



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:03 AM UTC

PDB ID : 6OPE / pdb_00006ope
Title : Crystal structure of tRNA^{Ala}(GGC) U32-A38 bound to near-cognate 70S A site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-24
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

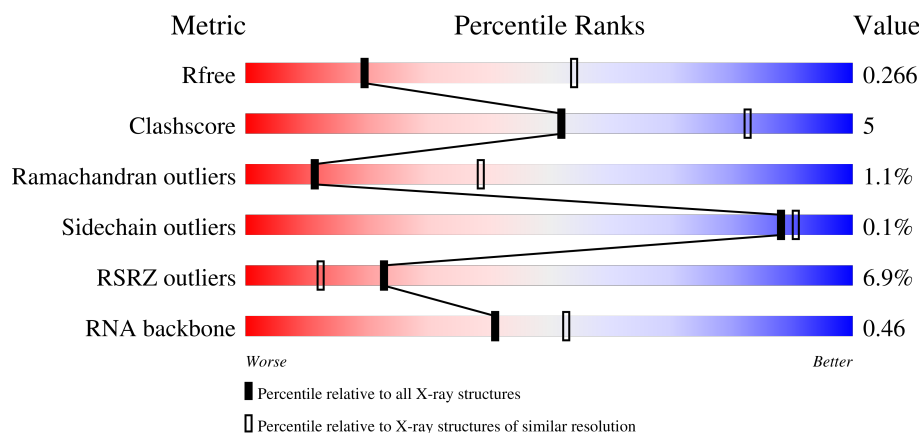
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	2% 66% 28% . .
1	XA	1522	% 68% 27% . .
2	QB	256	8% 71% 20% . 7%
2	XB	256	4% 72% 20% . 7%

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	QY	76	
24	XY	76	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	

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Mol	Chain	Length	Quality of chain
28	R3	60	
28	Y3	60	
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	122	
36	YB	122	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	
40	RG	182	

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Mol	Chain	Length	Quality of chain
40	YG	182	
41	RH	180	
41	YH	180	
42	RI	148	
42	YI	148	
43	RN	140	
43	YN	140	
44	RO	122	
44	YO	122	
45	RP	150	
45	YP	150	
46	RQ	141	
46	YQ	141	
47	RR	118	
47	YR	118	
48	RS	112	
48	YS	112	
49	RT	146	
49	YT	146	
50	RU	118	
50	YU	118	
51	RV	101	
51	YV	101	
52	RW	113	
52	YW	113	

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Mol	Chain	Length	Quality of chain
53	RX	96	
53	YX	96	
54	RY	110	
54	YY	110	
55	RZ	206	
55	YZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1601	-	-	-	X
56	MG	QA	1612	-	-	-	X
56	MG	QA	1618	-	-	-	X
56	MG	QA	1625	-	-	-	X
56	MG	QA	1628	-	-	-	X
56	MG	QA	1632	-	-	-	X
56	MG	QA	1638	-	-	-	X
56	MG	QA	1643	-	-	-	X
56	MG	QA	1658	-	-	-	X
56	MG	QX	102	-	-	-	X
56	MG	R9	101	-	-	-	X
56	MG	RA	3003	-	-	-	X
56	MG	RA	3011	-	-	-	X
56	MG	RA	3012	-	-	-	X
56	MG	RA	3013	-	-	-	X
56	MG	RA	3035	-	-	-	X
56	MG	RA	3051	-	-	-	X
56	MG	RA	3057	-	-	-	X
56	MG	RA	3067	-	-	-	X
56	MG	RA	3073	-	-	-	X
56	MG	RA	3112	-	-	-	X
56	MG	RA	3118	-	-	-	X
56	MG	RA	3120	-	-	-	X
56	MG	RA	3122	-	-	-	X
56	MG	RA	3126	-	-	-	X
56	MG	RA	3139	-	-	-	X
56	MG	RA	3142	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3146	-	-	-	X
56	MG	RA	3148	-	-	-	X
56	MG	RA	3149	-	-	-	X
56	MG	RA	3151	-	-	-	X
56	MG	RA	3159	-	-	-	X
56	MG	RA	3164	-	-	-	X
56	MG	RA	3166	-	-	-	X
56	MG	RA	3170	-	-	-	X
56	MG	RA	3173	-	-	-	X
56	MG	RA	3178	-	-	-	X
56	MG	RA	3180	-	-	-	X
56	MG	RA	3199	-	-	-	X
56	MG	RA	3202	-	-	-	X
56	MG	RA	3203	-	-	-	X
56	MG	RA	3206	-	-	-	X
56	MG	RA	3215	-	-	-	X
56	MG	RA	3217	-	-	-	X
56	MG	RA	3218	-	-	-	X
56	MG	RA	3223	-	-	-	X
56	MG	RA	3233	-	-	-	X
56	MG	RA	3236	-	-	-	X
56	MG	RA	3244	-	-	-	X
56	MG	RA	3249	-	-	-	X
56	MG	RA	3250	-	-	-	X
56	MG	RA	3252	-	-	-	X
56	MG	RA	3256	-	-	-	X
56	MG	RA	3262	-	-	-	X
56	MG	RA	3266	-	-	-	X
56	MG	RA	3277	-	-	-	X
56	MG	RA	3279	-	-	-	X
56	MG	XA	1607	-	-	-	X
56	MG	XA	1614	-	-	-	X
56	MG	XA	1619	-	-	-	X
56	MG	XA	1632	-	-	-	X
56	MG	XA	1646	-	-	-	X
56	MG	XA	1648	-	-	-	X
56	MG	XA	1654	-	-	-	X
56	MG	XA	1655	-	-	-	X
56	MG	XA	1660	-	-	-	X
56	MG	XA	1662	-	-	-	X
56	MG	XA	1667	-	-	-	X
56	MG	XA	1668	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XA	1671	-	-	-	X
56	MG	XA	1687	-	-	-	X
56	MG	XA	1691	-	-	-	X
56	MG	XA	1692	-	-	-	X
56	MG	XX	101	-	-	-	X
56	MG	YA	3035	-	-	-	X
56	MG	YA	3106	-	-	-	X
56	MG	YA	3111	-	-	-	X
56	MG	YA	3154	-	-	-	X
56	MG	YA	3155	-	-	-	X
56	MG	YA	3162	-	-	-	X
56	MG	YA	3163	-	-	-	X
56	MG	YA	3168	-	-	-	X
56	MG	YA	3172	-	-	-	X
56	MG	YA	3181	-	-	-	X
56	MG	YA	3182	-	-	-	X
56	MG	YA	3191	-	-	-	X
56	MG	YA	3193	-	-	-	X
56	MG	YA	3197	-	-	-	X
56	MG	YA	3202	-	-	-	X
56	MG	YA	3205	-	-	-	X
56	MG	YA	3206	-	-	-	X
56	MG	YA	3220	-	-	-	X
56	MG	YA	3233	-	-	-	X
56	MG	YA	3239	-	-	-	X
56	MG	YA	3246	-	-	-	X
56	MG	YA	3286	-	-	-	X
56	MG	YA	3288	-	-	-	X
56	MG	YA	3294	-	-	-	X
56	MG	YA	3313	-	-	-	X
56	MG	YA	3321	-	-	-	X
56	MG	YA	3323	-	-	-	X
56	MG	YA	3333	-	-	-	X
56	MG	YA	3337	-	-	-	X
56	MG	YA	3338	-	-	-	X
56	MG	YA	3340	-	-	-	X
56	MG	YA	3346	-	-	-	X
56	MG	YB	201	-	-	-	X
56	MG	YP	201	-	-	-	X
56	MG	YQ	203	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 294981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	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
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	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	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			396	177	82	119	18			
23	XX	18	Total	C	N	O	P	0	0	0
			396	177	82	119	18			

- Molecule 24 is a RNA chain called A-site tRNA^{Ala}(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	75	Total	C	N	O	P	0	0	0
			1602	714	288	525	75			
24	XY	75	Total	C	N	O	P	0	0	0
			1602	714	288	525	75			

- Molecule 25 is a protein called 50S ribosomal protein L27.

