98%)	178 (83%)	36 (17%)	3	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	11
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	9
29	RF	161/166 (97%)	140 (87%)	21 (13%)	6	38
29	YF	161/166 (97%)	140 (87%)	21 (13%)	6	38
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	27
30	YG	155/156 (99%)	130 (84%)	25 (16%)	3	27
31	RH	142/148 (96%)	114 (80%)	28 (20%)	2	15
31	YH	142/148 (96%)	114 (80%)	28 (20%)	2	15
32	RI	122/124 (98%)	94 (77%)	28 (23%)	1	9
32	YI	122/124 (98%)	92 (75%)	30 (25%)	1	8
33	RN	117/119 (98%)	98 (84%)	19 (16%)	3	26
33	YN	117/119 (98%)	98 (84%)	19 (16%)	3	26
34	RO	100/100 (100%)	90 (90%)	10 (10%)	11	52
34	YO	100/100 (100%)	90 (90%)	10 (10%)	11	52
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	9
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	9
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	26
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	3	26
37	RR	101/101 (100%)	84 (83%)	17 (17%)	3	24
37	YR	101/101 (100%)	84 (83%)	17 (17%)	3	24
38	RS	87/88 (99%)	74 (85%)	13 (15%)	4	30
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	30
39	RT	120/127 (94%)	97 (81%)	23 (19%)	2	16
39	YT	120/127 (94%)	97 (81%)	23 (19%)	2	16
40	RU	93/94 (99%)	80 (86%)	13 (14%)	5	34
40	YU	93/94 (99%)	80 (86%)	13 (14%)	5	34
41	RV	82/82 (100%)	71 (87%)	11 (13%)	6	36
41	YV	82/82 (100%)	71 (87%)	11 (13%)	6	36
42	RW	92/92 (100%)	77 (84%)	15 (16%)	3	26
42	YW	92/92 (100%)	77 (84%)	15 (16%)	3	26
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	30
44	RY	85/91 (93%)	70 (82%)	15 (18%)	3	21
44	YY	85/91 (93%)	70 (82%)	15 (18%)	3	21
45	RZ	162/179 (90%)	133 (82%)	29 (18%)	2	20
45	YZ	162/179 (90%)	131 (81%)	31 (19%)	2	16
46	R0	65/67 (97%)	58 (89%)	7 (11%)	9	48
46	Y0	65/67 (97%)	58 (89%)	7 (11%)	9	48
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	18
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	18
48	R2	64/67 (96%)	57 (89%)	7 (11%)	9	47
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	9	47
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	11
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	11
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	5
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	5
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	9
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	9
52	R6	48/52 (92%)	38 (79%)	10 (21%)	2	13
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	2	13
53	R7	42/42 (100%)	39 (93%)	3 (7%)	21	68
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	21	68
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	6
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	6
55	R9	34/34 (100%)	32 (94%)	2 (6%)	28	75
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	28	75
All	All	9702/10066 (96%)	8266 (85%)	1436 (15%)	4	31

5 of 1436 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	8	LEU
7	XG	111	ARG
45	YZ	141	VAL

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Mol	Chain	Res	Type
50	R4	50	VAL
2	XB	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
43	RX	55	ASN
2	XB	135	GLN
43	YX	55	ASN
43	RX	87	GLN
48	R2	47	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	385 (25%)	49 (3%)
1	XA	1498/1522 (98%)	378 (25%)	60 (4%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	5 (71%)	1 (14%)
23	XX	6/25 (24%)	3 (50%)	0
24	QY	13/18 (72%)	5 (38%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2879/2916 (98%)	835 (29%)	82 (2%)
25	YA	2880/2916 (98%)	865 (30%)	93 (3%)
26	RB	119/122 (97%)	32 (26%)	3 (2%)
26	YB	119/122 (97%)	42 (35%)	2 (1%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9186/9366 (98%)	2615 (28%)	294 (3%)

5 of 2615 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	7	G
1	QA	9	G
1	QA	10	A
1	QA	22	G
1	QA	32	A

5 of 294 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2848	G
1	XA	595	G
25	YA	2238	G
26	RB	108	C
1	XA	328	C

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	3.01	6 (25%)	34,39,42	3.50	12 (35%)
24	1MG	XY	37	24	24,26,27	3.01	6 (25%)	34,39,42	3.63	12 (35%)
56	PPU	Z6	76	25,56	38,40,41	2.43	9 (23%)	54,57,60	2.62	14 (25%)
56	PPU	Z8	76	25,56	38,40,41	2.42	8 (21%)	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
56	PPU	Z6	76	25,56	-	0/26/43/44	0/4/4/4
56	PPU	Z8	76	25,56	-	0/26/43/44	0/4/4/4

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.20	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.16	1.41	1.23
24	XY	37	1MG	C4-N3	8.22	1.49	1.35
24	QY	37	1MG	C4-N3	8.20	1.49	1.35
24	QY	37	1MG	C2-N1	7.44	1.47	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	XY	37	1MG	C6-C5-N7	-14.13	133.49	134.24
24	QY	37	1MG	C6-C5-N7	-13.30	133.53	134.24
24	XY	37	1MG	C6-N1-C2	12.01	124.00	120.71
24	QY	37	1MG	C6-N1-C2	11.88	123.97	120.71
