wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2023 – 08:02 PM EDT

PDB ID	:	4P6F
Title	:	Crystal structure of the peptolide 12C bound to bacterial ribosome
Authors	:	Fagan, C.E.; Dunham, C.M.
Deposited on	:	2014-03-24
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

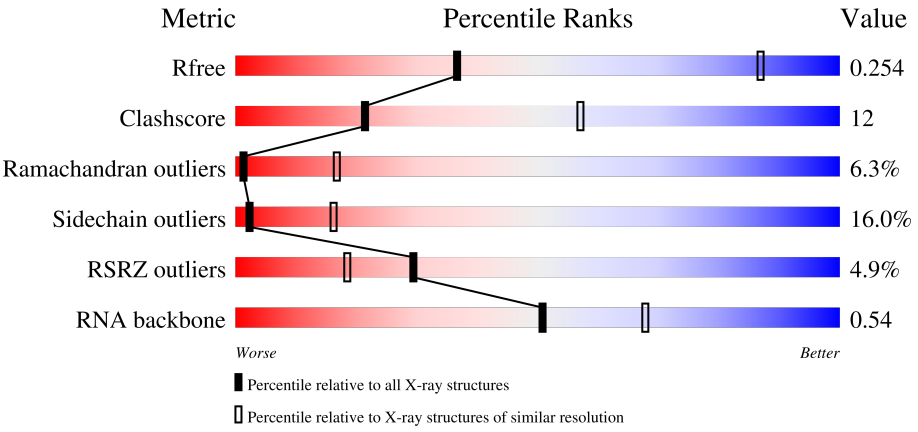
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	4% 54% 35% 9% ••
1	XA	1522	3% 56% 33% 9% •
2	QB	256	10% 48% 36% 7% • 7%
2	XB	256	5% 46% 36% 10% • 7%

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Mol	Chain	Length	Quality of chain
3	QC	239	9% 54% 29% 14%
3	XC	239	4% 54% 28% 14%
4	QD	209	% 51% 42% 5%
4	XD	209	% 65% 27% 6%
5	QE	162	4% 60% 31% 7%
5	XE	162	% 54% 35% 7%
6	QF	101	2% 61% 31% 8%
6	XF	101	5% 61% 35%
7	QG	156	6% 64% 32%
7	XG	156	3% 72% 24%
8	QH	138	62% 35%
8	XH	138	64% 30% 5%
9	QI	128	12% 56% 38%
9	XI	128	7% 55% 34% 9%
10	QJ	105	12% 45% 40% 10% 6%
10	XJ	105	10% 44% 41% 10% 6%
11	QK	129	5% 57% 31% 5% 8%
11	XK	129	3% 60% 30% 8%
12	QL	132	2% 49% 36% 8% 5%
12	XL	132	3% 51% 32% 10% 5%
13	QM	126	2% 47% 38% 11%
13	XM	126	2% 44% 41% 11%
14	QN	61	5% 44% 44% 10%
14	XN	61	51% 39% 8%
15	QO	89	3% 65% 28% 6%

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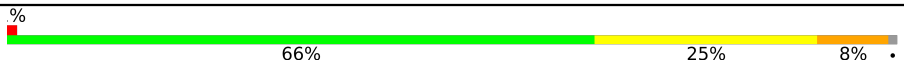
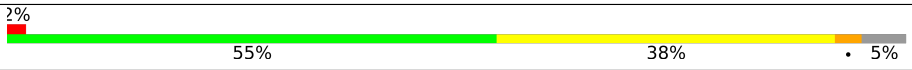
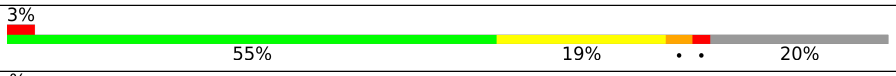
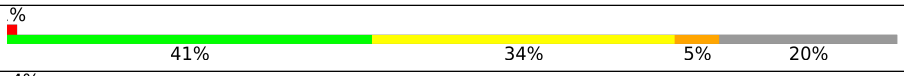
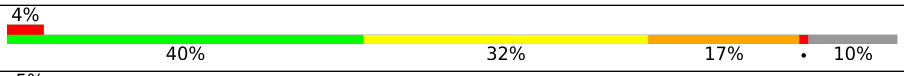
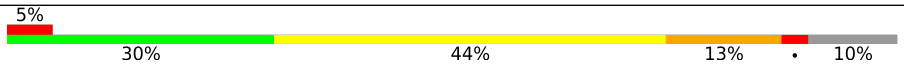
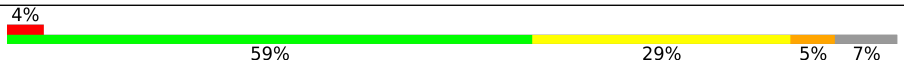
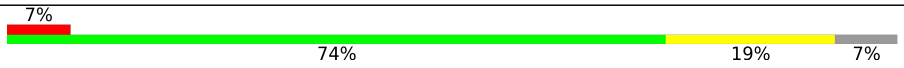
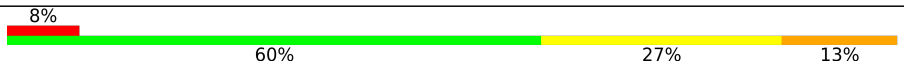
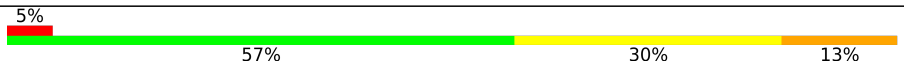
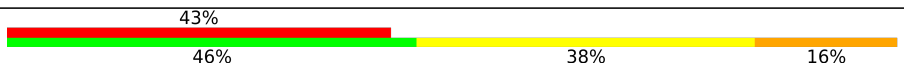
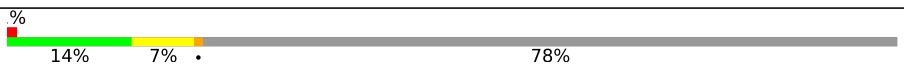
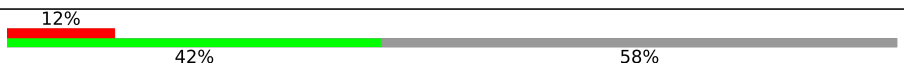
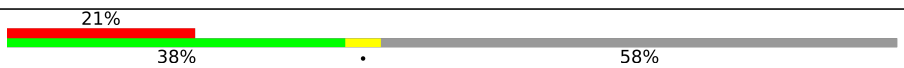
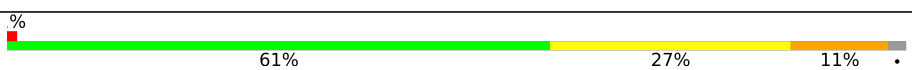
Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QW	76	
23	QY	76	
23	XW	76	
23	XY	76	
24	QX	24	
24	XX	24	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	

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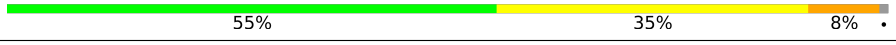
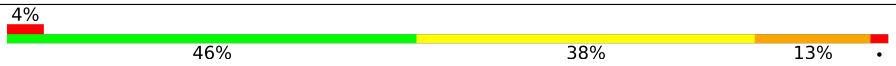
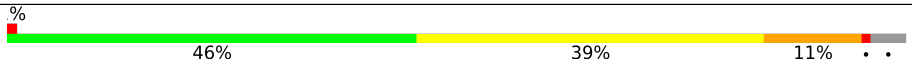
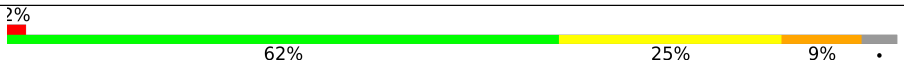
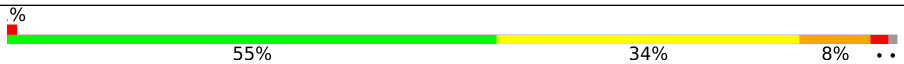
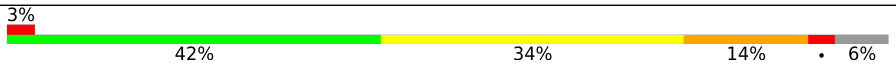
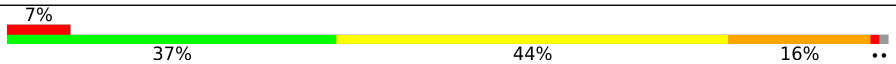
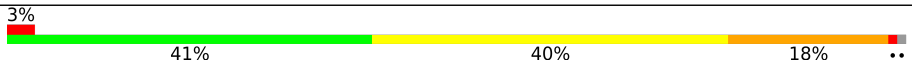
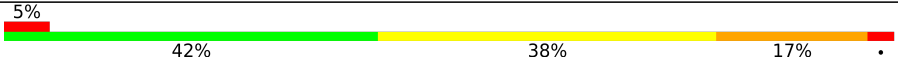
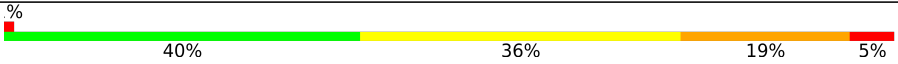
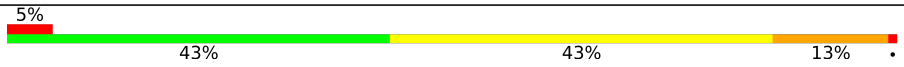
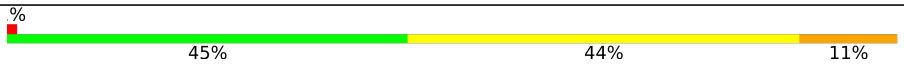
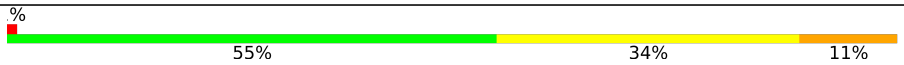
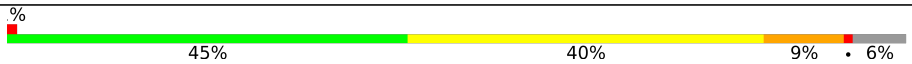
Mol	Chain	Length	Quality of chain
27	RD	276	
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39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

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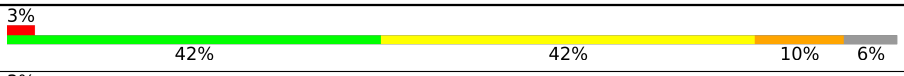
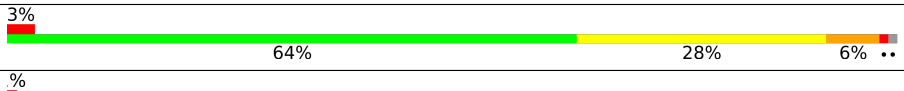
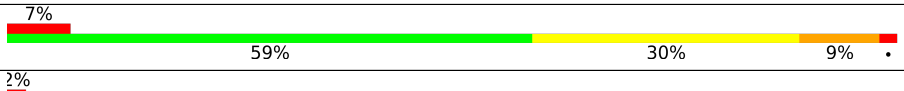
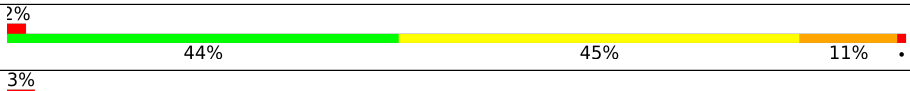
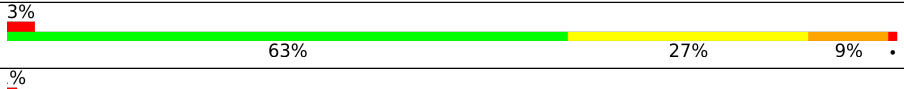
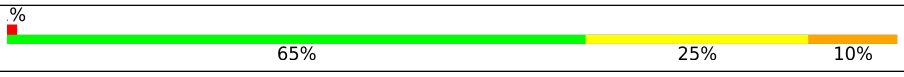
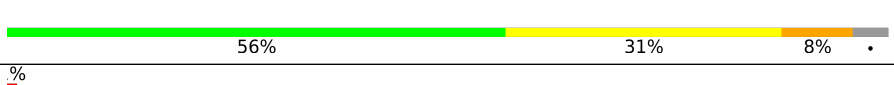
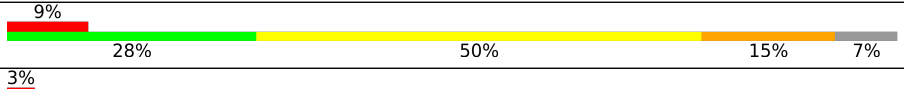
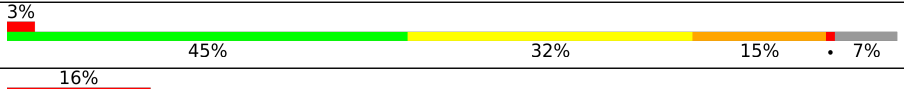
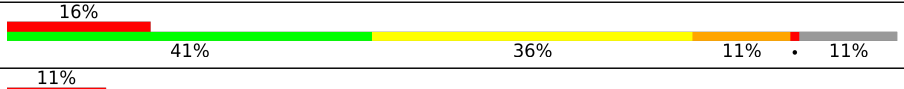
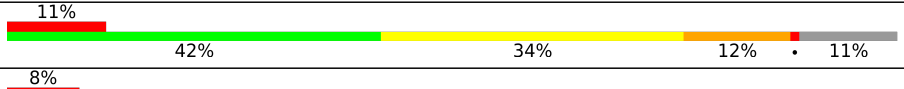
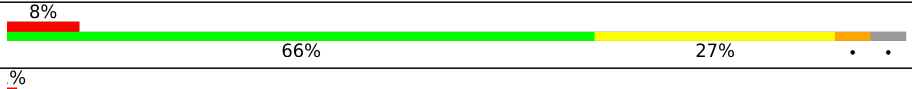
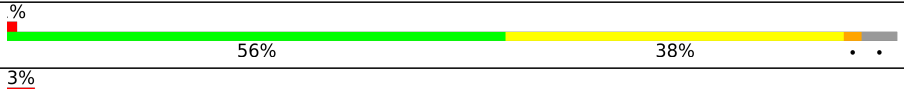
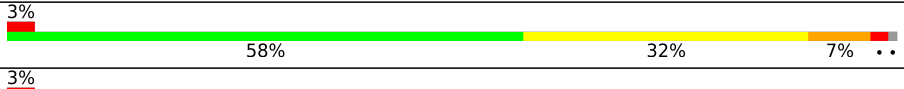
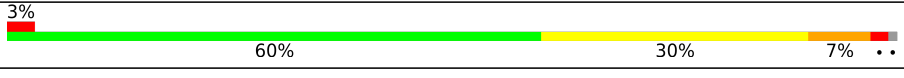
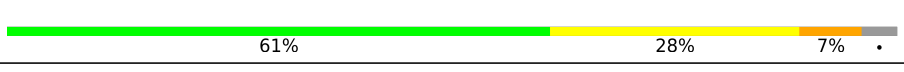
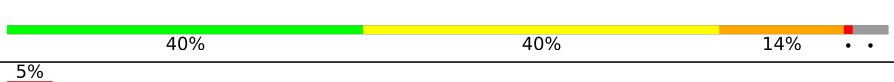
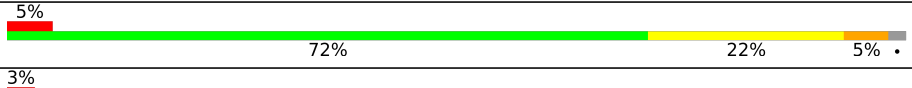
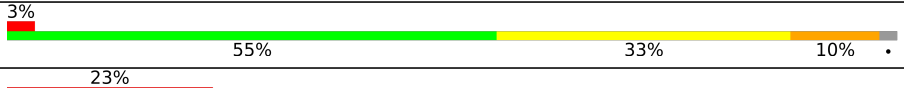
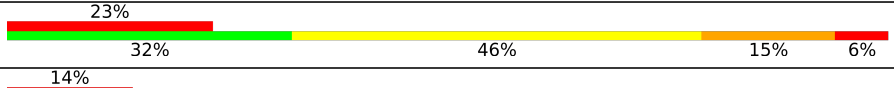
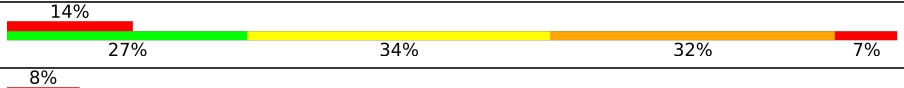
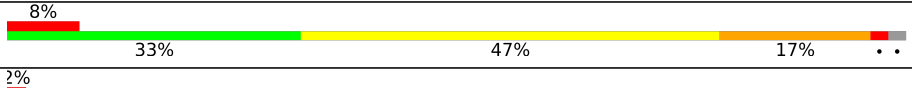
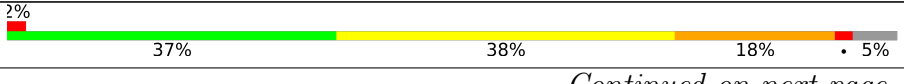
Mol	Chain	Length	Quality of chain
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	

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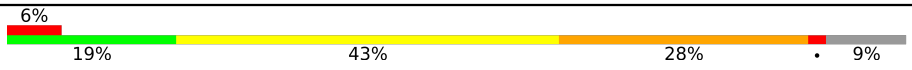
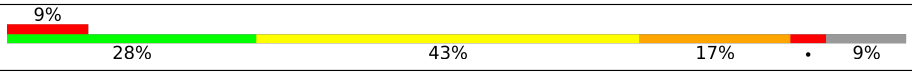
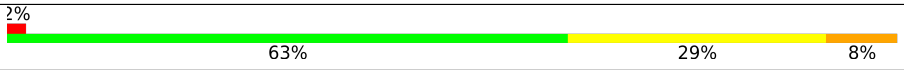
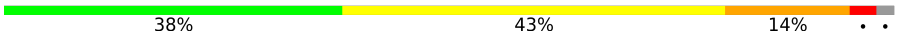
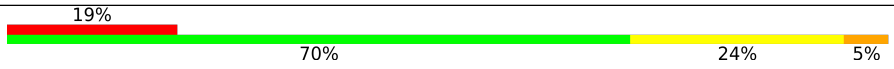
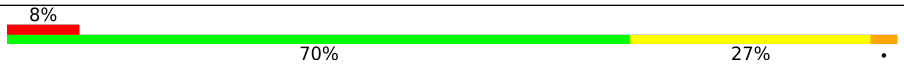
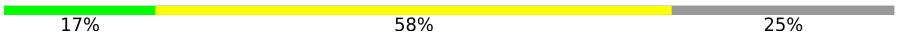
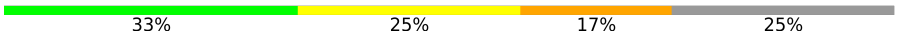
Mol	Chain	Length	Quality of chain
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z7	12	
56	Z8	12	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1603	-	-	-	X
57	MG	QA	1638	-	-	-	X
57	MG	QA	1644	-	-	-	X
57	MG	QA	1649	-	-	-	X
57	MG	QA	1655	-	-	-	X
57	MG	QA	1664	-	-	-	X
57	MG	R0	101	-	-	-	X
57	MG	R5	101	-	-	-	X
57	MG	RA	3002	-	-	-	X
57	MG	RA	3007	-	-	-	X
57	MG	RA	3044	-	-	-	X
57	MG	RA	3118	-	-	-	X
57	MG	RA	3127	-	-	-	X
57	MG	RA	3132	-	-	-	X
57	MG	RA	3138	-	-	-	X
57	MG	RA	3153	-	-	-	X
57	MG	RA	3157	-	-	-	X
57	MG	RA	3159	-	-	-	X
57	MG	RA	3161	-	-	-	X
57	MG	RA	3164	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3171	-	-	-	X
57	MG	RA	3175	-	-	-	X
57	MG	RA	3185	-	-	-	X
57	MG	RA	3196	-	-	-	X
57	MG	RA	3197	-	-	-	X
57	MG	RA	3201	-	-	-	X
57	MG	RA	3203	-	-	-	X
57	MG	RA	3206	-	-	-	X
57	MG	RA	3212	-	-	-	X
57	MG	RA	3216	-	-	-	X
57	MG	RA	3217	-	-	-	X
57	MG	RA	3218	-	-	-	X
57	MG	RA	3219	-	-	-	X
57	MG	RA	3220	-	-	-	X
57	MG	RA	3224	-	-	-	X
57	MG	RA	3225	-	-	-	X
57	MG	RA	3238	-	-	-	X
57	MG	RA	3239	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RP	204	-	-	-	X
57	MG	XA	1601	-	-	-	X
57	MG	XA	1608	-	-	-	X
57	MG	XA	1609	-	-	-	X
57	MG	XA	1634	-	-	-	X
57	MG	XA	1650	-	-	-	X
57	MG	XA	1662	-	-	-	X
57	MG	XA	1670	-	-	-	X
57	MG	XB	301	-	-	-	X
57	MG	XM	201	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3054	-	-	-	X
57	MG	YA	3125	-	-	-	X
57	MG	YA	3149	-	-	-	X
57	MG	YA	3153	-	-	-	X
57	MG	YA	3156	-	-	-	X
57	MG	YA	3161	-	-	-	X
57	MG	YA	3178	-	-	-	X
57	MG	YA	3190	-	-	-	X
57	MG	YA	3201	-	-	-	X
57	MG	YA	3210	-	-	-	X
57	MG	YA	3214	-	-	-	X
57	MG	YA	3228	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3231	-	-	-	X
57	MG	YA	3233	-	-	-	X
57	MG	YA	3243	-	-	-	X
57	MG	YA	3254	-	-	-	X
57	MG	YA	3258	-	-	-	X
57	MG	YA	3259	-	-	-	X
57	MG	YA	3274	-	-	-	X
57	MG	YB	201	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 295487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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 type Z.

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 Thx.

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

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

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

- Molecule 23 is a RNA chain called E-Site tRNA-Phe or A-Site tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total 1619	C 723	N 290	O 531	P 75	0	0	0
23	QY	17	Total 364	C 163	N 68	O 116	P 17	0	0	0
23	XW	76	Total 1619	C 723	N 290	O 531	P 75	0	0	0
23	XY	17	Total 364	C 163	N 68	O 116	P 17	0	0	0

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	10	Total 210	C 96	N 39	O 66	P 9	0	0	0
24	XX	10	Total 210	C 96	N 39	O 66	P 9	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	57	Total	C	N	O	S	0	0	0
			442	278	88	71	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	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 protein called T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	Z7	9	Total	C	N	O	0	0	0
			116	78	18	20			
56	Z8	9	Total	C	N	O	0	0	0
			116	78	18	20			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	67	Total	Mg	0	0
			67	67		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QV	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QY	1	Total Mg 1 1	0	0
57	RA	246	Total Mg 246 246	0	0
57	RB	2	Total Mg 2 2	0	0
57	RD	1	Total Mg 1 1	0	0
57	RE	1	Total Mg 1 1	0	0
57	RP	4	Total Mg 4 4	0	0
57	R0	1	Total Mg 1 1	0	0
57	R5	1	Total Mg 1 1	0	0
57	XA	71	Total Mg 71 71	0	0
57	XB	1	Total Mg 1 1	0	0
57	XM	1	Total Mg 1 1	0	0
57	XV	3	Total Mg 3 3	0	0
57	XX	1	Total Mg 1 1	0	0
57	XY	1	Total Mg 1 1	0	0
57	YA	278	Total Mg 278 278	0	0
57	YB	5	Total Mg 5 5	0	0
57	YD	1	Total Mg 1 1	0	0
57	YE	2	Total Mg 2 2	0	0
57	YP	1	Total Mg 1 1	0	0
57	YX	1	Total Mg 1 1	0	0
57	Y5	1	Total Mg 1 1	0	0

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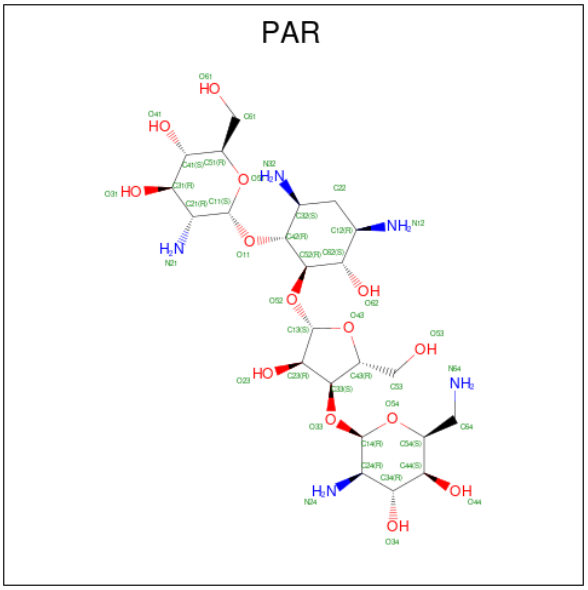
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	Y7	1	Total Mg 1 1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

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

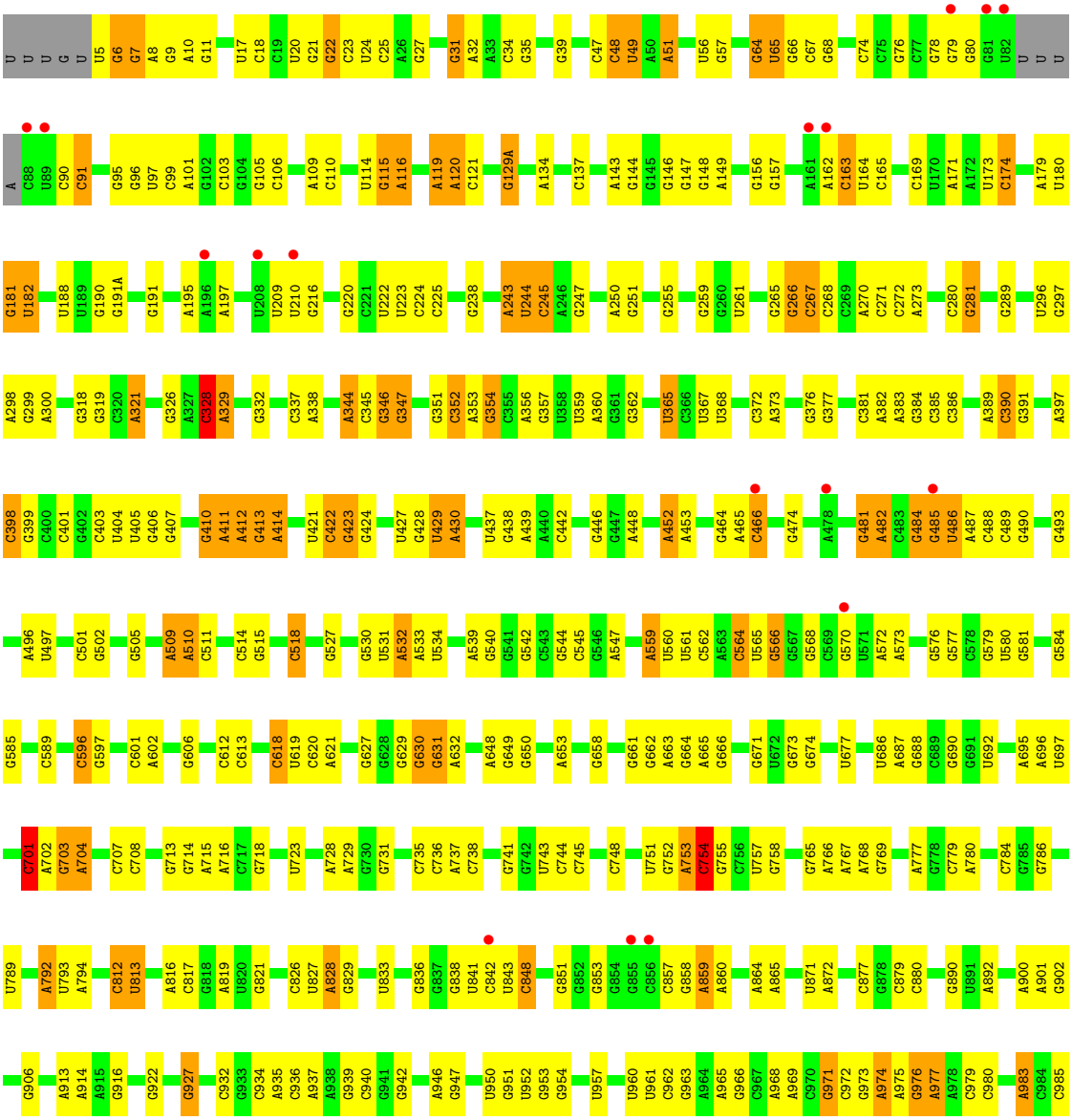
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QD	1	Total Zn 1 1	0	0
59	QN	1	Total Zn 1 1	0	0
59	R5	1	Total Zn 1 1	0	0
59	XD	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0
59	Y9	1	Total Zn 1 1	0	0

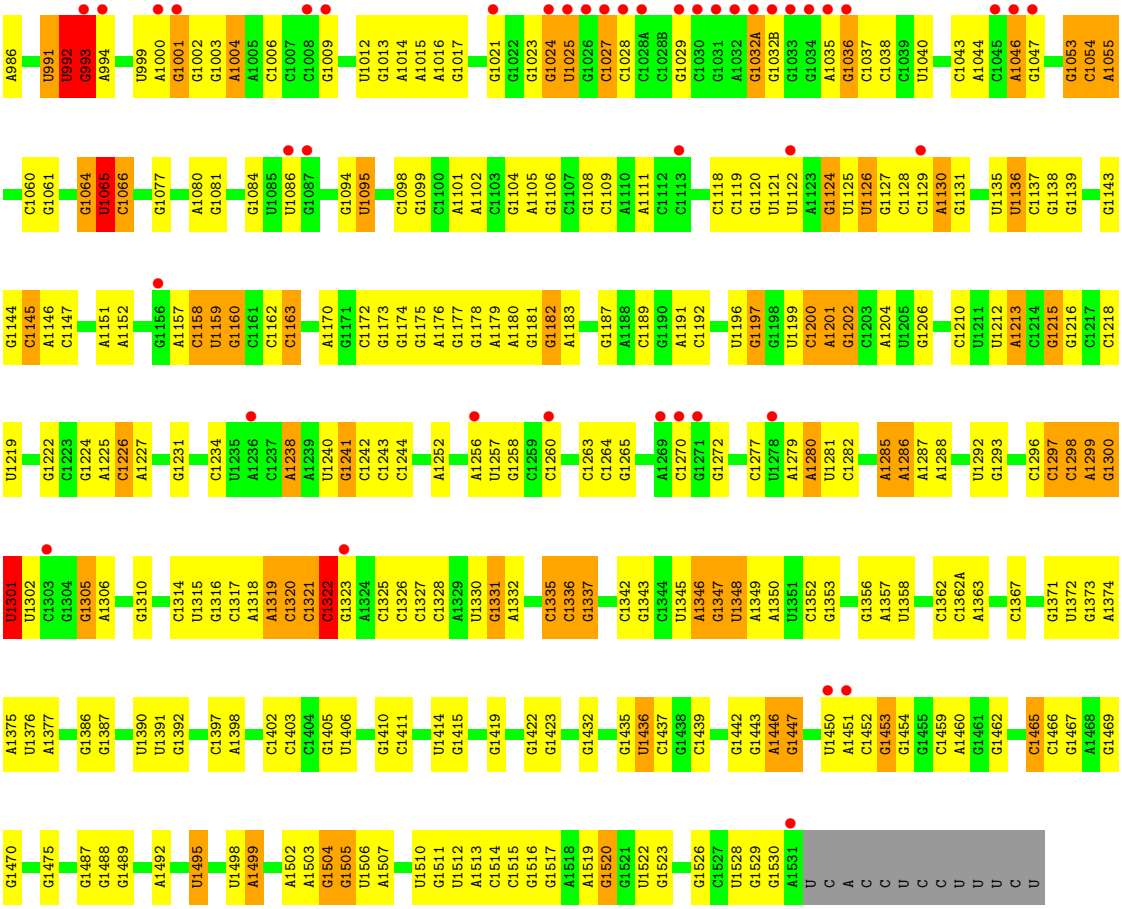
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