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

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	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
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

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

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

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

- Molecule 36 is a RNA chain called 5S rRNA.

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

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

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

- Molecule 42 is a protein called 50S ribosomal protein L9.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

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

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

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

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

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

- Molecule 55 is a protein called 50S ribosomal protein L25.

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	73	Total	Mg	0	0
			73	73		
56	QF	1	Total	Mg	0	0
			1	1		
56	QM	1	Total	Mg	0	0
			1	1		
56	QV	1	Total	Mg	0	0
			1	1		
56	QX	2	Total	Mg	0	0
			2	2		
56	R0	1	Total	Mg	0	0
			1	1		
56	R5	1	Total	Mg	0	0
			1	1		
56	R8	1	Total	Mg	0	0
			1	1		
56	R9	1	Total	Mg	0	0
			1	1		

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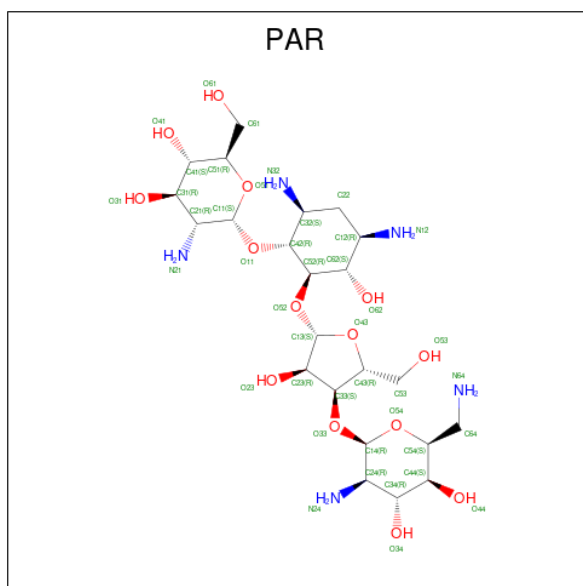
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RA	281	Total 281	Mg 281	0	0
56	RB	4	Total 4	Mg 4	0	0
56	RD	1	Total 1	Mg 1	0	0
56	RE	4	Total 4	Mg 4	0	0
56	RF	1	Total 1	Mg 1	0	0
56	RP	3	Total 3	Mg 3	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	XA	91	Total 91	Mg 91	0	0
56	XF	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	XV	2	Total 2	Mg 2	0	0
56	XX	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	Y2	1	Total 1	Mg 1	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	Y6	2	Total 2	Mg 2	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	Y9	1	Total 1	Mg 1	0	0
56	YA	347	Total 347	Mg 347	0	0

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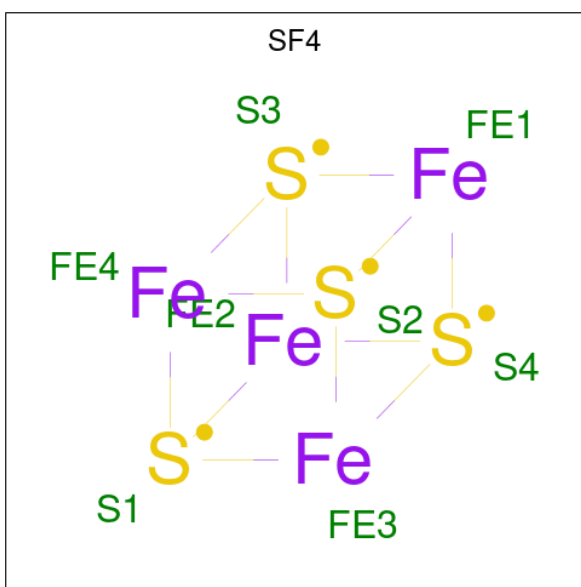
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YB	6	Total	Mg	0	0
			6	6		
56	YE	3	Total	Mg	0	0
			3	3		
56	YN	1	Total	Mg	0	0
			1	1		
56	YP	3	Total	Mg	0	0
			3	3		
56	YQ	3	Total	Mg	0	0
			3	3		
56	YR	1	Total	Mg	0	0
			1	1		
56	YX	1	Total	Mg	0	0
			1	1		

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

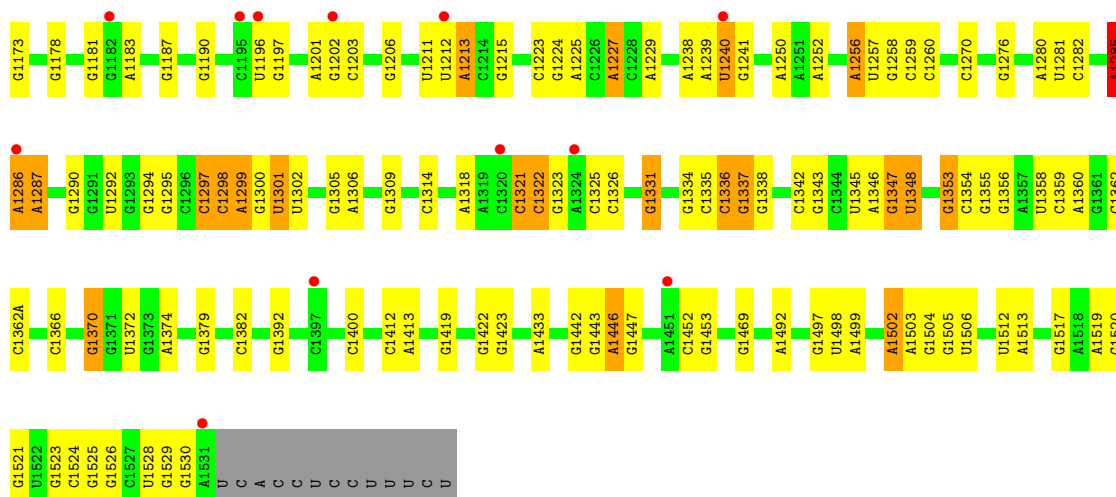
- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



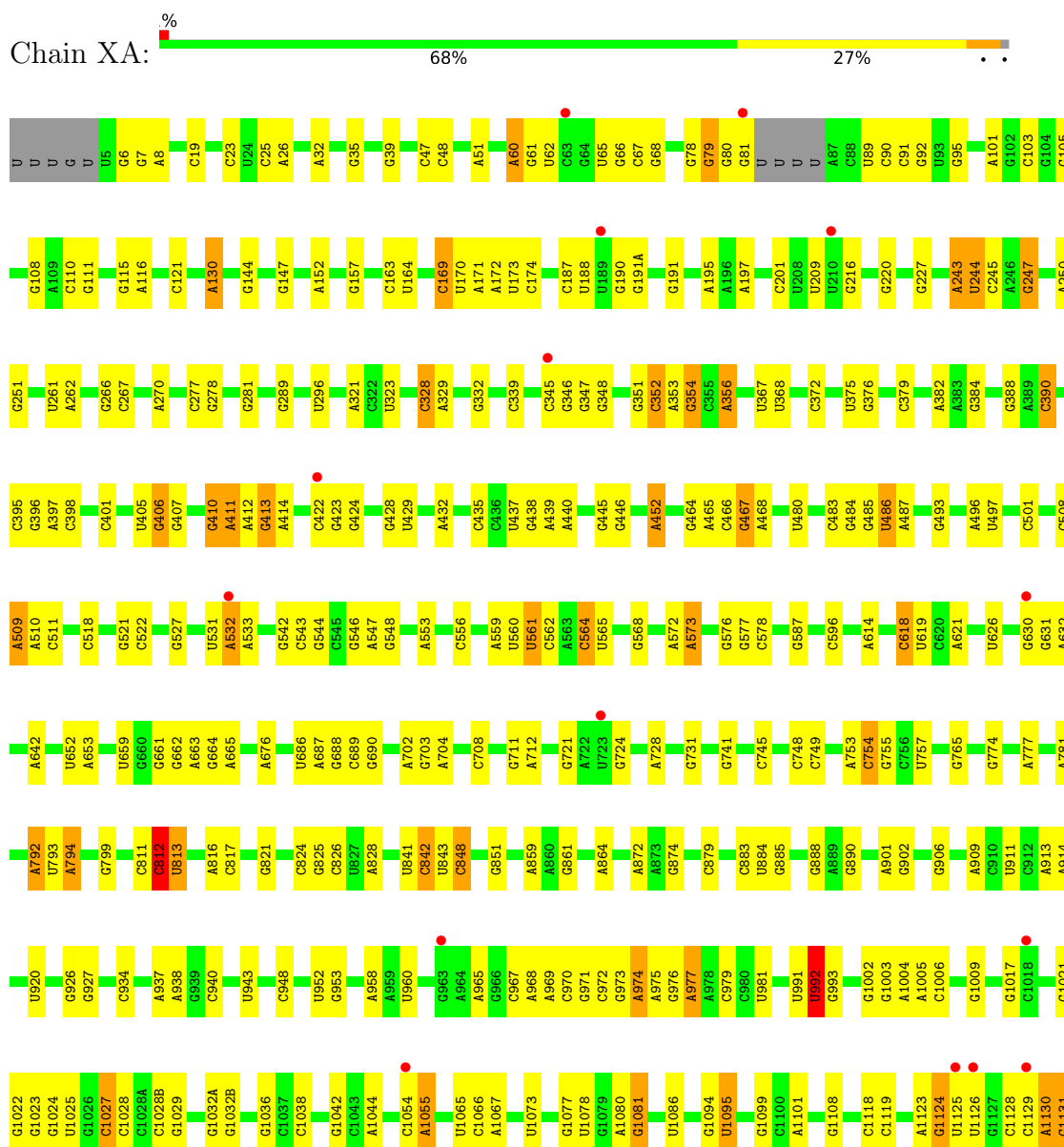
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