56	Z8	76	PPU	N3-C2-N1	-8.54	121.38	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 681 ligands modelled in this entry, 680 are monoatomic - leaving 1 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	$\# Z > 2$
59	A	XX	101	-	22,24,25	0.96	1 (4%)	32,35,38	1.12	3 (9%)

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
59	A	XX	101	-	-	0/8/25/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	XX	101	A	C1'-N9	2.36	1.56	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	XX	101	A	C1'-N9-C4	3.28	132.29	126.64
59	XX	101	A	C5-C6-N6	2.75	126.94	120.72
59	XX	101	A	C8-N9-C4	-2.54	104.89	106.96

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%)	-0.08	38 (2%) 54 41	3, 59, 153, 236	0
1	XA	1500/1522 (98%)	-0.13	33 (2%) 59 44	1, 53, 148, 240	0
2	QB	237/256 (92%)	0.43	13 (5%) 24 20	41, 113, 151, 177	0
2	XB	237/256 (92%)	0.29	5 (2%) 60 46	21, 96, 142, 157	0
3	QC	205/239 (85%)	0.42	13 (6%) 19 18	22, 104, 139, 161	0
3	XC	205/239 (85%)	0.09	3 (1%) 70 54	22, 79, 122, 161	0
4	QD	208/209 (99%)	0.12	3 (1%) 72 56	8, 69, 116, 153	0
4	XD	208/209 (99%)	0.23	4 (1%) 64 48	16, 74, 114, 159	0
5	QE	151/162 (93%)	0.49	3 (1%) 62 46	32, 95, 133, 161	0
5	XE	151/162 (93%)	0.02	0 100 100	20, 63, 108, 140	0
6	QF	101/101 (100%)	0.10	0 100 100	15, 68, 105, 139	0
6	XF	101/101 (100%)	0.33	2 (1%) 62 46	4, 66, 107, 134	0
7	QG	155/156 (99%)	0.30	8 (5%) 26 22	26, 89, 133, 154	0
7	XG	155/156 (99%)	0.28	7 (4%) 32 26	28, 83, 124, 148	0
8	QH	138/138 (100%)	0.15	1 (0%) 84 72	21, 79, 122, 132	0
8	XH	138/138 (100%)	0.04	0 100 100	14, 68, 108, 133	0
9	QI	127/128 (99%)	0.55	7 (5%) 24 20	49, 102, 138, 161	0
9	XI	127/128 (99%)	0.34	3 (2%) 56 42	13, 91, 134, 162	0
10	QJ	99/105 (94%)	0.98	18 (18%) 2 3	57, 108, 148, 192	0
10	XJ	99/105 (94%)	0.70	9 (9%) 9 11	40, 94, 140, 165	0
11	QK	119/129 (92%)	0.44	8 (6%) 17 17	25, 72, 127, 150	0
11	XK	119/129 (92%)	0.22	4 (3%) 43 33	4, 59, 109, 129	0
12	QL	125/132 (94%)	0.37	10 (8%) 12 13	15, 64, 124, 159	0
12	XL	125/132 (94%)	0.13	1 (0%) 83 69	6, 48, 102, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.36	4 (3%) 44 34	48, 101, 151, 159	0
13	XM	121/126 (96%)	0.26	4 (3%) 44 34	38, 85, 119, 158	0
14	QN	60/61 (98%)	0.77	2 (3%) 44 34	52, 108, 148, 159	0
14	XN	60/61 (98%)	0.20	0 100 100	33, 72, 116, 130	0
15	QO	88/89 (98%)	0.14	1 (1%) 77 61	17, 71, 119, 151	0
15	XO	88/89 (98%)	0.17	0 100 100	7, 59, 102, 127	0
16	QP	84/88 (95%)	0.12	1 (1%) 75 60	14, 59, 114, 134	0
16	XP	84/88 (95%)	0.17	2 (2%) 56 42	28, 68, 122, 176	0
17	QQ	100/105 (95%)	0.31	3 (3%) 48 36	30, 70, 116, 148	0
17	XQ	100/105 (95%)	0.28	2 (2%) 62 46	19, 71, 106, 144	0
18	QR	70/88 (79%)	0.19	1 (1%) 72 56	22, 70, 125, 150	0
18	XR	70/88 (79%)	0.13	1 (1%) 72 56	9, 65, 106, 140	0
19	QS	84/93 (90%)	0.96	11 (13%) 4 5	69, 116, 148, 161	0
19	XS	84/93 (90%)	0.31	3 (3%) 41 32	48, 87, 132, 145	0
20	QT	99/106 (93%)	0.29	2 (2%) 62 46	16, 73, 113, 135	0
20	XT	99/106 (93%)	0.40	5 (5%) 27 23	23, 77, 124, 157	0
21	QU	25/27 (92%)	1.96	9 (36%) 1 2	31, 92, 141, 158	0
21	XU	25/27 (92%)	1.38	6 (24%) 1 3	32, 83, 121, 143	0
22	QV	77/77 (100%)	0.18	1 (1%) 74 58	21, 85, 147, 180	0
22	XV	77/77 (100%)	0.16	3 (3%) 37 30	6, 64, 119, 169	0
23	QX	8/25 (32%)	0.70	2 (25%) 1 3	50, 74, 138, 138	0
23	XX	7/25 (28%)	0.68	0 100 100	18, 51, 81, 90	0
24	QY	14/18 (77%)	1.45	3 (21%) 1 3	106, 175, 223, 238	0
24	XY	14/18 (77%)	1.86	3 (21%) 1 3	55, 149, 189, 217	0
25	RA	2882/2916 (98%)	-0.12	108 (3%) 39 31	0, 30, 174, 252	0
25	YA	2883/2916 (98%)	-0.20	89 (3%) 47 36	0, 20, 159, 242	0
26	RB	120/122 (98%)	0.08	0 100 100	39, 82, 133, 170	0
26	YB	120/122 (98%)	-0.08	1 (0%) 83 69	16, 68, 104, 146	0
27	RD	272/276 (98%)	0.03	2 (0%) 84 72	0, 34, 82, 147	0
27	YD	272/276 (98%)	-0.04	0 100 100	0, 18, 64, 125	0
28	RE	205/206 (99%)	0.08	2 (0%) 79 64	1, 49, 112, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.08	4 (1%) 62 46	0, 47, 104, 155	0
29	RF	202/210 (96%)	-0.00	1 (0%) 88 77	0, 55, 108, 143	0
29	YF	202/210 (96%)	-0.05	0 100 100	0, 32, 96, 124	0
30	RG	181/182 (99%)	0.87	18 (9%) 8 10	39, 113, 160, 177	0
30	YG	181/182 (99%)	0.38	6 (3%) 44 34	18, 92, 131, 177	0
31	RH	170/180 (94%)	0.85	15 (8%) 10 12	45, 112, 156, 177	0
31	YH	170/180 (94%)	0.14	1 (0%) 86 74	11, 66, 116, 131	0
32	RI	146/148 (98%)	0.07	4 (2%) 52 39	3, 77, 124, 177	0
32	YI	146/148 (98%)	0.02	2 (1%) 72 56	3, 64, 125, 140	0
33	RN	138/140 (98%)	0.24	1 (0%) 84 72	6, 61, 118, 144	0
33	YN	138/140 (98%)	-0.04	0 100 100	4, 45, 98, 131	0
34	RO	122/122 (100%)	-0.04	0 100 100	2, 42, 80, 107	0
34	YO	122/122 (100%)	-0.04	0 100 100	2, 41, 82, 126	0
35	RP	150/150 (100%)	0.27	8 (5%) 25 22	1, 58, 130, 158	0
35	YP	150/150 (100%)	0.13	2 (1%) 74 58	1, 46, 101, 160	0
36	RQ	141/141 (100%)	0.17	3 (2%) 60 46	3, 58, 103, 133	0
36	YQ	141/141 (100%)	0.01	0 100 100	0, 47, 97, 115	0
37	RR	118/118 (100%)	-0.08	0 100 100	1, 34, 87, 136	0