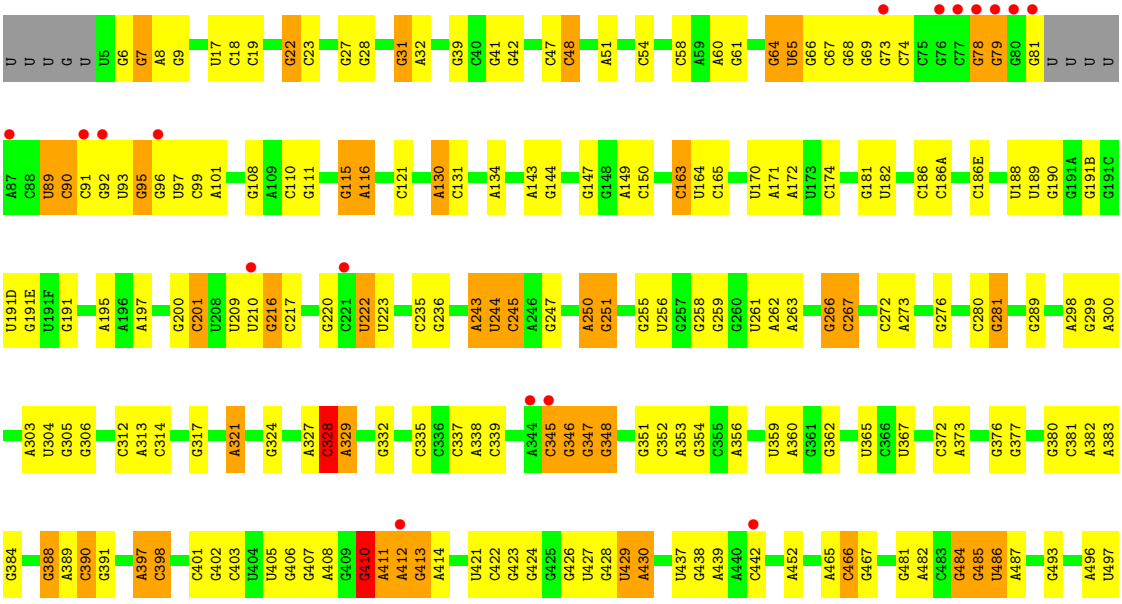
Chain QA: 

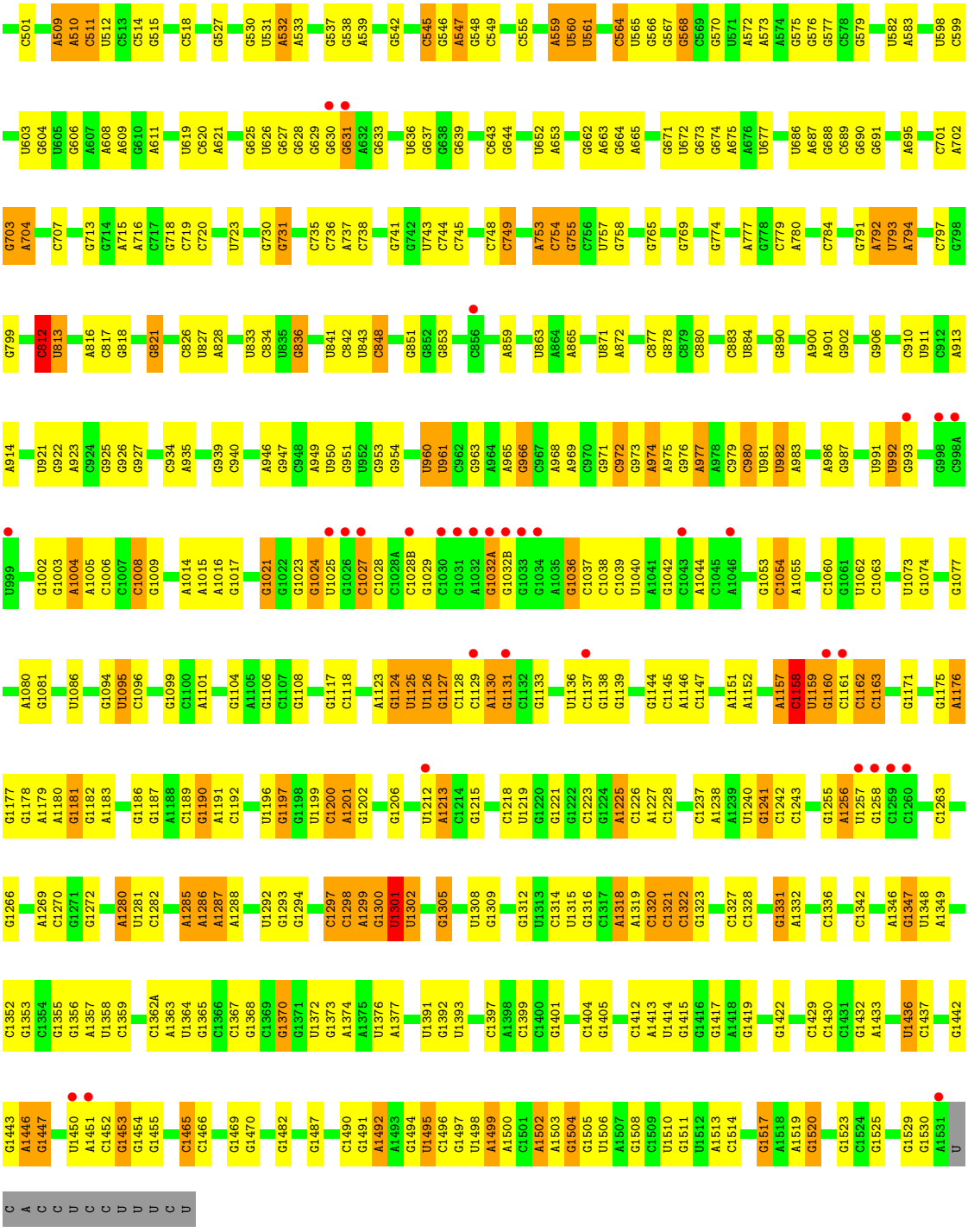




• Molecule 1: 16S ribosomal RNA

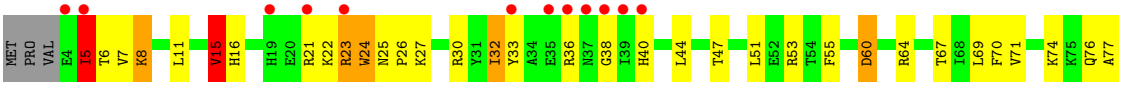
Chain XA:

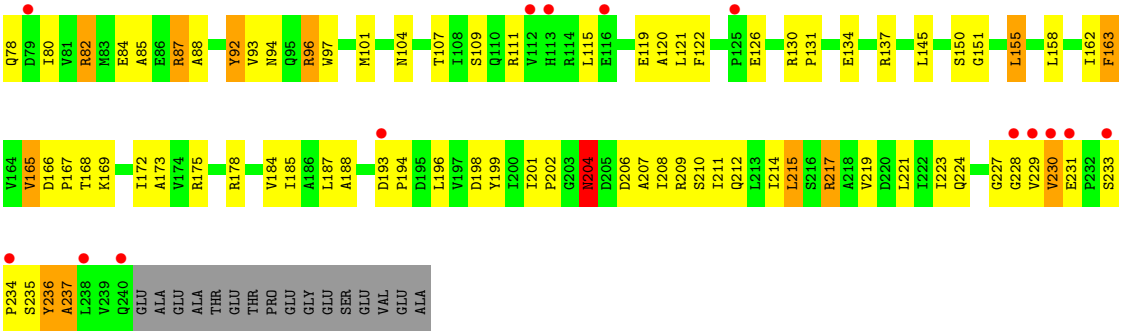




• Molecule 2: 30S ribosomal protein S2

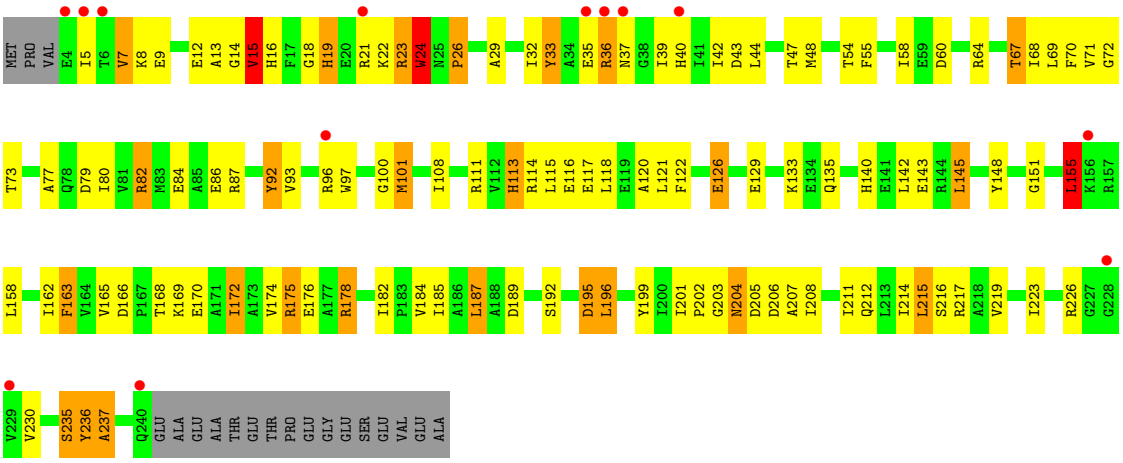
Chain QB:





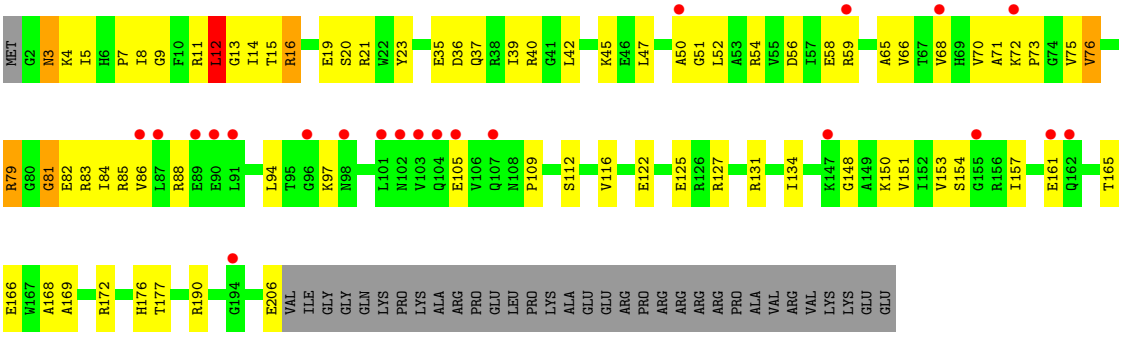
• Molecule 2: 30S ribosomal protein S2

Chain XB:



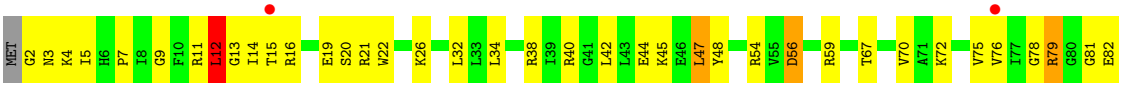
• Molecule 3: 30S ribosomal protein S3

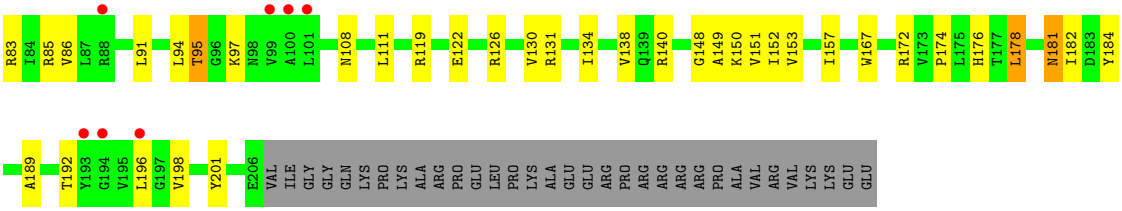
Chain QC:



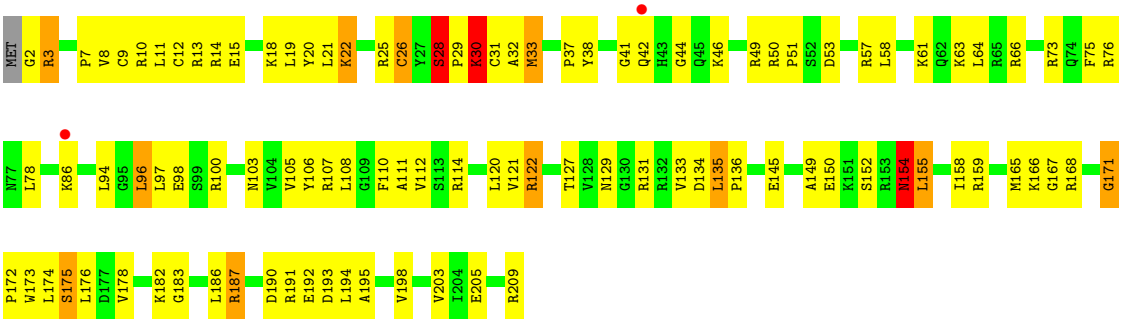
• Molecule 3: 30S ribosomal protein S3

Chain XC:

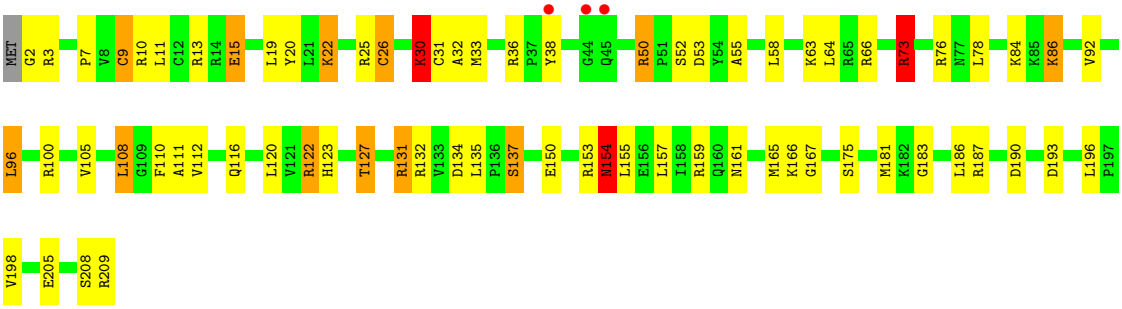




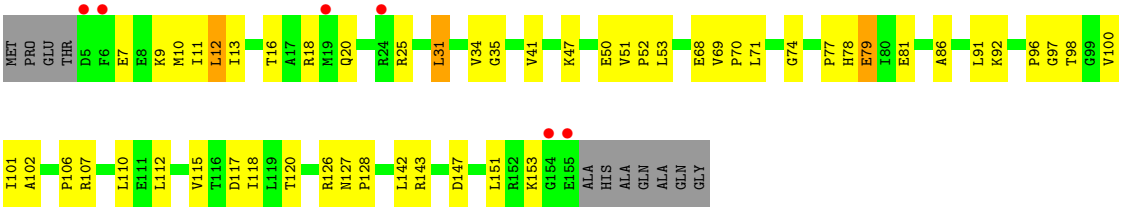
• Molecule 4: 30S ribosomal protein S4



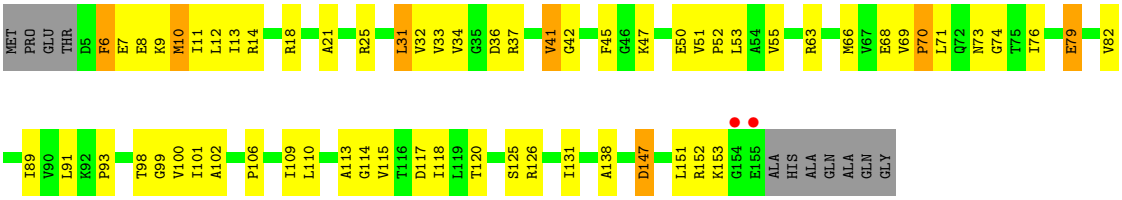
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

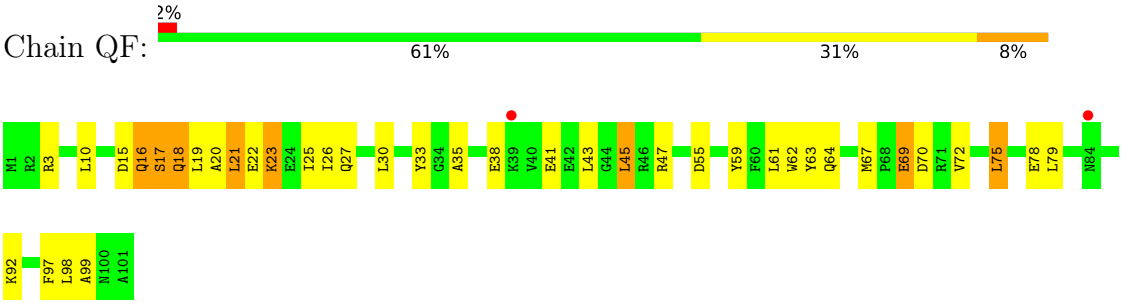


• Molecule 5: 30S ribosomal protein S5



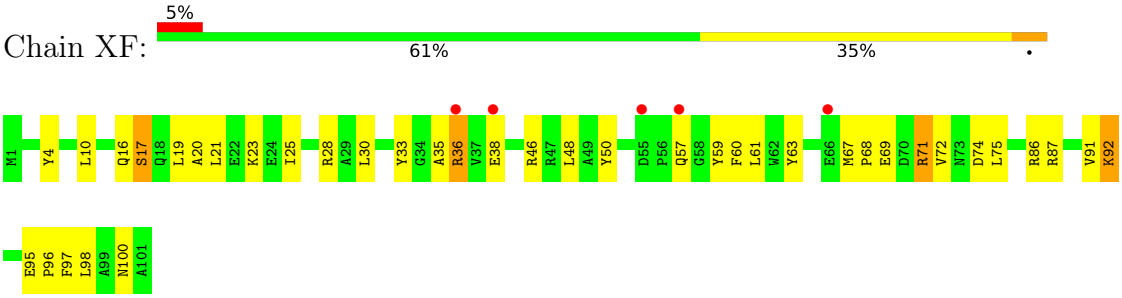
• Molecule 6: 30S ribosomal protein S6

Chain QF:



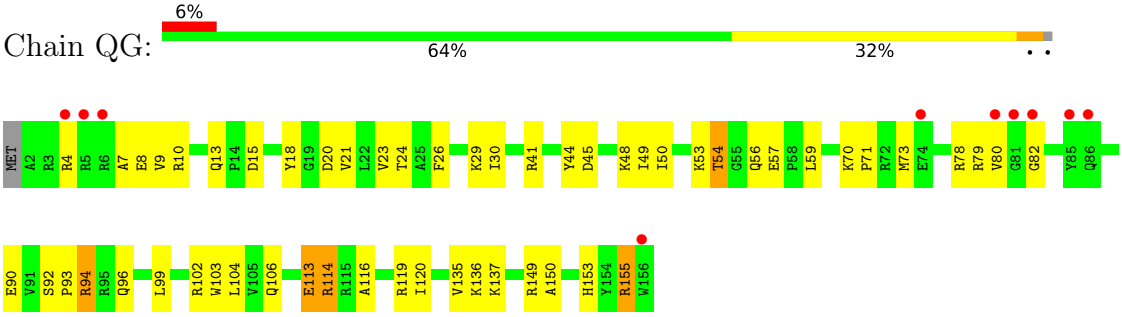
• Molecule 6: 30S ribosomal protein S6

Chain XF:



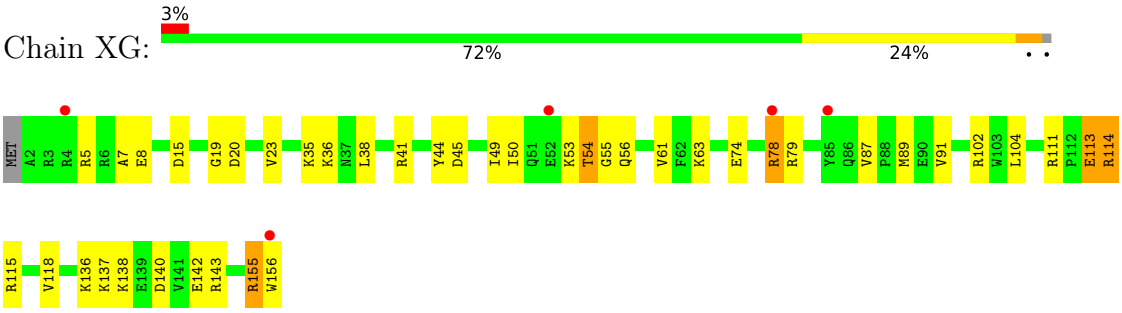
• Molecule 7: 30S ribosomal protein S7

Chain QG:



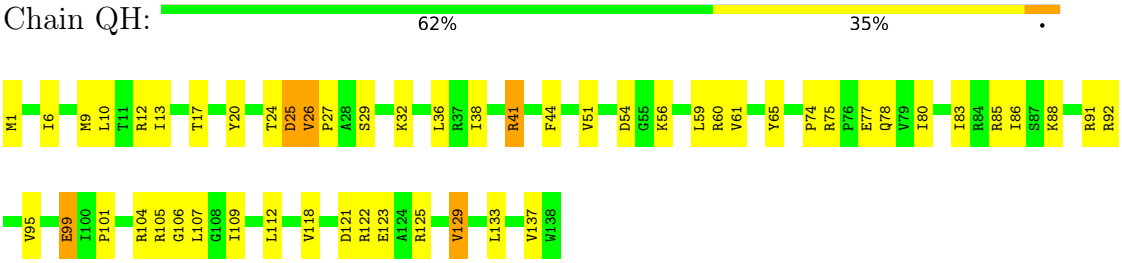
• Molecule 7: 30S ribosomal protein S7

Chain XG:



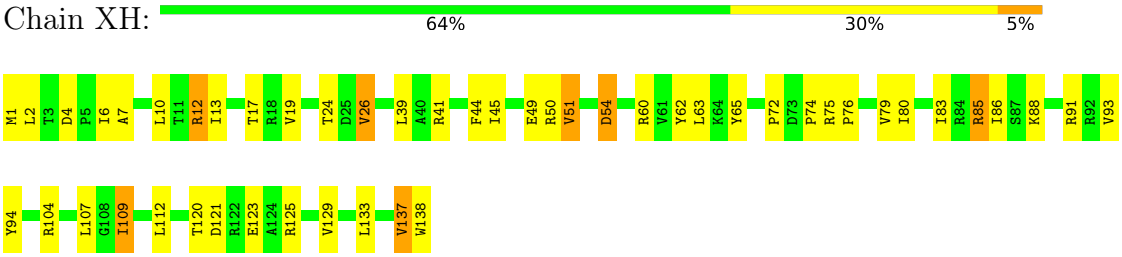
• Molecule 8: 30S ribosomal protein S8

Chain QH:



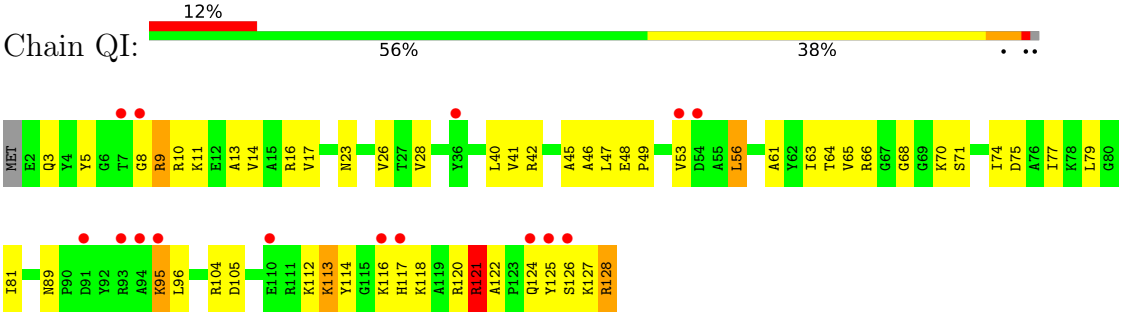
• Molecule 8: 30S ribosomal protein S8

Chain XH:



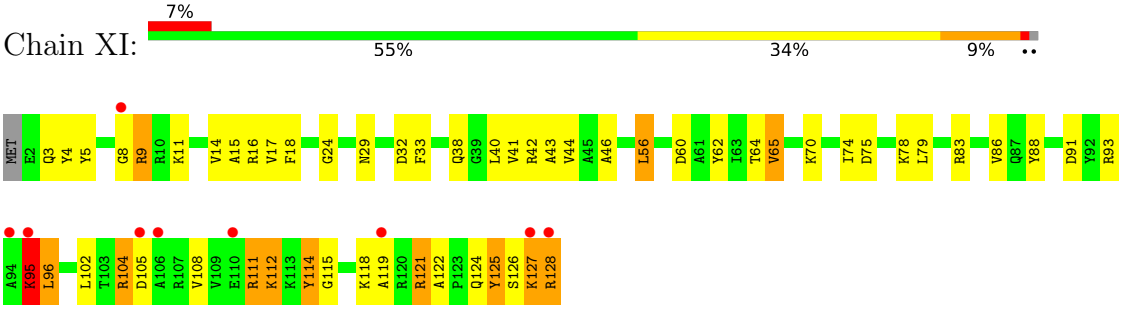
• Molecule 9: 30S ribosomal protein S9

Chain QI:



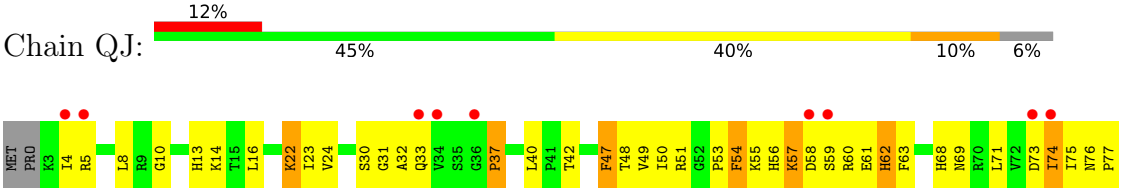
• Molecule 9: 30S ribosomal protein S9

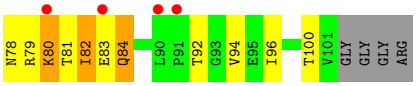
Chain XI:



• Molecule 10: 30S ribosomal protein S10

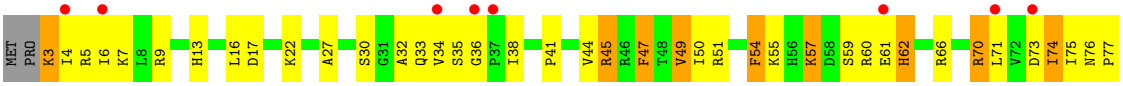
Chain QJ:

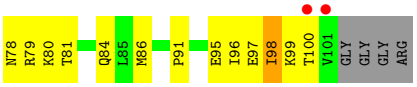




• Molecule 10: 30S ribosomal protein S10

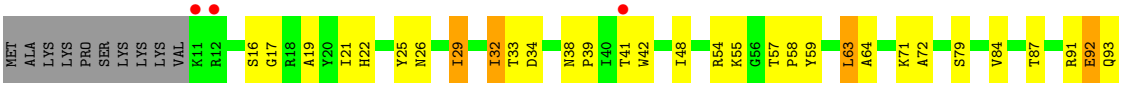
Chain XJ:

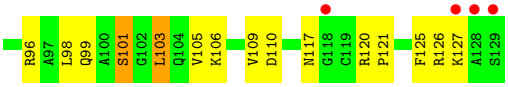




• Molecule 11: 30S ribosomal protein S11

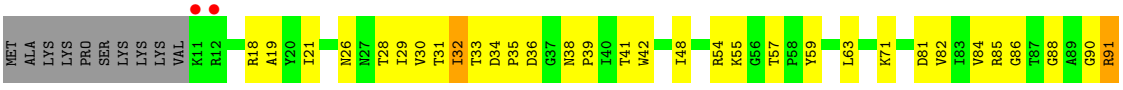
Chain QK:

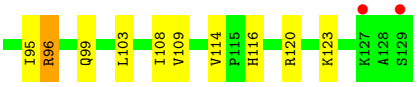




• Molecule 11: 30S ribosomal protein S11

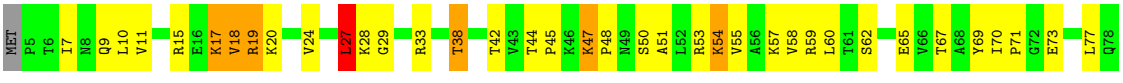
Chain XK:

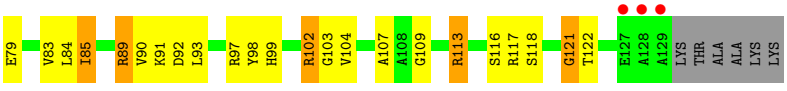




• Molecule 12: 30S ribosomal protein S12

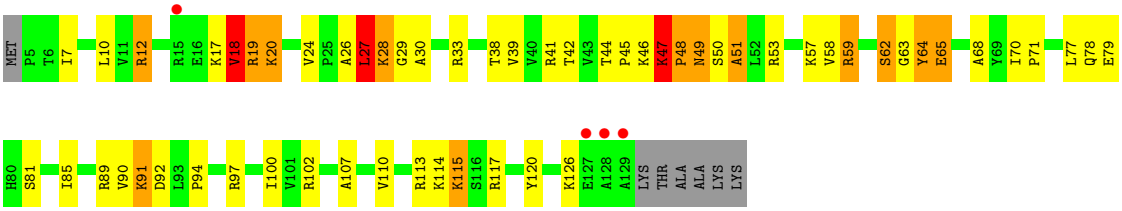
Chain QL:



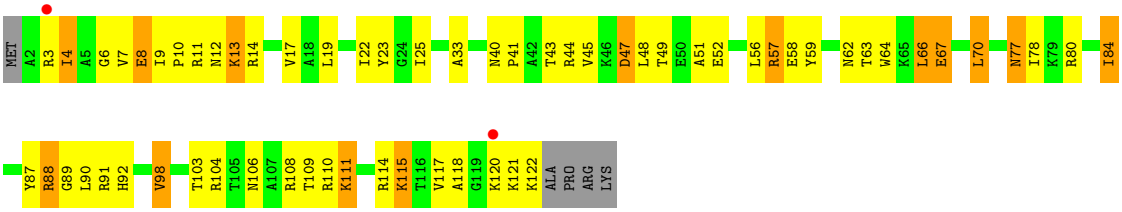


• Molecule 12: 30S ribosomal protein S12

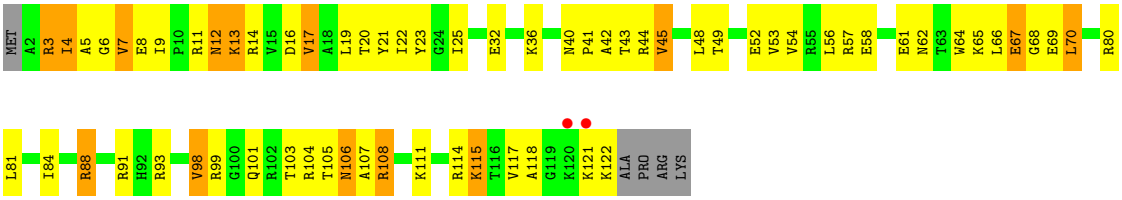
Chain XL:



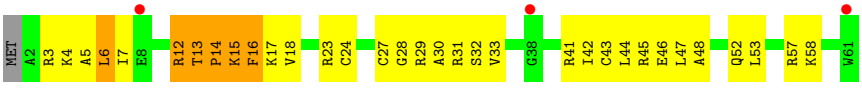
• Molecule 13: 30S ribosomal protein S13



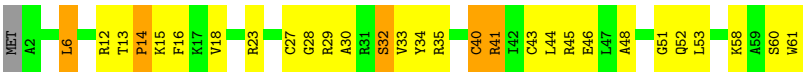
• Molecule 13: 30S ribosomal protein S13