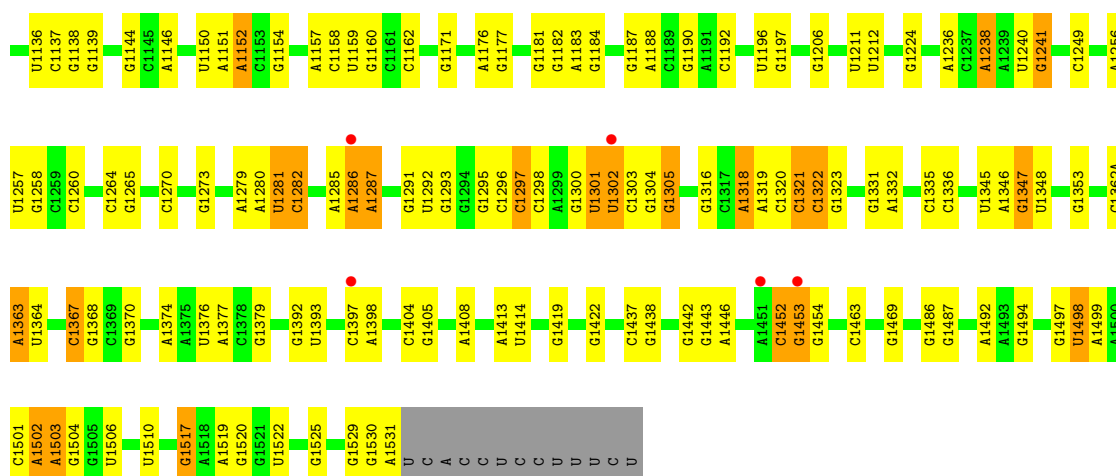
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

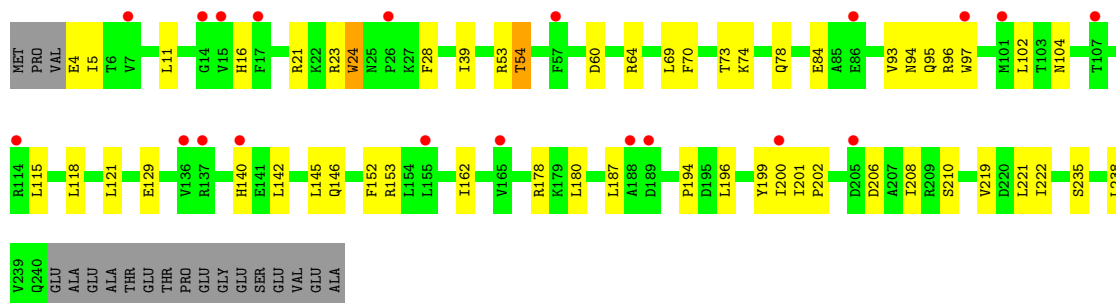
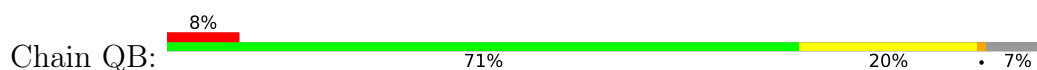


• Molecule 1: 16S rRNA

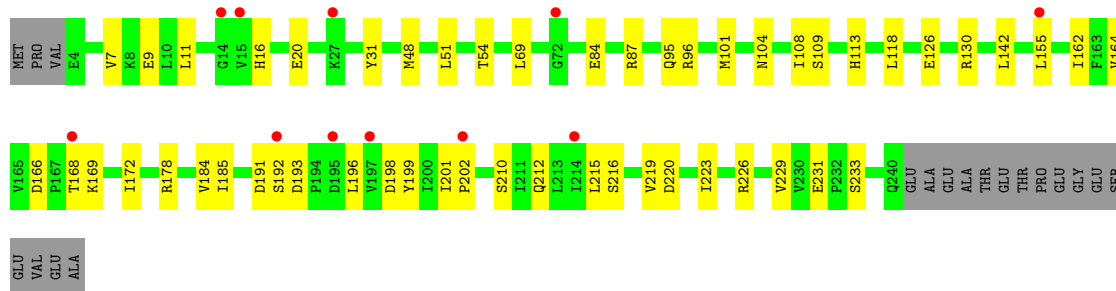
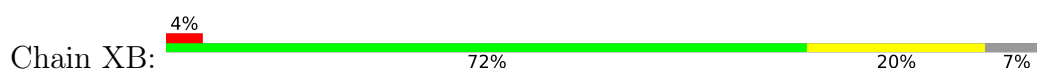




• Molecule 2: 30S ribosomal protein S2

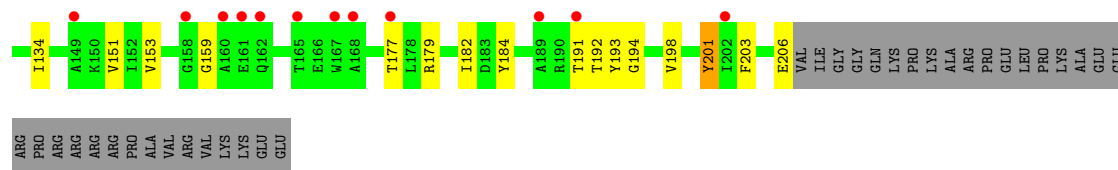


• Molecule 2: 30S ribosomal protein S2

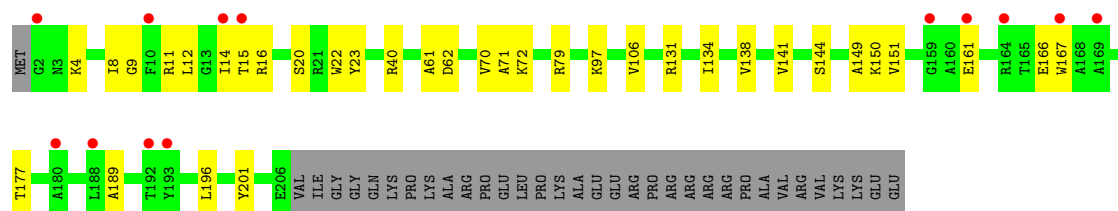
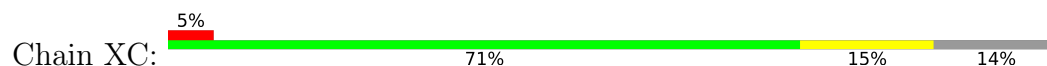