37	YR	118/118 (100%)	0.03	1 (0%) 83 69	2, 38, 98, 136	0
38	RS	111/112 (99%)	0.19	0 100 100	23, 83, 117, 138	0
38	YS	111/112 (99%)	0.22	0 100 100	13, 73, 115, 168	0
39	RT	137/146 (93%)	0.20	0 100 100	8, 58, 130, 152	0
39	YT	137/146 (93%)	0.11	3 (2%) 59 44	9, 56, 122, 170	0
40	RU	117/118 (99%)	0.12	2 (1%) 67 52	1, 49, 113, 166	0
40	YU	117/118 (99%)	-0.12	2 (1%) 67 52	1, 31, 97, 145	0
41	RV	101/101 (100%)	0.13	1 (0%) 79 64	1, 68, 120, 193	0
41	YV	101/101 (100%)	0.02	1 (0%) 79 64	1, 45, 97, 171	0
42	RW	113/113 (100%)	0.18	3 (2%) 52 39	2, 34, 95, 131	0
42	YW	113/113 (100%)	0.07	1 (0%) 81 67	1, 24, 84, 155	0
43	RX	92/96 (95%)	0.14	2 (2%) 59 44	4, 44, 91, 131	0
43	YX	92/96 (95%)	0.17	0 100 100	1, 25, 64, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.58	5 (4%) 28 23	10, 84, 138, 174	0
44	YY	102/110 (92%)	-0.03	2 (1%) 62 46	2, 50, 106, 160	0
45	RZ	183/206 (88%)	0.27	3 (1%) 68 53	20, 88, 136, 160	0
45	YZ	183/206 (88%)	0.17	4 (2%) 59 44	20, 78, 137, 167	0
46	R0	82/85 (96%)	-0.07	1 (1%) 75 60	6, 44, 83, 137	0
46	Y0	82/85 (96%)	-0.07	0 100 100	2, 32, 70, 88	0
47	R1	97/98 (98%)	0.53	5 (5%) 26 22	2, 47, 126, 202	0
47	Y1	97/98 (98%)	0.34	6 (6%) 20 18	0, 32, 114, 142	0
48	R2	69/72 (95%)	0.06	1 (1%) 72 56	8, 72, 116, 128	0
48	Y2	69/72 (95%)	-0.05	0 100 100	0, 39, 97, 137	0
49	R3	59/60 (98%)	0.26	3 (5%) 27 23	7, 60, 126, 152	0
49	Y3	59/60 (98%)	-0.11	0 100 100	3, 40, 87, 128	0
50	R4	71/71 (100%)	0.98	12 (16%) 2 4	78, 145, 193, 235	0
50	Y4	71/71 (100%)	0.62	5 (7%) 16 15	69, 122, 166, 194	0
51	R5	59/60 (98%)	0.41	6 (10%) 7 9	4, 39, 139, 166	0
51	Y5	59/60 (98%)	0.27	2 (3%) 43 33	1, 40, 132, 156	0
52	R6	49/54 (90%)	1.84	18 (36%) 1 2	48, 122, 152, 191	0
52	Y6	49/54 (90%)	0.81	4 (8%) 12 12	47, 108, 148, 175	0
53	R7	49/49 (100%)	0.19	1 (2%) 62 46	1, 27, 75, 161	0
53	Y7	49/49 (100%)	0.23	1 (2%) 62 46	1, 15, 84, 140	0
54	R8	64/65 (98%)	0.25	2 (3%) 47 36	4, 41, 94, 153	0
54	Y8	64/65 (98%)	0.13	0 100 100	2, 34, 85, 138	0
55	R9	37/37 (100%)	3.09	24 (64%) 0 1	53, 103, 154, 162	0
55	Y9	37/37 (100%)	2.80	29 (78%) 0 1	60, 98, 136, 154	0
56	Z6	3/3 (100%)	3.40	1 (33%) 1 2	15, 15, 17, 30	0
56	Z8	3/3 (100%)	4.20	1 (33%) 1 2	10, 10, 19, 22	0
All	All	20874/21494 (97%)	0.09	681 (3%) 44 34	0, 55, 139, 252	0

The worst 5 of 681 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	2173	A	12.6
56	Z8	76	PPU	11.6

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Mol	Chain	Res	Type	RSRZ
25	RA	1058	G	11.2
25	RA	1057	A	10.6
25	RA	1094	U	10.3

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
24	1MG	QY	37	24/25	0.19	-	130,130,130,130	0
24	1MG	XY	37	24/25	0.23	-	56,56,56,56	0
56	PPU	Z8	76	37/38	0.38	-	10,10,10,10	0
56	PPU	Z6	76	37/38	0.32	-	14,14,14,14	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
57	MG	YA	3180	1/1	0.51	-	38,38,38,38	0
57	MG	YA	3161	1/1	0.20	-	1,1,1,1	0
57	MG	YA	3017	1/1	0.18	-	1,1,1,1	0
57	MG	XA	1627	1/1	0.27	-	14,14,14,14	0
57	MG	RA	3128	1/1	0.47	-	7,7,7,7	0
57	MG	YA	3091	1/1	0.38	-	13,13,13,13	0
57	MG	YA	3032	1/1	0.31	-	1,1,1,1	0
57	MG	YA	3226	1/1	0.40	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3073	1/1	0.40	-	2,2,2,2	0
57	MG	QA	1644	1/1	0.29	-	4,4,4,4	0
57	MG	RA	3186	1/1	0.19	-	8,8,8,8	0
57	MG	QA	1618	1/1	0.53	-	3,3,3,3	0
57	MG	YA	3196	1/1	0.54	-	1,1,1,1	0
57	MG	YA	3191	1/1	0.07	-	7,7,7,7	0
57	MG	YA	3148	1/1	0.11	-	7,7,7,7	0
57	MG	RA	3063	1/1	0.94	-	3,3,3,3	0
57	MG	YA	3166	1/1	0.33	-	4,4,4,4	0
57	MG	RA	3158	1/1	0.25	-	15,15,15,15	0
57	MG	XA	1642	1/1	0.62	-	5,5,5,5	0
57	MG	YA	3115	1/1	0.35	-	4,4,4,4	0
57	MG	RA	3034	1/1	0.93	-	9,9,9,9	0
57	MG	XA	1651	1/1	0.27	-	25,25,25,25	0
57	MG	YA	3205	1/1	0.13	-	10,10,10,10	0
57	MG	RA	3053	1/1	0.15	-	2,2,2,2	0
57	MG	RA	3003	1/1	1.01	-	5,5,5,5	0
57	MG	RA	3121	1/1	0.74	-	5,5,5,5	0
57	MG	YA	3265	1/1	1.06	-	4,4,4,4	0
57	MG	YA	3051	1/1	0.42	-	3,3,3,3	0
57	MG	RA	3111	1/1	0.43	-	11,11,11,11	0
57	MG	XA	1648	1/1	0.54	-	3,3,3,3	0
57	MG	YA	3242	1/1	0.76	-	4,4,4,4	0
57	MG	YA	3026	1/1	1.18	-	1,1,1,1	0
57	MG	XA	1666	1/1	0.27	-	50,50,50,50	0
57	MG	YA	3024	1/1	0.46	-	50,50,50,50	0
57	MG	RA	3154	1/1	0.11	-	11,11,11,11	0
57	MG	QA	1604	1/1	0.26	-	0,0,0,0	0
57	MG	RA	3210	1/1	0.18	-	45,45,45,45	0
57	MG	YA	3108	1/1	0.49	-	1,1,1,1	0
57	MG	RA	3120	1/1	0.23	-	1,1,1,1	0
57	MG	YA	3055	1/1	0.28	-	0,0,0,0	0
57	MG	XA	1632	1/1	0.82	-	14,14,14,14	0
57	MG	RA	3118	1/1	0.23	-	2,2,2,2	0
57	MG	RA	3193	1/1	0.34	-	22,22,22,22	0
57	MG	YA	3208	1/1	0.20	-	15,15,15,15	0
57	MG	YA	3245	1/1	0.29	-	2,2,2,2	0
57	MG	RA	3194	1/1	0.23	-	6,6,6,6	0
57	MG	RA	3151	1/1	0.34	-	9,9,9,9	0
57	MG	YA	3128	1/1	0.53	-	12,12,12,12	0
57	MG	YA	3018	1/1	0.68	-	3,3,3,3	0
57	MG	RA	3011	1/1	0.19	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1665	1/1	0.53	-	7,7,7,7	0
57	MG	RA	3004	1/1	0.95	-	10,10,10,10	0
57	MG	XA	1622	1/1	0.11	-	7,7,7,7	0