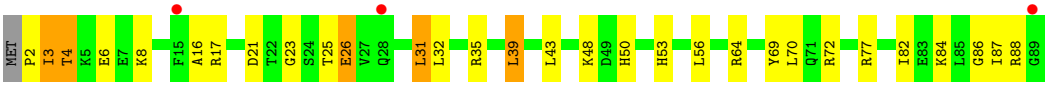
• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 14: 30S ribosomal protein S14 type Z

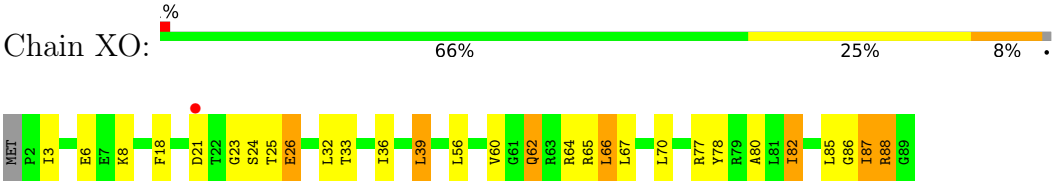


• Molecule 15: 30S ribosomal protein S15



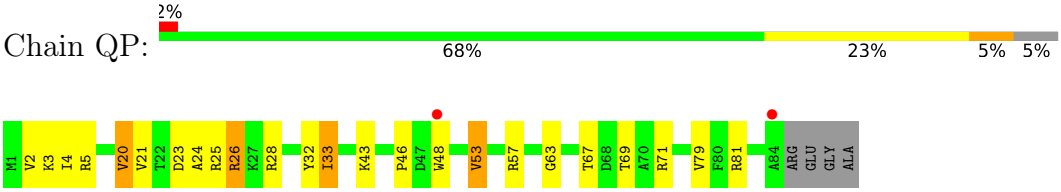
• Molecule 15: 30S ribosomal protein S15

Chain XO:



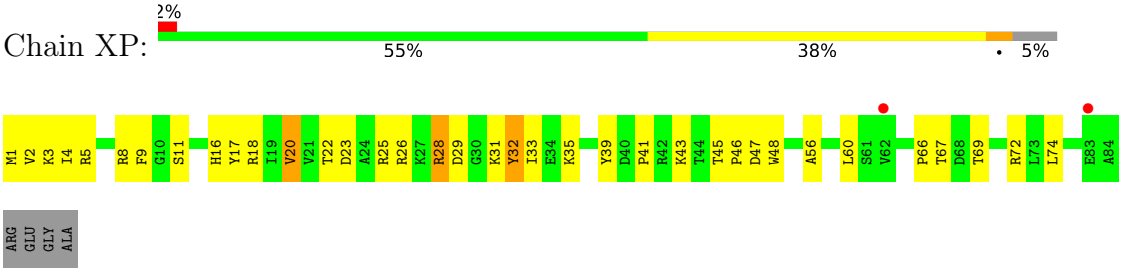
• Molecule 16: 30S ribosomal protein S16

Chain QP:



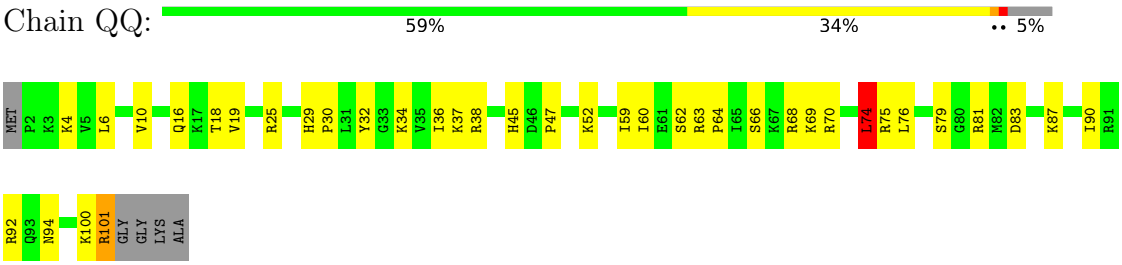
• Molecule 16: 30S ribosomal protein S16

Chain XP:



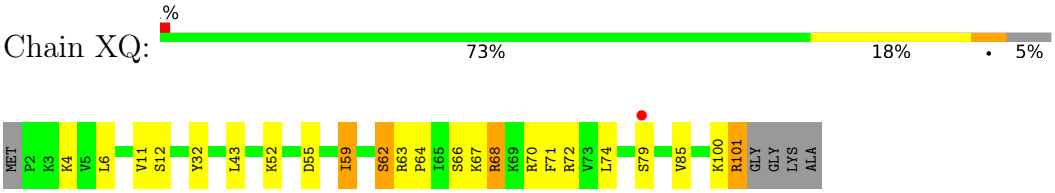
• Molecule 17: 30S ribosomal protein S17

Chain QQ:



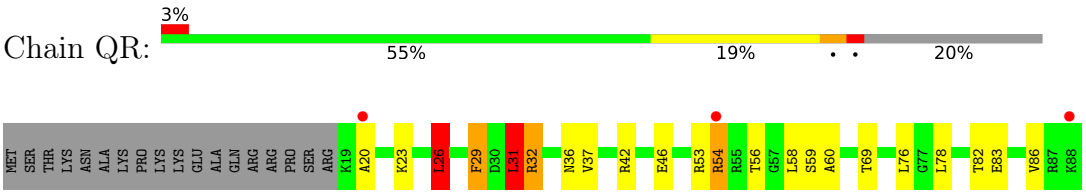
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



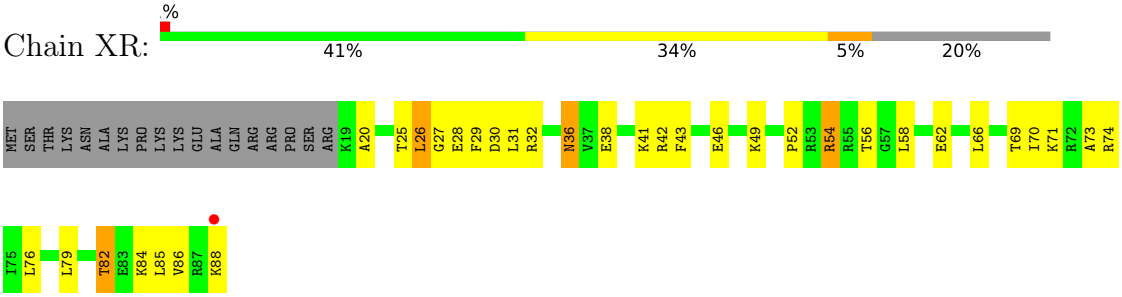
• Molecule 18: 30S ribosomal protein S18

Chain QR:



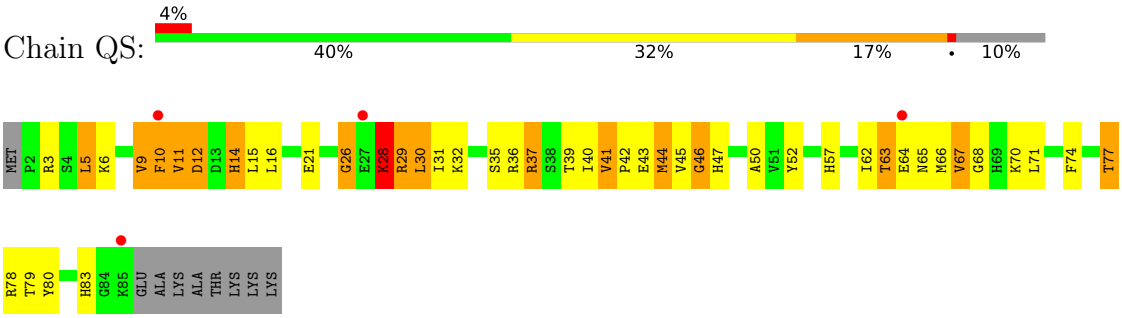
• Molecule 18: 30S ribosomal protein S18

Chain XR:



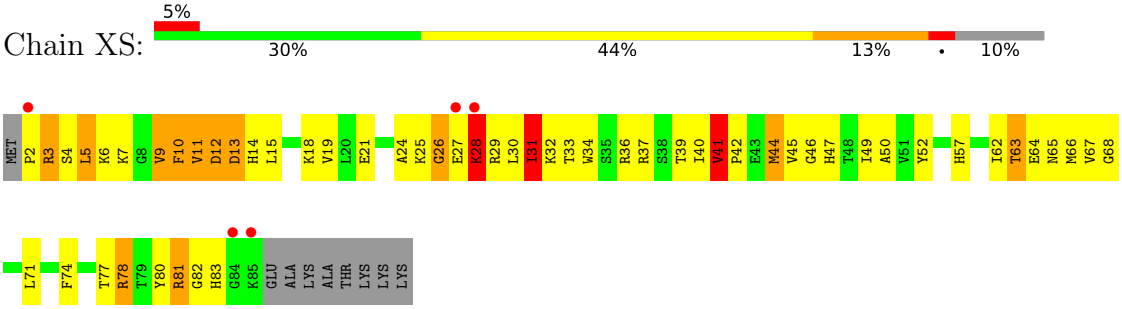
• Molecule 19: 30S ribosomal protein S19

Chain QS:



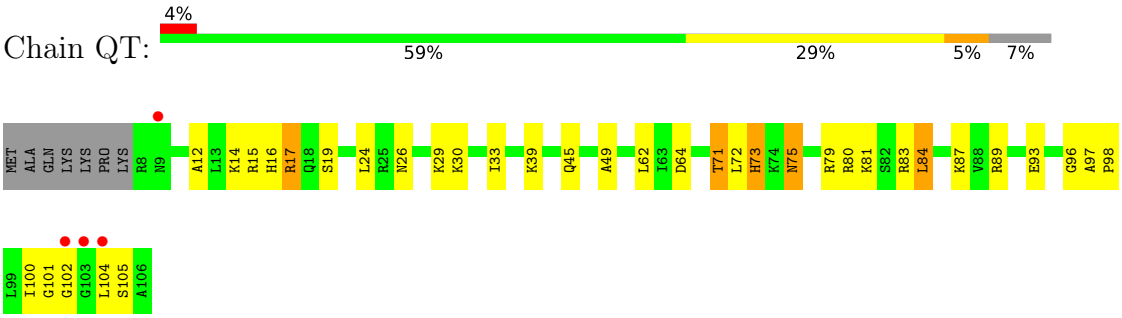
• Molecule 19: 30S ribosomal protein S19

Chain XS:



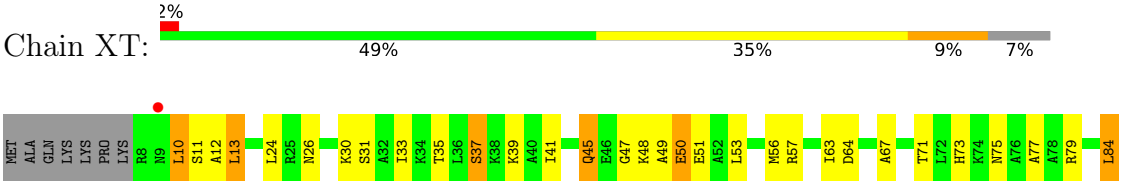
• Molecule 20: 30S ribosomal protein S20

Chain QT:



• Molecule 20: 30S ribosomal protein S20

Chain XT:

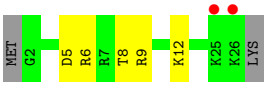


• Molecule 21: 30S ribosomal protein Thx

Chain QU:

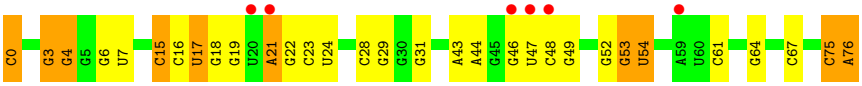
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



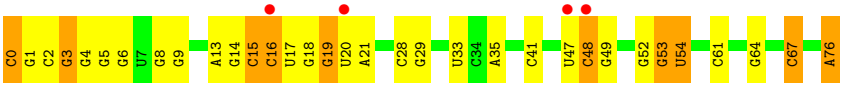
• Molecule 22: tRNA-fMet

Chain QV:



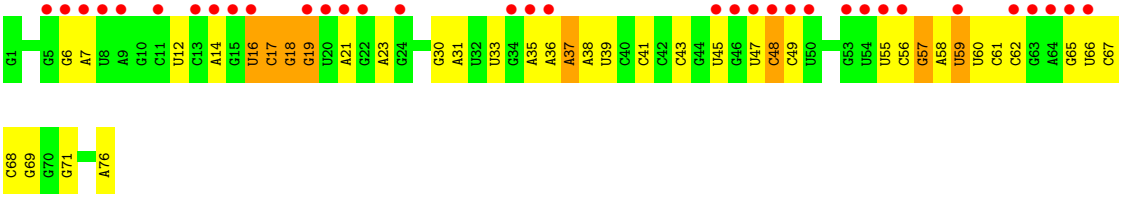
• Molecule 22: tRNA-fMet

Chain XV:



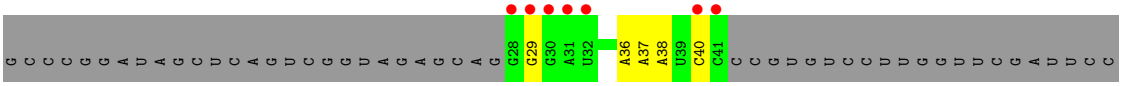
• Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

Chain QW:



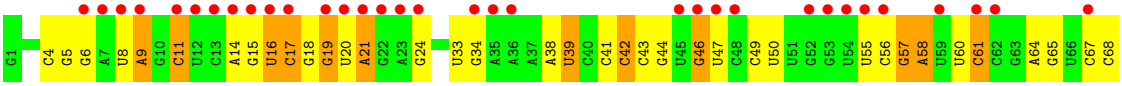
• Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

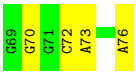
Chain QY:



• Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

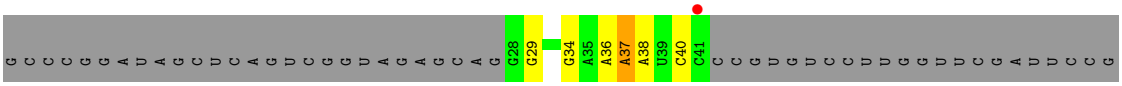
Chain XW:





• Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

Chain XY:

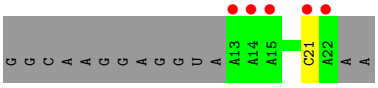


• Molecule 24: mRNA

Chain QX:

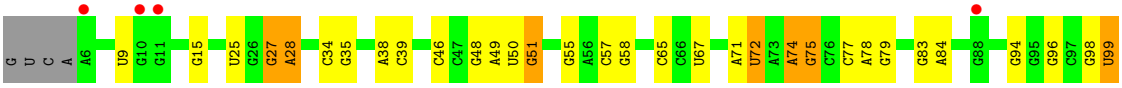
• Molecule 24: mRNA

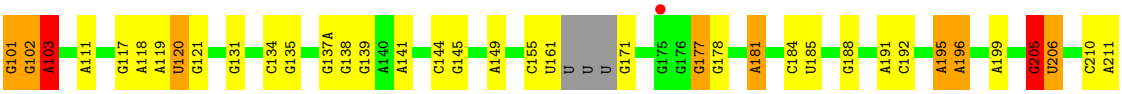
Chain XX:

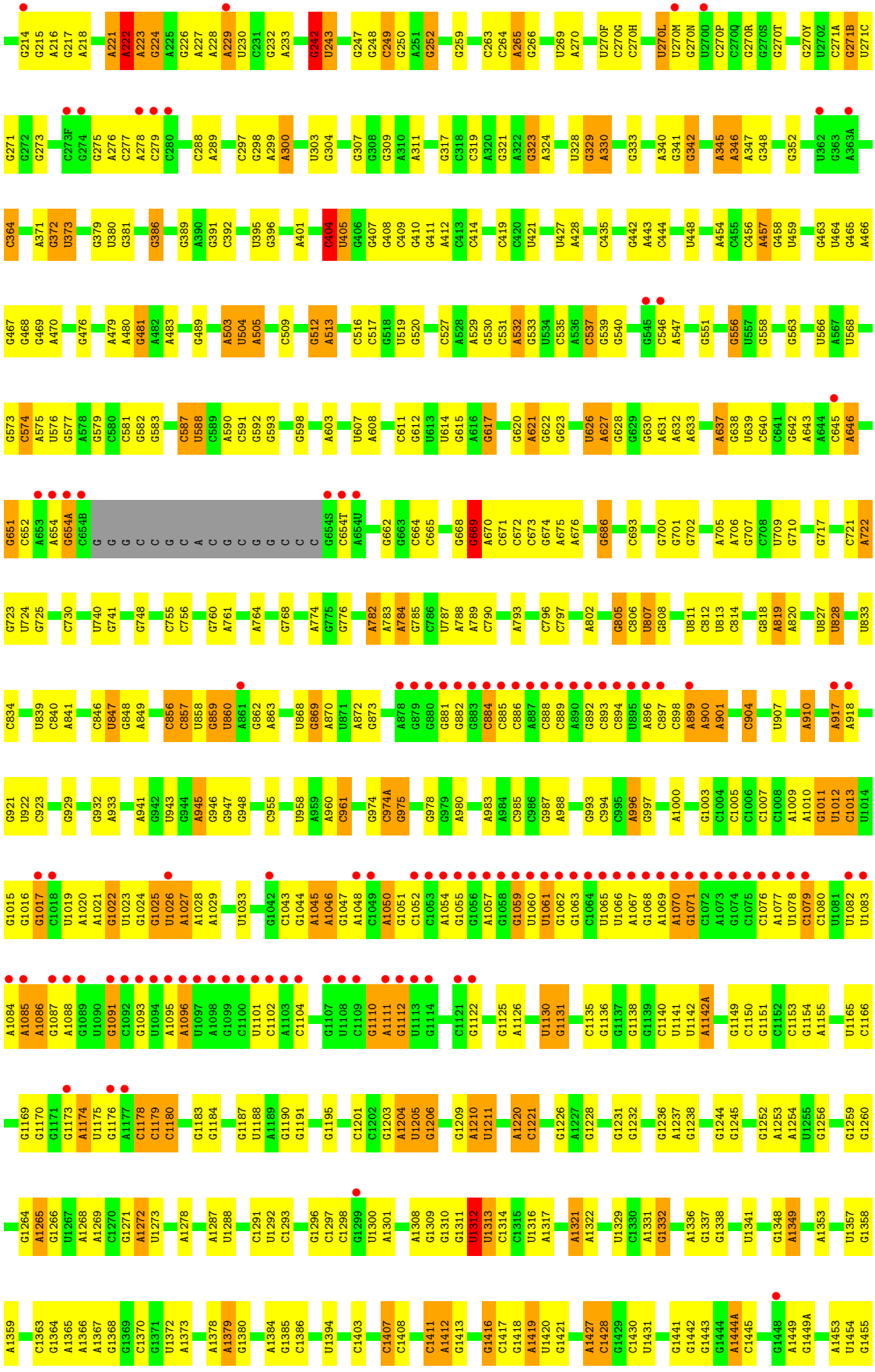


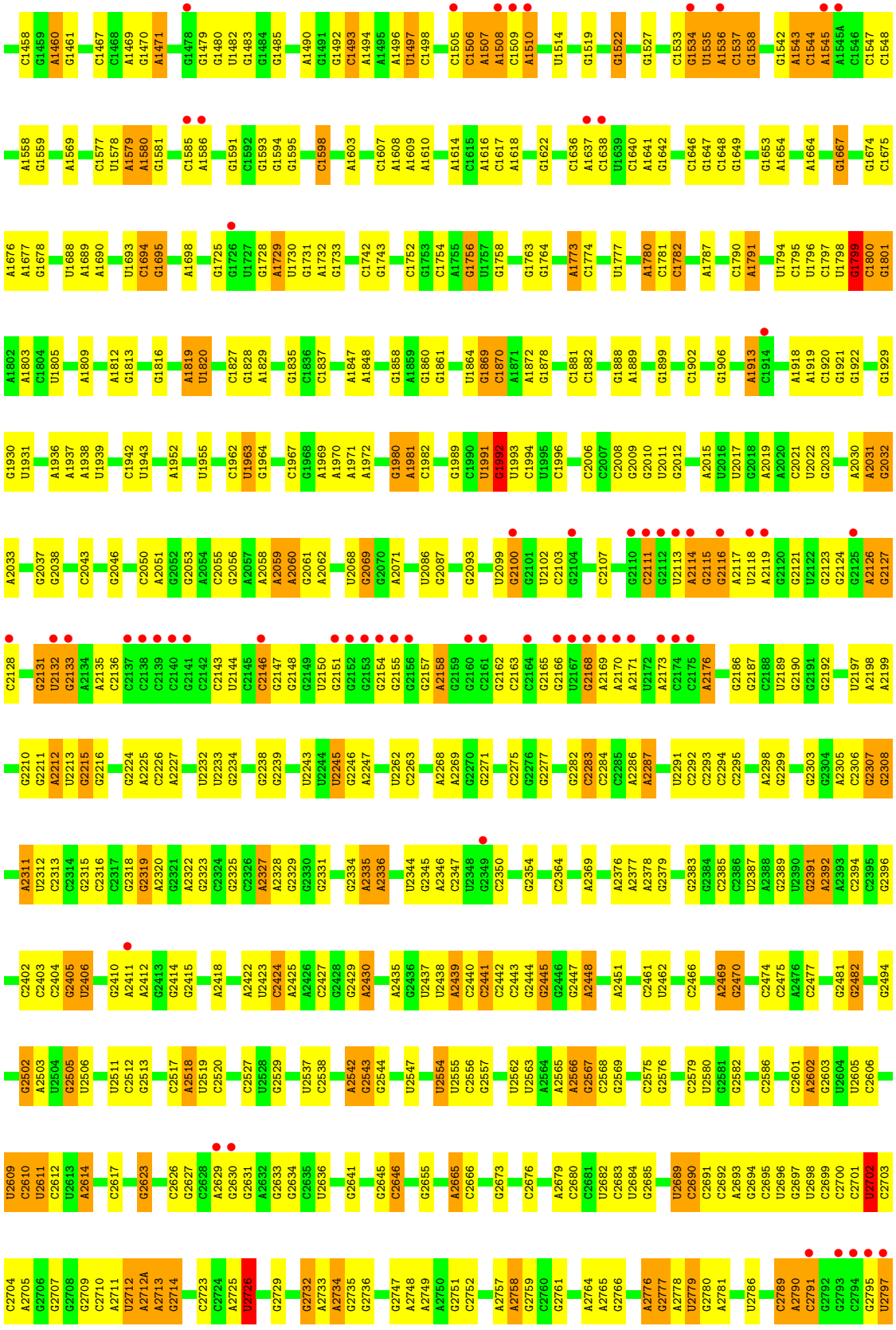
• Molecule 25: 23S ribosomal RNA

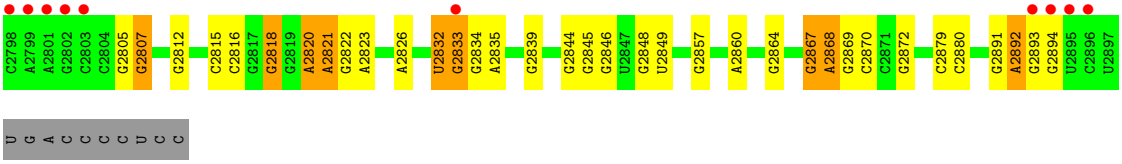
Chain RA:





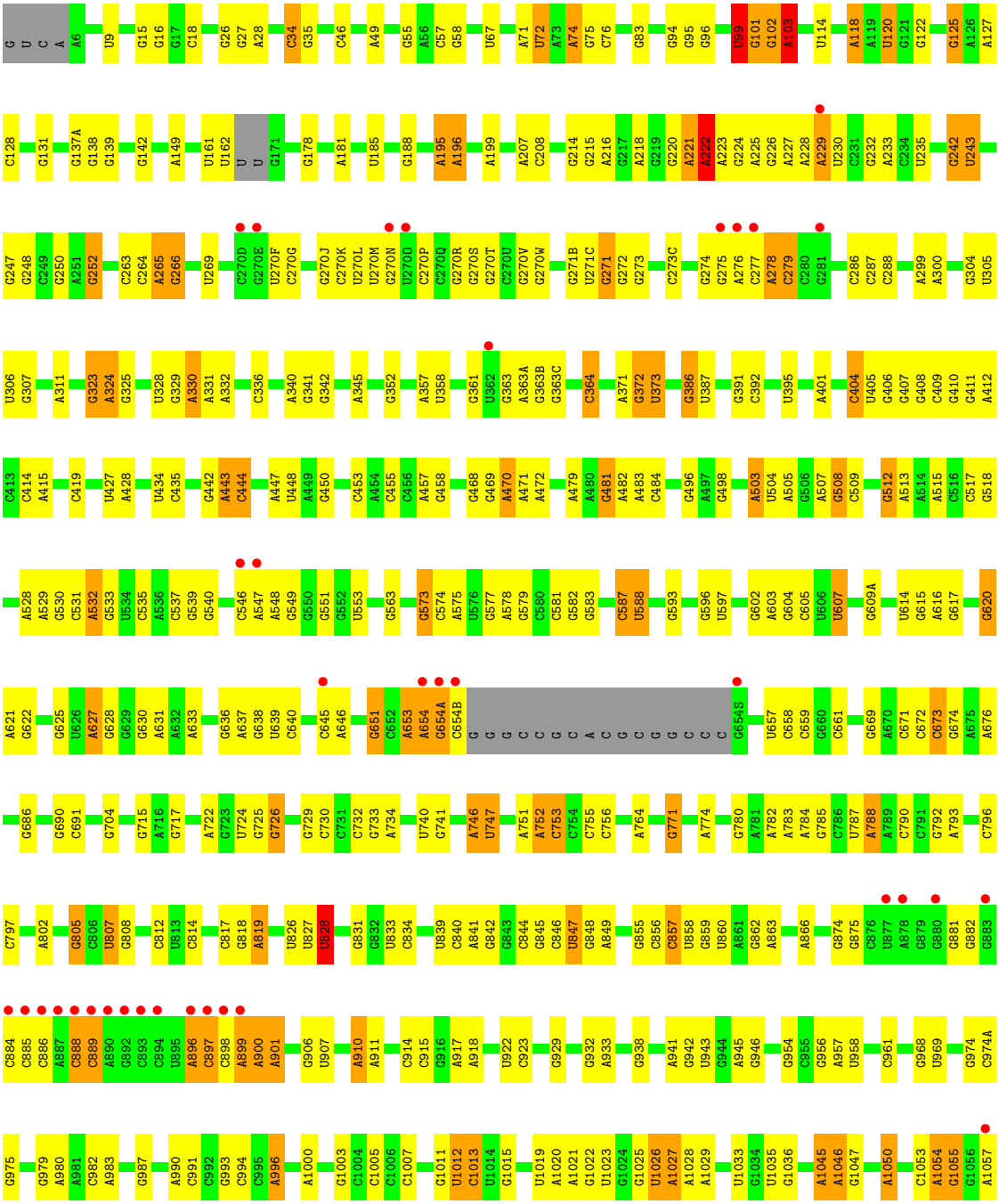


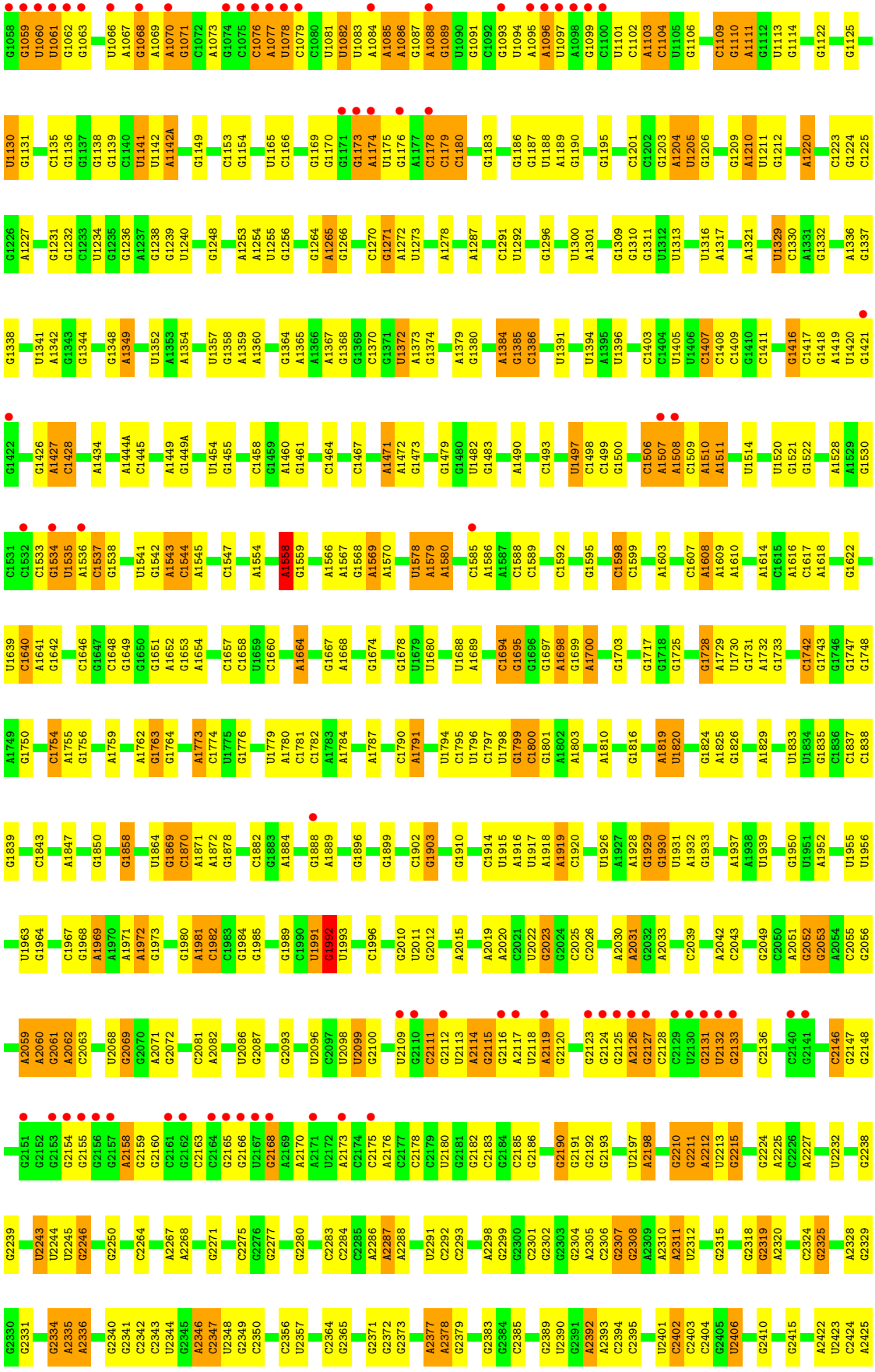


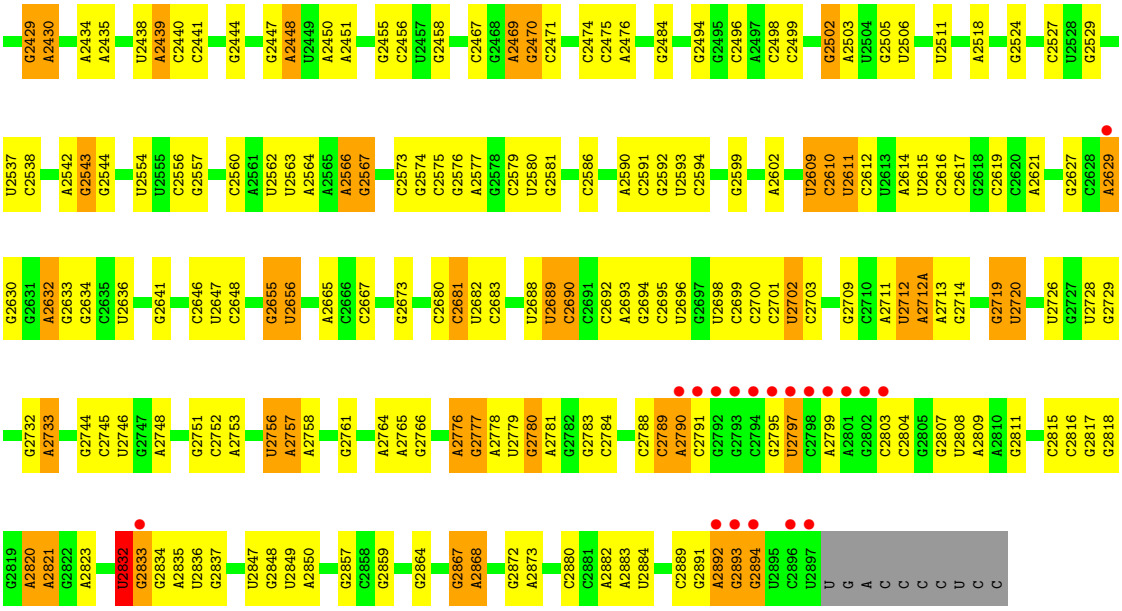


• Molecule 25: 23S ribosomal RNA

Chain YA:

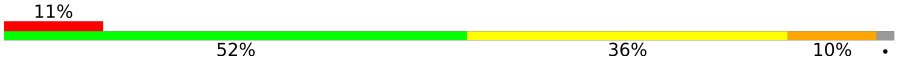


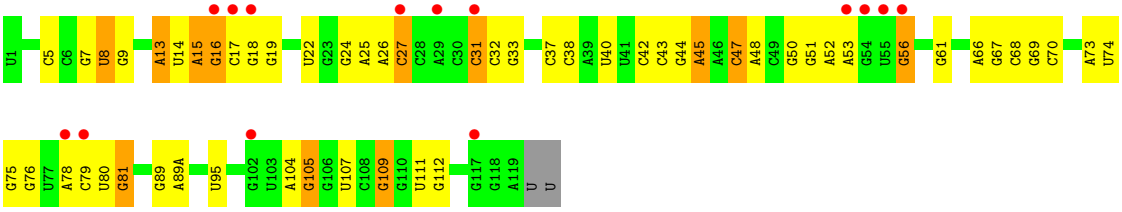




• Molecule 26: 5S ribosomal RNA

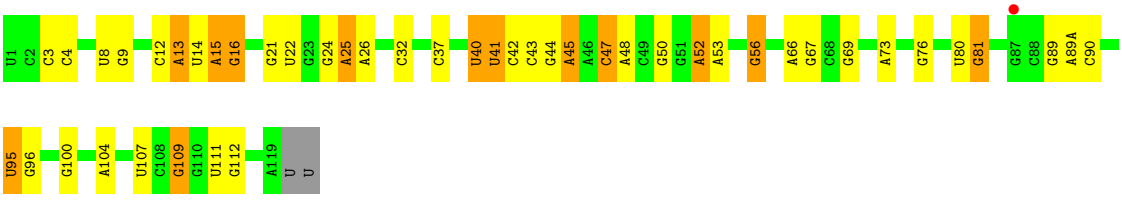
Chain RB:





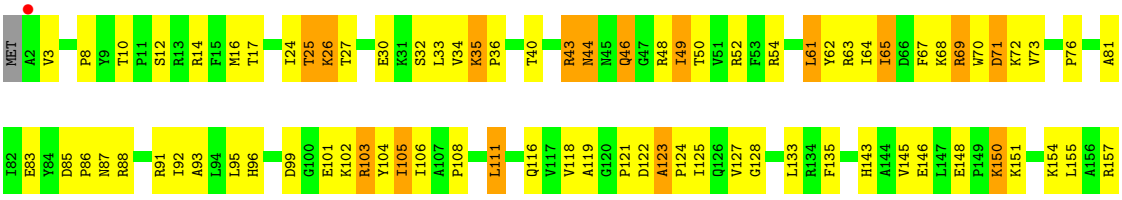
• Molecule 26: 5S ribosomal RNA

Chain YB:



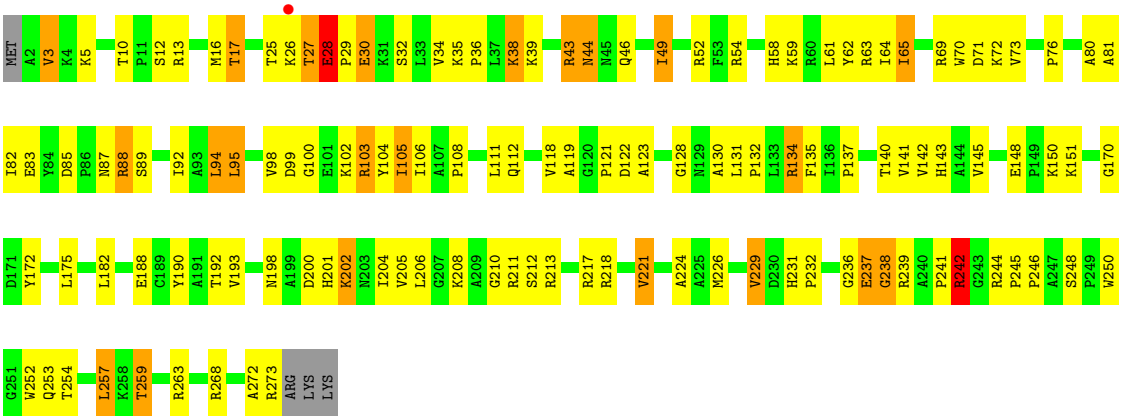
• Molecule 27: 50S ribosomal protein L2

Chain RD:



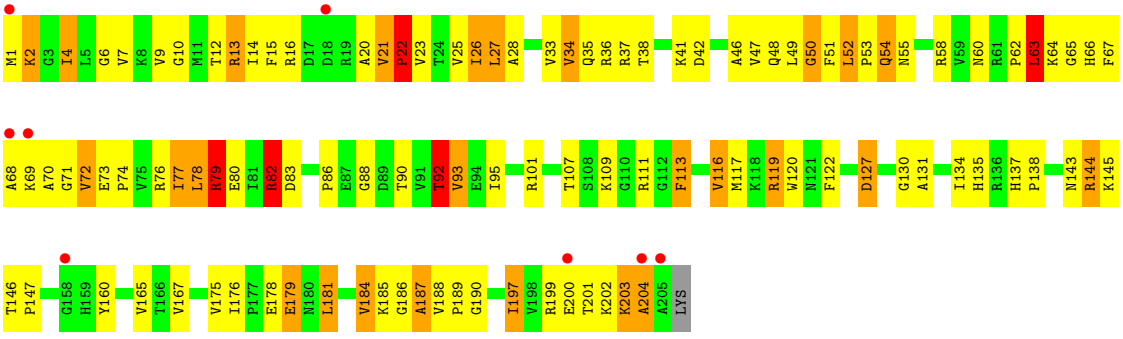
• Molecule 27: 50S ribosomal protein L2

Chain YD:



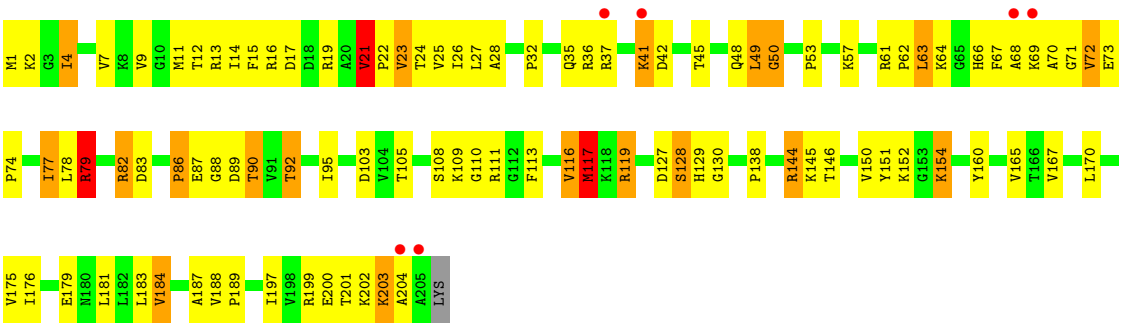
• Molecule 28: 50S ribosomal protein L3

Chain RE:



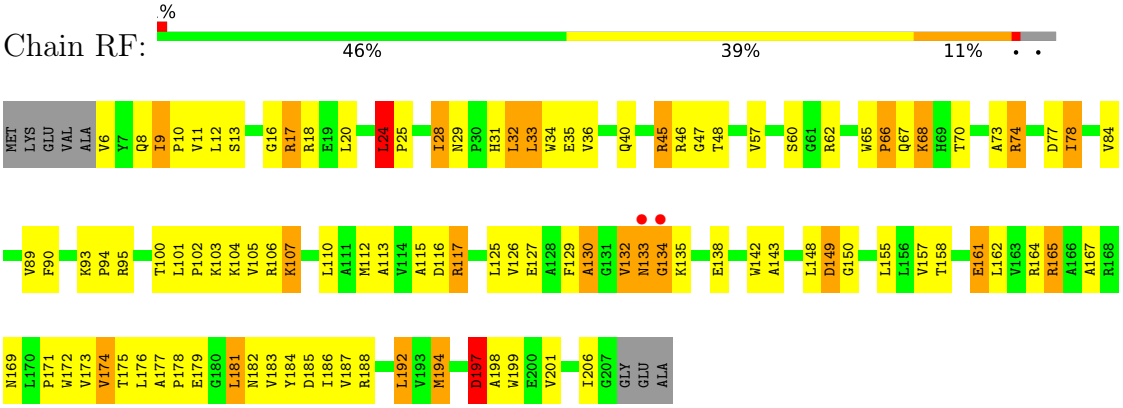
• Molecule 28: 50S ribosomal protein L3

Chain YE:



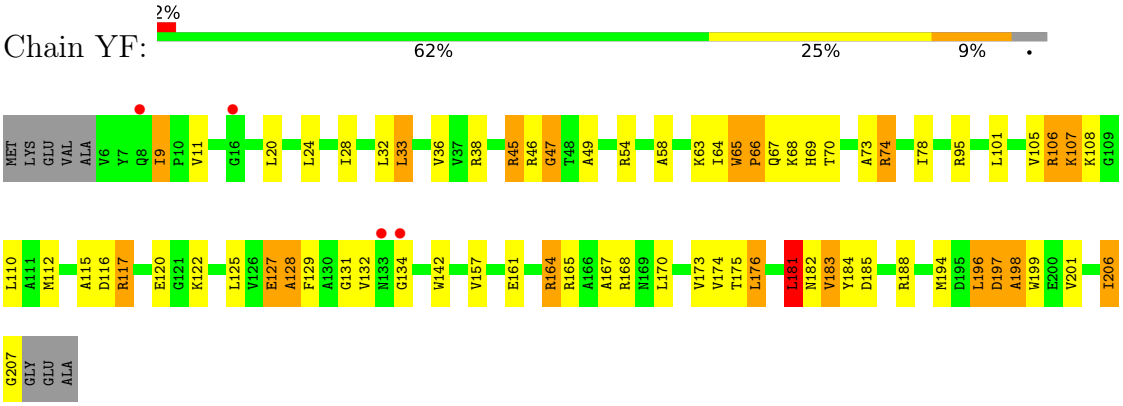
• Molecule 29: 50S ribosomal protein L4

Chain RF:



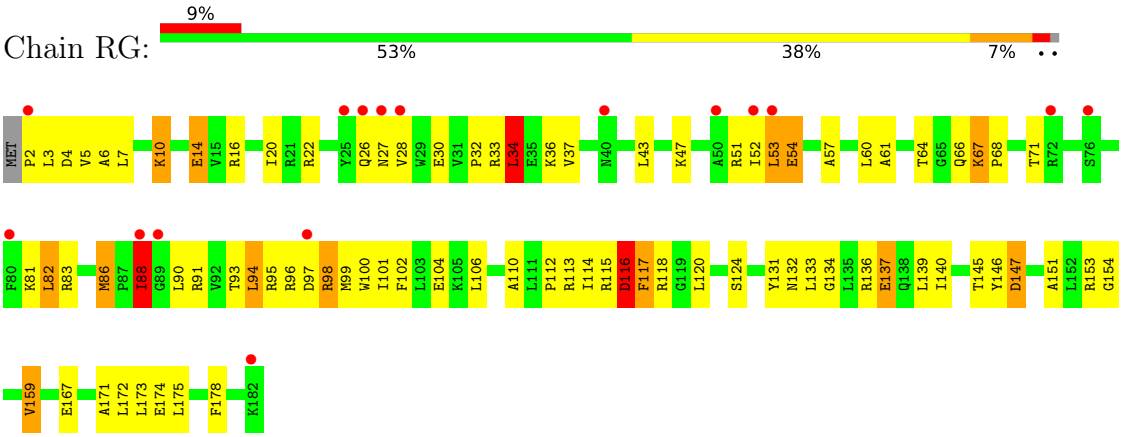
• Molecule 29: 50S ribosomal protein L4

Chain YF:



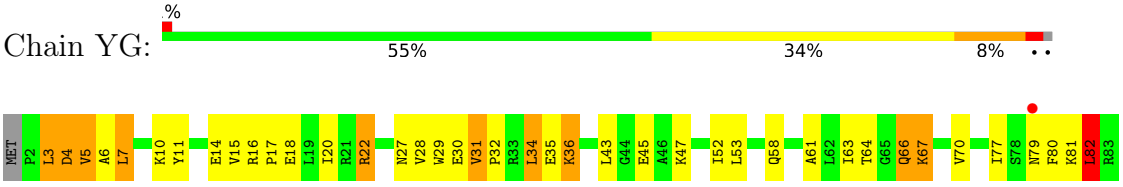
• Molecule 30: 50S ribosomal protein L5

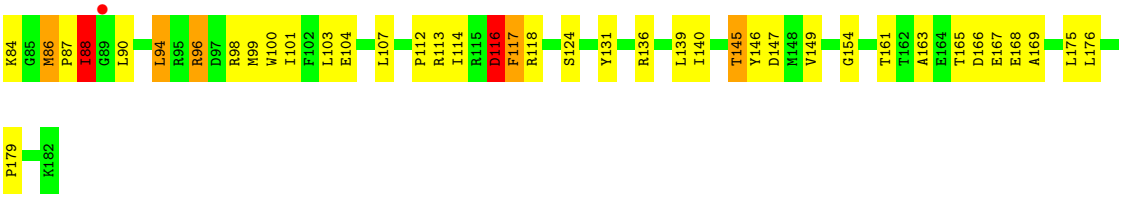
Chain RG:



• Molecule 30: 50S ribosomal protein L5

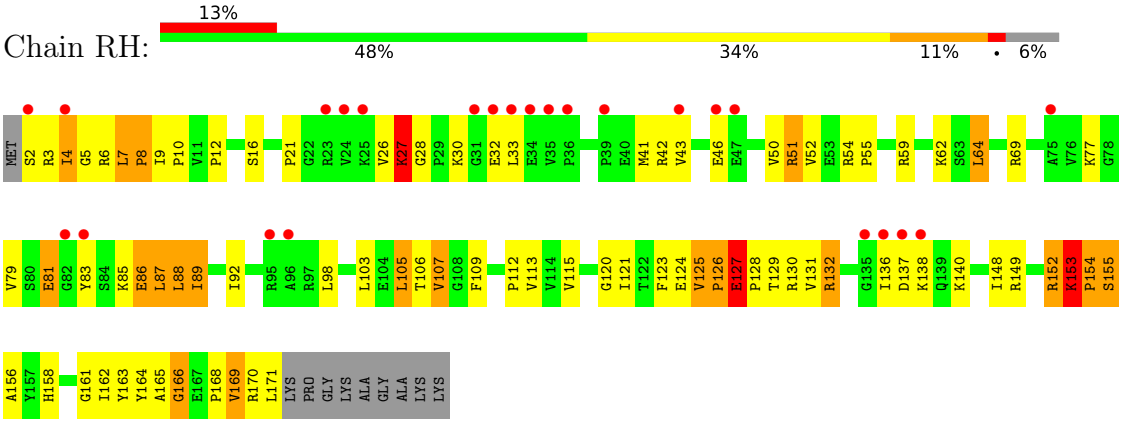
Chain YG:





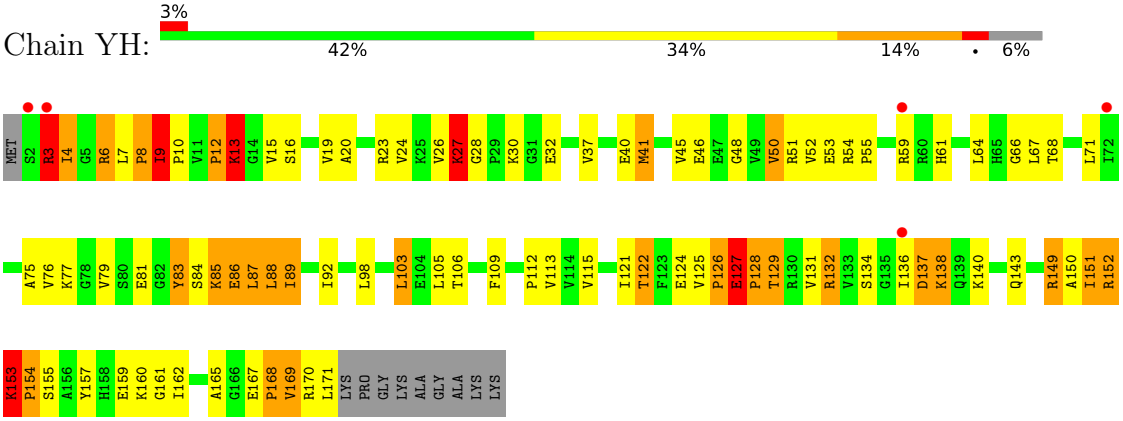
- Molecule 31: 50S ribosomal protein L6

Chain RH:



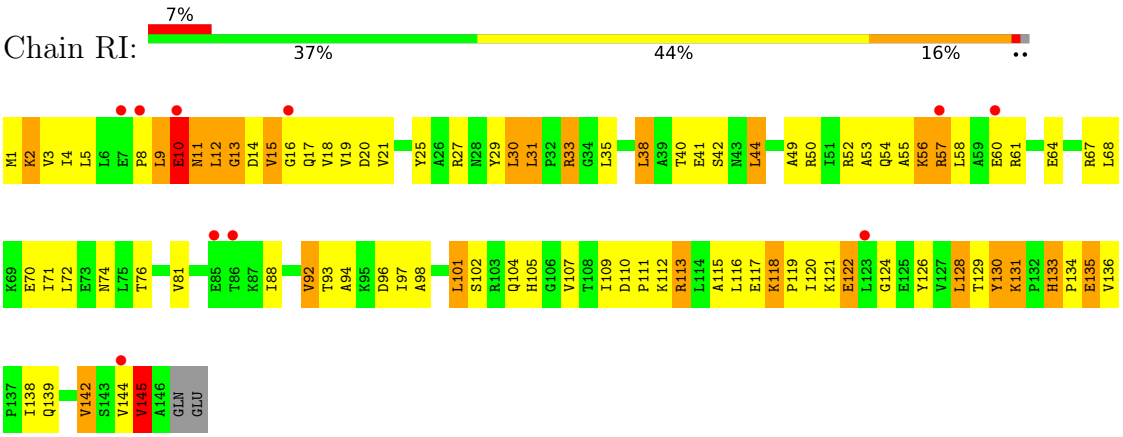
- Molecule 31: 50S ribosomal protein L6

Chain YH:



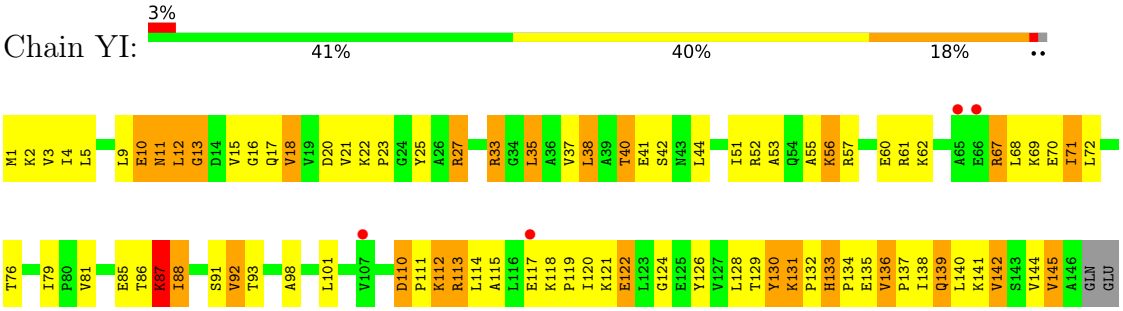
- Molecule 32: 50S ribosomal protein L9

Chain RI:



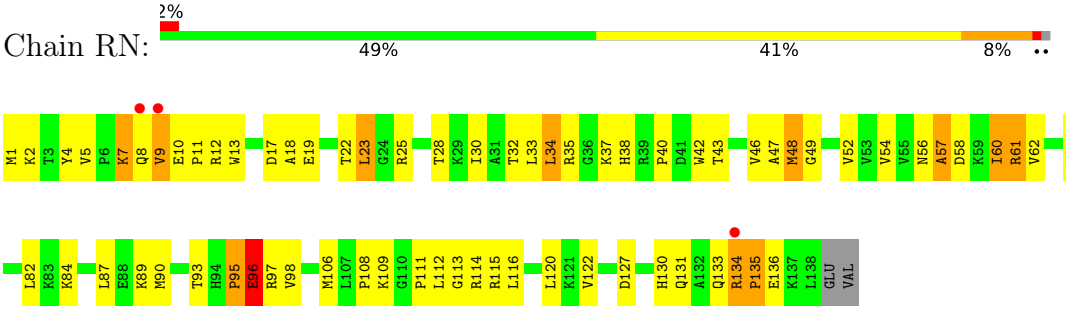
- Molecule 32: 50S ribosomal protein L9

Chain YI:



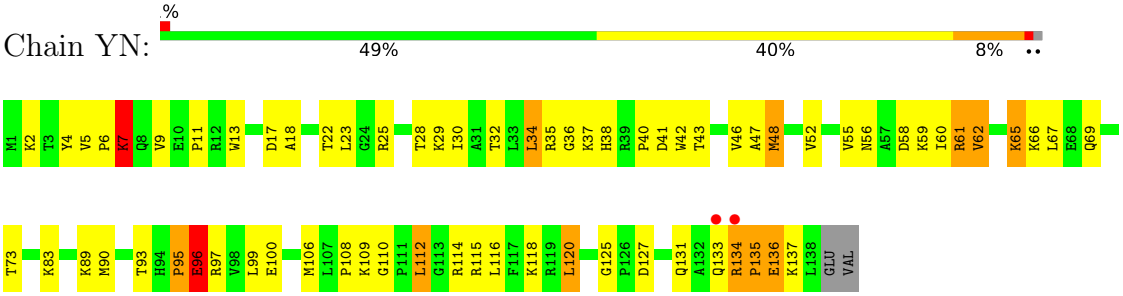
• Molecule 33: 50S ribosomal protein L13

Chain RN:



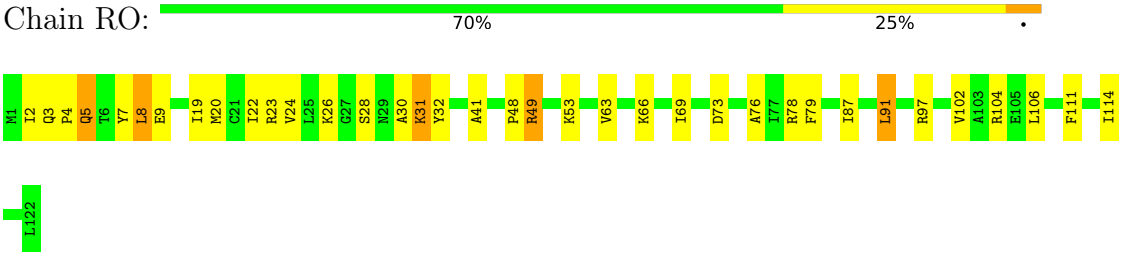
• Molecule 33: 50S ribosomal protein L13

Chain YN:



• Molecule 34: 50S ribosomal protein L14

Chain RO:

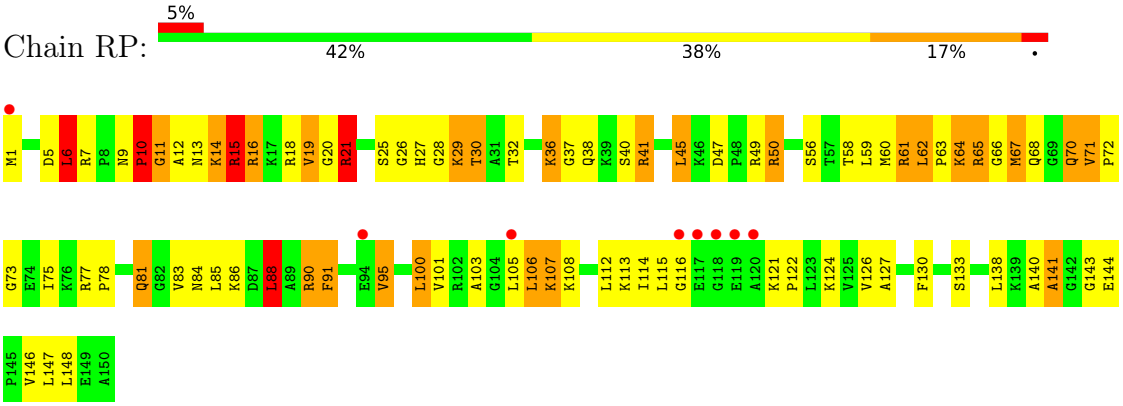


• Molecule 34: 50S ribosomal protein L14

Chain YO:

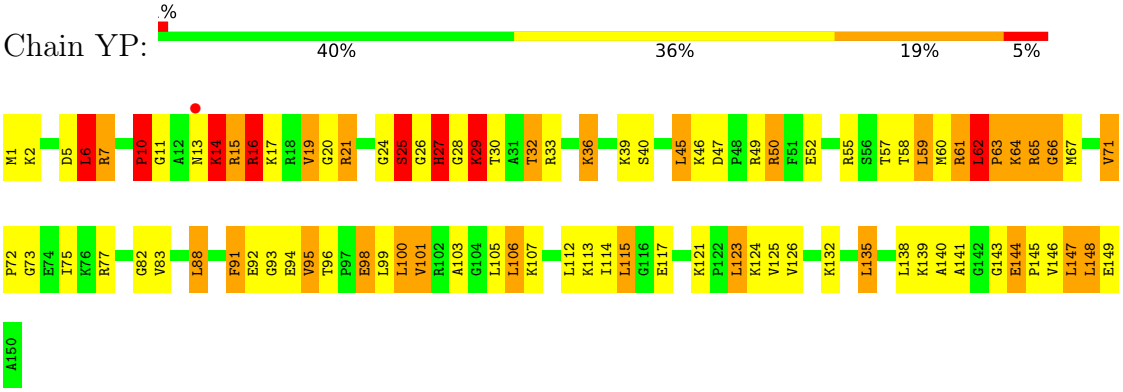
• Molecule 35: 50S ribosomal protein L15

Chain RP:



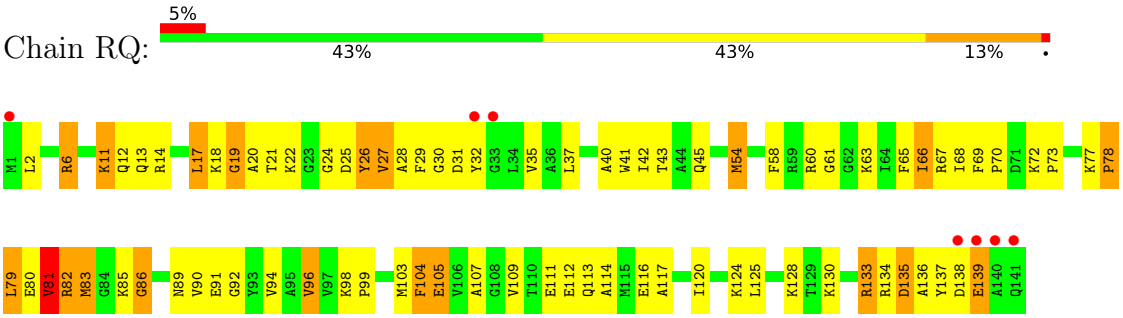
• Molecule 35: 50S ribosomal protein L15

Chain YP:



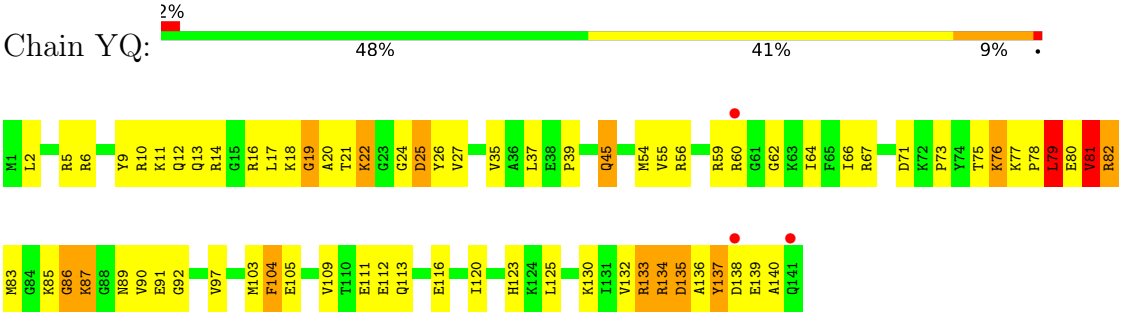
• Molecule 36: 50S ribosomal protein L16

Chain RQ:



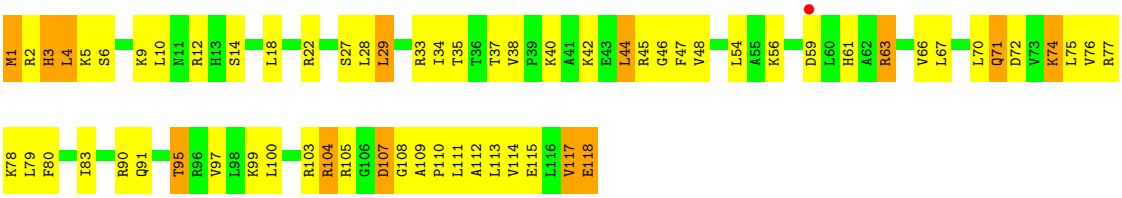
• Molecule 36: 50S ribosomal protein L16

Chain YQ:



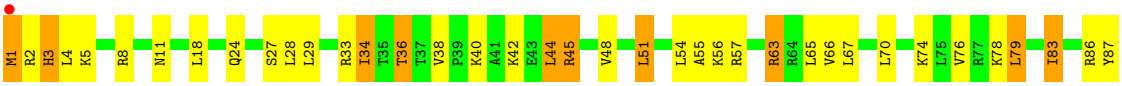
• Molecule 37: 50S ribosomal protein L17

Chain RR:



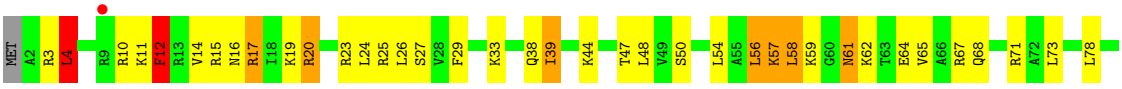
• Molecule 37: 50S ribosomal protein L17

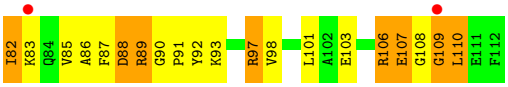
Chain YR:



• Molecule 38: 50S ribosomal protein L18

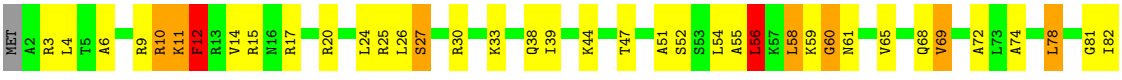
Chain RS:





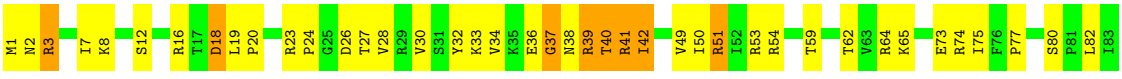
• Molecule 38: 50S ribosomal protein L18

Chain YS:



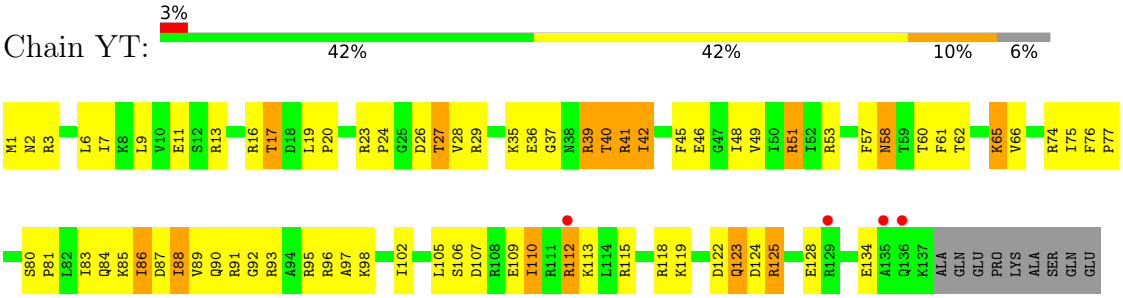
• Molecule 39: 50S ribosomal protein L19

Chain RT:



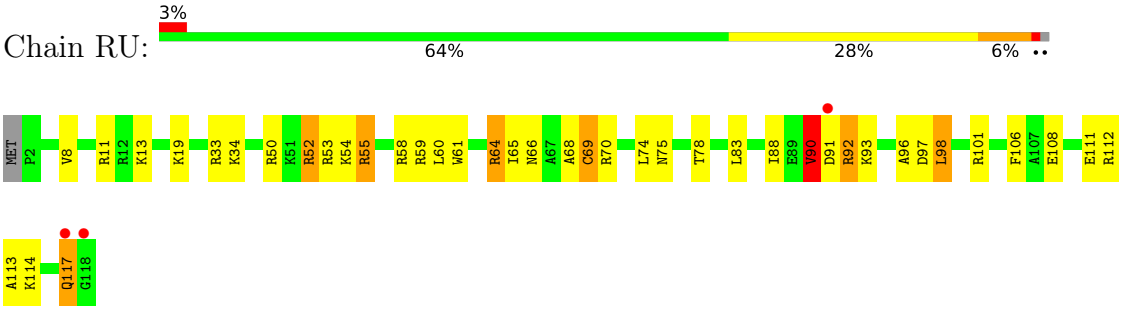
• Molecule 39: 50S ribosomal protein L19

Chain YT:



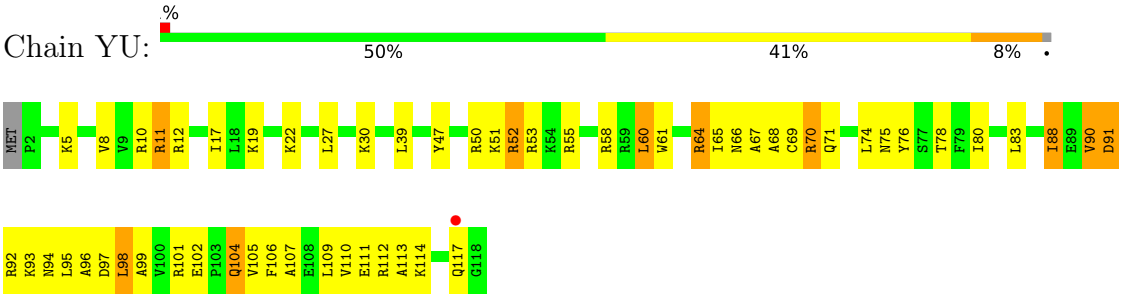
• Molecule 40: 50S ribosomal protein L20

Chain RU:



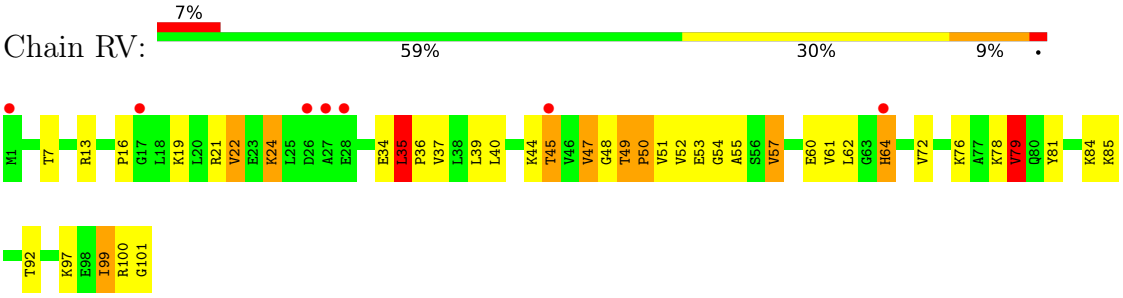
• Molecule 40: 50S ribosomal protein L20

Chain YU:



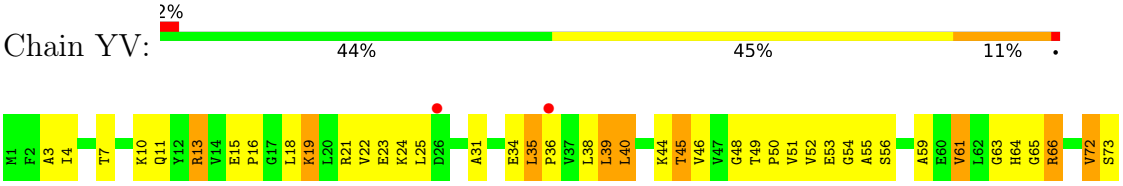
• Molecule 41: 50S ribosomal protein L21

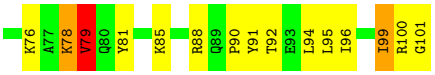
Chain RV:



• Molecule 41: 50S ribosomal protein L21

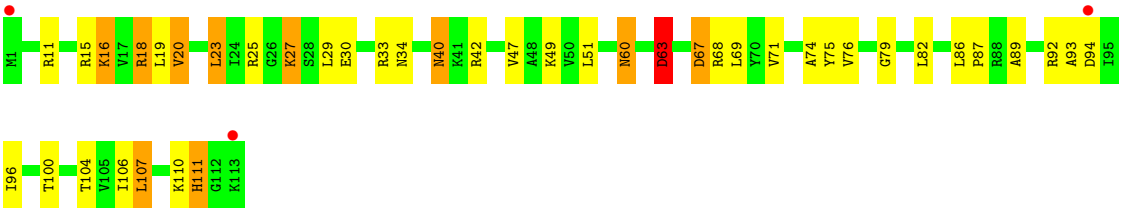
Chain YV:





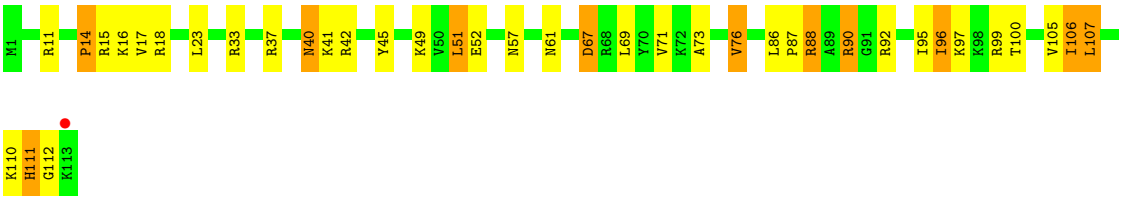
• Molecule 42: 50S ribosomal protein L22

Chain RW:



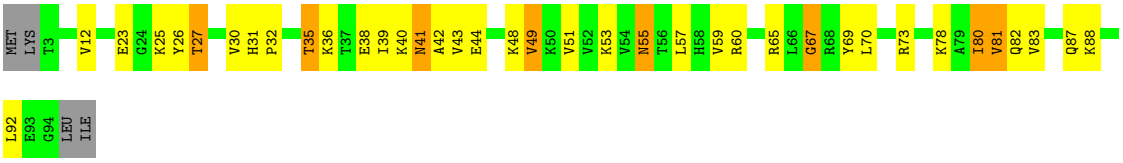
• Molecule 42: 50S ribosomal protein L22

Chain YW:



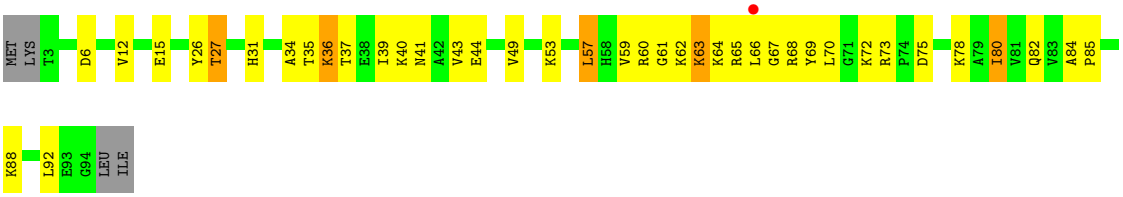
• Molecule 43: 50S ribosomal protein L23

Chain RX:



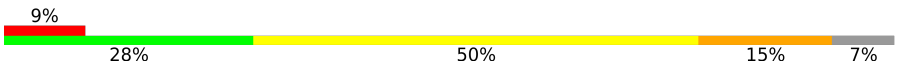
• Molecule 43: 50S ribosomal protein L23

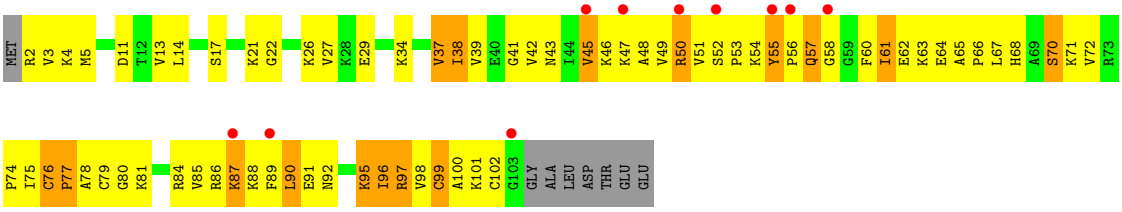
Chain YX:

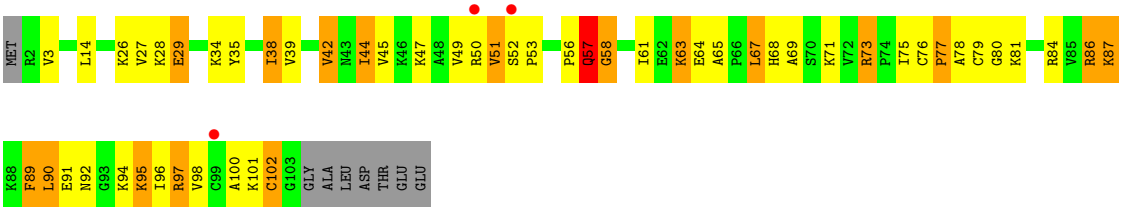


• Molecule 44: 50S ribosomal protein L24

Chain RY:





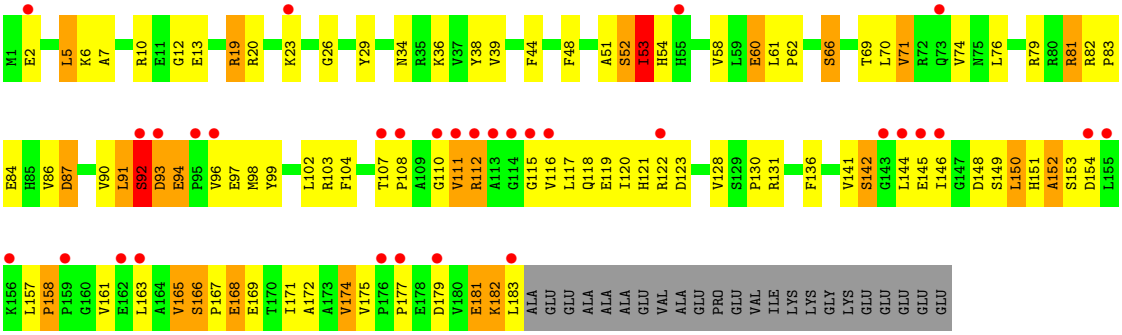


• Molecule 44: 50S ribosomal protein L24

Chain YY:

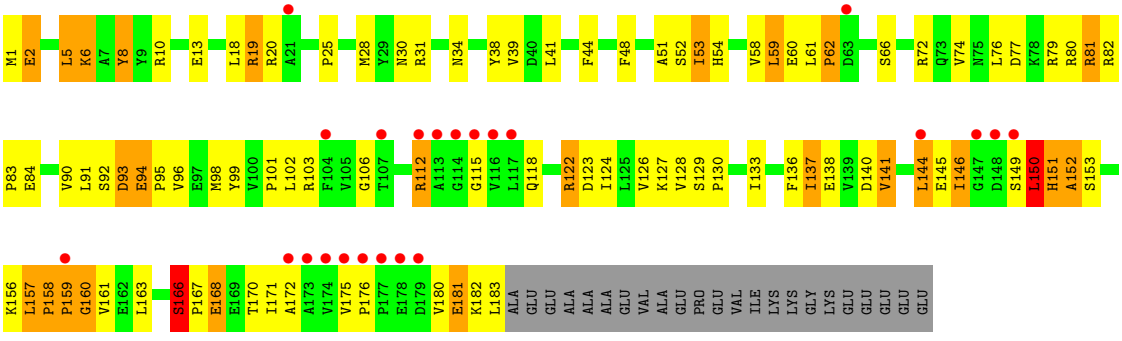
• Molecule 45: 50S ribosomal protein L25

Chain RZ:



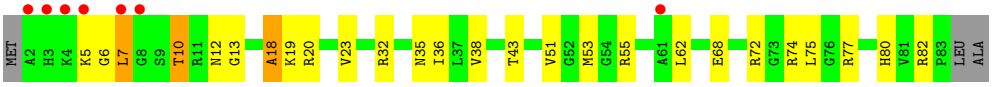
• Molecule 45: 50S ribosomal protein L25

Chain YZ:



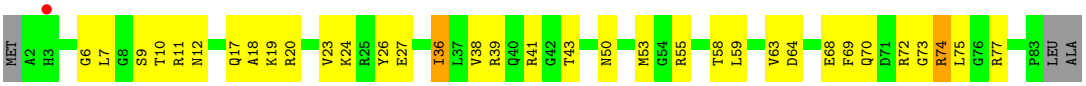
• Molecule 46: 50S ribosomal protein L27

Chain R0:



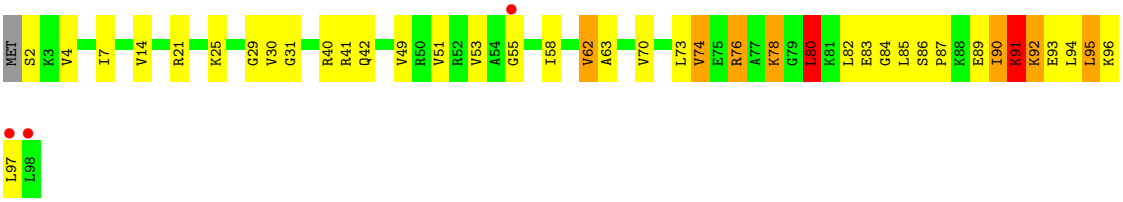
• Molecule 46: 50S ribosomal protein L27

Chain Y0:



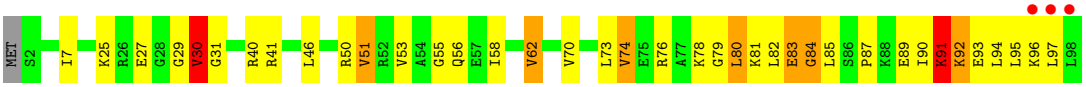
• Molecule 47: 50S ribosomal protein L28

Chain R1:



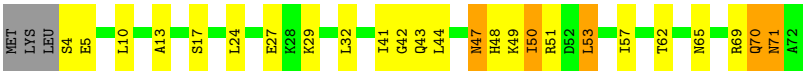
• Molecule 47: 50S ribosomal protein L28

Chain Y1:



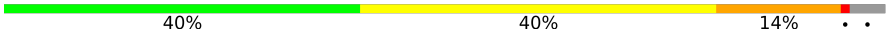
• Molecule 48: 50S ribosomal protein L29

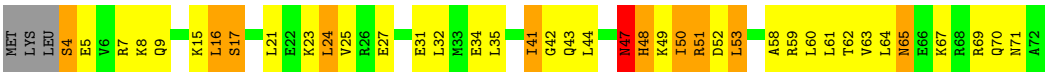
Chain R2:



• Molecule 48: 50S ribosomal protein L29

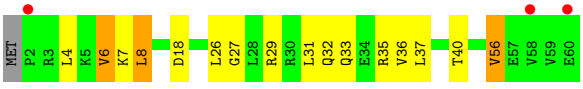
Chain Y2:





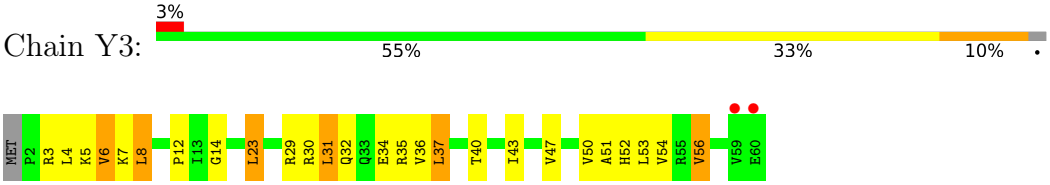
• Molecule 49: 50S ribosomal protein L30

Chain R3:



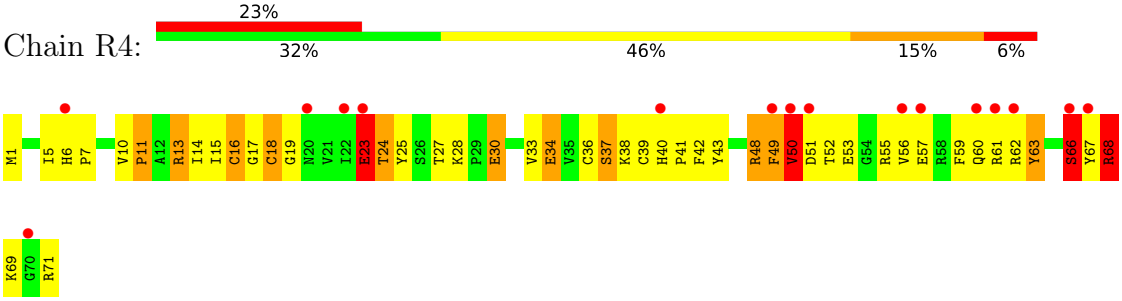
• Molecule 49: 50S ribosomal protein L30

Chain Y3:



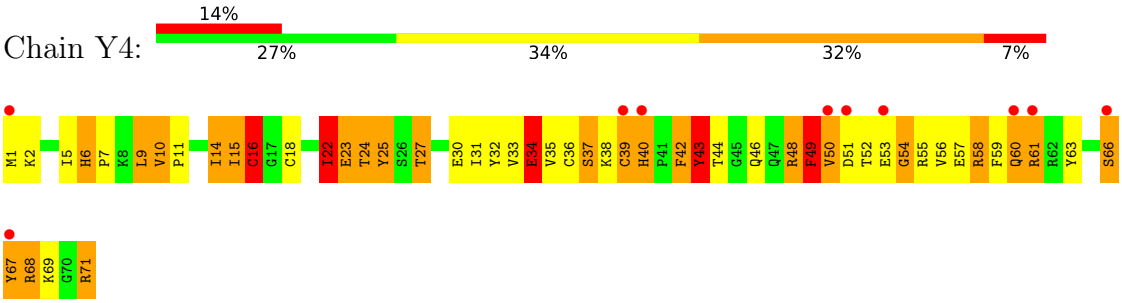
• Molecule 50: 50S ribosomal protein L31

Chain R4:



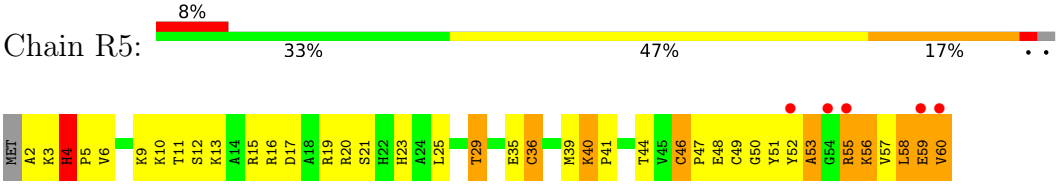
• Molecule 50: 50S ribosomal protein L31

Chain Y4:



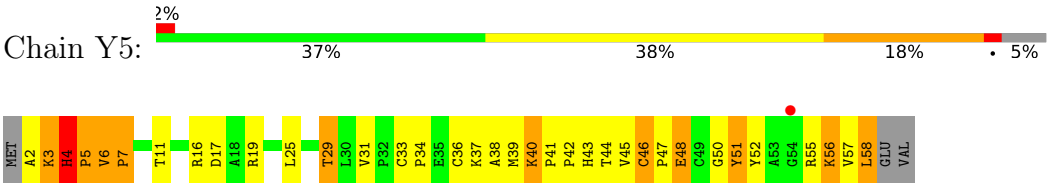
• Molecule 51: 50S ribosomal protein L32

Chain R5:



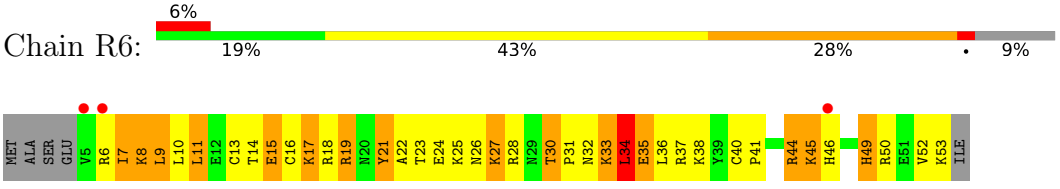
• Molecule 51: 50S ribosomal protein L32

Chain Y5:



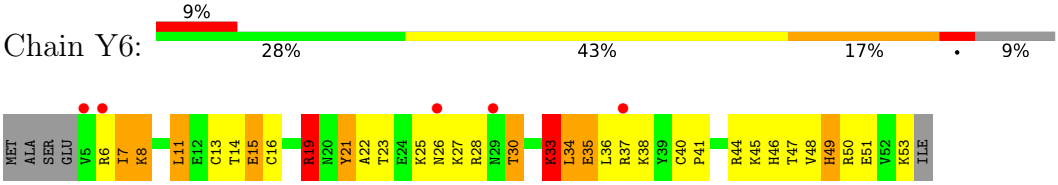
• Molecule 52: 50S ribosomal protein L33

Chain R6:



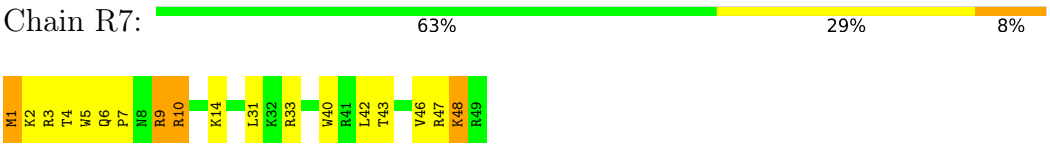
• Molecule 52: 50S ribosomal protein L33

Chain Y6:



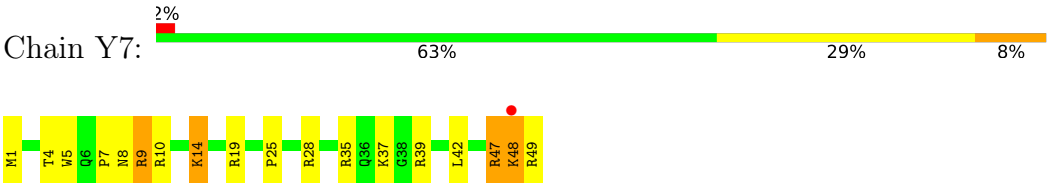
• Molecule 53: 50S ribosomal protein L34

Chain R7:



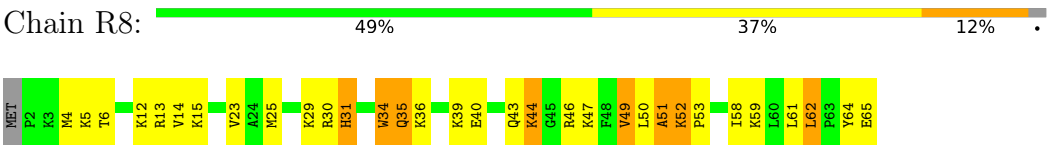
• Molecule 53: 50S ribosomal protein L34

Chain Y7:



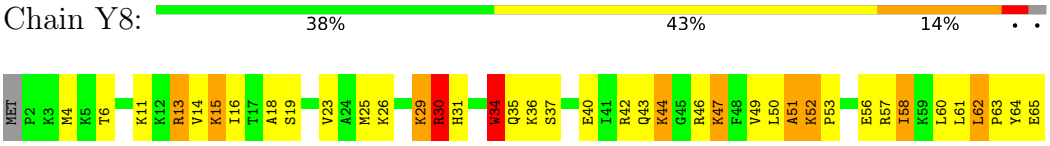
• Molecule 54: 50S ribosomal protein L35

Chain R8:



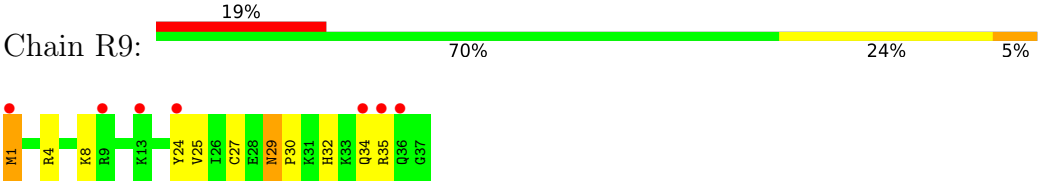
• Molecule 54: 50S ribosomal protein L35

Chain Y8:



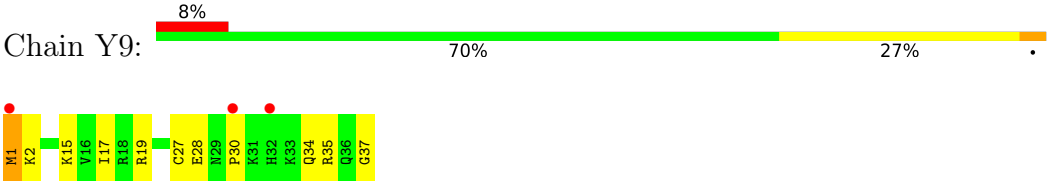
• Molecule 55: 50S ribosomal protein L36

Chain R9:



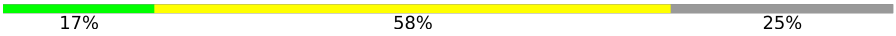
• Molecule 55: 50S ribosomal protein L36

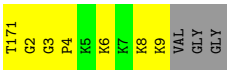
Chain Y9:



• Molecule 56: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

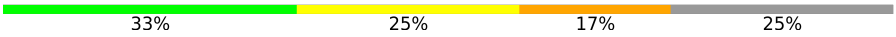
Chain Z7:

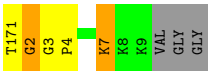




• Molecule 56: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

Chain Z8:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.24Å 443.46Å 618.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.60 34.94 – 3.61	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.79-3.60) 98.0 (34.94-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 3.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.222 , 0.254 0.224 , 0.254	Depositor DCC
R_{free} test set	28952 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å^2)	104.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 79.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	295487	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: T17, ZN, PAR, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	QA	0.23	0/36098	0.81	32/56341 (0.1%)
1	XA	0.24	0/36101	0.81	18/56346 (0.0%)
2	QB	0.31	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.53	0/2195
3	XC	0.37	0/1629	0.56	0/2195
4	QD	0.45	0/1733	0.62	1/2318 (0.0%)
4	XD	0.39	0/1733	0.60	0/2318
5	QE	0.35	0/1171	0.56	0/1576
5	XE	0.39	0/1171	0.59	0/1576
6	QF	0.39	0/856	0.57	0/1154
6	XF	0.39	0/856	0.61	0/1154
7	QG	0.33	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.51	0/1709
8	QH	0.33	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.35	0/814	0.60	0/1095
11	QK	0.37	0/900	0.57	0/1213
11	XK	0.39	0/900	0.58	0/1213
12	QL	0.37	0/991	0.61	0/1327
12	XL	0.50	1/991 (0.1%)	0.77	2/1327 (0.2%)
13	QM	0.32	0/974	0.59	0/1303
13	XM	0.36	0/974	0.63	0/1303
14	QN	0.40	0/501	0.60	0/664
14	XN	0.42	0/501	0.66	0/664
15	QO	0.35	0/745	0.53	0/992
15	XO	0.39	0/745	0.54	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.35	0/847	0.53	0/1131
17	XQ	0.35	0/847	0.54	0/1131
18	QR	0.35	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.60	0/768
19	QS	0.33	0/689	0.60	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.36	0/765	0.64	0/1007
20	XT	0.31	0/765	0.60	0/1007
21	QU	0.31	0/221	0.53	0/288
21	XU	0.32	0/221	0.61	0/288
22	QV	0.32	1/1836 (0.1%)	0.80	0/2859
22	XV	0.33	1/1836 (0.1%)	0.81	1/2859 (0.0%)
23	QW	0.19	0/1809	0.79	0/2819
23	QY	0.17	0/406	0.73	0/628
23	XW	0.20	0/1809	0.80	0/2819
23	XY	0.20	0/406	0.74	0/628
24	QX	0.19	0/235	0.71	0/364
24	XX	0.18	0/235	0.65	0/364
25	RA	0.26	0/69521	0.81	28/108529 (0.0%)
25	YA	0.29	0/69543	0.83	41/108563 (0.0%)
26	RB	0.26	0/2878	0.88	7/4490 (0.2%)
26	YB	0.29	0/2878	0.91	11/4490 (0.2%)
27	RD	0.51	0/2165	0.70	0/2919
27	YD	0.57	0/2165	0.77	1/2919 (0.0%)
28	RE	0.46	1/1601 (0.1%)	0.73	3/2160 (0.1%)
28	YE	0.48	1/1601 (0.1%)	0.74	2/2160 (0.1%)
29	RF	0.45	1/1620 (0.1%)	0.64	1/2194 (0.0%)
29	YF	0.48	0/1620	0.71	1/2194 (0.0%)
30	RG	0.31	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	0/2016
31	RH	0.33	1/1332 (0.1%)	0.73	2/1802 (0.1%)
31	YH	0.50	1/1332 (0.1%)	0.76	2/1802 (0.1%)
32	RI	0.40	0/1151	0.75	1/1558 (0.1%)
32	YI	0.38	0/1151	0.66	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.43	0/1131	0.64	0/1525
34	RO	0.41	0/943	0.62	1/1269 (0.1%)
34	YO	0.50	0/943	0.65	0/1269
35	RP	0.48	1/1162 (0.1%)	0.83	1/1544 (0.1%)
35	YP	0.55	2/1162 (0.2%)	0.93	4/1544 (0.3%)
36	RQ	0.44	0/1143	0.71	1/1527 (0.1%)
36	YQ	0.56	0/1143	0.78	0/1527
37	RR	0.42	0/982	0.69	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	YR	0.45	0/982	0.73	0/1312
38	RS	0.36	0/892	0.64	0/1187
38	YS	0.39	0/892	0.71	0/1187
39	RT	0.41	0/1155	0.63	0/1542
39	YT	0.44	0/1155	0.67	0/1542
40	RU	0.40	0/982	0.65	0/1306
40	YU	0.50	0/982	0.69	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.46	0/790	0.73	1/1057 (0.1%)
42	RW	0.50	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.50	0/739	0.66	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.45	0/798	0.69	0/1064
45	RZ	0.34	0/1493	0.60	0/2026
45	YZ	0.45	2/1493 (0.1%)	0.68	4/2026 (0.2%)
46	R0	0.45	0/657	0.65	0/874
46	Y0	0.48	0/657	0.69	0/874
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.39	0/583	0.65	0/771
48	Y2	0.52	0/583	0.73	0/771
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.41	0/474	0.59	0/635
50	R4	0.33	0/594	0.68	0/795
50	Y4	0.37	0/594	0.69	0/795
51	R5	0.43	0/473	0.78	0/639
51	Y5	0.68	3/456 (0.7%)	0.89	3/617 (0.5%)
52	R6	0.35	0/431	0.69	0/575
52	Y6	0.37	0/431	0.68	0/575
53	R7	0.49	0/438	0.68	0/575
53	Y7	0.57	0/438	0.71	0/575
54	R8	0.55	0/525	0.79	0/691
54	Y8	0.58	0/525	0.82	0/691
55	R9	0.26	0/310	0.45	0/407
55	Y9	0.32	0/310	0.48	0/407
56	Z7	0.22	0/56	0.45	0/70
56	Z8	0.25	0/56	0.45	0/70
All	All	0.32	16/320246 (0.0%)	0.78	173/478995 (0.0%)