• Molecule 3: 30S ribosomal protein S3

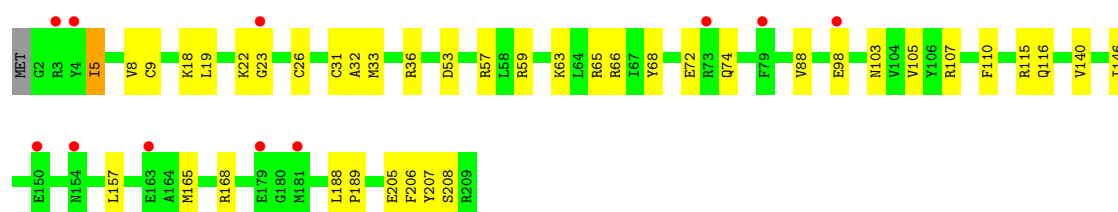
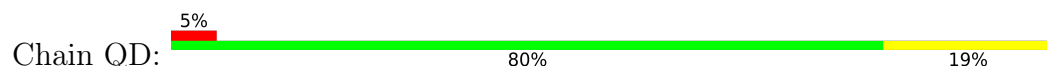




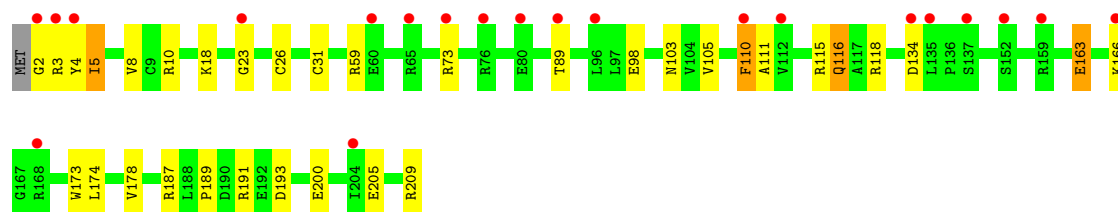
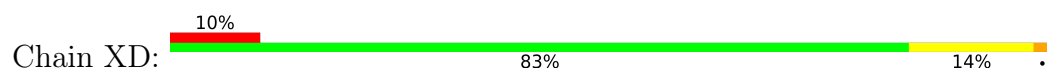
• Molecule 3: 30S ribosomal protein S3



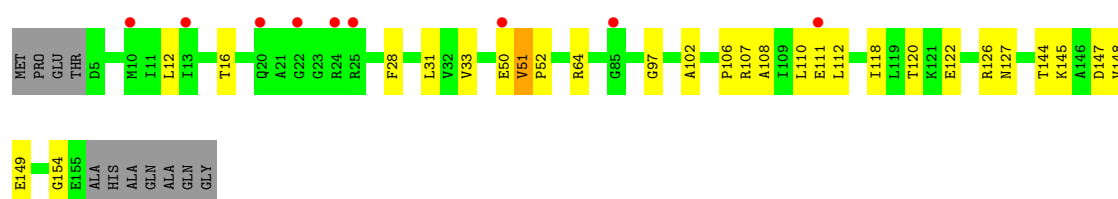
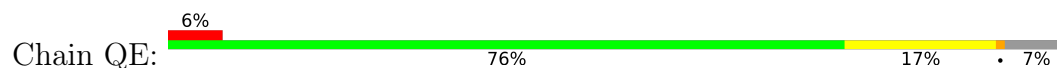
• Molecule 4: 30S ribosomal protein S4