57	MG	YA	3111	1/1	0.20	-	15,15,15,15	0
57	MG	YA	3044	1/1	0.32	-	6,6,6,6	0
57	MG	YA	3162	1/1	0.22	-	0,0,0,0	0
57	MG	YA	3154	1/1	0.23	-	1,1,1,1	0
57	MG	YA	3178	1/1	0.19	-	2,2,2,2	0
57	MG	YA	3075	1/1	0.26	-	0,0,0,0	0
57	MG	YA	3117	1/1	0.93	-	6,6,6,6	0
57	MG	QA	1636	1/1	0.11	-	16,16,16,16	0
57	MG	RA	3179	1/1	0.34	-	4,4,4,4	0
57	MG	RA	3088	1/1	0.59	-	15,15,15,15	0
57	MG	RA	3049	1/1	1.22	-	13,13,13,13	0
57	MG	YA	3143	1/1	0.15	-	8,8,8,8	0
57	MG	XA	1635	1/1	0.56	-	4,4,4,4	0
57	MG	YA	3257	1/1	0.22	-	3,3,3,3	0
57	MG	RA	3012	1/1	0.52	-	4,4,4,4	0
57	MG	YA	3213	1/1	0.15	-	19,19,19,19	0
57	MG	YA	3218	1/1	0.34	-	5,5,5,5	0
57	MG	RA	3138	1/1	0.82	-	29,29,29,29	0
57	MG	RA	3065	1/1	0.37	-	7,7,7,7	0
57	MG	YA	3255	1/1	1.25	-	0,0,0,0	0
57	MG	RA	3032	1/1	1.06	-	50,50,50,50	0
57	MG	YA	3155	1/1	0.38	-	7,7,7,7	0
57	MG	YA	3224	1/1	0.40	-	0,0,0,0	0
57	MG	RA	3205	1/1	0.32	-	12,12,12,12	0
57	MG	RA	3220	1/1	0.29	-	26,26,26,26	0
57	MG	RA	3144	1/1	0.27	-	0,0,0,0	0
57	MG	XA	1631	1/1	0.20	-	31,31,31,31	0
57	MG	RA	3109	1/1	0.21	-	8,8,8,8	0
57	MG	QA	1650	1/1	0.68	-	11,11,11,11	0
57	MG	RA	3191	1/1	0.30	-	67,67,67,67	0
57	MG	RA	3236	1/1	0.43	-	0,0,0,0	0
57	MG	RA	3020	1/1	0.72	-	50,50,50,50	0
57	MG	YA	3207	1/1	0.84	-	7,7,7,7	0
57	MG	RA	3052	1/1	0.87	-	50,50,50,50	0
57	MG	RA	3123	1/1	0.12	-	7,7,7,7	0
57	MG	YA	3006	1/1	0.55	-	3,3,3,3	0
57	MG	XA	1664	1/1	0.27	-	8,8,8,8	0
57	MG	RA	3100	1/1	0.17	-	2,2,2,2	0
57	MG	QA	1655	1/1	0.56	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3133	1/1	0.18	-	0,0,0,0	0
57	MG	YA	3199	1/1	0.10	-	55,55,55,55	0
57	MG	QA	1663	1/1	0.08	-	47,47,47,47	0
58	ZN	XD	301	1/1	0.42	-	50,50,50,50	0
57	MG	QA	1607	1/1	0.11	-	13,13,13,13	0
57	MG	RA	3081	1/1	0.71	-	1,1,1,1	0
57	MG	R0	101	1/1	0.30	-	0,0,0,0	0
57	MG	QA	1614	1/1	0.50	-	9,9,9,9	0
57	MG	YA	3109	1/1	0.34	-	2,2,2,2	0
57	MG	YA	3156	1/1	0.69	-	2,2,2,2	0
57	MG	RA	3038	1/1	0.32	-	8,8,8,8	0
57	MG	XA	1607	1/1	0.33	-	16,16,16,16	0
57	MG	RA	3208	1/1	0.59	-	15,15,15,15	0
58	ZN	R9	101	1/1	0.42	-	145,145,145,145	0
57	MG	RA	3181	1/1	0.17	-	3,3,3,3	0
57	MG	YA	3041	1/1	0.71	-	0,0,0,0	0
57	MG	YA	3233	1/1	0.18	-	7,7,7,7	0
57	MG	YA	3103	1/1	0.17	-	5,5,5,5	0
57	MG	YA	3010	1/1	0.36	-	5,5,5,5	0
57	MG	YA	3023	1/1	0.31	-	2,2,2,2	0
57	MG	YA	3101	1/1	0.57	-	2,2,2,2	0
57	MG	RE	302	1/1	0.25	-	1,1,1,1	0
57	MG	YA	3133	1/1	0.12	-	1,1,1,1	0
57	MG	YA	3266	1/1	0.23	-	2,2,2,2	0
57	MG	RA	3001	1/1	0.55	-	3,3,3,3	0
57	MG	RA	3215	1/1	0.24	-	27,27,27,27	0
57	MG	RA	3051	1/1	0.46	-	7,7,7,7	0
57	MG	YA	3138	1/1	0.15	-	0,0,0,0	0
57	MG	RA	3083	1/1	0.40	-	6,6,6,6	0
57	MG	XA	1658	1/1	0.44	-	9,9,9,9	0
57	MG	RA	3149	1/1	0.15	-	20,20,20,20	0
57	MG	XA	1617	1/1	0.24	-	15,15,15,15	0
57	MG	QA	1648	1/1	0.36	-	12,12,12,12	0
57	MG	RA	3026	1/1	0.59	-	50,50,50,50	0
57	MG	QA	1611	1/1	0.32	-	6,6,6,6	0
57	MG	RA	3070	1/1	0.93	-	0,0,0,0	0
57	MG	YA	3056	1/1	0.18	-	5,5,5,5	0
57	MG	QA	1602	1/1	0.81	-	12,12,12,12	0
57	MG	RA	3098	1/1	0.58	-	14,14,14,14	0
57	MG	YA	3189	1/1	0.48	-	6,6,6,6	0
57	MG	XA	1609	1/1	0.53	-	10,10,10,10	0
57	MG	RA	3091	1/1	0.40	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3247	1/1	0.43	-	14,14,14,14	0
57	MG	RA	3155	1/1	0.42	-	10,10,10,10	0
57	MG	RA	3048	1/1	0.20	-	3,3,3,3	0
57	MG	YA	3164	1/1	0.39	-	8,8,8,8	0
57	MG	RA	3188	1/1	0.31	-	5,5,5,5	0
57	MG	RA	3219	1/1	0.81	-	40,40,40,40	0
57	MG	RA	3168	1/1	0.40	-	1,1,1,1	0
57	MG	YA	3014	1/1	1.20	-	50,50,50,50	0
57	MG	XA	1654	1/1	0.31	-	26,26,26,26	0
57	MG	YA	3012	1/1	1.53	-	50,50,50,50	0
57	MG	YA	3177	1/1	0.20	-	3,3,3,3	0
57	MG	RA	3196	1/1	0.21	-	0,0,0,0	0
57	MG	R8	101	1/1	0.33	-	0,0,0,0	0
57	MG	QA	1646	1/1	0.58	-	10,10,10,10	0
57	MG	RA	3019	1/1	0.39	-	8,8,8,8	0
57	MG	XA	1663	1/1	0.49	-	15,15,15,15	0
57	MG	RA	3235	1/1	0.63	-	1,1,1,1	0
57	MG	YA	3136	1/1	0.16	-	21,21,21,21	0
57	MG	XA	1621	1/1	0.33	-	3,3,3,3	0
57	MG	XA	1630	1/1	0.70	-	10,10,10,10	0
57	MG	YA	3254	1/1	0.62	-	2,2,2,2	0
57	MG	XA	1633	1/1	0.22	-	3,3,3,3	0
57	MG	RA	3239	1/1	0.43	-	14,14,14,14	0
57	MG	YA	3067	1/1	0.29	-	5,5,5,5	0
57	MG	QA	1637	1/1	0.34	-	0,0,0,0	0
57	MG	YA	3015	1/1	1.12	-	50,50,50,50	0
57	MG	YA	3058	1/1	0.50	-	15,15,15,15	0
57	MG	YA	3013	1/1	0.55	-	5,5,5,5	0
57	MG	YA	3228	1/1	0.49	-	17,17,17,17	0
57	MG	RA	3029	1/1	0.34	-	1,1,1,1	0
57	MG	YA	3102	1/1	0.47	-	14,14,14,14	0
57	MG	XA	1603	1/1	0.61	-	8,8,8,8	0
57	MG	RA	3233	1/1	0.62	-	2,2,2,2	0
57	MG	RR	202	1/1	0.29	-	0,0,0,0	0
57	MG	YA	3140	1/1	0.26	-	12,12,12,12	0
57	MG	RA	3167	1/1	0.21	-	3,3,3,3	0
57	MG	RA	3094	1/1	0.45	-	0,0,0,0	0
57	MG	YA	3047	1/1	0.54	-	3,3,3,3	0
57	MG	YA	3082	1/1	0.26	-	3,3,3,3	0
57	MG	YA	3087	1/1	0.64	-	11,11,11,11	0
57	MG	XA	1626	1/1	0.17	-	6,6,6,6	0
57	MG	XA	1656	1/1	1.08	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XX	102	1/1	0.09	-	50,50,50,50	0
57	MG	YA	3078	1/1	0.32	-	2,2,2,2	0
57	MG	YA	3187	1/1	0.16	-	2,2,2,2	0