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
12	QL	0	1
12	XL	0	1
29	YF	0	1
31	RH	0	1
31	YH	0	1
38	YS	0	1
45	YZ	0	1
48	Y2	0	1
50	R4	0	1
54	R8	0	2
54	Y8	0	2
All	All	0	13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.61	1.48	1.61
22	XV	0	C	OP3-P	-10.59	1.48	1.61
35	YP	63	PRO	N-CD	6.16	1.56	1.47
45	YZ	159	PRO	N-CD	5.60	1.55	1.47
35	RP	10	PRO	N-CD	5.58	1.55	1.47

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	RH	125	VAL	C-N-CD	-17.76	81.53	120.60
25	YA	771	G	C2-N3-C4	-10.26	106.77	111.90
36	RQ	77	LYS	C-N-CD	-8.42	102.08	120.60
25	YA	771	G	N9-C4-C5	-8.13	102.15	105.40
25	YA	673	C	C2-N3-C4	-7.98	115.91	119.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
50	R4	38	LYS	Peptide
54	R8	30	ARG	Peptide
54	R8	35	GLN	Peptide
31	RH	153	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	479	0
1	XA	32249	0	16279	433	0
2	QB	1924	0	1975	62	0
2	XB	1924	0	1975	83	0
3	QC	1605	0	1668	49	0
3	XC	1605	0	1668	57	0
4	QD	1703	0	1763	93	0
4	XD	1703	0	1765	50	1
5	QE	1155	0	1213	28	0
5	XE	1155	0	1213	42	0
6	QF	843	0	857	29	0
6	XF	843	0	857	40	0
7	QG	1257	0	1296	46	0
7	XG	1257	0	1296	24	0
8	QH	1116	0	1175	38	0
8	XH	1116	0	1177	28	0
9	QI	1010	0	1037	37	0
9	XI	1010	0	1037	49	0
10	QJ	801	0	849	51	0
10	XJ	801	0	849	42	0
11	QK	885	0	904	36	0
11	XK	885	0	904	37	0
12	QL	975	0	1062	39	0
12	XL	975	0	1062	50	0
13	QM	964	0	1034	64	0
13	XM	964	0	1034	61	0
14	QN	492	0	529	27	0
14	XN	492	0	529	18	0
15	QO	734	0	771	20	0
15	XO	734	0	771	18	0
16	QP	705	0	725	16	0
16	XP	705	0	725	25	0
17	QQ	834	0	904	23	0
17	XQ	834	0	904	14	0
18	QR	574	0	644	10	0
18	XR	574	0	644	25	0
19	QS	674	0	699	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	74	0
20	QT	763	0	861	20	0
20	XT	763	0	861	35	0
21	QU	217	0	234	11	0
21	XU	217	0	234	2	0
22	QV	1644	0	835	17	0
22	XV	1644	0	836	18	0
23	QW	1619	0	822	25	0
23	QY	364	0	186	2	0
23	XW	1619	0	822	30	0
23	XY	364	0	186	2	0
24	QX	210	0	109	0	0
24	XX	210	0	109	1	0
25	RA	62071	0	31284	759	1
25	YA	62091	0	31294	730	0
26	RB	2573	0	1306	41	0
26	YB	2573	0	1306	34	0
27	RD	2115	0	2195	95	0
27	YD	2115	0	2195	139	0
28	RE	1568	0	1634	92	0
28	YE	1568	0	1634	72	0
29	RF	1585	0	1632	85	0
29	YF	1585	0	1632	62	0
30	RG	1474	0	1535	65	0
30	YG	1474	0	1535	62	0
31	RH	1307	0	1382	74	0
31	YH	1307	0	1382	89	0
32	RI	1136	0	1223	75	0
32	YI	1136	0	1223	52	0
33	RN	1104	0	1180	41	0
33	YN	1104	0	1180	50	0
34	RO	933	0	996	23	0
34	YO	933	0	996	21	0
35	RP	1145	0	1226	82	0
35	YP	1145	0	1228	88	0
36	RQ	1122	0	1179	57	0
36	YQ	1122	0	1178	50	0
37	RR	968	0	1033	49	0
37	YR	968	0	1033	35	0
38	RS	882	0	943	42	0
38	YS	882	0	943	45	0
39	RT	1141	0	1202	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	YT	1141	0	1202	53	0
40	RU	964	0	1022	31	0
40	YU	964	0	1022	52	0
41	RV	779	0	852	20	0
41	YV	779	0	852	43	0
42	RW	900	0	964	24	0
42	YW	900	0	964	27	0
43	RX	725	0	778	29	0
43	YX	725	0	778	23	0
44	RY	785	0	878	48	0
44	YY	785	0	878	40	0
45	RZ	1461	0	1493	64	0
45	YZ	1461	0	1493	80	0
46	R0	648	0	672	21	0
46	Y0	648	0	672	31	0
47	R1	763	0	848	29	0
47	Y1	763	0	848	28	0
48	R2	581	0	629	15	0
48	Y2	581	0	629	23	0
49	R3	469	0	518	6	0
49	Y3	469	0	518	15	0
50	R4	581	0	574	77	0
50	Y4	581	0	574	98	0
51	R5	459	0	476	68	0
51	Y5	442	0	465	35	0
52	R6	424	0	450	26	0
52	Y6	424	0	450	32	0
53	R7	430	0	480	20	0
53	Y7	430	0	480	15	0
54	R8	517	0	582	30	0
54	Y8	517	0	582	40	0
55	R9	307	0	338	8	0
55	Y9	307	0	336	8	0
56	Z7	116	0	134	13	0
56	Z8	116	0	133	5	0
57	QA	67	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QV	2	0	0	0	0
57	QY	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	RA	246	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	1	0	0	0	0
57	RP	4	0	0	0	0
57	XA	71	0	0	0	0
57	XB	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	3	0	0	0	0
57	XX	1	0	0	0	0
57	XY	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	278	0	0	0	0
57	YB	5	0	0	0	0
57	YD	1	0	0	0	0
57	YE	2	0	0	0	0
57	YP	1	0	0	0	0
57	YX	1	0	0	0	0
58	QA	42	0	45	1	0
58	XA	42	0	45	4	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	R5	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	295487	0	200229	5889	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5889 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YQ:134:ARG:CZ	45:YZ:122:ARG:HH21	1.34	1.39
28:YE:14:ILE:HG22	28:YE:21:VAL:CG2	1.56	1.35
27:YD:121:PRO:HB3	27:YD:135:PHE:CE2	1.64	1.31
28:YE:14:ILE:CG2	28:YE:21:VAL:HG23	1.62	1.29
31:RH:125:VAL:HG12	31:RH:126:PRO:CD	1.64	1.25

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	Interatomic distance (Å)	Clash overlap (Å)
25:RA:2197:U:OP1	4:XD:159:ARG:NH2[4_555]	2.05	0.15

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	173 (74%)	45 (19%)	17 (7%)	1 13
2	XB	235/256 (92%)	177 (75%)	43 (18%)	15 (6%)	1 17
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	4 33
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	10 47
4	QD	206/209 (99%)	177 (86%)	22 (11%)	7 (3%)	3 31
4	XD	206/209 (99%)	178 (86%)	23 (11%)	5 (2%)	6 37
5	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	3 31
5	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	7 41
6	QF	99/101 (98%)	93 (94%)	3 (3%)	3 (3%)	4 33
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100 100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	12 50
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12 50
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	22 61
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4 33
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3 26
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	4 31
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	4 32
10	XJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	2 20
11	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	5 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	XK	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	9 45
12	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	1 18
12	XL	123/132 (93%)	97 (79%)	14 (11%)	12 (10%)	0 8
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1 12
13	XM	119/126 (94%)	94 (79%)	15 (13%)	10 (8%)	1 10
14	QN	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	1 14
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0 7
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13 51
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6 38
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	13 51
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	13 51
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7 41
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100 100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2 23
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10 47
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0 4
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0 4
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1 17
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	1 17
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2 24
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2 24
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2 23
27	YD	270/276 (98%)	228 (84%)	33 (12%)	9 (3%)	4 31
28	RE	203/206 (98%)	148 (73%)	35 (17%)	20 (10%)	0 8
28	YE	203/206 (98%)	144 (71%)	42 (21%)	17 (8%)	1 10
29	RF	200/210 (95%)	170 (85%)	18 (9%)	12 (6%)	1 17
29	YF	200/210 (95%)	168 (84%)	24 (12%)	8 (4%)	3 26
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1 11
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1 15
31	RH	168/180 (93%)	116 (69%)	33 (20%)	19 (11%)	0 6
31	YH	168/180 (93%)	124 (74%)	23 (14%)	21 (12%)	0 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	RI	144/148 (97%)	104 (72%)	27 (19%)	13 (9%)	1 9
32	YI	144/148 (97%)	107 (74%)	20 (14%)	17 (12%)	0 5
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1 9
33	YN	136/140 (97%)	105 (77%)	17 (12%)	14 (10%)	0 7
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9 45
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	9 45
35	RP	148/150 (99%)	106 (72%)	28 (19%)	14 (10%)	0 8
35	YP	148/150 (99%)	108 (73%)	22 (15%)	18 (12%)	0 5
36	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0 5
36	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0 4
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2 24
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2 20
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0 7
38	YS	109/112 (97%)	79 (72%)	17 (16%)	13 (12%)	0 5
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1 9
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1 13
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3 30
40	YU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3 30
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1 17
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1 11
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3 29
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	8 43
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6 39
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6 39
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0 3
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0 5
45	RZ	181/206 (88%)	126 (70%)	34 (19%)	21 (12%)	0 6
45	YZ	181/206 (88%)	125 (69%)	38 (21%)	18 (10%)	0 8
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	12 50
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100 100
47	R1	95/98 (97%)	76 (80%)	10 (10%)	9 (10%)	0 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1 17
48	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1 12
48	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1 9
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3 30
49	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8 43
50	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0 0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0 0
51	R5	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	2 19
51	Y5	55/60 (92%)	45 (82%)	9 (16%)	1 (2%)	8 43
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0 0
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0 2
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7 40
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7 40
54	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1 11
54	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1 16
55	R9	35/37 (95%)	35 (100%)	0	0	100 100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
56	Z7	7/12 (58%)	5 (71%)	2 (29%)	0	100 100
56	Z8	7/12 (58%)	3 (43%)	3 (43%)	1 (14%)	0 4
All	All	11482/12152 (94%)	9247 (80%)	1516 (13%)	719 (6%)	1 17

5 of 719 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
6	QF	16	GLN

5.3.2 Protein sidechains (i)

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%)	171 (83%)	34 (17%)	2 15
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5 26
3	QC	159/188 (85%)	145 (91%)	14 (9%)	10 40
3	XC	159/188 (85%)	146 (92%)	13 (8%)	11 42
4	QD	180/181 (99%)	157 (87%)	23 (13%)	4 24
4	XD	180/181 (99%)	152 (84%)	28 (16%)	2 18
5	QE	116/123 (94%)	104 (90%)	12 (10%)	7 34
5	XE	116/123 (94%)	104 (90%)	12 (10%)	7 34
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4 23
6	XF	90/90 (100%)	81 (90%)	9 (10%)	7 35
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8 37
7	XG	126/127 (99%)	114 (90%)	12 (10%)	8 37
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11 42
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6 32
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2 12
9	XI	98/99 (99%)	80 (82%)	18 (18%)	1 10
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4 23
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	2 14
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7 35
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7 35
12	QL	104/109 (95%)	87 (84%)	17 (16%)	2 15
12	XL	104/109 (95%)	92 (88%)	12 (12%)	5 29
13	QM	97/101 (96%)	73 (75%)	24 (25%)	0 4
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1 8
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1 10
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3 21
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9 40
15	XO	79/80 (99%)	69 (87%)	10 (13%)	4 24
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4 25
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	11 42
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18 53
18	QR	61/77 (79%)	50 (82%)	11 (18%)	1 11
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3 19
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1 9
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1 6
20	QT	76/82 (93%)	67 (88%)	9 (12%)	5 28
20	XT	76/82 (93%)	66 (87%)	10 (13%)	4 23
21	QU	20/22 (91%)	20 (100%)	0	100 100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24 59
27	RD	214/218 (98%)	176 (82%)	38 (18%)	2 11
27	YD	214/218 (98%)	180 (84%)	34 (16%)	2 16
28	RE	165/166 (99%)	126 (76%)	39 (24%)	1 5
28	YE	165/166 (99%)	135 (82%)	30 (18%)	1 10
29	RF	161/166 (97%)	132 (82%)	29 (18%)	1 11
29	YF	161/166 (97%)	137 (85%)	24 (15%)	3 19
30	RG	155/156 (99%)	134 (86%)	21 (14%)	4 23
30	YG	155/156 (99%)	134 (86%)	21 (14%)	4 23
31	RH	142/148 (96%)	120 (84%)	22 (16%)	2 18
31	YH	142/148 (96%)	116 (82%)	26 (18%)	1 10
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1 8
32	YI	122/124 (98%)	92 (75%)	30 (25%)	0 4
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2 13
33	YN	117/119 (98%)	96 (82%)	21 (18%)	2 11
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7 35
34	YO	100/100 (100%)	89 (89%)	11 (11%)	6 31
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0 4
35	YP	116/116 (100%)	81 (70%)	35 (30%)	0 2
36	RQ	111/111 (100%)	94 (85%)	17 (15%)	2 18
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2 13
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	YR	101/101 (100%)	80 (79%)	21 (21%)	1 7
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1 7
38	YS	87/88 (99%)	68 (78%)	19 (22%)	1 6
39	RT	120/127 (94%)	102 (85%)	18 (15%)	3 19
39	YT	120/127 (94%)	98 (82%)	22 (18%)	1 10
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3 19
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2 13
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1 9
41	YV	82/82 (100%)	67 (82%)	15 (18%)	1 10
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1 7
42	YW	92/92 (100%)	75 (82%)	17 (18%)	1 10
43	RX	74/78 (95%)	63 (85%)	11 (15%)	3 19
43	YX	74/78 (95%)	60 (81%)	14 (19%)	1 9
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0 4
44	YY	85/91 (93%)	64 (75%)	21 (25%)	0 4
45	RZ	162/179 (90%)	132 (82%)	30 (18%)	1 10
45	YZ	162/179 (90%)	133 (82%)	29 (18%)	2 11
46	R0	65/67 (97%)	60 (92%)	5 (8%)	13 45
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	9 39
47	R1	82/83 (99%)	73 (89%)	9 (11%)	6 31
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3 20
48	R2	64/67 (96%)	57 (89%)	7 (11%)	6 32
48	Y2	64/67 (96%)	47 (73%)	17 (27%)	0 3
49	R3	51/52 (98%)	45 (88%)	6 (12%)	5 28
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	2 17
50	R4	63/63 (100%)	45 (71%)	18 (29%)	0 3
50	Y4	63/63 (100%)	43 (68%)	20 (32%)	0 2
51	R5	51/52 (98%)	36 (71%)	15 (29%)	0 2
51	Y5	49/52 (94%)	36 (74%)	13 (26%)	0 3
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0 3
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	R7	42/42 (100%)	34 (81%)	8 (19%)	1 9
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2 14
54	R8	54/55 (98%)	44 (82%)	10 (18%)	1 10
54	Y8	54/55 (98%)	41 (76%)	13 (24%)	0 4
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19 55
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19 55
56	Z7	5/7 (71%)	5 (100%)	0	100 100
56	Z8	5/7 (71%)	4 (80%)	1 (20%)	1 8
All	All	9710/10080 (96%)	8152 (84%)	1558 (16%)	2 16

5 of 1558 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	XL	17	LYS
31	YH	88	LEU
13	XM	114	ARG
11	XK	116	HIS
27	YD	106	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	XB	204	ASN
10	XJ	78	ASN
19	QS	47	HIS
38	RS	34	HIS
43	RX	55	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	267 (17%)	43 (2%)
1	XA	1498/1522 (98%)	277 (18%)	38 (2%)
22	QV	76/77 (98%)	19 (25%)	1 (1%)
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QW	75/76 (98%)	16 (21%)	0
23	QY	15/76 (19%)	3 (20%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	XW	75/76 (98%)	19 (25%)	0
23	XY	15/76 (19%)	4 (26%)	0
24	QX	9/24 (37%)	0	0
24	XX	9/24 (37%)	0	0
25	RA	2879/2915 (98%)	567 (19%)	57 (1%)
25	YA	2880/2915 (98%)	563 (19%)	57 (1%)
26	RB	119/122 (97%)	21 (17%)	1 (0%)
26	YB	119/122 (97%)	21 (17%)	1 (0%)
All	All	9344/9624 (97%)	1794 (19%)	199 (2%)

5 of 1794 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 199 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	410	G
25	YA	195	A
1	XA	481	G
1	XA	991	U
25	YA	372	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 704 ligands modelled in this entry, 702 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	PAR	XA	1672	-	45,45,45	1.53	7 (15%)	64,67,67	1.26	5 (7%)
58	PAR	QA	1667	-	45,45,45	1.55	7 (15%)	64,67,67	1.17	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	XA	1672	-	-	5/18/94/94	0/4/4/4
58	PAR	QA	1667	-	-	5/18/94/94	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1667	PAR	C64-C54	5.11	1.59	1.52
58	XA	1672	PAR	C64-C54	5.01	1.58	1.52
58	QA	1667	PAR	C52-C42	3.12	1.58	1.52
58	XA	1672	PAR	C52-C42	3.05	1.58	1.52
58	XA	1672	PAR	O54-C14	3.01	1.49	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	XA	1672	PAR	C14-O54-C54	4.10	121.73	113.69
58	QA	1667	PAR	C14-O54-C54	4.04	121.62	113.69
58	QA	1667	PAR	O52-C13-C23	3.57	115.35	107.96
58	QA	1667	PAR	O33-C14-C24	3.49	114.23	108.22
58	XA	1672	PAR	O54-C54-C64	3.38	112.29	106.01

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

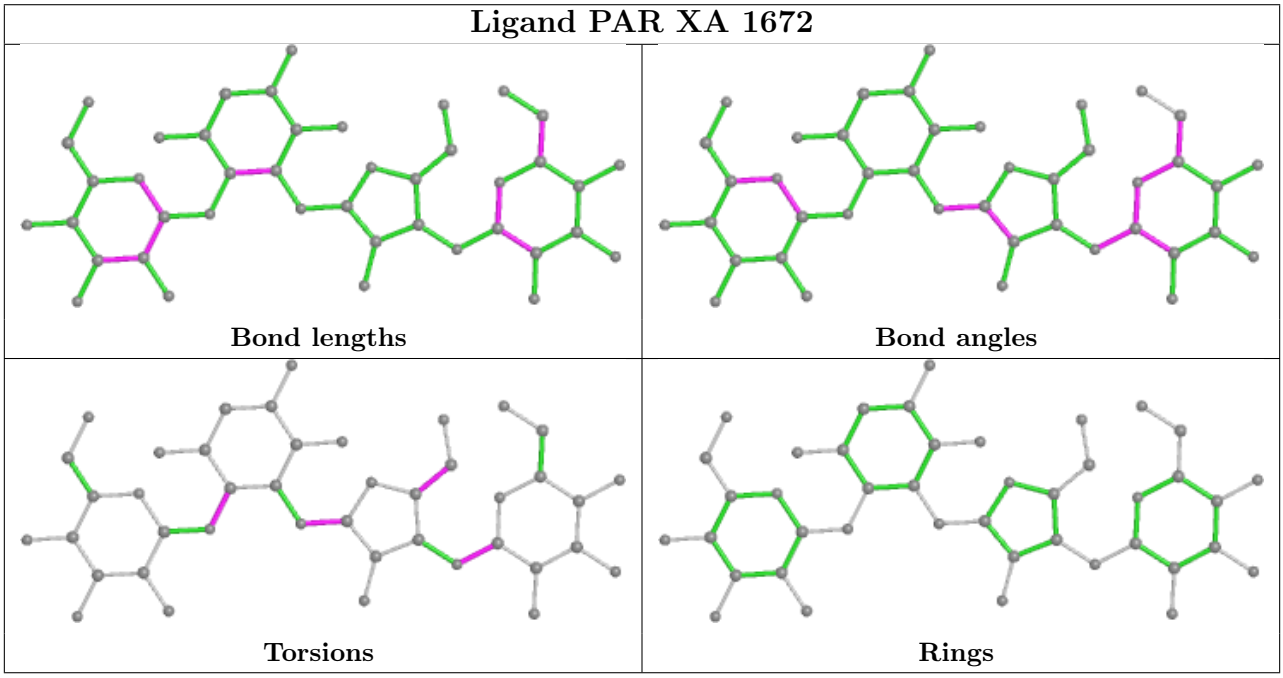
Mol	Chain	Res	Type	Atoms
58	XA	1672	PAR	O43-C43-C53-O53
58	XA	1672	PAR	C33-C43-C53-O53
58	QA	1667	PAR	C33-C43-C53-O53
58	QA	1667	PAR	O43-C43-C53-O53
58	QA	1667	PAR	C41-C51-C61-O61

There are no ring outliers.

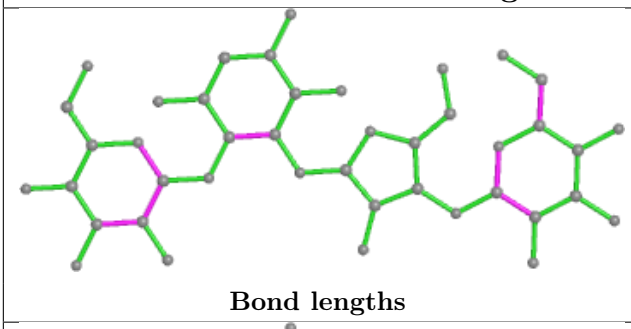
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1672	PAR	4	0
58	QA	1667	PAR	1	0

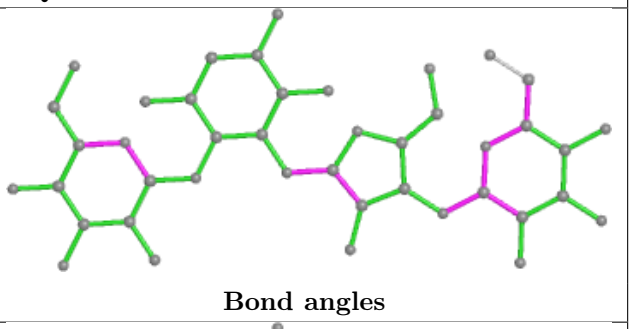
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



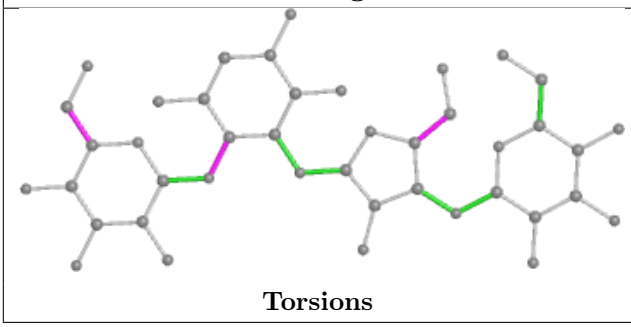
Ligand PAR QA 1667



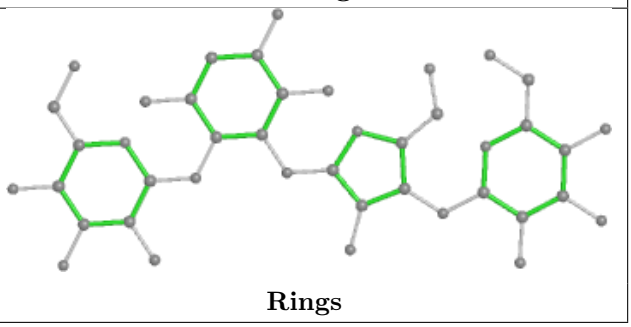
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.27	61 (4%) 37 24	68, 102, 211, 576	0
1	XA	1500/1522 (98%)	0.22	50 (3%) 46 31	57, 88, 196, 440	0
2	QB	237/256 (92%)	0.44	26 (10%) 5 3	106, 186, 344, 418	0
2	XB	237/256 (92%)	0.15	13 (5%) 25 15	88, 156, 283, 529	0
3	QC	205/239 (85%)	0.57	22 (10%) 6 3	103, 172, 294, 429	0
3	XC	205/239 (85%)	0.13	9 (4%) 34 21	80, 124, 195, 316	0
4	QD	208/209 (99%)	-0.04	2 (0%) 82 70	85, 114, 192, 458	0
4	XD	208/209 (99%)	-0.00	3 (1%) 75 61	71, 109, 190, 368	0
5	QE	151/162 (93%)	0.14	6 (3%) 38 25	90, 128, 201, 260	0
5	XE	151/162 (93%)	-0.01	2 (1%) 77 63	72, 101, 185, 236	0
6	QF	101/101 (100%)	-0.02	2 (1%) 65 49	80, 109, 175, 310	0
6	XF	101/101 (100%)	0.12	5 (4%) 28 18	73, 107, 161, 559	0
7	QG	155/156 (99%)	0.20	10 (6%) 18 11	83, 150, 262, 534	0
7	XG	155/156 (99%)	-0.03	5 (3%) 47 32	76, 129, 209, 334	0
8	QH	138/138 (100%)	-0.05	0 100 100	92, 133, 195, 285	0
8	XH	138/138 (100%)	-0.09	0 100 100	80, 113, 165, 331	0
9	QI	127/128 (99%)	0.56	15 (11%) 4 3	96, 189, 303, 476	0
9	XI	127/128 (99%)	0.32	9 (7%) 16 9	76, 153, 232, 396	0
10	QJ	99/105 (94%)	0.71	13 (13%) 3 2	107, 196, 431, 583	0
10	XJ	99/105 (94%)	0.55	10 (10%) 7 4	85, 164, 316, 369	0
11	QK	119/129 (92%)	0.16	7 (5%) 22 13	77, 112, 201, 335	0
11	XK	119/129 (92%)	0.02	4 (3%) 45 30	67, 105, 181, 251	0
12	QL	125/132 (94%)	0.04	3 (2%) 59 42	79, 101, 176, 309	0
12	XL	125/132 (94%)	-0.01	4 (3%) 47 32	55, 78, 146, 341	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	0.09	2 (1%) 70 55	101, 160, 265, 447	0
13	XM	121/126 (96%)	-0.02	2 (1%) 70 55	78, 126, 200, 488	0
14	QN	60/61 (98%)	0.40	3 (5%) 28 18	117, 157, 211, 250	0
14	XN	60/61 (98%)	-0.01	0 100 100	89, 106, 151, 194	0
15	QO	88/89 (98%)	0.08	3 (3%) 45 30	77, 113, 167, 241	0
15	XO	88/89 (98%)	-0.02	1 (1%) 80 68	69, 101, 153, 171	0
16	QP	84/88 (95%)	0.09	2 (2%) 59 42	85, 102, 164, 241	0
16	XP	84/88 (95%)	0.09	2 (2%) 59 42	87, 111, 187, 400	0
17	QQ	100/105 (95%)	0.03	0 100 100	82, 107, 157, 336	0
17	XQ	100/105 (95%)	0.01	1 (1%) 82 70	71, 105, 171, 330	0
18	QR	70/88 (79%)	-0.00	3 (4%) 35 22	83, 114, 185, 205	0
18	XR	70/88 (79%)	0.04	1 (1%) 75 61	77, 112, 187, 227	0
19	QS	84/93 (90%)	0.38	4 (4%) 30 19	109, 181, 257, 381	0
19	XS	84/93 (90%)	0.07	5 (5%) 21 12	80, 133, 207, 286	0
20	QT	99/106 (93%)	0.10	4 (4%) 38 25	87, 122, 208, 237	0
20	XT	99/106 (93%)	0.22	2 (2%) 65 49	87, 136, 211, 236	0
21	QU	25/27 (92%)	1.05	5 (20%) 1 0	112, 155, 238, 264	0
21	XU	25/27 (92%)	0.37	2 (8%) 12 7	102, 128, 202, 210	0
22	QV	77/77 (100%)	0.46	6 (7%) 13 8	91, 114, 175, 228	0
22	XV	77/77 (100%)	0.15	4 (5%) 27 17	70, 91, 164, 210	0
23	QW	76/76 (100%)	2.07	34 (44%) 0 0	91, 205, 292, 361	0
23	QY	17/76 (22%)	1.59	9 (52%) 0 0	120, 132, 201, 212	0
23	XW	76/76 (100%)	2.27	33 (43%) 0 0	88, 196, 373, 402	0
23	XY	17/76 (22%)	0.66	1 (5%) 22 13	94, 101, 177, 187	0
24	QX	10/24 (41%)	1.59	3 (30%) 0 0	102, 106, 257, 377	0
24	XX	10/24 (41%)	1.88	5 (50%) 0 0	94, 99, 237, 284	0
25	RA	2882/2915 (98%)	0.37	190 (6%) 18 10	53, 82, 254, 563	0
25	YA	2883/2915 (98%)	0.19	127 (4%) 34 21	39, 64, 217, 437	0
26	RB	120/122 (98%)	0.65	14 (11%) 4 3	119, 162, 204, 242	0
26	YB	120/122 (98%)	0.18	1 (0%) 86 75	71, 106, 119, 200	0
27	RD	272/276 (98%)	-0.27	1 (0%) 92 86	54, 74, 127, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	YD	272/276 (98%)	-0.30	1 (0%) 92 86	40, 66, 120, 213	0
28	RE	205/206 (99%)	0.06	8 (3%) 39 25	55, 94, 188, 447	0
28	YE	205/206 (99%)	0.02	6 (2%) 51 35	43, 78, 167, 453	0
29	RF	202/210 (96%)	-0.10	2 (0%) 82 70	54, 110, 191, 469	0
29	YF	202/210 (96%)	-0.25	4 (1%) 65 49	39, 71, 138, 248	0
30	RG	181/182 (99%)	0.54	16 (8%) 10 6	122, 192, 303, 490	0
30	YG	181/182 (99%)	0.07	2 (1%) 80 68	82, 117, 183, 391	0
31	RH	170/180 (94%)	0.75	24 (14%) 2 2	113, 199, 359, 517	0
31	YH	170/180 (94%)	0.15	5 (2%) 51 35	65, 114, 180, 363	0
32	RI	146/148 (98%)	0.23	10 (6%) 17 10	73, 155, 265, 529	0
32	YI	146/148 (98%)	0.05	4 (2%) 54 38	62, 143, 271, 559	0
33	RN	138/140 (98%)	-0.07	3 (2%) 62 45	64, 110, 186, 302	0
33	YN	138/140 (98%)	-0.28	2 (1%) 75 61	49, 78, 167, 266	0
34	RO	122/122 (100%)	-0.25	0 100 100	63, 94, 139, 155	0
34	YO	122/122 (100%)	-0.28	0 100 100	51, 68, 115, 146	0
35	RP	150/150 (100%)	0.10	8 (5%) 26 16	61, 122, 202, 369	0
35	YP	150/150 (100%)	-0.20	1 (0%) 87 78	42, 81, 157, 361	0
36	RQ	141/141 (100%)	0.18	7 (4%) 28 18	80, 122, 205, 332	0
36	YQ	141/141 (100%)	-0.21	3 (2%) 63 48	56, 73, 148, 430	0
37	RR	118/118 (100%)	-0.20	1 (0%) 86 75	61, 86, 134, 160	0
37	YR	118/118 (100%)	-0.18	1 (0%) 86 75	51, 71, 120, 207	0
38	RS	111/112 (99%)	0.23	3 (2%) 54 38	109, 160, 253, 420	0
38	YS	111/112 (99%)	-0.03	0 100 100	73, 102, 175, 285	0
39	RT	137/146 (93%)	-0.14	2 (1%) 73 60	70, 107, 263, 350	0
39	YT	137/146 (93%)	-0.11	4 (2%) 51 35	60, 84, 192, 451	0
40	RU	117/118 (99%)	0.01	3 (2%) 56 40	62, 106, 174, 287	0
40	YU	117/118 (99%)	-0.27	1 (0%) 84 73	47, 71, 134, 425	0
41	RV	101/101 (100%)	0.27	7 (6%) 16 10	64, 129, 225, 419	0
41	YV	101/101 (100%)	-0.08	2 (1%) 65 49	46, 89, 172, 424	0
42	RW	113/113 (100%)	-0.11	3 (2%) 54 38	55, 75, 154, 298	0
42	YW	113/113 (100%)	-0.15	1 (0%) 84 73	42, 67, 139, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	RX	92/96 (95%)	-0.04	0 100 100	67, 95, 161, 200	0
43	YX	92/96 (95%)	-0.03	1 (1%) 80 68	50, 72, 129, 260	0
44	RY	102/110 (92%)	0.39	10 (9%) 7 4	79, 132, 238, 489	0
44	YY	102/110 (92%)	-0.04	3 (2%) 51 35	63, 103, 175, 385	0
45	RZ	183/206 (88%)	0.93	32 (17%) 1 1	123, 195, 338, 497	0
45	YZ	183/206 (88%)	0.63	23 (12%) 3 2	76, 148, 434, 554	0
46	R0	82/85 (96%)	0.27	7 (8%) 10 6	69, 114, 152, 188	0
46	Y0	82/85 (96%)	-0.02	1 (1%) 79 66	47, 70, 126, 171	0
47	R1	97/98 (98%)	0.34	3 (3%) 49 33	58, 95, 208, 261	0
47	Y1	97/98 (98%)	0.06	3 (3%) 49 33	45, 72, 181, 340	0
48	R2	69/72 (95%)	-0.21	0 100 100	80, 129, 215, 245	0
48	Y2	69/72 (95%)	-0.06	0 100 100	60, 88, 176, 274	0
49	R3	59/60 (98%)	0.22	3 (5%) 28 17	82, 121, 199, 517	0
49	Y3	59/60 (98%)	-0.02	2 (3%) 45 30	55, 76, 140, 319	0
50	R4	71/71 (100%)	1.27	16 (22%) 0 0	132, 252, 520, 577	0
50	Y4	71/71 (100%)	0.79	10 (14%) 2 2	103, 196, 455, 567	0
51	R5	59/60 (98%)	0.25	5 (8%) 10 6	46, 95, 288, 394	0
51	Y5	57/60 (95%)	0.11	1 (1%) 68 53	23, 73, 267, 342	0
52	R6	49/54 (90%)	0.66	3 (6%) 21 12	88, 156, 225, 300	0
52	Y6	49/54 (90%)	0.63	5 (10%) 6 4	53, 118, 199, 327	0
53	R7	49/49 (100%)	-0.26	0 100 100	38, 65, 157, 188	0
53	Y7	49/49 (100%)	-0.18	1 (2%) 65 49	26, 48, 108, 212	0
54	R8	64/65 (98%)	-0.02	0 100 100	53, 93, 152, 285	0
54	Y8	64/65 (98%)	-0.14	0 100 100	29, 61, 107, 272	0
55	R9	37/37 (100%)	1.31	7 (18%) 1 0	92, 141, 227, 400	0
55	Y9	37/37 (100%)	0.79	3 (8%) 12 7	45, 101, 162, 378	0
56	Z7	8/12 (66%)	0.80	0 100 100	115, 174, 254, 280	0
56	Z8	8/12 (66%)	0.43	0 100 100	124, 137, 204, 234	0
All	All	21045/21776 (96%)	0.20	1024 (4%) 29 18	23, 99, 241, 583	0