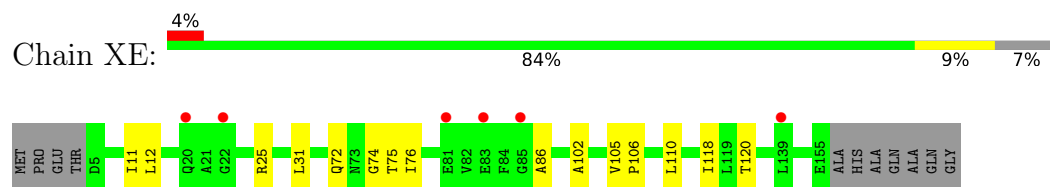
• Molecule 4: 30S ribosomal protein S4



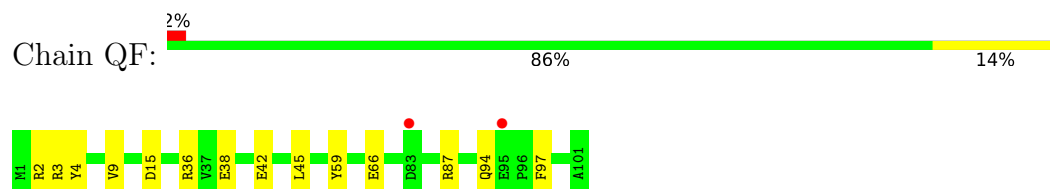
• Molecule 5: 30S ribosomal protein S5



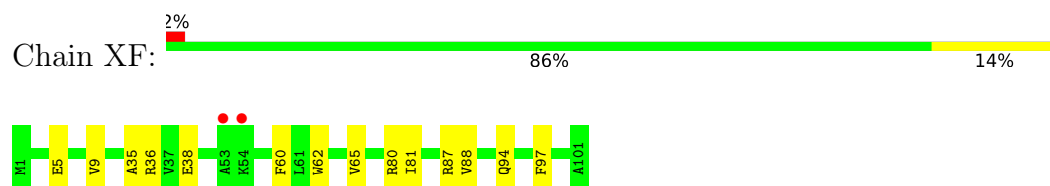
- Molecule 5: 30S ribosomal protein S5



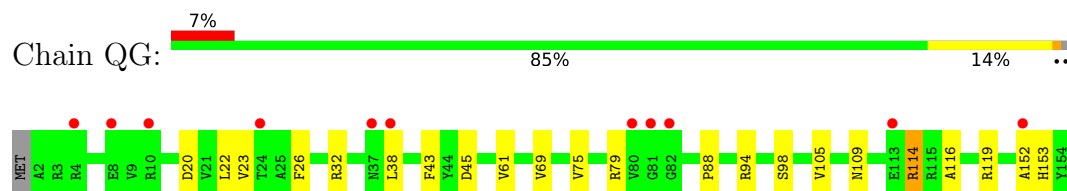
- Molecule 6: 30S ribosomal protein S6



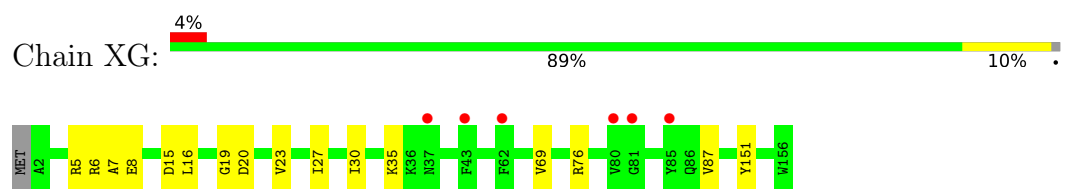
- Molecule 6: 30S ribosomal protein S6



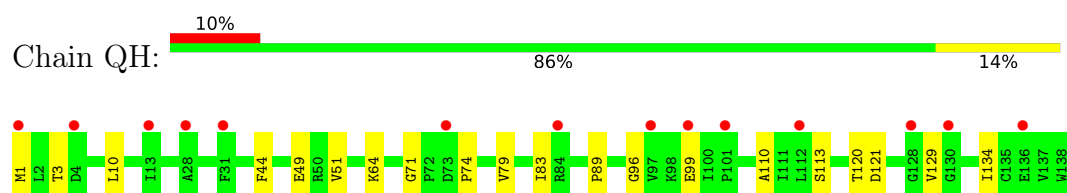
- Molecule 7: 30S ribosomal protein S7



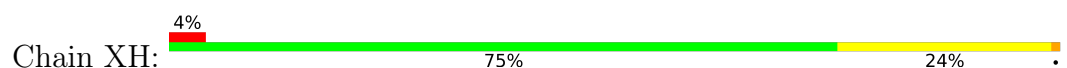
- Molecule 7: 30S ribosomal protein S7

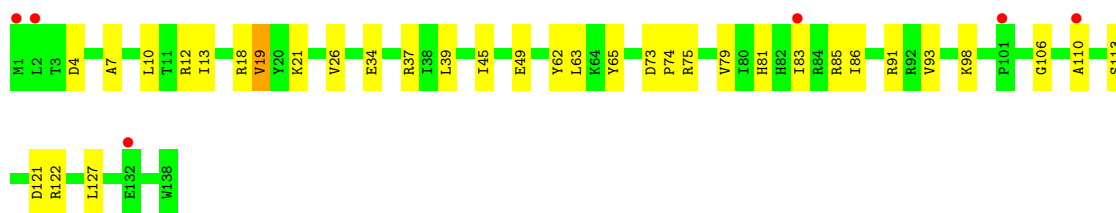


- Molecule 8: 30S ribosomal protein S8

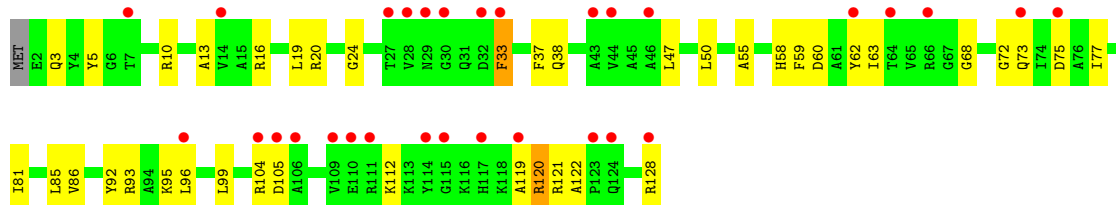


- Molecule 8: 30S ribosomal protein S8

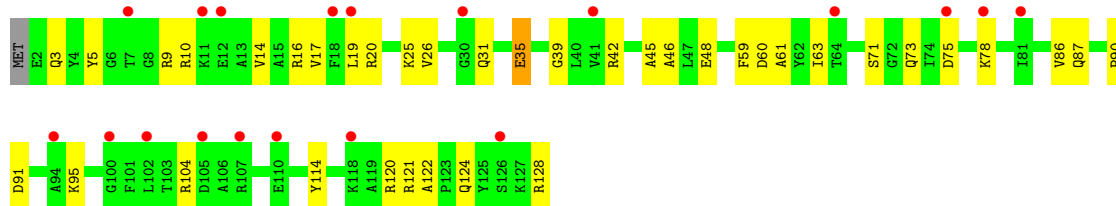




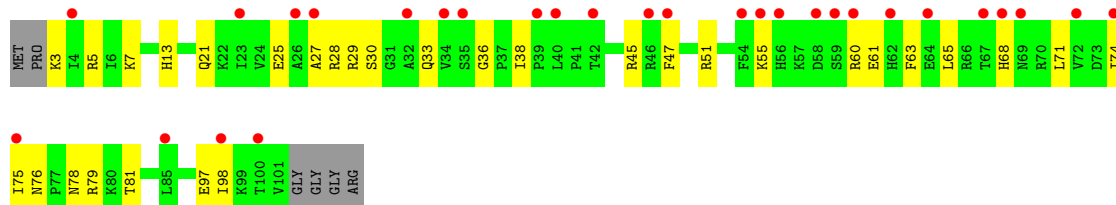
• Molecule 9: 30S ribosomal protein S9



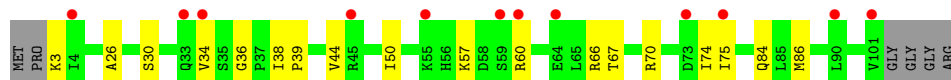
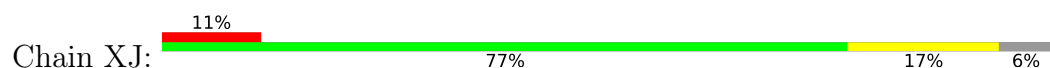
• Molecule 9: 30S ribosomal protein S9



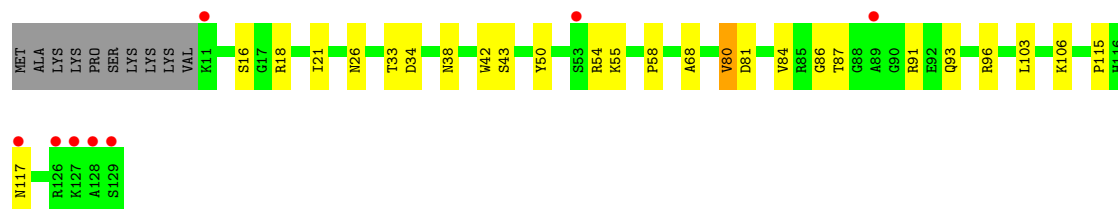
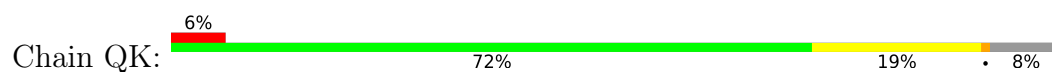
• Molecule 10: 30S ribosomal protein S10



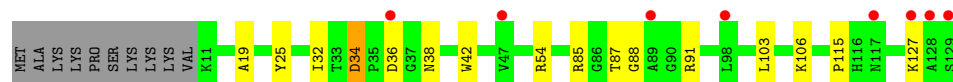
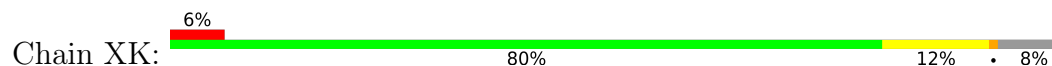
• Molecule 10: 30S ribosomal protein S10



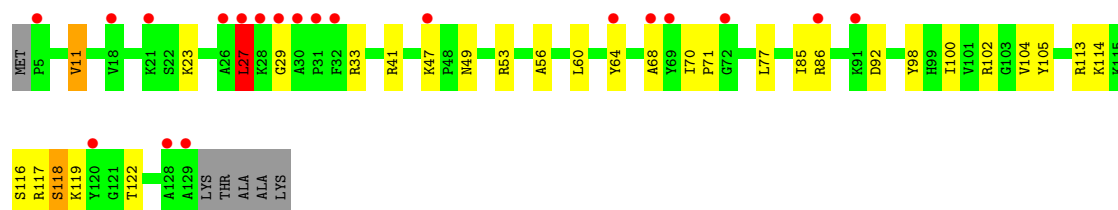
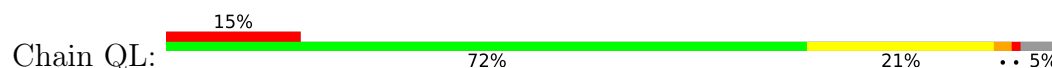
• Molecule 11: 30S ribosomal protein S11



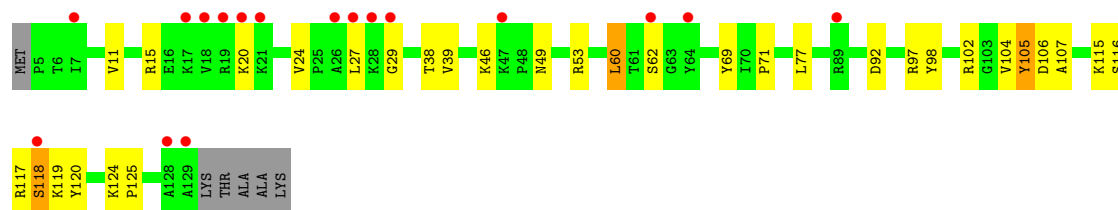
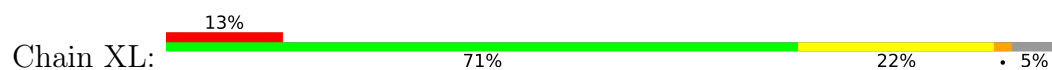
- Molecule 11: 30S ribosomal protein S11