57	MG	RA	3165	1/1	0.45	-	13,13,13,13	0
57	MG	QA	1605	1/1	1.06	-	7,7,7,7	0
57	MG	YA	3110	1/1	0.11	-	2,2,2,2	0
57	MG	YA	3120	1/1	0.58	-	8,8,8,8	0
57	MG	YA	3119	1/1	0.78	-	8,8,8,8	0
57	MG	YA	3221	1/1	0.46	-	18,18,18,18	0
57	MG	YA	3168	1/1	0.35	-	41,41,41,41	0
57	MG	XA	1638	1/1	0.39	-	20,20,20,20	0
57	MG	RA	3037	1/1	0.48	-	5,5,5,5	0
57	MG	YA	3065	1/1	0.14	-	5,5,5,5	0
57	MG	RA	3101	1/1	0.48	-	11,11,11,11	0
57	MG	QA	1653	1/1	0.08	-	67,67,67,67	0
57	MG	YA	3193	1/1	0.23	-	3,3,3,3	0
57	MG	YA	3262	1/1	0.58	-	8,8,8,8	0
57	MG	YA	3197	1/1	0.16	-	1,1,1,1	0
57	MG	XA	1619	1/1	0.30	-	5,5,5,5	0
57	MG	YA	3034	1/1	0.48	-	2,2,2,2	0
57	MG	RA	3182	1/1	0.22	-	4,4,4,4	0
57	MG	XA	1606	1/1	0.58	-	10,10,10,10	0
57	MG	YA	3098	1/1	0.29	-	1,1,1,1	0
57	MG	YA	3165	1/1	0.22	-	11,11,11,11	0
57	MG	XA	1647	1/1	0.37	-	1,1,1,1	0
57	MG	RA	3116	1/1	0.50	-	9,9,9,9	0
57	MG	YA	3170	1/1	0.14	-	8,8,8,8	0
57	MG	YA	3069	1/1	0.52	-	2,2,2,2	0
57	MG	YA	3074	1/1	0.18	-	11,11,11,11	0
57	MG	YA	3020	1/1	0.89	-	0,0,0,0	0
57	MG	QA	1638	1/1	0.69	-	34,34,34,34	0
57	MG	RA	3084	1/1	0.18	-	4,4,4,4	0
57	MG	YA	3145	1/1	0.35	-	9,9,9,9	0
57	MG	QA	1632	1/1	0.14	-	42,42,42,42	0
57	MG	YA	3022	1/1	0.29	-	1,1,1,1	0
57	MG	XA	1628	1/1	0.52	-	10,10,10,10	0
57	MG	YA	3076	1/1	1.28	-	50,50,50,50	0
57	MG	RA	3018	1/1	0.72	-	6,6,6,6	0
57	MG	YA	3202	1/1	0.24	-	1,1,1,1	0
57	MG	RA	3043	1/1	0.19	-	10,10,10,10	0
57	MG	YA	3174	1/1	0.22	-	40,40,40,40	0
57	MG	RA	3211	1/1	0.26	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3183	1/1	0.52	-	16,16,16,16	0
57	MG	YA	3185	1/1	0.15	-	2,2,2,2	0
57	MG	XA	1661	1/1	0.17	-	2,2,2,2	0
57	MG	RA	3189	1/1	0.18	-	4,4,4,4	0
57	MG	XA	1637	1/1	0.42	-	25,25,25,25	0
57	MG	RA	3125	1/1	0.41	-	1,1,1,1	0
57	MG	RA	3166	1/1	0.26	-	34,34,34,34	0
57	MG	YA	3060	1/1	0.57	-	10,10,10,10	0
57	MG	RA	3068	1/1	0.13	-	6,6,6,6	0
57	MG	YA	3238	1/1	0.22	-	11,11,11,11	0
57	MG	XA	1605	1/1	0.56	-	3,3,3,3	0
57	MG	RA	3218	1/1	0.33	-	23,23,23,23	0
57	MG	YA	3192	1/1	0.53	-	11,11,11,11	0
57	MG	RA	3058	1/1	0.76	-	3,3,3,3	0
57	MG	YA	3043	1/1	1.07	-	2,2,2,2	0
57	MG	YA	3246	1/1	0.33	-	7,7,7,7	0
57	MG	RA	3102	1/1	0.19	-	4,4,4,4	0
57	MG	YA	3003	1/1	0.18	-	2,2,2,2	0
57	MG	YA	3123	1/1	0.16	-	18,18,18,18	0
57	MG	XA	1668	1/1	0.23	-	18,18,18,18	0
57	MG	RA	3127	1/1	0.24	-	0,0,0,0	0
57	MG	RA	3159	1/1	0.23	-	6,6,6,6	0
57	MG	QA	1626	1/1	0.38	-	57,57,57,57	0
57	MG	RA	3228	1/1	0.47	-	11,11,11,11	0
57	MG	RA	3199	1/1	0.83	-	6,6,6,6	0
57	MG	YA	3134	1/1	0.60	-	11,11,11,11	0
57	MG	RA	3147	1/1	0.29	-	9,9,9,9	0
57	MG	YB	201	1/1	0.28	-	7,7,7,7	0
57	MG	RA	3229	1/1	1.51	-	50,50,50,50	0
57	MG	RA	3093	1/1	0.49	-	10,10,10,10	0
57	MG	RA	3115	1/1	0.41	-	6,6,6,6	0
57	MG	YA	3149	1/1	0.19	-	15,15,15,15	0
57	MG	QA	1609	1/1	0.74	-	4,4,4,4	0
57	MG	YA	3157	1/1	0.61	-	0,0,0,0	0
57	MG	RA	3198	1/1	0.20	-	12,12,12,12	0
57	MG	RA	3113	1/1	0.15	-	0,0,0,0	0
57	MG	RA	3002	1/1	0.83	-	6,6,6,6	0
57	MG	RF	301	1/1	0.38	-	2,2,2,2	0
57	MG	RA	3024	1/1	0.23	-	16,16,16,16	0
57	MG	YA	3054	1/1	0.20	-	1,1,1,1	0
57	MG	XA	1671	1/1	0.20	-	3,3,3,3	0
57	MG	XA	1649	1/1	0.21	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3139	1/1	0.34	-	7,7,7,7	0
57	MG	QA	1629	1/1	0.86	-	0,0,0,0	0
57	MG	QA	1658	1/1	0.22	-	16,16,16,16	0
57	MG	YA	3253	1/1	0.61	-	6,6,6,6	0
57	MG	QA	1661	1/1	0.35	-	64,64,64,64	0
57	MG	YA	3268	1/1	0.45	-	6,6,6,6	0
57	MG	RA	3077	1/1	0.53	-	0,0,0,0	0
57	MG	YA	3172	1/1	1.41	-	1,1,1,1	0
57	MG	RA	3017	1/1	0.43	-	11,11,11,11	0
57	MG	RA	3153	1/1	0.35	-	15,15,15,15	0
57	MG	XA	1659	1/1	0.30	-	0,0,0,0	0
57	MG	RA	3042	1/1	0.18	-	2,2,2,2	0
57	MG	RA	3078	1/1	0.33	-	3,3,3,3	0
57	MG	RA	3027	1/1	0.51	-	13,13,13,13	0
57	MG	RA	3160	1/1	0.35	-	4,4,4,4	0
57	MG	YA	3084	1/1	0.30	-	17,17,17,17	0
57	MG	RA	3072	1/1	0.43	-	3,3,3,3	0
57	MG	RA	3062	1/1	1.87	-	50,50,50,50	0
57	MG	YA	3112	1/1	0.12	-	21,21,21,21	0
57	MG	XA	1662	1/1	0.91	-	11,11,11,11	0
57	MG	YA	3105	1/1	0.28	-	4,4,4,4	0
57	MG	YA	3045	1/1	0.55	-	13,13,13,13	0
57	MG	RA	3216	1/1	0.56	-	7,7,7,7	0
57	MG	RA	3022	1/1	0.33	-	4,4,4,4	0
57	MG	RA	3201	1/1	0.69	-	10,10,10,10	0
57	MG	YA	3209	1/1	0.27	-	15,15,15,15	0
57	MG	YA	3096	1/1	0.52	-	3,3,3,3	0
57	MG	RA	3173	1/1	0.49	-	48,48,48,48	0
57	MG	QA	1640	1/1	0.40	-	9,9,9,9	0
57	MG	YA	3092	1/1	0.26	-	12,12,12,12	0
57	MG	YA	3169	1/1	0.15	-	6,6,6,6	0
57	MG	RA	3136	1/1	0.35	-	0,0,0,0	0
57	MG	QA	1608	1/1	0.10	-	10,10,10,10	0
57	MG	RA	3169	1/1	0.24	-	16,16,16,16	0
57	MG	XA	1672	1/1	0.39	-	0,0,0,0	0
57	MG	YA	3217	1/1	0.20	-	35,35,35,35	0
57	MG	XA	1636	1/1	0.38	-	3,3,3,3	0
57	MG	YA	3042	1/1	0.55	-	2,2,2,2	0
57	MG	RA	3013	1/1	0.55	-	4,4,4,4	0
57	MG	RA	3213	1/1	0.47	-	8,8,8,8	0
57	MG	RA	3140	1/1	0.63	-	9,9,9,9	0
57	MG	QA	1623	1/1	0.45	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1615	1/1	0.68	-	4,4,4,4	0
57	MG	RA	3089	1/1	0.60	-	11,11,11,11	0
57	MG	YA	3070	1/1	0.44	-	15,15,15,15	0