The worst 5 of 1024 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	YE	205	ALA	22.8
1	QA	1032	A	16.7
25	RA	1100	C	16.6
25	RA	1068	G	15.9
23	XW	20	U	14.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3206	1/1	-0.03	0.75	140,140,140,140	0
57	MG	RA	3201	1/1	0.08	1.74	128,128,128,128	0
57	MG	RA	3215	1/1	0.09	0.35	68,68,68,68	0
57	MG	RA	3225	1/1	0.19	0.67	161,161,161,161	0
57	MG	R0	101	1/1	0.29	0.61	78,78,78,78	0
57	MG	RA	3219	1/1	0.30	0.78	138,138,138,138	0
57	MG	RA	3217	1/1	0.33	0.66	133,133,133,133	0
57	MG	RD	301	1/1	0.34	1.06	91,91,91,91	0
57	MG	YA	3178	1/1	0.37	0.50	64,64,64,64	0
57	MG	XA	1662	1/1	0.38	0.71	61,61,61,61	0
57	MG	XA	1650	1/1	0.39	0.68	60,60,60,60	0
57	MG	RA	3152	1/1	0.40	0.30	50,50,50,50	0
57	MG	QA	1649	1/1	0.41	0.62	104,104,104,104	0
57	MG	RA	3224	1/1	0.41	0.61	91,91,91,91	0
57	MG	RA	3220	1/1	0.42	0.60	83,83,83,83	0
57	MG	QA	1664	1/1	0.42	0.52	78,78,78,78	0
57	MG	RA	3161	1/1	0.45	1.15	76,76,76,76	0
57	MG	RA	3218	1/1	0.46	1.01	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1644	1/1	0.46	0.50	114,114,114,114	0
57	MG	YA	3149	1/1	0.47	1.62	106,106,106,106	0
57	MG	QA	1633	1/1	0.47	0.16	143,143,143,143	0
57	MG	YA	3169	1/1	0.48	0.28	93,93,93,93	0
57	MG	RA	3164	1/1	0.48	0.75	82,82,82,82	0
57	MG	YA	3155	1/1	0.49	0.25	44,44,44,44	0
57	MG	YA	3229	1/1	0.51	0.35	36,36,36,36	0
57	MG	XA	1634	1/1	0.53	0.54	98,98,98,98	0
57	MG	YA	3153	1/1	0.53	0.78	63,63,63,63	0
57	MG	QA	1603	1/1	0.55	2.24	66,66,66,66	0
57	MG	RA	3159	1/1	0.57	0.75	72,72,72,72	0
57	MG	RA	3216	1/1	0.58	0.70	110,110,110,110	0
57	MG	XA	1666	1/1	0.58	0.30	55,55,55,55	0
57	MG	YA	3165	1/1	0.59	0.34	77,77,77,77	0
57	MG	YA	3141	1/1	0.60	0.39	69,69,69,69	0
57	MG	QA	1632	1/1	0.60	0.15	69,69,69,69	0
57	MG	QH	201	1/1	0.61	0.38	105,105,105,105	0
57	MG	YA	3224	1/1	0.61	0.19	44,44,44,44	0
57	MG	RA	3002	1/1	0.61	1.24	70,70,70,70	0
57	MG	YA	3254	1/1	0.61	0.65	61,61,61,61	0
57	MG	RA	3196	1/1	0.62	0.41	108,108,108,108	0
57	MG	RA	3007	1/1	0.62	0.55	59,59,59,59	0
57	MG	RA	3127	1/1	0.62	0.45	74,74,74,74	0
57	MG	YA	3274	1/1	0.62	0.61	57,57,57,57	0
57	MG	RA	3156	1/1	0.63	0.22	48,48,48,48	0
57	MG	YA	3158	1/1	0.64	0.34	69,69,69,69	0
57	MG	RA	3139	1/1	0.65	0.27	70,70,70,70	0
57	MG	RA	3157	1/1	0.65	0.53	54,54,54,54	0
57	MG	RA	3138	1/1	0.65	1.69	95,95,95,95	0
57	MG	YA	3201	1/1	0.65	0.42	61,61,61,61	0
57	MG	XA	1601	1/1	0.66	0.66	29,29,29,29	0
57	MG	QA	1655	1/1	0.67	0.62	74,74,74,74	0
57	MG	YA	3156	1/1	0.68	0.40	58,58,58,58	0
57	MG	RA	3136	1/1	0.68	0.39	105,105,105,105	0
57	MG	RA	3118	1/1	0.69	0.63	44,44,44,44	0
57	MG	YA	3243	1/1	0.69	0.44	60,60,60,60	0
57	MG	YA	3210	1/1	0.69	0.43	135,135,135,135	0
57	MG	YA	3259	1/1	0.69	0.62	40,40,40,40	0
57	MG	RA	3044	1/1	0.69	1.29	75,75,75,75	0
57	MG	RA	3213	1/1	0.70	0.25	62,62,62,62	0
57	MG	YB	201	1/1	0.70	0.45	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3179	1/1	0.71	0.29	44,44,44,44	0
57	MG	QA	1629	1/1	0.71	0.35	85,85,85,85	0
57	MG	RA	3212	1/1	0.71	0.54	89,89,89,89	0
57	MG	XA	1628	1/1	0.71	0.25	41,41,41,41	0
57	MG	RA	3175	1/1	0.71	0.96	57,57,57,57	0
57	MG	XA	1664	1/1	0.72	0.25	51,51,51,51	0
57	MG	RA	3153	1/1	0.72	0.46	79,79,79,79	0
57	MG	XA	1608	1/1	0.72	0.69	119,119,119,119	0
57	MG	XA	1670	1/1	0.73	0.45	47,47,47,47	0
57	MG	YA	3233	1/1	0.73	0.60	58,58,58,58	0
57	MG	YA	3132	1/1	0.73	0.24	56,56,56,56	0
57	MG	RA	3151	1/1	0.73	0.26	69,69,69,69	0
57	MG	XA	1607	1/1	0.73	0.24	53,53,53,53	0
57	MG	QA	1626	1/1	0.73	0.22	156,156,156,156	0
57	MG	YA	3228	1/1	0.73	0.67	59,59,59,59	0
57	MG	XA	1651	1/1	0.74	0.39	111,111,111,111	0
57	MG	XA	1653	1/1	0.74	0.33	83,83,83,83	0
57	MG	RP	204	1/1	0.74	0.42	183,183,183,183	0
57	MG	QA	1639	1/1	0.74	0.32	49,49,49,49	0
57	MG	YA	3161	1/1	0.75	0.58	43,43,43,43	0
57	MG	YA	3258	1/1	0.75	1.08	68,68,68,68	0
57	MG	QA	1651	1/1	0.75	0.31	49,49,49,49	0
57	MG	YA	3012	1/1	0.75	0.97	36,36,36,36	0
57	MG	QA	1638	1/1	0.75	0.45	63,63,63,63	0
57	MG	RA	3238	1/1	0.76	0.45	51,51,51,51	0
57	MG	R5	101	1/1	0.76	1.48	291,291,291,291	0
57	MG	RA	3239	1/1	0.76	0.95	90,90,90,90	0
57	MG	RA	3099	1/1	0.76	0.32	48,48,48,48	0
57	MG	RA	3197	1/1	0.76	0.62	84,84,84,84	0
57	MG	YA	3054	1/1	0.76	0.67	65,65,65,65	0
57	MG	YA	3231	1/1	0.77	0.60	79,79,79,79	0
57	MG	YA	3016	1/1	0.77	0.20	31,31,31,31	0
57	MG	YA	3135	1/1	0.77	0.37	65,65,65,65	0
57	MG	RA	3191	1/1	0.77	0.22	34,34,34,34	0
57	MG	RA	3101	1/1	0.78	0.31	56,56,56,56	0
57	MG	RA	3189	1/1	0.78	0.25	96,96,96,96	0
57	MG	YA	3084	1/1	0.78	0.23	71,71,71,71	0
57	MG	YA	3125	1/1	0.78	0.67	60,60,60,60	0
57	MG	QA	1653	1/1	0.78	0.18	79,79,79,79	0
57	MG	RA	3158	1/1	0.79	0.25	56,56,56,56	0
57	MG	RA	3171	1/1	0.79	0.45	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1648	1/1	0.79	0.21	75,75,75,75	0
57	MG	YA	3167	1/1	0.79	0.31	69,69,69,69	0
57	MG	XB	301	1/1	0.79	0.59	87,87,87,87	0
57	MG	QA	1660	1/1	0.79	0.32	193,193,193,193	0
57	MG	QA	1628	1/1	0.79	0.24	103,103,103,103	0
57	MG	YA	3186	1/1	0.79	0.18	64,64,64,64	0
57	MG	YA	3190	1/1	0.79	0.57	51,51,51,51	0
57	MG	RA	3203	1/1	0.79	0.53	74,74,74,74	0
57	MG	XA	1609	1/1	0.79	0.42	35,35,35,35	0
57	MG	XM	201	1/1	0.80	0.45	173,173,173,173	0
57	MG	YA	3227	1/1	0.80	0.57	121,121,121,121	0
57	MG	RA	3185	1/1	0.80	0.64	48,48,48,48	0
57	MG	XA	1663	1/1	0.80	0.34	75,75,75,75	0
57	MG	YA	3150	1/1	0.80	0.36	114,114,114,114	0
57	MG	XA	1614	1/1	0.80	0.31	153,153,153,153	0
57	MG	YA	3237	1/1	0.80	0.54	52,52,52,52	0
57	MG	YA	3071	1/1	0.80	0.19	37,37,37,37	0
57	MG	QA	1607	1/1	0.80	0.36	124,124,124,124	0
57	MG	YA	3256	1/1	0.80	0.31	128,128,128,128	0
57	MG	YA	3195	1/1	0.80	0.26	88,88,88,88	0
57	MG	RA	3132	1/1	0.80	0.42	66,66,66,66	0
57	MG	XA	1659	1/1	0.80	0.50	102,102,102,102	0
57	MG	YA	3214	1/1	0.80	0.44	244,244,244,244	0
57	MG	RA	3068	1/1	0.81	0.82	45,45,45,45	0
57	MG	YA	3204	1/1	0.81	0.48	182,182,182,182	0
57	MG	RA	3114	1/1	0.81	0.24	37,37,37,37	0
57	MG	YA	3006	1/1	0.81	0.70	59,59,59,59	0
57	MG	YA	3140	1/1	0.81	0.26	33,33,33,33	0
57	MG	RA	3011	1/1	0.81	0.64	52,52,52,52	0
57	MG	QA	1640	1/1	0.82	0.36	78,78,78,78	0
57	MG	RA	3214	1/1	0.82	0.32	119,119,119,119	0
57	MG	QA	1624	1/1	0.82	0.95	68,68,68,68	0
57	MG	RA	3190	1/1	0.82	0.37	107,107,107,107	0
57	MG	YA	3211	1/1	0.82	0.38	72,72,72,72	0
57	MG	YA	3177	1/1	0.82	0.60	51,51,51,51	0
57	MG	RA	3025	1/1	0.82	0.10	34,34,34,34	0
57	MG	RA	3123	1/1	0.82	0.28	55,55,55,55	0
57	MG	RA	3240	1/1	0.82	0.60	70,70,70,70	0
57	MG	RA	3245	1/1	0.82	0.83	128,128,128,128	0
57	MG	YA	3144	1/1	0.83	0.26	62,62,62,62	0
57	MG	XA	1638	1/1	0.83	0.10	59,59,59,59	0
57	MG	QA	1618	1/1	0.83	0.52	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QF	201	1/1	0.83	0.54	166,166,166,166	0
57	MG	RA	3246	1/1	0.83	0.28	198,198,198,198	0
57	MG	RA	3182	1/1	0.83	0.34	92,92,92,92	0
57	MG	RA	3228	1/1	0.83	0.81	25,25,25,25	0
57	MG	YA	3263	1/1	0.83	0.58	60,60,60,60	0
57	MG	YA	3273	1/1	0.83	0.86	55,55,55,55	0
57	MG	RA	3133	1/1	0.83	0.41	118,118,118,118	0
57	MG	RA	3165	1/1	0.83	0.58	82,82,82,82	0
57	MG	YB	204	1/1	0.83	0.59	37,37,37,37	0
57	MG	YA	3239	1/1	0.84	0.20	85,85,85,85	0
57	MG	RA	3130	1/1	0.84	0.17	64,64,64,64	0
57	MG	RA	3004	1/1	0.84	0.51	39,39,39,39	0
57	MG	RA	3177	1/1	0.84	0.81	72,72,72,72	0
57	MG	XA	1661	1/1	0.84	0.96	75,75,75,75	0
57	MG	RA	3001	1/1	0.84	0.82	44,44,44,44	0
57	MG	QA	1615	1/1	0.84	0.54	88,88,88,88	0
57	MG	RA	3223	1/1	0.84	0.15	113,113,113,113	0
57	MG	YA	3166	1/1	0.84	1.29	74,74,74,74	0
57	MG	RA	3186	1/1	0.84	0.68	72,72,72,72	0
57	MG	YA	3206	1/1	0.84	0.38	88,88,88,88	0
57	MG	RA	3208	1/1	0.85	0.47	74,74,74,74	0
57	MG	RA	3176	1/1	0.85	0.27	25,25,25,25	0
57	MG	RA	3089	1/1	0.85	0.34	114,114,114,114	0
57	MG	YA	3199	1/1	0.85	0.25	54,54,54,54	0
57	MG	RA	3008	1/1	0.85	0.77	62,62,62,62	0
57	MG	XA	1629	1/1	0.85	0.42	104,104,104,104	0
57	MG	YA	3116	1/1	0.85	1.00	89,89,89,89	0
57	MG	XA	1631	1/1	0.85	0.23	68,68,68,68	0
57	MG	RA	3010	1/1	0.85	0.50	89,89,89,89	0
57	MG	RA	3063	1/1	0.85	1.00	43,43,43,43	0
57	MG	RA	3230	1/1	0.85	0.82	92,92,92,92	0
57	MG	RA	3188	1/1	0.85	0.42	103,103,103,103	0
57	MG	YA	3003	1/1	0.85	0.29	42,42,42,42	0
57	MG	QA	1623	1/1	0.85	0.44	79,79,79,79	0
57	MG	YE	301	1/1	0.85	0.55	47,47,47,47	0
57	MG	YA	3223	1/1	0.86	0.17	59,59,59,59	0
57	MG	RA	3178	1/1	0.86	0.30	99,99,99,99	0
57	MG	QA	1620	1/1	0.86	0.26	80,80,80,80	0
57	MG	RA	3155	1/1	0.86	0.68	71,71,71,71	0
57	MG	YA	3133	1/1	0.86	0.14	50,50,50,50	0
57	MG	YA	3265	1/1	0.86	0.37	41,41,41,41	0
57	MG	XA	1669	1/1	0.86	0.28	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1645	1/1	0.86	0.21	25,25,25,25	0
57	MG	RA	3173	1/1	0.86	0.13	38,38,38,38	0
57	MG	XA	1649	1/1	0.86	0.28	61,61,61,61	0
57	MG	YA	3219	1/1	0.86	0.50	105,105,105,105	0
57	MG	RA	3116	1/1	0.87	0.28	30,30,30,30	0
57	MG	YA	3249	1/1	0.87	0.28	27,27,27,27	0
57	MG	YA	3217	1/1	0.87	0.42	76,76,76,76	0
57	MG	YA	3185	1/1	0.87	0.16	61,61,61,61	0
57	MG	RA	3082	1/1	0.87	0.66	61,61,61,61	0
57	MG	RA	3168	1/1	0.87	0.65	44,44,44,44	0
57	MG	YA	3137	1/1	0.87	0.19	27,27,27,27	0
57	MG	RA	3244	1/1	0.87	0.28	35,35,35,35	0
57	MG	YA	3267	1/1	0.87	0.65	59,59,59,59	0
57	MG	RA	3140	1/1	0.87	0.27	74,74,74,74	0
57	MG	XA	1655	1/1	0.87	0.80	53,53,53,53	0
57	MG	YA	3275	1/1	0.87	0.79	35,35,35,35	0
57	MG	RA	3233	1/1	0.87	0.23	33,33,33,33	0
57	MG	YB	202	1/1	0.87	0.80	70,70,70,70	0
57	MG	RA	3234	1/1	0.87	0.38	48,48,48,48	0
57	MG	XX	101	1/1	0.87	0.39	64,64,64,64	0
57	MG	RA	3067	1/1	0.88	0.31	85,85,85,85	0
57	MG	RA	3242	1/1	0.88	0.71	67,67,67,67	0
57	MG	RA	3243	1/1	0.88	0.64	32,32,32,32	0
57	MG	QA	1614	1/1	0.88	0.65	76,76,76,76	0
57	MG	YA	3194	1/1	0.88	0.73	49,49,49,49	0
57	MG	YA	3148	1/1	0.88	0.74	28,28,28,28	0
57	MG	XA	1620	1/1	0.88	0.29	83,83,83,83	0
57	MG	RA	3143	1/1	0.88	0.33	69,69,69,69	0
57	MG	RA	3229	1/1	0.88	0.36	88,88,88,88	0
57	MG	RA	3147	1/1	0.88	0.28	120,120,120,120	0
57	MG	RA	3050	1/1	0.88	0.36	46,46,46,46	0
57	MG	YA	3082	1/1	0.88	0.23	44,44,44,44	0
57	MG	XA	1635	1/1	0.88	0.74	74,74,74,74	0
57	MG	YA	3164	1/1	0.88	0.31	72,72,72,72	0
57	MG	RA	3211	1/1	0.88	0.42	67,67,67,67	0
57	MG	XA	1667	1/1	0.88	0.64	75,75,75,75	0
57	MG	YA	3128	1/1	0.88	0.15	52,52,52,52	0
57	MG	XA	1668	1/1	0.88	0.40	136,136,136,136	0
57	MG	RA	3193	1/1	0.88	0.21	87,87,87,87	0
57	MG	QA	1646	1/1	0.88	0.09	65,65,65,65	0
57	MG	YA	3041	1/1	0.89	0.39	35,35,35,35	0
57	MG	YA	3044	1/1	0.89	0.74	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3181	1/1	0.89	0.21	49,49,49,49	0
57	MG	YA	3070	1/1	0.89	0.20	50,50,50,50	0
57	MG	YA	3191	1/1	0.89	0.20	39,39,39,39	0
57	MG	RA	3144	1/1	0.89	0.50	70,70,70,70	0
57	MG	YA	3244	1/1	0.89	0.52	75,75,75,75	0
57	MG	YA	3074	1/1	0.89	0.25	33,33,33,33	0
57	MG	QA	1647	1/1	0.89	0.29	67,67,67,67	0
57	MG	YA	3200	1/1	0.89	0.44	58,58,58,58	0
57	MG	XA	1652	1/1	0.89	0.30	104,104,104,104	0
57	MG	YA	3094	1/1	0.89	0.60	60,60,60,60	0
57	MG	RA	3172	1/1	0.89	0.27	43,43,43,43	0
57	MG	YA	3163	1/1	0.89	0.20	48,48,48,48	0
57	MG	YA	3266	1/1	0.89	0.54	64,64,64,64	0
57	MG	RA	3148	1/1	0.89	0.33	90,90,90,90	0
57	MG	XA	1656	1/1	0.89	0.60	89,89,89,89	0
57	MG	QA	1634	1/1	0.89	0.75	53,53,53,53	0
57	MG	RA	3075	1/1	0.89	0.74	46,46,46,46	0
57	MG	QA	1625	1/1	0.89	0.82	92,92,92,92	0
57	MG	YA	3174	1/1	0.89	0.16	53,53,53,53	0
57	MG	QA	1602	1/1	0.89	0.45	39,39,39,39	0
57	MG	RA	3195	1/1	0.89	0.23	102,102,102,102	0
57	MG	QA	1643	1/1	0.90	0.39	67,67,67,67	0
57	MG	RA	3226	1/1	0.90	0.41	63,63,63,63	0
57	MG	YA	3036	1/1	0.90	0.29	38,38,38,38	0
57	MG	RA	3061	1/1	0.90	0.16	64,64,64,64	0
57	MG	YA	3238	1/1	0.90	0.18	36,36,36,36	0
57	MG	RA	3088	1/1	0.90	0.36	59,59,59,59	0
57	MG	RA	3174	1/1	0.90	0.33	36,36,36,36	0
57	MG	YA	3055	1/1	0.90	0.54	43,43,43,43	0
57	MG	XA	1640	1/1	0.90	0.86	43,43,43,43	0
57	MG	QA	1637	1/1	0.90	0.13	53,53,53,53	0
57	MG	YA	3152	1/1	0.90	0.48	57,57,57,57	0
57	MG	RA	3091	1/1	0.90	0.61	73,73,73,73	0
57	MG	YA	3080	1/1	0.90	0.85	53,53,53,53	0
57	MG	XA	1604	1/1	0.90	1.07	64,64,64,64	0
57	MG	YA	3264	1/1	0.90	0.39	75,75,75,75	0
57	MG	RA	3160	1/1	0.90	0.26	39,39,39,39	0
57	MG	QA	1656	1/1	0.90	0.35	87,87,87,87	0
57	MG	YA	3101	1/1	0.90	0.38	30,30,30,30	0
57	MG	YA	3272	1/1	0.90	0.29	78,78,78,78	0
57	MG	YA	3102	1/1	0.90	0.14	27,27,27,27	0
57	MG	QA	1627	1/1	0.90	0.27	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3118	1/1	0.90	0.50	35,35,35,35	0
57	MG	RA	3069	1/1	0.90	0.48	49,49,49,49	0
57	MG	RA	3167	1/1	0.90	0.18	54,54,54,54	0
57	MG	YA	3170	1/1	0.90	0.65	38,38,38,38	0
57	MG	RA	3115	1/1	0.90	0.41	82,82,82,82	0
57	MG	RA	3094	1/1	0.91	0.89	28,28,28,28	0
57	MG	RA	3194	1/1	0.91	0.45	51,51,51,51	0
57	MG	YA	3072	1/1	0.91	0.25	30,30,30,30	0
57	MG	YA	3157	1/1	0.91	0.23	42,42,42,42	0
57	MG	QA	1601	1/1	0.91	0.36	36,36,36,36	0
57	MG	QA	1613	1/1	0.91	0.64	57,57,57,57	0
57	MG	RA	3109	1/1	0.91	0.21	51,51,51,51	0
57	MG	RA	3200	1/1	0.91	0.31	76,76,76,76	0
57	MG	RA	3111	1/1	0.91	0.20	48,48,48,48	0
57	MG	XA	1671	1/1	0.91	0.28	76,76,76,76	0
57	MG	RA	3039	1/1	0.91	0.43	36,36,36,36	0
57	MG	YA	3105	1/1	0.91	0.32	31,31,31,31	0
57	MG	RA	3073	1/1	0.91	0.32	70,70,70,70	0
57	MG	XV	102	1/1	0.91	0.30	61,61,61,61	0
57	MG	YA	3124	1/1	0.91	0.31	84,84,84,84	0
57	MG	RA	3041	1/1	0.91	0.34	32,32,32,32	0
57	MG	RA	3005	1/1	0.91	0.63	31,31,31,31	0
57	MG	YA	3257	1/1	0.91	0.88	42,42,42,42	0
57	MG	RA	3232	1/1	0.91	0.33	40,40,40,40	0
57	MG	QA	1658	1/1	0.91	0.34	71,71,71,71	0
57	MG	QY	101	1/1	0.91	0.18	83,83,83,83	0
57	MG	YA	3024	1/1	0.91	0.47	33,33,33,33	0
57	MG	YA	3139	1/1	0.91	0.96	57,57,57,57	0
57	MG	RA	3170	1/1	0.91	0.18	55,55,55,55	0
57	MG	YA	3196	1/1	0.91	0.27	34,34,34,34	0
57	MG	YA	3270	1/1	0.91	0.83	57,57,57,57	0
57	MG	YA	3037	1/1	0.91	0.37	50,50,50,50	0
57	MG	YA	3143	1/1	0.91	0.47	60,60,60,60	0
57	MG	RA	3128	1/1	0.91	0.37	91,91,91,91	0
57	MG	XA	1660	1/1	0.91	0.17	77,77,77,77	0
57	MG	YA	3277	1/1	0.91	0.37	42,42,42,42	0
57	MG	YA	3047	1/1	0.91	0.59	26,26,26,26	0
57	MG	XA	1621	1/1	0.91	0.55	46,46,46,46	0
57	MG	YA	3151	1/1	0.91	0.26	28,28,28,28	0
57	MG	YD	301	1/1	0.91	0.33	42,42,42,42	0
57	MG	QA	1605	1/1	0.91	1.01	44,44,44,44	0
57	MG	QA	1654	1/1	0.92	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3019	1/1	0.92	0.46	25,25,25,25	0
57	MG	RA	3112	1/1	0.92	0.33	78,78,78,78	0
57	MG	QA	1666	1/1	0.92	0.50	57,57,57,57	0
57	MG	XA	1630	1/1	0.92	0.53	33,33,33,33	0
57	MG	YA	3039	1/1	0.92	0.29	59,59,59,59	0
57	MG	YA	3230	1/1	0.92	0.23	45,45,45,45	0
57	MG	RA	3006	1/1	0.92	0.48	25,25,25,25	0
57	MG	YA	3173	1/1	0.92	0.16	37,37,37,37	0
57	MG	YA	3235	1/1	0.92	0.35	63,63,63,63	0
57	MG	YA	3134	1/1	0.92	0.29	39,39,39,39	0
57	MG	YA	3175	1/1	0.92	0.53	38,38,38,38	0
57	MG	YA	3176	1/1	0.92	0.27	106,106,106,106	0
57	MG	YA	3240	1/1	0.92	0.86	52,52,52,52	0
57	MG	YA	3242	1/1	0.92	0.87	46,46,46,46	0
57	MG	RA	3047	1/1	0.92	0.46	26,26,26,26	0
57	MG	QA	1612	1/1	0.92	0.45	44,44,44,44	0
57	MG	YA	3246	1/1	0.92	0.52	32,32,32,32	0
57	MG	RA	3162	1/1	0.92	0.14	72,72,72,72	0
57	MG	YA	3251	1/1	0.92	1.05	52,52,52,52	0
57	MG	YA	3180	1/1	0.92	0.28	79,79,79,79	0
57	MG	YA	3184	1/1	0.92	0.15	37,37,37,37	0
57	MG	QA	1641	1/1	0.92	0.20	76,76,76,76	0
57	MG	YA	3065	1/1	0.92	0.27	53,53,53,53	0
57	MG	RA	3184	1/1	0.92	0.16	48,48,48,48	0
57	MG	YA	3261	1/1	0.92	0.62	70,70,70,70	0
57	MG	YA	3262	1/1	0.92	0.63	63,63,63,63	0
57	MG	XA	1647	1/1	0.92	0.42	49,49,49,49	0
57	MG	QA	1652	1/1	0.92	0.81	77,77,77,77	0
57	MG	RA	3166	1/1	0.92	0.84	59,59,59,59	0
57	MG	RA	3150	1/1	0.92	0.13	42,42,42,42	0
57	MG	RA	3097	1/1	0.92	0.52	44,44,44,44	0
57	MG	XV	103	1/1	0.92	1.07	54,54,54,54	0
57	MG	YA	3088	1/1	0.92	0.35	26,26,26,26	0
57	MG	YA	3202	1/1	0.92	0.30	54,54,54,54	0
57	MG	QA	1631	1/1	0.92	0.40	72,72,72,72	0
57	MG	QA	1662	1/1	0.92	0.19	100,100,100,100	0
57	MG	XA	1619	1/1	0.92	0.37	46,46,46,46	0
57	MG	YA	3278	1/1	0.92	0.26	85,85,85,85	0
57	MG	RA	3026	1/1	0.92	0.78	33,33,33,33	0
57	MG	YA	3212	1/1	0.92	0.18	38,38,38,38	0
57	MG	YA	3160	1/1	0.92	0.19	89,89,89,89	0
57	MG	YA	3115	1/1	0.92	0.31	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3218	1/1	0.92	0.17	58,58,58,58	0
57	MG	YE	302	1/1	0.92	0.35	31,31,31,31	0
58	PAR	QA	1667	42/42	0.92	0.20	72,72,72,72	0
57	MG	RA	3056	1/1	0.93	0.43	38,38,38,38	0
57	MG	XA	1625	1/1	0.93	0.16	53,53,53,53	0
57	MG	YA	3181	1/1	0.93	0.22	32,32,32,32	0
57	MG	YA	3183	1/1	0.93	0.63	67,67,67,67	0
57	MG	RB	201	1/1	0.93	0.13	79,79,79,79	0
57	MG	QA	1609	1/1	0.93	0.11	154,154,154,154	0
57	MG	YA	3145	1/1	0.93	0.20	35,35,35,35	0
57	MG	YA	3188	1/1	0.93	0.43	39,39,39,39	0
57	MG	YA	3147	1/1	0.93	0.21	75,75,75,75	0
57	MG	YA	3076	1/1	0.93	0.69	25,25,25,25	0
57	MG	XA	1657	1/1	0.93	0.59	65,65,65,65	0
57	MG	YA	3252	1/1	0.93	0.38	42,42,42,42	0
57	MG	XA	1658	1/1	0.93	0.53	101,101,101,101	0
57	MG	RP	202	1/1	0.93	0.46	64,64,64,64	0
57	MG	RA	3180	1/1	0.93	0.16	86,86,86,86	0
57	MG	QA	1657	1/1	0.93	0.43	112,112,112,112	0
57	MG	YA	3099	1/1	0.93	0.55	32,32,32,32	0
57	MG	QA	1616	1/1	0.93	0.20	81,81,81,81	0
57	MG	YA	3203	1/1	0.93	0.24	139,139,139,139	0
57	MG	YA	3030	1/1	0.93	0.67	36,36,36,36	0
57	MG	RA	3045	1/1	0.93	0.18	27,27,27,27	0
57	MG	XA	1639	1/1	0.93	0.10	71,71,71,71	0
57	MG	QV	102	1/1	0.93	0.24	69,69,69,69	0
57	MG	RA	3048	1/1	0.93	0.36	47,47,47,47	0
57	MG	YA	3213	1/1	0.93	0.15	54,54,54,54	0
57	MG	RA	3031	1/1	0.93	0.50	52,52,52,52	0
57	MG	YA	3216	1/1	0.93	0.18	72,72,72,72	0
57	MG	YA	3045	1/1	0.93	0.51	47,47,47,47	0
57	MG	RA	3076	1/1	0.93	0.48	28,28,28,28	0
57	MG	YA	3130	1/1	0.93	0.27	84,84,84,84	0
57	MG	YA	3131	1/1	0.93	0.69	55,55,55,55	0
57	MG	YA	3048	1/1	0.93	0.39	58,58,58,58	0
57	MG	YA	3053	1/1	0.93	0.62	51,51,51,51	0
57	MG	YB	203	1/1	0.93	0.30	91,91,91,91	0
57	MG	RA	3131	1/1	0.93	0.19	57,57,57,57	0
57	MG	RA	3078	1/1	0.93	0.72	54,54,54,54	0
57	MG	YA	3063	1/1	0.93	0.40	27,27,27,27	0
57	MG	YA	3138	1/1	0.93	0.50	34,34,34,34	0
57	MG	Y5	101	1/1	0.93	1.04	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3227	1/1	0.93	1.24	40,40,40,40	0
58	PAR	XA	1672	42/42	0.93	0.26	66,66,66,66	0
59	ZN	R5	102	1/1	0.93	0.07	306,306,306,306	0
57	MG	RA	3043	1/1	0.94	0.22	47,47,47,47	0
57	MG	RA	3231	1/1	0.94	0.63	29,29,29,29	0
57	MG	RA	3149	1/1	0.94	0.26	29,29,29,29	0
57	MG	YA	3142	1/1	0.94	0.72	50,50,50,50	0
57	MG	RA	3066	1/1	0.94	0.27	37,37,37,37	0
57	MG	YA	3002	1/1	0.94	0.47	37,37,37,37	0
57	MG	YA	3075	1/1	0.94	0.25	42,42,42,42	0
57	MG	RA	3129	1/1	0.94	0.64	45,45,45,45	0
57	MG	YA	3077	1/1	0.94	0.32	32,32,32,32	0
57	MG	QA	1665	1/1	0.94	0.47	82,82,82,82	0
57	MG	RA	3009	1/1	0.94	0.36	68,68,68,68	0
57	MG	YA	3015	1/1	0.94	0.59	29,29,29,29	0
57	MG	RA	3046	1/1	0.94	0.73	35,35,35,35	0
57	MG	YA	3260	1/1	0.94	0.54	67,67,67,67	0
57	MG	RA	3241	1/1	0.94	0.35	46,46,46,46	0
57	MG	YA	3096	1/1	0.94	0.76	53,53,53,53	0
57	MG	RA	3027	1/1	0.94	0.23	29,29,29,29	0
57	MG	RA	3028	1/1	0.94	0.41	39,39,39,39	0
57	MG	QA	1635	1/1	0.94	0.28	58,58,58,58	0
57	MG	YA	3104	1/1	0.94	0.18	39,39,39,39	0
57	MG	RA	3221	1/1	0.94	0.39	50,50,50,50	0
57	MG	YA	3269	1/1	0.94	0.25	69,69,69,69	0
57	MG	YA	3110	1/1	0.94	0.28	45,45,45,45	0
57	MG	YA	3271	1/1	0.94	1.04	84,84,84,84	0
57	MG	YA	3113	1/1	0.94	0.32	50,50,50,50	0
57	MG	RA	3053	1/1	0.94	0.46	33,33,33,33	0
57	MG	XA	1633	1/1	0.94	0.31	47,47,47,47	0
57	MG	YA	3043	1/1	0.94	0.82	27,27,27,27	0
57	MG	YA	3276	1/1	0.94	0.40	37,37,37,37	0
57	MG	YA	3168	1/1	0.94	0.15	69,69,69,69	0
57	MG	RA	3055	1/1	0.94	0.77	34,34,34,34	0
57	MG	RA	3142	1/1	0.94	0.30	38,38,38,38	0
57	MG	YA	3172	1/1	0.94	0.15	62,62,62,62	0
57	MG	YA	3046	1/1	0.94	0.63	38,38,38,38	0
57	MG	RE	301	1/1	0.94	0.29	58,58,58,58	0
57	MG	RA	3084	1/1	0.94	0.35	28,28,28,28	0
57	MG	RA	3205	1/1	0.94	0.12	40,40,40,40	0
57	MG	XA	1641	1/1	0.94	0.38	74,74,74,74	0
57	MG	QA	1621	1/1	0.94	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3056	1/1	0.94	0.24	33,33,33,33	0
57	MG	RA	3019	1/1	0.94	0.34	61,61,61,61	0
57	MG	YA	3064	1/1	0.94	0.22	29,29,29,29	0
57	MG	QA	1619	1/1	0.95	0.26	68,68,68,68	0
57	MG	QA	1650	1/1	0.95	0.46	91,91,91,91	0
57	MG	XA	1665	1/1	0.95	0.52	74,74,74,74	0
57	MG	RA	3192	1/1	0.95	0.29	250,250,250,250	0
57	MG	YA	3222	1/1	0.95	0.12	71,71,71,71	0
57	MG	QA	1661	1/1	0.95	0.09	126,126,126,126	0
57	MG	RA	3134	1/1	0.95	0.33	31,31,31,31	0
57	MG	RA	3135	1/1	0.95	0.55	53,53,53,53	0
57	MG	QA	1668	1/1	0.95	0.09	101,101,101,101	0
57	MG	RA	3105	1/1	0.95	0.23	43,43,43,43	0
57	MG	RA	3071	1/1	0.95	0.22	51,51,51,51	0
57	MG	RA	3237	1/1	0.95	0.42	29,29,29,29	0
57	MG	YA	3232	1/1	0.95	0.15	28,28,28,28	0
57	MG	RA	3003	1/1	0.95	0.47	28,28,28,28	0
57	MG	RA	3169	1/1	0.95	0.20	47,47,47,47	0
57	MG	YA	3085	1/1	0.95	0.44	44,44,44,44	0
57	MG	YA	3087	1/1	0.95	0.44	29,29,29,29	0
57	MG	RA	3141	1/1	0.95	0.37	45,45,45,45	0
57	MG	YA	3091	1/1	0.95	0.21	37,37,37,37	0
57	MG	YA	3241	1/1	0.95	0.25	54,54,54,54	0
57	MG	YA	3093	1/1	0.95	0.49	24,24,24,24	0
57	MG	XY	101	1/1	0.95	0.17	74,74,74,74	0
57	MG	RA	3051	1/1	0.95	0.38	27,27,27,27	0
57	MG	RA	3033	1/1	0.95	0.47	49,49,49,49	0
57	MG	YA	3100	1/1	0.95	0.48	40,40,40,40	0
57	MG	YA	3004	1/1	0.95	0.41	50,50,50,50	0
57	MG	RA	3210	1/1	0.95	0.41	74,74,74,74	0
57	MG	RA	3054	1/1	0.95	0.22	85,85,85,85	0
57	MG	YA	3013	1/1	0.95	0.87	28,28,28,28	0
57	MG	XA	1642	1/1	0.95	0.54	41,41,41,41	0
57	MG	XA	1643	1/1	0.95	0.18	56,56,56,56	0
57	MG	YA	3114	1/1	0.95	0.26	27,27,27,27	0
57	MG	RA	3145	1/1	0.95	0.23	43,43,43,43	0
57	MG	YA	3020	1/1	0.95	0.82	34,34,34,34	0
57	MG	RA	3081	1/1	0.95	0.35	28,28,28,28	0
57	MG	YA	3120	1/1	0.95	0.32	54,54,54,54	0
57	MG	YA	3121	1/1	0.95	0.23	32,32,32,32	0
57	MG	YA	3122	1/1	0.95	0.70	30,30,30,30	0
57	MG	YA	3123	1/1	0.95	0.29	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3117	1/1	0.95	0.29	84,84,84,84	0
57	MG	QA	1645	1/1	0.95	0.12	55,55,55,55	0
57	MG	RA	3122	1/1	0.95	0.89	45,45,45,45	0
57	MG	YA	3192	1/1	0.95	0.19	57,57,57,57	0
57	MG	RA	3015	1/1	0.95	0.50	26,26,26,26	0
57	MG	YA	3040	1/1	0.95	0.54	28,28,28,28	0
57	MG	RA	3124	1/1	0.95	0.17	61,61,61,61	0
57	MG	RA	3126	1/1	0.95	0.22	58,58,58,58	0
57	MG	XA	1654	1/1	0.95	0.45	39,39,39,39	0
57	MG	RA	3154	1/1	0.95	0.43	42,42,42,42	0
57	MG	YA	3136	1/1	0.95	0.24	39,39,39,39	0
57	MG	RA	3086	1/1	0.95	0.77	53,53,53,53	0
57	MG	XA	1603	1/1	0.95	0.42	43,43,43,43	0
57	MG	YA	3205	1/1	0.95	0.30	78,78,78,78	0
57	MG	RA	3057	1/1	0.95	0.46	133,133,133,133	0
57	MG	YA	3207	1/1	0.95	0.24	116,116,116,116	0
57	MG	YA	3208	1/1	0.95	0.19	51,51,51,51	0
57	MG	XA	1605	1/1	0.95	0.65	45,45,45,45	0
57	MG	XA	1606	1/1	0.95	0.54	76,76,76,76	0
57	MG	Y7	101	1/1	0.95	0.24	40,40,40,40	0
57	MG	QA	1663	1/1	0.95	0.17	40,40,40,40	0
57	MG	RA	3021	1/1	0.95	0.29	29,29,29,29	0
59	ZN	QD	301	1/1	0.95	0.23	59,59,59,59	0
59	ZN	QN	101	1/1	0.95	0.12	127,127,127,127	0
57	MG	YA	3060	1/1	0.95	0.42	35,35,35,35	0
57	MG	RB	202	1/1	0.96	0.08	100,100,100,100	0
57	MG	YA	3058	1/1	0.96	0.42	31,31,31,31	0
57	MG	YA	3059	1/1	0.96	0.14	45,45,45,45	0
57	MG	YA	3182	1/1	0.96	0.07	53,53,53,53	0
57	MG	QA	1611	1/1	0.96	0.20	28,28,28,28	0
57	MG	RA	3100	1/1	0.96	0.28	43,43,43,43	0
57	MG	RA	3222	1/1	0.96	0.38	49,49,49,49	0
57	MG	RA	3040	1/1	0.96	0.26	35,35,35,35	0
57	MG	RA	3102	1/1	0.96	0.48	30,30,30,30	0
57	MG	RA	3083	1/1	0.96	0.15	50,50,50,50	0
57	MG	RA	3108	1/1	0.96	0.25	43,43,43,43	0
57	MG	RA	3198	1/1	0.96	0.23	49,49,49,49	0
57	MG	YA	3255	1/1	0.96	0.64	34,34,34,34	0
57	MG	RA	3199	1/1	0.96	0.68	56,56,56,56	0
57	MG	YA	3009	1/1	0.96	0.62	25,25,25,25	0
57	MG	QA	1617	1/1	0.96	0.27	48,48,48,48	0
57	MG	YA	3198	1/1	0.96	0.15	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3085	1/1	0.96	0.32	55,55,55,55	0
57	MG	RA	3202	1/1	0.96	0.67	32,32,32,32	0
57	MG	RA	3070	1/1	0.96	0.34	58,58,58,58	0
57	MG	YA	3018	1/1	0.96	0.53	48,48,48,48	0
57	MG	YA	3086	1/1	0.96	0.52	28,28,28,28	0
57	MG	RA	3087	1/1	0.96	0.49	54,54,54,54	0
57	MG	RA	3137	1/1	0.96	0.33	42,42,42,42	0
57	MG	YA	3089	1/1	0.96	0.48	53,53,53,53	0
57	MG	YA	3022	1/1	0.96	0.38	45,45,45,45	0
57	MG	XA	1616	1/1	0.96	0.27	25,25,25,25	0
57	MG	YA	3209	1/1	0.96	0.38	52,52,52,52	0
57	MG	YA	3027	1/1	0.96	0.20	38,38,38,38	0
57	MG	RA	3049	1/1	0.96	0.43	49,49,49,49	0
57	MG	YA	3031	1/1	0.96	0.73	37,37,37,37	0
57	MG	YA	3032	1/1	0.96	0.29	28,28,28,28	0
57	MG	RA	3029	1/1	0.96	0.27	35,35,35,35	0
57	MG	RA	3062	1/1	0.96	0.81	28,28,28,28	0
57	MG	XA	1624	1/1	0.96	0.58	42,42,42,42	0
57	MG	RA	3093	1/1	0.96	0.53	34,34,34,34	0
57	MG	YA	3107	1/1	0.96	0.49	26,26,26,26	0
57	MG	XA	1627	1/1	0.96	0.25	43,43,43,43	0
57	MG	YA	3042	1/1	0.96	0.42	45,45,45,45	0
57	MG	QA	1659	1/1	0.96	0.40	70,70,70,70	0
57	MG	RA	3163	1/1	0.96	0.28	38,38,38,38	0
57	MG	RA	3187	1/1	0.96	0.33	49,49,49,49	0
57	MG	RA	3095	1/1	0.96	0.43	34,34,34,34	0
57	MG	RA	3096	1/1	0.96	0.27	36,36,36,36	0
57	MG	RA	3016	1/1	0.96	0.47	39,39,39,39	0
57	MG	YA	3052	1/1	0.96	0.56	41,41,41,41	0
57	MG	RA	3146	1/1	0.96	0.17	137,137,137,137	0
57	MG	XA	1636	1/1	0.96	0.28	36,36,36,36	0
57	MG	XA	1637	1/1	0.96	0.19	59,59,59,59	0
57	MG	XA	1611	1/1	0.97	0.28	28,28,28,28	0
57	MG	YA	3073	1/1	0.97	0.36	37,37,37,37	0
57	MG	XA	1613	1/1	0.97	0.19	50,50,50,50	0
57	MG	RA	3017	1/1	0.97	0.32	52,52,52,52	0
57	MG	YA	3146	1/1	0.97	0.25	48,48,48,48	0
57	MG	YA	3017	1/1	0.97	0.30	31,31,31,31	0
57	MG	YA	3220	1/1	0.97	0.55	45,45,45,45	0
57	MG	XA	1615	1/1	0.97	0.42	29,29,29,29	0
57	MG	YA	3078	1/1	0.97	0.47	51,51,51,51	0
57	MG	RA	3018	1/1	0.97	0.55	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3225	1/1	0.97	0.39	67,67,67,67	0
57	MG	YA	3226	1/1	0.97	0.16	74,74,74,74	0
57	MG	YA	3081	1/1	0.97	1.05	31,31,31,31	0
57	MG	XA	1617	1/1	0.97	0.18	40,40,40,40	0
57	MG	YA	3021	1/1	0.97	0.38	24,24,24,24	0
57	MG	RA	3034	1/1	0.97	0.85	42,42,42,42	0
57	MG	YA	3023	1/1	0.97	0.31	39,39,39,39	0
57	MG	RA	3036	1/1	0.97	0.43	29,29,29,29	0
57	MG	RA	3120	1/1	0.97	0.11	49,49,49,49	0
57	MG	YA	3159	1/1	0.97	0.39	34,34,34,34	0
57	MG	YA	3236	1/1	0.97	0.33	52,52,52,52	0
57	MG	YA	3028	1/1	0.97	0.32	25,25,25,25	0
57	MG	XA	1623	1/1	0.97	0.15	42,42,42,42	0
57	MG	YA	3092	1/1	0.97	0.30	25,25,25,25	0
57	MG	RA	3037	1/1	0.97	0.41	32,32,32,32	0
57	MG	RA	3038	1/1	0.97	0.29	29,29,29,29	0
57	MG	YA	3095	1/1	0.97	0.17	49,49,49,49	0
57	MG	YA	3033	1/1	0.97	0.54	28,28,28,28	0
57	MG	YA	3098	1/1	0.97	0.57	29,29,29,29	0
57	MG	YA	3245	1/1	0.97	0.53	25,25,25,25	0
57	MG	YA	3034	1/1	0.97	0.39	27,27,27,27	0
57	MG	YA	3247	1/1	0.97	1.06	29,29,29,29	0
57	MG	XA	1626	1/1	0.97	0.43	59,59,59,59	0
57	MG	YA	3250	1/1	0.97	0.62	52,52,52,52	0
57	MG	YA	3171	1/1	0.97	0.62	33,33,33,33	0
57	MG	RA	3098	1/1	0.97	0.21	65,65,65,65	0
57	MG	YA	3038	1/1	0.97	0.19	50,50,50,50	0
57	MG	RA	3125	1/1	0.97	0.13	48,48,48,48	0
57	MG	RA	3079	1/1	0.97	0.28	48,48,48,48	0
57	MG	YA	3106	1/1	0.97	0.52	42,42,42,42	0
57	MG	QV	101	1/1	0.97	0.14	48,48,48,48	0
57	MG	YA	3108	1/1	0.97	0.37	33,33,33,33	0
57	MG	YA	3109	1/1	0.97	0.18	30,30,30,30	0
57	MG	RA	3020	1/1	0.97	0.75	33,33,33,33	0
57	MG	YA	3111	1/1	0.97	0.24	63,63,63,63	0
57	MG	XA	1632	1/1	0.97	0.45	41,41,41,41	0
57	MG	QA	1642	1/1	0.97	0.36	56,56,56,56	0
57	MG	RA	3103	1/1	0.97	0.41	41,41,41,41	0
57	MG	RP	201	1/1	0.97	0.19	166,166,166,166	0
57	MG	YA	3117	1/1	0.97	0.20	39,39,39,39	0
57	MG	RA	3022	1/1	0.97	0.17	30,30,30,30	0
57	MG	YA	3189	1/1	0.97	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3012	1/1	0.97	0.33	45,45,45,45	0
57	MG	YA	3049	1/1	0.97	0.41	27,27,27,27	0
57	MG	YA	3051	1/1	0.97	0.46	26,26,26,26	0
57	MG	YA	3193	1/1	0.97	0.42	230,230,230,230	0
57	MG	RA	3013	1/1	0.97	0.43	27,27,27,27	0
57	MG	RA	3110	1/1	0.97	0.14	50,50,50,50	0
57	MG	RA	3179	1/1	0.97	0.14	113,113,113,113	0
57	MG	YA	3127	1/1	0.97	0.15	39,39,39,39	0
57	MG	RA	3014	1/1	0.97	0.21	64,64,64,64	0
57	MG	YA	3129	1/1	0.97	0.11	59,59,59,59	0
57	MG	YA	3001	1/1	0.97	0.75	38,38,38,38	0
57	MG	QA	1622	1/1	0.97	0.20	103,103,103,103	0
57	MG	YB	205	1/1	0.97	0.19	231,231,231,231	0
57	MG	RA	3113	1/1	0.97	0.69	34,34,34,34	0
57	MG	RA	3209	1/1	0.97	0.09	57,57,57,57	0
57	MG	YA	3062	1/1	0.97	0.42	51,51,51,51	0
57	MG	YX	101	1/1	0.97	0.21	196,196,196,196	0
57	MG	QA	1604	1/1	0.97	0.30	30,30,30,30	0
57	MG	YA	3007	1/1	0.97	0.23	40,40,40,40	0
57	MG	RA	3235	1/1	0.97	0.28	59,59,59,59	0
57	MG	YA	3067	1/1	0.97	0.29	37,37,37,37	0
57	MG	YA	3069	1/1	0.97	0.43	29,29,29,29	0
57	MG	YA	3011	1/1	0.97	0.42	29,29,29,29	0
57	MG	RA	3236	1/1	0.97	0.85	46,46,46,46	0
59	ZN	Y9	300	1/1	0.97	0.08	101,101,101,101	0
57	MG	XV	101	1/1	0.98	0.28	49,49,49,49	0
57	MG	RA	3030	1/1	0.98	0.27	35,35,35,35	0
57	MG	RA	3119	1/1	0.98	0.43	76,76,76,76	0
57	MG	XA	1644	1/1	0.98	0.32	60,60,60,60	0
57	MG	RA	3080	1/1	0.98	0.81	75,75,75,75	0
57	MG	YA	3187	1/1	0.98	0.41	73,73,73,73	0
57	MG	RA	3121	1/1	0.98	0.27	69,69,69,69	0
57	MG	RA	3024	1/1	0.98	0.31	28,28,28,28	0
57	MG	QA	1630	1/1	0.98	0.14	101,101,101,101	0
57	MG	XA	1618	1/1	0.98	0.32	37,37,37,37	0
57	MG	YA	3248	1/1	0.98	0.32	27,27,27,27	0
57	MG	YA	3090	1/1	0.98	0.17	30,30,30,30	0
57	MG	YA	3005	1/1	0.98	0.22	26,26,26,26	0
57	MG	RA	3042	1/1	0.98	0.29	53,53,53,53	0
57	MG	RA	3052	1/1	0.98	0.27	27,27,27,27	0
57	MG	YA	3253	1/1	0.98	0.90	55,55,55,55	0
57	MG	QA	1606	1/1	0.98	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3197	1/1	0.98	0.12	42,42,42,42	0
57	MG	YA	3010	1/1	0.98	0.48	33,33,33,33	0
57	MG	YA	3050	1/1	0.98	0.35	25,25,25,25	0
57	MG	YA	3097	1/1	0.98	0.16	29,29,29,29	0
57	MG	XA	1622	1/1	0.98	0.12	49,49,49,49	0
57	MG	RA	3104	1/1	0.98	0.44	42,42,42,42	0
57	MG	RA	3035	1/1	0.98	0.53	43,43,43,43	0
57	MG	YA	3014	1/1	0.98	0.39	29,29,29,29	0
57	MG	RA	3106	1/1	0.98	0.21	32,32,32,32	0
57	MG	YA	3103	1/1	0.98	0.59	31,31,31,31	0
57	MG	YA	3154	1/1	0.98	0.20	40,40,40,40	0
57	MG	RA	3107	1/1	0.98	0.19	45,45,45,45	0
57	MG	YA	3057	1/1	0.98	0.79	33,33,33,33	0
57	MG	QA	1636	1/1	0.98	0.13	44,44,44,44	0
57	MG	RP	203	1/1	0.98	0.18	381,381,381,381	0
57	MG	QA	1610	1/1	0.98	0.25	34,34,34,34	0
57	MG	YA	3061	1/1	0.98	0.12	26,26,26,26	0
57	MG	QA	1608	1/1	0.98	0.11	36,36,36,36	0
57	MG	YA	3215	1/1	0.98	0.37	61,61,61,61	0
57	MG	YA	3162	1/1	0.98	0.14	35,35,35,35	0
57	MG	RA	3090	1/1	0.98	0.46	40,40,40,40	0
57	MG	YA	3112	1/1	0.98	0.27	47,47,47,47	0
57	MG	RA	3074	1/1	0.98	0.18	51,51,51,51	0
57	MG	XA	1602	1/1	0.98	0.27	36,36,36,36	0
57	MG	YA	3221	1/1	0.98	0.37	40,40,40,40	0
57	MG	YA	3066	1/1	0.98	0.73	42,42,42,42	0
57	MG	RA	3207	1/1	0.98	0.28	156,156,156,156	0
57	MG	YA	3068	1/1	0.98	0.46	42,42,42,42	0
57	MG	YA	3026	1/1	0.98	0.98	30,30,30,30	0
57	MG	YA	3119	1/1	0.98	0.32	52,52,52,52	0
57	MG	RA	3092	1/1	0.98	0.46	71,71,71,71	0
57	MG	YP	201	1/1	0.98	0.49	380,380,380,380	0
57	MG	RA	3183	1/1	0.98	0.07	67,67,67,67	0
57	MG	YA	3029	1/1	0.98	0.76	39,39,39,39	0
57	MG	RA	3058	1/1	0.98	0.29	49,49,49,49	0
57	MG	RA	3059	1/1	0.98	0.34	30,30,30,30	0
57	MG	RA	3077	1/1	0.98	0.23	52,52,52,52	0
57	MG	RA	3060	1/1	0.98	0.26	44,44,44,44	0
57	MG	XA	1610	1/1	0.98	0.29	32,32,32,32	0
57	MG	YA	3035	1/1	0.98	0.51	42,42,42,42	0
59	ZN	XN	101	1/1	0.98	0.16	76,76,76,76	0
57	MG	YA	3079	1/1	0.98	0.26	26,26,26,26	0