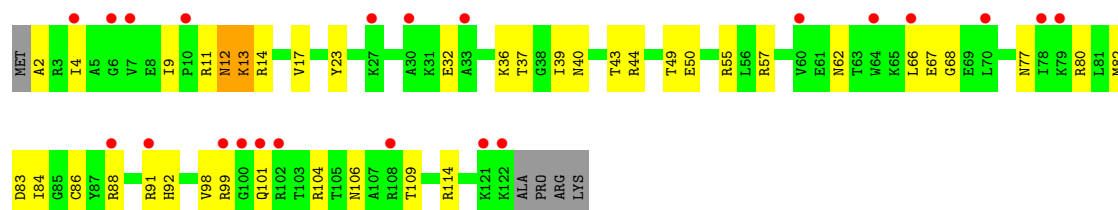
- Molecule 12: 30S ribosomal protein S12



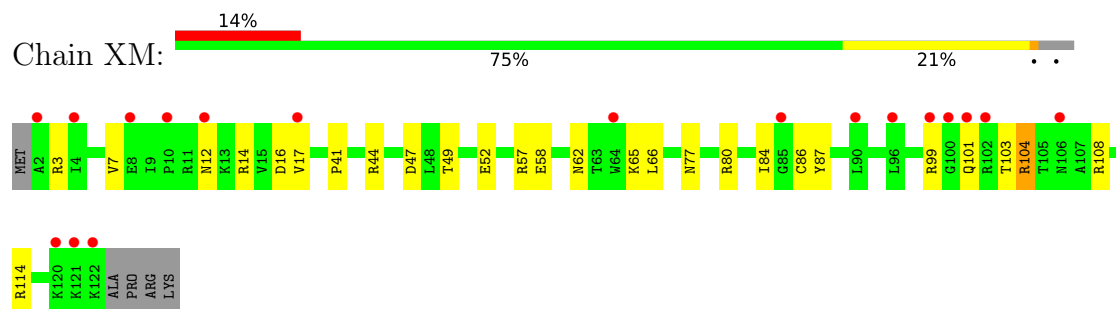
- Molecule 12: 30S ribosomal protein S12



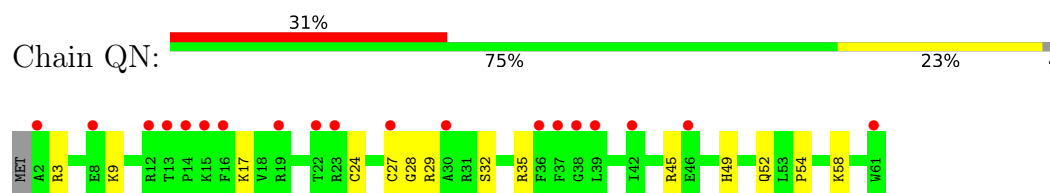
- Molecule 13: 30S ribosomal protein S13



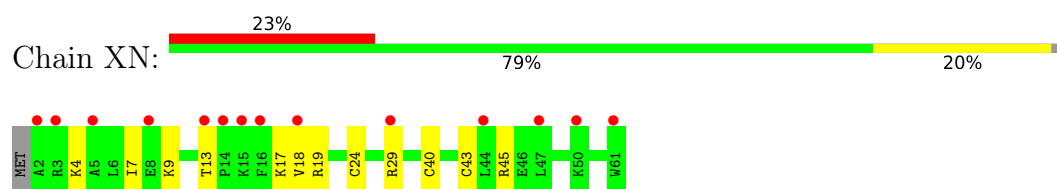
- Molecule 13: 30S ribosomal protein S13



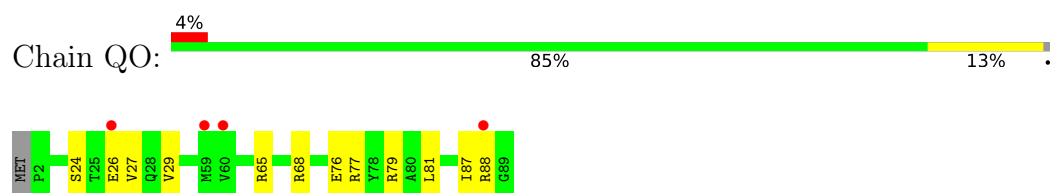
- Molecule 14: 30S ribosomal protein S14 type Z



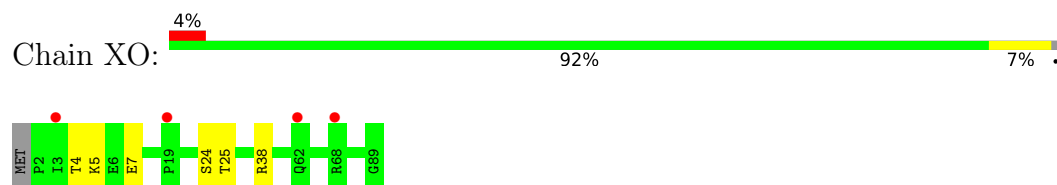
- Molecule 14: 30S ribosomal protein S14 type Z



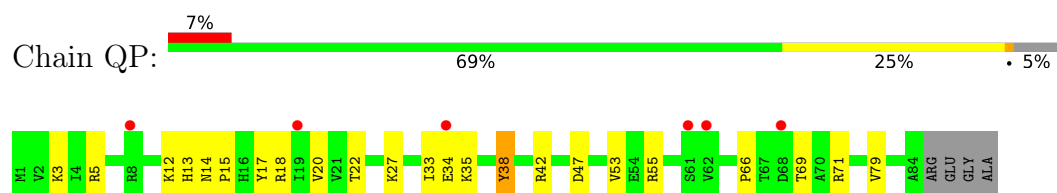
- Molecule 15: 30S ribosomal protein S15



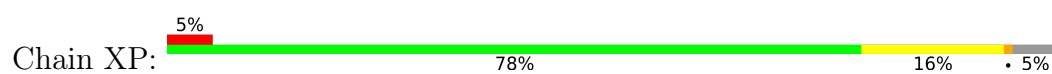
- Molecule 15: 30S ribosomal protein S15



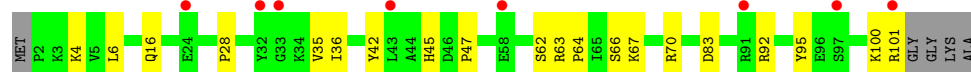
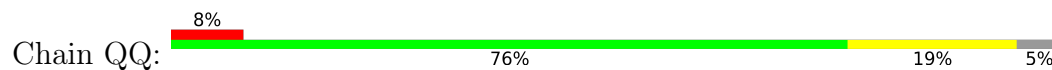
- Molecule 16: 30S ribosomal protein S16



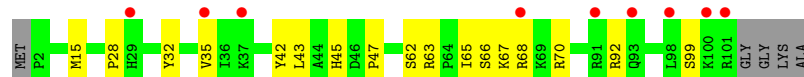
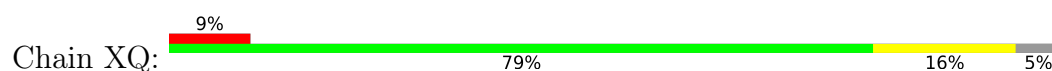
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



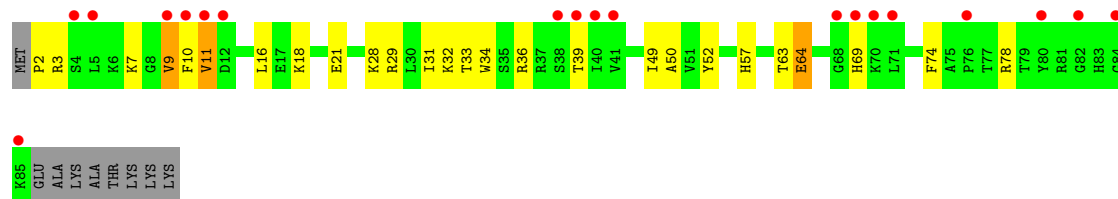
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