57	MG	YA	3029	1/1	0.88	-	10,10,10,10	0
57	MG	RA	3030	1/1	0.34	-	5,5,5,5	0
57	MG	YA	3152	1/1	0.61	-	5,5,5,5	0
57	MG	QA	1656	1/1	0.12	-	30,30,30,30	0
57	MG	QA	1619	1/1	0.42	-	4,4,4,4	0
57	MG	R5	101	1/1	0.54	-	5,5,5,5	0
57	MG	XA	1657	1/1	0.48	-	8,8,8,8	0
57	MG	YA	3061	1/1	0.12	-	17,17,17,17	0
57	MG	RA	3092	1/1	0.52	-	7,7,7,7	0
57	MG	YA	3248	1/1	0.38	-	0,0,0,0	0
57	MG	YA	3256	1/1	0.37	-	7,7,7,7	0
57	MG	YA	3107	1/1	0.60	-	15,15,15,15	0
57	MG	QA	1631	1/1	0.44	-	26,26,26,26	0
57	MG	YA	3122	1/1	0.34	-	3,3,3,3	0
57	MG	RA	3041	1/1	0.43	-	4,4,4,4	0
57	MG	YA	3158	1/1	0.33	-	6,6,6,6	0
57	MG	XA	1667	1/1	0.27	-	17,17,17,17	0
57	MG	YA	3001	1/1	1.17	-	50,50,50,50	0
57	MG	YA	3049	1/1	0.91	-	50,50,50,50	0
57	MG	YA	3186	1/1	0.59	-	11,11,11,11	0
57	MG	YA	3097	1/1	0.67	-	5,5,5,5	0
57	MG	RA	3114	1/1	0.33	-	1,1,1,1	0
57	MG	YA	3062	1/1	0.38	-	6,6,6,6	0
57	MG	XA	1615	1/1	0.28	-	6,6,6,6	0
57	MG	RA	3230	1/1	0.76	-	5,5,5,5	0
57	MG	YA	3137	1/1	0.21	-	10,10,10,10	0
57	MG	RA	3184	1/1	0.25	-	8,8,8,8	0
57	MG	RA	3157	1/1	0.50	-	0,0,0,0	0
57	MG	RA	3054	1/1	0.28	-	3,3,3,3	0
57	MG	XA	1644	1/1	0.16	-	5,5,5,5	0
57	MG	YA	3008	1/1	0.35	-	10,10,10,10	0
57	MG	YA	3240	1/1	0.16	-	72,72,72,72	0
57	MG	RA	3150	1/1	0.49	-	37,37,37,37	0
57	MG	YA	3040	1/1	0.49	-	10,10,10,10	0
57	MG	RP	201	1/1	1.18	-	21,21,21,21	0
57	MG	QF	201	1/1	1.06	-	36,36,36,36	0
57	MG	RA	3064	1/1	0.21	-	5,5,5,5	0
57	MG	RA	3110	1/1	0.55	-	3,3,3,3	0
57	MG	RA	3056	1/1	0.36	-	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3045	1/1	0.12	-	1,1,1,1	0
57	MG	XA	1652	1/1	0.24	-	66,66,66,66	0
57	MG	YA	3036	1/1	0.31	-	2,2,2,2	0
57	MG	RA	3225	1/1	0.25	-	10,10,10,10	0
57	MG	YA	3153	1/1	0.40	-	20,20,20,20	0
57	MG	QA	1659	1/1	0.23	-	4,4,4,4	0
57	MG	RA	3016	1/1	0.36	-	8,8,8,8	0
57	MG	QA	1660	1/1	0.72	-	2,2,2,2	0
57	MG	RA	3214	1/1	0.31	-	5,5,5,5	0
57	MG	RA	3146	1/1	0.15	-	5,5,5,5	0
57	MG	XA	1650	1/1	0.28	-	18,18,18,18	0
57	MG	RA	3067	1/1	0.26	-	2,2,2,2	0
57	MG	YA	3007	1/1	0.17	-	7,7,7,7	0
57	MG	YA	3200	1/1	0.96	-	4,4,4,4	0
57	MG	RA	3080	1/1	0.35	-	21,21,21,21	0
57	MG	QA	1625	1/1	0.27	-	0,0,0,0	0
57	MG	RA	3238	1/1	0.46	-	16,16,16,16	0
57	MG	YA	3188	1/1	0.53	-	1,1,1,1	0
57	MG	YA	3195	1/1	0.43	-	9,9,9,9	0
57	MG	YA	3267	1/1	0.40	-	4,4,4,4	0
57	MG	XA	1660	1/1	0.14	-	24,24,24,24	0
57	MG	XV	101	1/1	0.43	-	14,14,14,14	0
57	MG	RA	3047	1/1	0.59	-	5,5,5,5	0
57	MG	QA	1651	1/1	0.20	-	9,9,9,9	0
58	ZN	QN	101	1/1	0.13	-	104,104,104,104	0
57	MG	RA	3163	1/1	1.05	-	12,12,12,12	0
57	MG	YA	3085	1/1	0.51	-	13,13,13,13	0
58	ZN	Y9	101	1/1	0.46	-	138,138,138,138	0
57	MG	RA	3099	1/1	0.22	-	10,10,10,10	0
57	MG	RA	3074	1/1	0.14	-	8,8,8,8	0
57	MG	RA	3161	1/1	0.13	-	1,1,1,1	0
57	MG	XA	1669	1/1	0.21	-	38,38,38,38	0
57	MG	YA	3114	1/1	0.34	-	13,13,13,13	0
57	MG	RA	3203	1/1	0.40	-	24,24,24,24	0
57	MG	RA	3204	1/1	0.26	-	18,18,18,18	0
59	A	XX	101	22/23	0.31	-	91,91,91,91	0
57	MG	YA	3227	1/1	0.27	-	0,0,0,0	0
57	MG	YQ	201	1/1	0.22	-	99,99,99,99	0
57	MG	RA	3050	1/1	0.58	-	11,11,11,11	0
57	MG	YA	3100	1/1	0.94	-	6,6,6,6	0
57	MG	RA	3190	1/1	0.18	-	16,16,16,16	0
57	MG	YA	3088	1/1	0.64	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3134	1/1	0.12	-	25,25,25,25	0
57	MG	XA	1623	1/1	0.17	-	14,14,14,14	0
57	MG	RA	3223	1/1	0.28	-	47,47,47,47	0
57	MG	YA	3035	1/1	0.31	-	9,9,9,9	0
57	MG	RA	3212	1/1	0.48	-	1,1,1,1	0
57	MG	XA	1624	1/1	0.54	-	3,3,3,3	0
57	MG	YA	3079	1/1	0.24	-	4,4,4,4	0
57	MG	QA	1643	1/1	0.30	-	33,33,33,33	0
57	MG	YA	3236	1/1	0.27	-	5,5,5,5	0
57	MG	YA	3212	1/1	0.23	-	8,8,8,8	0
57	MG	RA	3129	1/1	0.14	-	31,31,31,31	0
57	MG	RA	3175	1/1	0.13	-	1,1,1,1	0
57	MG	RA	3105	1/1	0.46	-	11,11,11,11	0
57	MG	RA	3135	1/1	0.17	-	7,7,7,7	0
57	MG	YA	3269	1/1	0.80	-	1,1,1,1	0
57	MG	YA	3206	1/1	0.37	-	26,26,26,26	0
57	MG	RA	3082	1/1	0.32	-	0,0,0,0	0
57	MG	XA	1645	1/1	0.27	-	1,1,1,1	0
57	MG	YA	3201	1/1	0.63	-	9,9,9,9	0
57	MG	QA	1621	1/1	0.12	-	5,5,5,5	0
57	MG	RB	202	1/1	0.09	-	4,4,4,4	0
57	MG	YA	3086	1/1	0.76	-	6,6,6,6	0
57	MG	YA	3072	1/1	0.21	-	2,2,2,2	0
57	MG	XA	1601	1/1	0.98	-	1,1,1,1	0
57	MG	YA	3223	1/1	0.37	-	34,34,34,34	0
57	MG	XA	1614	1/1	0.14	-	26,26,26,26	0
57	MG	Y5	101	1/1	0.43	-	6,6,6,6	0
57	MG	XA	1608	1/1	0.14	-	37,37,37,37	0
57	MG	XA	1613	1/1	0.08	-	0,0,0,0	0
57	MG	YA	3028	1/1	0.40	-	6,6,6,6	0
57	MG	YA	3225	1/1	0.18	-	10,10,10,10	0
57	MG	RA	3015	1/1	0.69	-	5,5,5,5	0
57	MG	RA	3035	1/1	0.41	-	11,11,11,11	0
57	MG	YA	3064	1/1	0.33	-	8,8,8,8	0
57	MG	RA	3172	1/1	0.45	-	4,4,4,4	0
57	MG	YA	3259	1/1	0.75	-	8,8,8,8	0
57	MG	YA	3125	1/1	0.39	-	12,12,12,12	0
57	MG	Y7	101	1/1	0.61	-	15,15,15,15	0
57	MG	RA	3187	1/1	0.45	-	3,3,3,3	0
57	MG	RA	3066	1/1	0.52	-	6,6,6,6	0
57	MG	RA	3142	1/1	0.54	-	36,36,36,36	0
57	MG	YA	3182	1/1	0.15	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3053	1/1	0.56	-	4,4,4,4	0
57	MG	RA	3152	1/1	0.12	-	4,4,4,4	0