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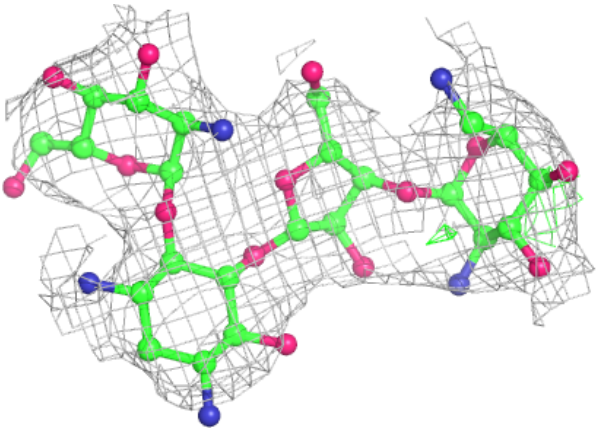
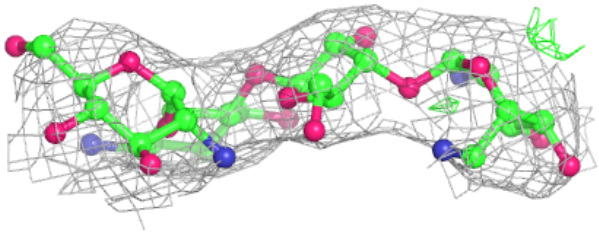
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3268	1/1	0.99	0.29	66,66,66,66	0
57	MG	RA	3065	1/1	0.99	0.41	29,29,29,29	0
57	MG	RA	3023	1/1	0.99	0.17	32,32,32,32	0
57	MG	RA	3204	1/1	0.99	0.20	167,167,167,167	0
57	MG	XA	1612	1/1	0.99	0.18	37,37,37,37	0
57	MG	YA	3126	1/1	0.99	0.40	46,46,46,46	0
57	MG	RA	3072	1/1	0.99	0.26	54,54,54,54	0
57	MG	XA	1646	1/1	0.99	0.14	49,49,49,49	0
57	MG	YA	3025	1/1	0.99	0.42	31,31,31,31	0
57	MG	YA	3234	1/1	0.99	0.10	147,147,147,147	0
57	MG	RA	3032	1/1	0.99	0.49	29,29,29,29	0
57	MG	QA	1648	1/1	0.99	0.07	93,93,93,93	0
57	MG	YA	3083	1/1	0.99	0.54	50,50,50,50	0
59	ZN	XD	301	1/1	0.99	0.31	52,52,52,52	0
57	MG	RA	3064	1/1	0.99	0.27	48,48,48,48	0
57	MG	YA	3008	1/1	0.99	0.33	48,48,48,48	0

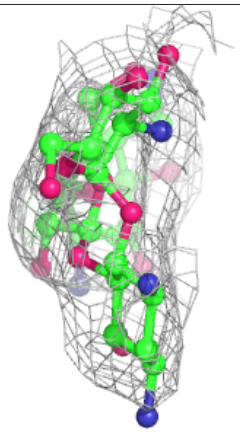
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR QA 1667:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

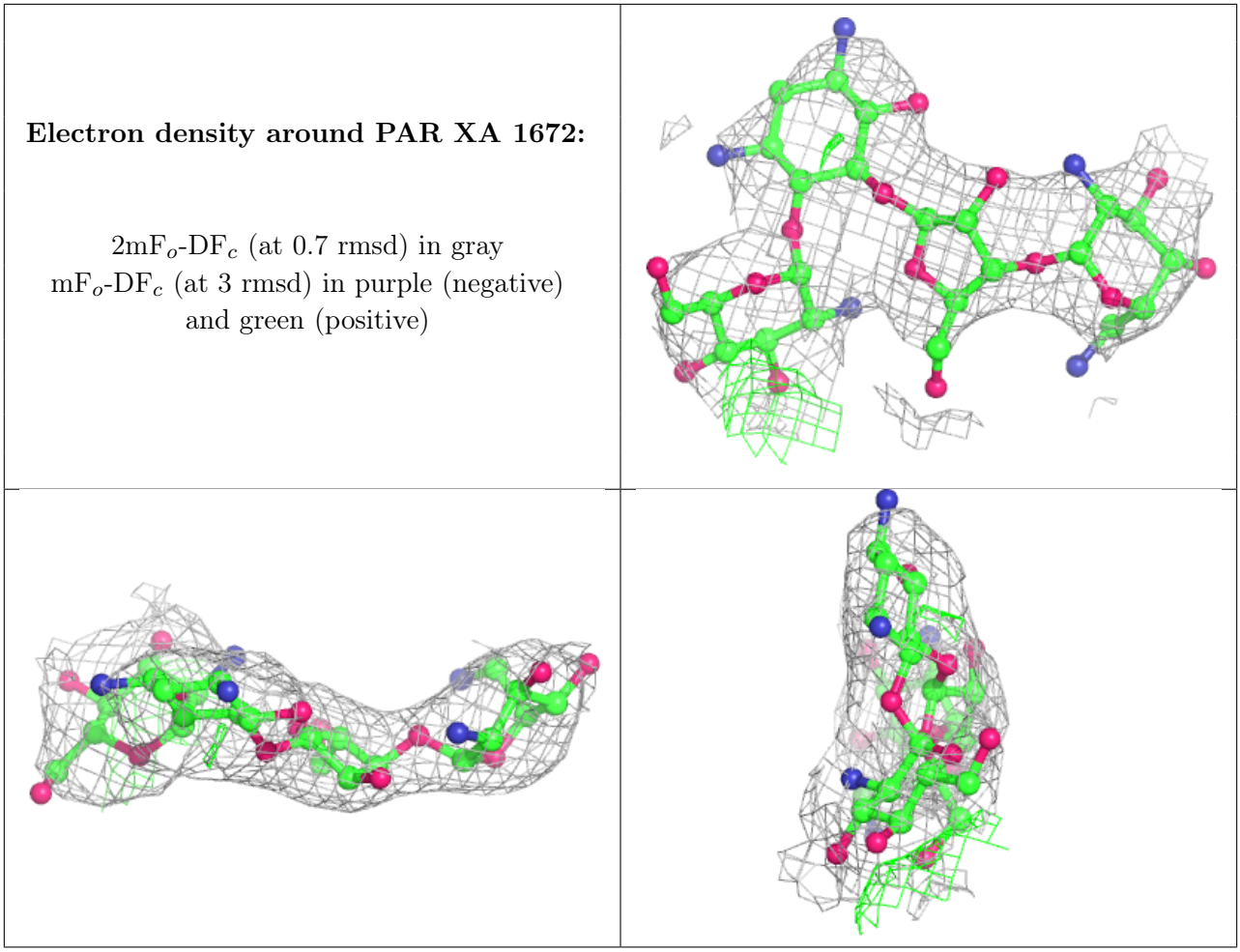






Electron density around PAR XA 1672:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.