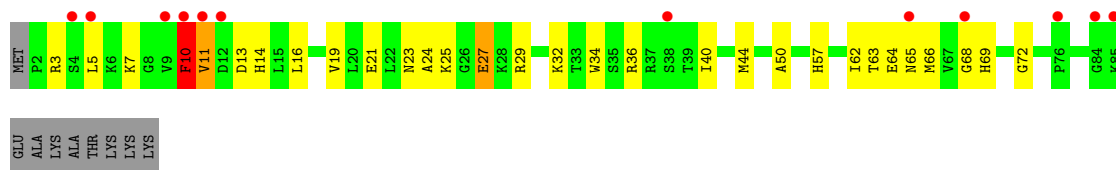


- Molecule 19: 30S ribosomal protein S19

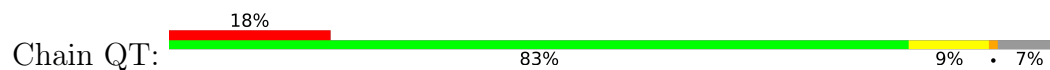


- Molecule 19: 30S ribosomal protein S19

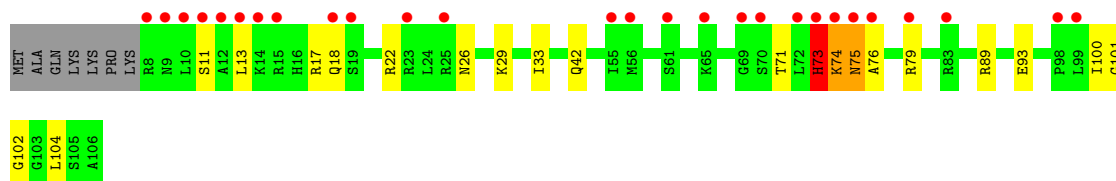
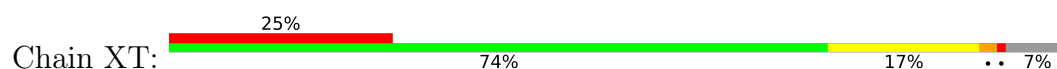




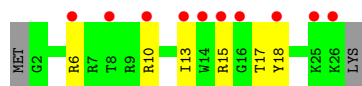
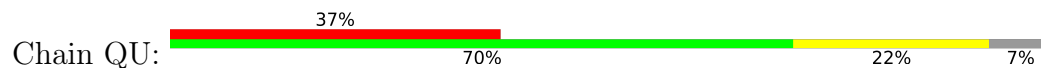
- Molecule 20: 30S ribosomal protein S20



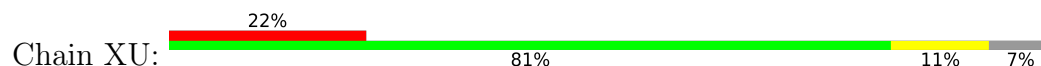
- Molecule 20: 30S ribosomal protein S20



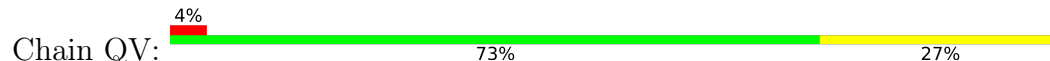
- Molecule 21: 30S ribosomal protein Thx



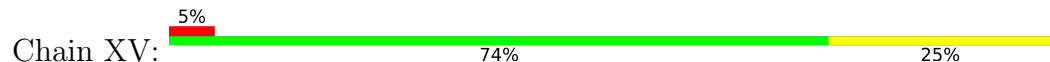
- Molecule 21: 30S ribosomal protein Thx

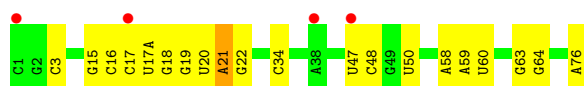


- Molecule 22: P-site tRNAfMet

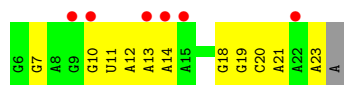


- Molecule 22: P-site tRNAfMet

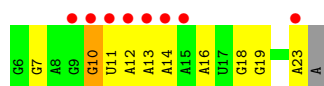




- Molecule 23: mRNA



- Molecule 23: mRNA



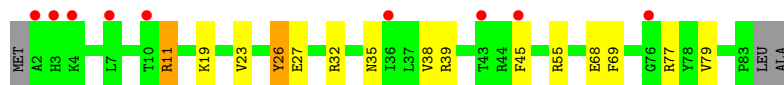
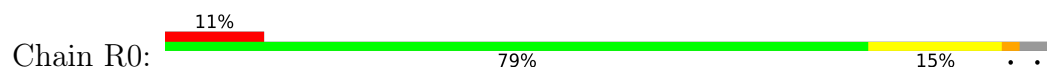
- Molecule 24: A-site tRNAAla(GGC) U32-A38



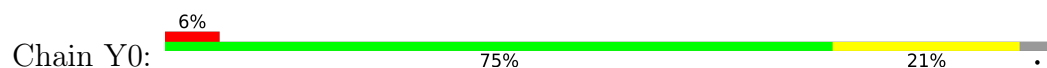
- Molecule 24: A-site tRNAAla(GGC) U32-A38



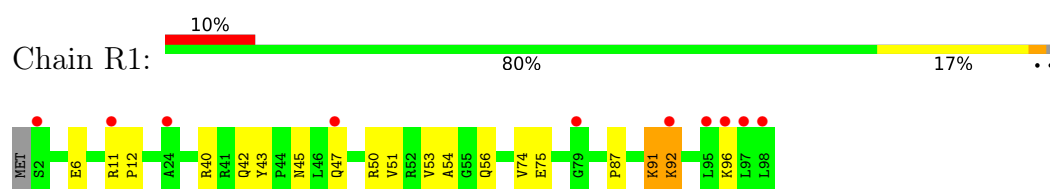
- Molecule 25: 50S ribosomal protein L27



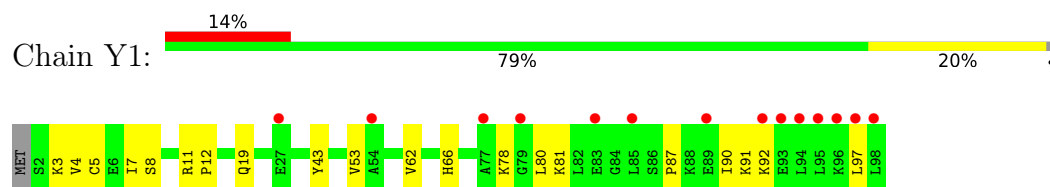
- Molecule 25: 50S ribosomal protein L27



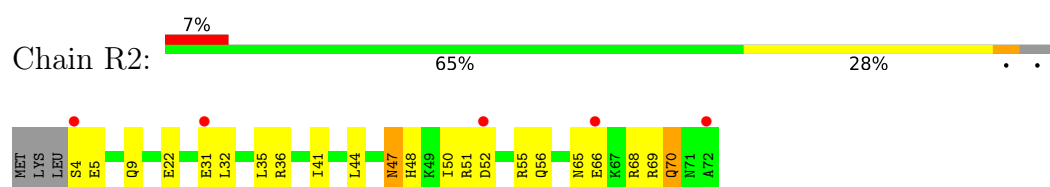
- Molecule 26: 50S ribosomal protein L28



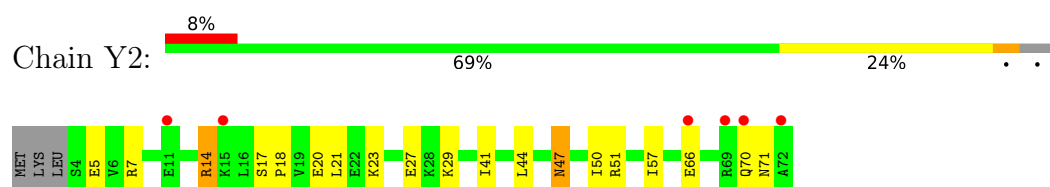
- Molecule 26: 50S ribosomal protein L28