57	MG	YA	3127	1/1	0.28	-	2,2,2,2	0
57	MG	XA	1602	1/1	0.16	-	7,7,7,7	0
57	MG	YA	3099	1/1	0.75	-	10,10,10,10	0
57	MG	QA	1610	1/1	0.24	-	7,7,7,7	0
57	MG	YA	3116	1/1	0.43	-	3,3,3,3	0
57	MG	YA	3190	1/1	0.22	-	21,21,21,21	0
57	MG	RA	3112	1/1	0.19	-	6,6,6,6	0
57	MG	RA	3234	1/1	0.37	-	9,9,9,9	0
57	MG	RA	3176	1/1	0.32	-	3,3,3,3	0
57	MG	RA	3237	1/1	1.28	-	1,1,1,1	0
57	MG	XA	1604	1/1	0.92	-	10,10,10,10	0
57	MG	RA	3090	1/1	0.19	-	75,75,75,75	0
57	MG	YA	3204	1/1	0.12	-	11,11,11,11	0
57	MG	YA	3160	1/1	0.40	-	1,1,1,1	0
57	MG	RA	3108	1/1	0.08	-	0,0,0,0	0
57	MG	RA	3185	1/1	0.15	-	9,9,9,9	0
57	MG	RA	3025	1/1	0.15	-	3,3,3,3	0
57	MG	RA	3192	1/1	0.26	-	21,21,21,21	0
58	ZN	QD	301	1/1	0.35	-	50,50,50,50	0
57	MG	YA	3077	1/1	0.30	-	2,2,2,2	0
57	MG	YA	3090	1/1	0.40	-	1,1,1,1	0
57	MG	QA	1630	1/1	0.15	-	7,7,7,7	0
57	MG	YA	3216	1/1	0.25	-	19,19,19,19	0
57	MG	YA	3244	1/1	0.09	-	9,9,9,9	0
57	MG	YA	3046	1/1	0.35	-	3,3,3,3	0
57	MG	QA	1652	1/1	0.15	-	12,12,12,12	0
57	MG	RA	3124	1/1	0.42	-	10,10,10,10	0
57	MG	QA	1627	1/1	0.24	-	10,10,10,10	0
57	MG	YA	3151	1/1	0.18	-	5,5,5,5	0
57	MG	YA	3237	1/1	0.34	-	7,7,7,7	0
57	MG	RA	3046	1/1	0.84	-	50,50,50,50	0
57	MG	YA	3011	1/1	0.32	-	0,0,0,0	0
57	MG	QA	1613	1/1	0.61	-	15,15,15,15	0
57	MG	RR	201	1/1	0.25	-	13,13,13,13	0
57	MG	YA	3093	1/1	0.35	-	7,7,7,7	0
57	MG	YA	3229	1/1	0.27	-	3,3,3,3	0
57	MG	RA	3060	1/1	0.31	-	6,6,6,6	0
57	MG	QA	1620	1/1	0.37	-	6,6,6,6	0
57	MG	YA	3094	1/1	0.86	-	11,11,11,11	0
57	MG	XB	301	1/1	0.22	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3055	1/1	0.92	-	5,5,5,5	0
57	MG	YA	3131	1/1	0.42	-	3,3,3,3	0
57	MG	RA	3007	1/1	0.34	-	16,16,16,16	0
57	MG	RA	3095	1/1	0.75	-	1,1,1,1	0
57	MG	RA	3178	1/1	0.33	-	1,1,1,1	0
57	MG	YP	201	1/1	0.14	-	94,94,94,94	0
57	MG	RA	3031	1/1	0.68	-	5,5,5,5	0
57	MG	RA	3164	1/1	0.17	-	4,4,4,4	0
57	MG	QA	1635	1/1	0.51	-	13,13,13,13	0
57	MG	YA	3118	1/1	0.29	-	14,14,14,14	0
57	MG	RA	3059	1/1	0.47	-	11,11,11,11	0
57	MG	YA	3019	1/1	0.50	-	5,5,5,5	0
57	MG	YA	3210	1/1	0.65	-	3,3,3,3	0
57	MG	YA	3211	1/1	0.50	-	7,7,7,7	0
57	MG	YA	3066	1/1	0.65	-	7,7,7,7	0
57	MG	XA	1640	1/1	0.12	-	75,75,75,75	0
57	MG	RA	3096	1/1	0.55	-	4,4,4,4	0
57	MG	YA	3033	1/1	0.43	-	4,4,4,4	0
57	MG	YA	3030	1/1	0.98	-	5,5,5,5	0
57	MG	XA	1612	1/1	0.19	-	19,19,19,19	0
57	MG	XA	1646	1/1	0.30	-	7,7,7,7	0
57	MG	QA	1641	1/1	0.23	-	7,7,7,7	0
57	MG	XA	1653	1/1	0.42	-	8,8,8,8	0
57	MG	RA	3119	1/1	0.42	-	3,3,3,3	0
57	MG	YA	3163	1/1	0.17	-	4,4,4,4	0
57	MG	QA	1622	1/1	0.32	-	14,14,14,14	0
57	MG	YA	3231	1/1	0.11	-	45,45,45,45	0
57	MG	YA	3203	1/1	0.16	-	53,53,53,53	0
57	MG	YA	3144	1/1	0.12	-	4,4,4,4	0
57	MG	RA	3170	1/1	0.96	-	5,5,5,5	0
57	MG	RA	3177	1/1	0.72	-	7,7,7,7	0
57	MG	YA	3126	1/1	0.38	-	7,7,7,7	0
57	MG	RA	3061	1/1	0.16	-	53,53,53,53	0
57	MG	RA	3174	1/1	0.49	-	4,4,4,4	0
57	MG	RA	3107	1/1	0.19	-	10,10,10,10	0
57	MG	QA	1639	1/1	0.15	-	3,3,3,3	0
57	MG	XA	1611	1/1	0.34	-	7,7,7,7	0
58	ZN	XN	101	1/1	0.19	-	84,84,84,84	0
57	MG	YA	3159	1/1	0.19	-	6,6,6,6	0
57	MG	YA	3095	1/1	0.45	-	2,2,2,2	0
57	MG	RE	301	1/1	0.25	-	12,12,12,12	0
57	MG	RA	3132	1/1	0.13	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3142	1/1	0.55	-	19,19,19,19	0
57	MG	YA	3104	1/1	0.55	-	10,10,10,10	0
57	MG	RA	3097	1/1	0.49	-	2,2,2,2	0
57	MG	QA	1633	1/1	0.63	-	4,4,4,4	0
57	MG	RA	3231	1/1	0.25	-	14,14,14,14	0
57	MG	YA	3171	1/1	0.42	-	13,13,13,13	0
57	MG	YA	3222	1/1	0.18	-	8,8,8,8	0
57	MG	YA	3252	1/1	0.65	-	8,8,8,8	0
57	MG	RA	3104	1/1	0.21	-	3,3,3,3	0
57	MG	RA	3023	1/1	0.28	-	16,16,16,16	0
57	MG	YA	3113	1/1	0.19	-	1,1,1,1	0
57	MG	RA	3137	1/1	0.42	-	10,10,10,10	0
57	MG	RA	3008	1/1	0.53	-	0,0,0,0	0
57	MG	RA	3076	1/1	0.60	-	7,7,7,7	0
57	MG	YA	3004	1/1	0.41	-	12,12,12,12	0
57	MG	RA	3141	1/1	0.23	-	2,2,2,2	0
57	MG	RA	3130	1/1	0.60	-	2,2,2,2	0
57	MG	YA	3009	1/1	0.74	-	8,8,8,8	0
57	MG	XM	201	1/1	0.11	-	85,85,85,85	0
57	MG	RB	201	1/1	0.14	-	8,8,8,8	0
57	MG	RA	3206	1/1	0.29	-	3,3,3,3	0
57	MG	RA	3202	1/1	0.13	-	16,16,16,16	0
57	MG	YA	3147	1/1	0.55	-	4,4,4,4	0
57	MG	QA	1654	1/1	0.14	-	17,17,17,17	0
57	MG	YA	3184	1/1	0.34	-	7,7,7,7	0
57	MG	RA	3057	1/1	0.30	-	2,2,2,2	0
57	MG	YA	3243	1/1	0.42	-	32,32,32,32	0
57	MG	YA	3198	1/1	0.25	-	51,51,51,51	0
57	MG	RA	3033	1/1	0.61	-	50,50,50,50	0
57	MG	YA	3258	1/1	0.44	-	1,1,1,1	0
57	MG	QH	201	1/1	0.19	-	47,47,47,47	0
57	MG	RA	3224	1/1	0.40	-	5,5,5,5	0
57	MG	QA	1662	1/1	0.24	-	37,37,37,37	0
57	MG	QM	201	1/1	0.15	-	44,44,44,44	0
57	MG	YA	3135	1/1	0.23	-	6,6,6,6	0
57	MG	YA	3234	1/1	0.58	-	17,17,17,17	0
57	MG	YA	3215	1/1	0.18	-	14,14,14,14	0
57	MG	RA	3232	1/1	0.45	-	13,13,13,13	0
57	MG	YA	3146	1/1	0.42	-	0,0,0,0	0
57	MG	QA	1603	1/1	0.88	-	14,14,14,14	0
57	MG	RA	3197	1/1	0.59	-	3,3,3,3	0
57	MG	RA	3006	1/1	1.03	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3261	1/1	0.27	-	4,4,4,4	0
57	MG	YA	3263	1/1	0.76	-	4,4,4,4	0
57	MG	YA	3081	1/1	0.40	-	9,9,9,9	0
57	MG	YA	3059	1/1	0.33	-	5,5,5,5	0
57	MG	XA	1625	1/1	0.18	-	5,5,5,5	0
57	MG	YA	3106	1/1	0.27	-	8,8,8,8	0
57	MG	RA	3122	1/1	0.59	-	5,5,5,5	0
57	MG	YA	3005	1/1	0.23	-	3,3,3,3	0
57	MG	RA	3207	1/1	0.24	-	11,11,11,11	0
57	MG	XA	1616	1/1	0.29	-	1,1,1,1	0
57	MG	YA	3141	1/1	0.59	-	0,0,0,0	0
57	MG	YA	3181	1/1	0.30	-	3,3,3,3	0
57	MG	YA	3031	1/1	0.58	-	0,0,0,0	0
57	MG	RA	3156	1/1	0.11	-	9,9,9,9	0
57	MG	YA	3251	1/1	0.15	-	9,9,9,9	0
57	MG	YA	3167	1/1	0.56	-	2,2,2,2	0
57	MG	YA	3038	1/1	0.18	-	7,7,7,7	0
57	MG	RA	3227	1/1	0.54	-	22,22,22,22	0
57	MG	YA	3232	1/1	0.36	-	2,2,2,2	0
57	MG	RA	3009	1/1	0.39	-	10,10,10,10	0
57	MG	RA	3028	1/1	0.49	-	14,14,14,14	0
57	MG	YA	3073	1/1	0.25	-	1,1,1,1	0
57	MG	QA	1612	1/1	0.48	-	7,7,7,7	0
57	MG	RA	3221	1/1	0.33	-	22,22,22,22	0
57	MG	QX	101	1/1	0.41	-	4,4,4,4	0
57	MG	QA	1664	1/1	0.41	-	54,54,54,54	0
57	MG	YA	3071	1/1	0.21	-	28,28,28,28	0
57	MG	YA	3176	1/1	0.48	-	6,6,6,6	0
57	MG	YE	301	1/1	0.18	-	0,0,0,0	0
57	MG	QA	1634	1/1	0.19	-	7,7,7,7	0
57	MG	YA	3021	1/1	0.42	-	12,12,12,12	0
57	MG	YA	3260	1/1	0.98	-	50,50,50,50	0
57	MG	XA	1641	1/1	1.12	-	21,21,21,21	0
57	MG	YA	3050	1/1	0.51	-	50,50,50,50	0
57	MG	YA	3121	1/1	0.46	-	62,62,62,62	0
57	MG	YA	3068	1/1	0.51	-	2,2,2,2	0
57	MG	RA	3040	1/1	0.39	-	14,14,14,14	0
57	MG	XA	1639	1/1	0.14	-	5,5,5,5	0
57	MG	YA	3027	1/1	0.12	-	1,1,1,1	0
57	MG	QA	1649	1/1	0.39	-	6,6,6,6	0
57	MG	QA	1601	1/1	0.39	-	9,9,9,9	0
57	MG	YA	3214	1/1	0.24	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3016	1/1	0.23	-	6,6,6,6	0
57	MG	YA	3230	1/1	0.14	-	8,8,8,8	0
57	MG	RA	3162	1/1	0.23	-	2,2,2,2	0
57	MG	RA	3044	1/1	0.91	-	10,10,10,10	0
57	MG	YA	3048	1/1	0.19	-	4,4,4,4	0
57	MG	QA	1624	1/1	0.57	-	0,0,0,0	0
57	MG	QA	1647	1/1	0.28	-	33,33,33,33	0
57	MG	YA	3220	1/1	0.66	-	33,33,33,33	0
57	MG	RA	3075	1/1	0.20	-	3,3,3,3	0
57	MG	YA	3194	1/1	0.19	-	0,0,0,0	0
57	MG	RA	3131	1/1	0.70	-	9,9,9,9	0
57	MG	XA	1634	1/1	0.56	-	0,0,0,0	0
57	MG	RA	3039	1/1	0.42	-	10,10,10,10	0
57	MG	YA	3129	1/1	0.74	-	15,15,15,15	0
57	MG	RA	3036	1/1	0.86	-	6,6,6,6	0
57	MG	RA	3171	1/1	0.17	-	12,12,12,12	0
57	MG	YA	3002	1/1	1.04	-	50,50,50,50	0
57	MG	YA	3150	1/1	0.43	-	4,4,4,4	0
57	MG	XA	1655	1/1	0.28	-	9,9,9,9	0
57	MG	RA	3087	1/1	0.91	-	11,11,11,11	0
57	MG	RA	3195	1/1	0.23	-	24,24,24,24	0
57	MG	QA	1617	1/1	0.20	-	4,4,4,4	0
57	MG	YA	3173	1/1	0.26	-	35,35,35,35	0
57	MG	RA	3085	1/1	0.80	-	5,5,5,5	0
57	MG	YA	3264	1/1	0.16	-	9,9,9,9	0
57	MG	YA	3052	1/1	0.71	-	14,14,14,14	0
57	MG	YA	3039	1/1	0.27	-	6,6,6,6	0
57	MG	YA	3124	1/1	0.21	-	9,9,9,9	0
57	MG	YA	3239	1/1	0.20	-	5,5,5,5	0
57	MG	QV	101	1/1	0.23	-	1,1,1,1	0
57	MG	YA	3250	1/1	1.21	-	11,11,11,11	0
57	MG	RA	3217	1/1	0.34	-	74,74,74,74	0
57	MG	RA	3139	1/1	0.23	-	2,2,2,2	0
57	MG	XA	1670	1/1	0.15	-	43,43,43,43	0
57	MG	QA	1657	1/1	0.14	-	7,7,7,7	0
57	MG	XA	1643	1/1	0.33	-	5,5,5,5	0
57	MG	YA	3025	1/1	0.19	-	4,4,4,4	0
57	MG	RA	3126	1/1	0.45	-	2,2,2,2	0
57	MG	RA	3183	1/1	0.42	-	57,57,57,57	0
57	MG	YA	3249	1/1	0.37	-	10,10,10,10	0
57	MG	RA	3226	1/1	0.37	-	9,9,9,9	0
57	MG	QA	1642	1/1	0.50	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3021	1/1	0.19	-	2,2,2,2	0
57	MG	YA	3037	1/1	0.22	-	13,13,13,13	0
57	MG	RA	3079	1/1	0.64	-	5,5,5,5	0
57	MG	YA	3235	1/1	0.25	-	3,3,3,3	0
57	MG	YA	3130	1/1	0.22	-	20,20,20,20	0
57	MG	YB	202	1/1	0.66	-	24,24,24,24	0
57	MG	RA	3071	1/1	0.24	-	1,1,1,1	0
57	MG	RA	3010	1/1	0.57	-	14,14,14,14	0
57	MG	RA	3222	1/1	0.31	-	14,14,14,14	0
57	MG	XA	1618	1/1	0.49	-	3,3,3,3	0
57	MG	QA	1606	1/1	0.15	-	16,16,16,16	0
57	MG	RA	3005	1/1	0.66	-	12,12,12,12	0
57	MG	QA	1645	1/1	0.14	-	38,38,38,38	0
57	MG	RA	3180	1/1	0.11	-	6,6,6,6	0
57	MG	YA	3241	1/1	0.21	-	5,5,5,5	0
57	MG	RA	3117	1/1	0.18	-	25,25,25,25	0
57	MG	QA	1616	1/1	0.13	-	29,29,29,29	0
57	MG	RA	3014	1/1	0.28	-	13,13,13,13	0
57	MG	YA	3083	1/1	0.46	-	9,9,9,9	0
57	MG	YA	3219	1/1	0.16	-	7,7,7,7	0
57	MG	RA	3145	1/1	0.46	-	3,3,3,3	0
57	MG	RA	3209	1/1	0.29	-	17,17,17,17	0
57	MG	YB	203	1/1	0.15	-	37,37,37,37	0
57	MG	YA	3175	1/1	0.24	-	9,9,9,9	0
57	MG	RA	3086	1/1	0.24	-	0,0,0,0	0
57	MG	YA	3089	1/1	0.44	-	5,5,5,5	0
57	MG	RA	3069	1/1	0.81	-	4,4,4,4	0
57	MG	RA	3143	1/1	0.31	-	7,7,7,7	0
57	MG	YA	3057	1/1	0.84	-	4,4,4,4	0
57	MG	RD	301	1/1	0.51	-	1,1,1,1	0
57	MG	RA	3106	1/1	0.41	-	13,13,13,13	0
57	MG	RA	3103	1/1	0.49	-	9,9,9,9	0
57	MG	RA	3148	1/1	0.30	-	5,5,5,5	0
57	MG	YA	3179	1/1	0.25	-	0,0,0,0	0
57	MG	YA	3132	1/1	0.10	-	5,5,5,5	0
57	MG	RA	3200	1/1	0.16	-	1,1,1,1	0
57	MG	XA	1610	1/1	0.22	-	3,3,3,3	0
57	MG	XA	1620	1/1	0.17	-	2,2,2,2	0
57	MG	QA	1628	1/1	0.19	-	8,8,8,8	0
57	MG	YA	3080	1/1	1.45	-	50,50,50,50	0
57	MG	YA	3063	1/1	0.29	-	11,11,11,11	0
57	MG	XV	102	1/1	0.65	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1629	1/1	0.15	-	8,8,8,8	0

6.5 Other polymers ⓘ

There are no such residues in this entry.