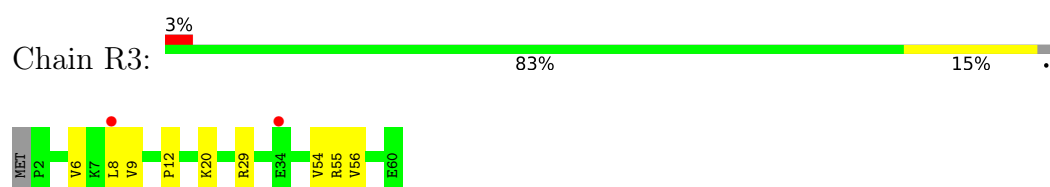
- Molecule 27: 50S ribosomal protein L29



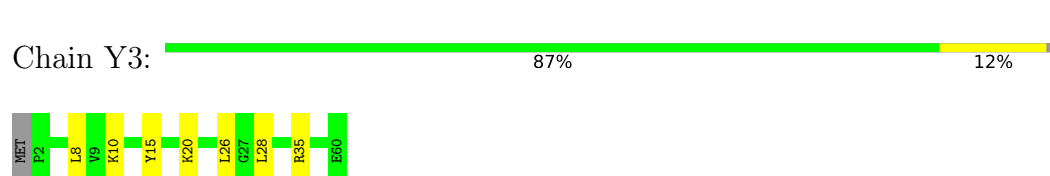
- Molecule 27: 50S ribosomal protein L29



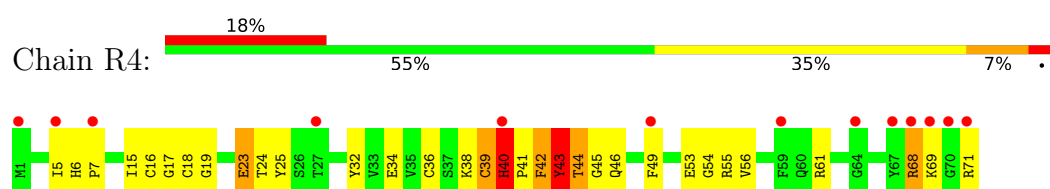
- Molecule 28: 50S ribosomal protein L30



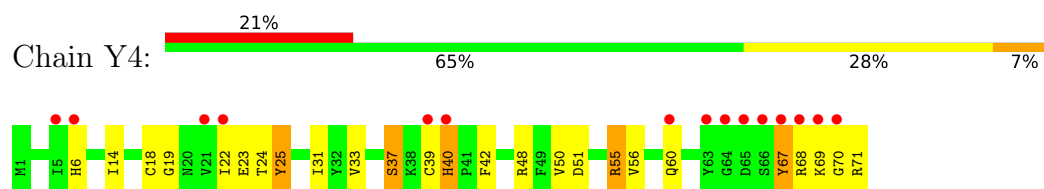
- Molecule 28: 50S ribosomal protein L30



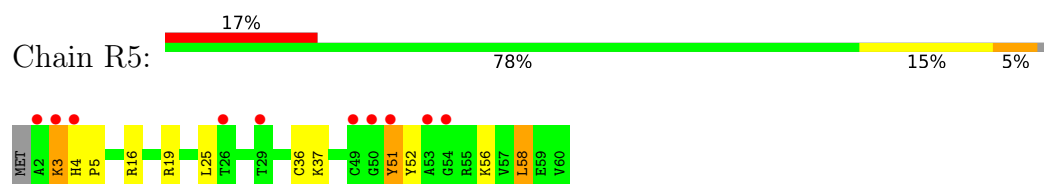
- Molecule 29: 50S ribosomal protein L31



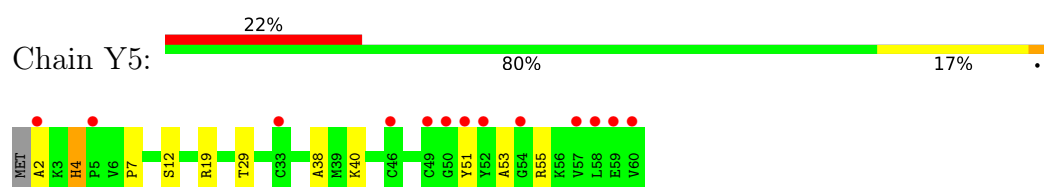
• Molecule 29: 50S ribosomal protein L31



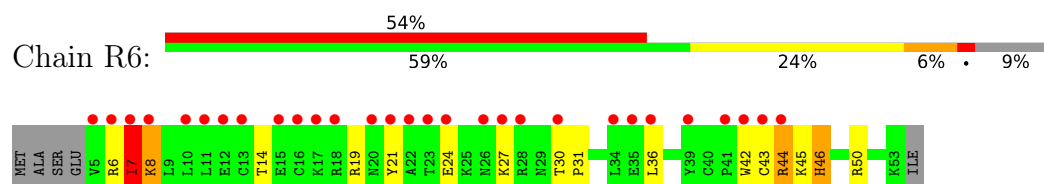
• Molecule 30: 50S ribosomal protein L32



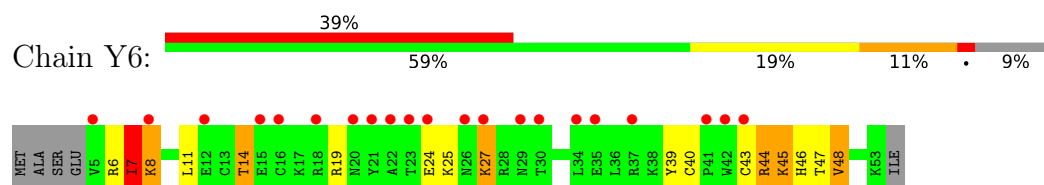
• Molecule 30: 50S ribosomal protein L32



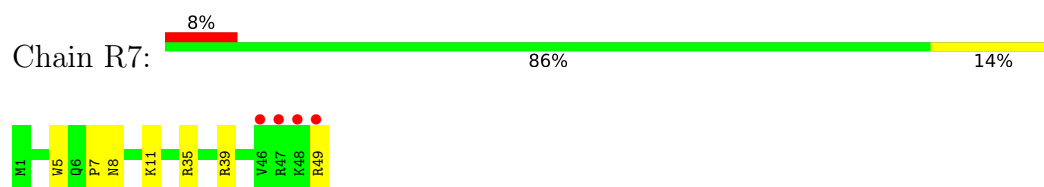
• Molecule 31: 50S ribosomal protein L33



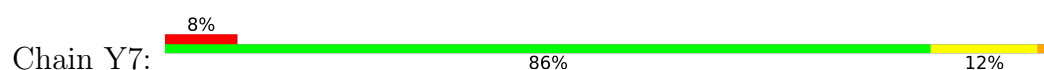
• Molecule 31: 50S ribosomal protein L33

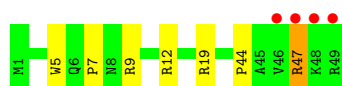


• Molecule 32: 50S ribosomal protein L34

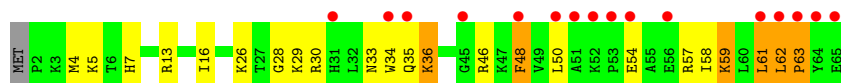


• Molecule 32: 50S ribosomal protein L34





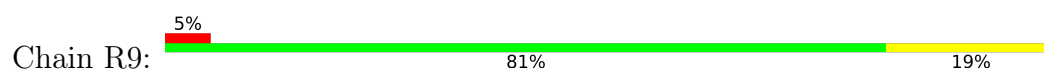
- Molecule 33: 50S ribosomal protein L35



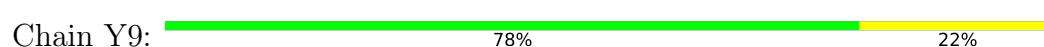
- Molecule 33: 50S ribosomal protein L35



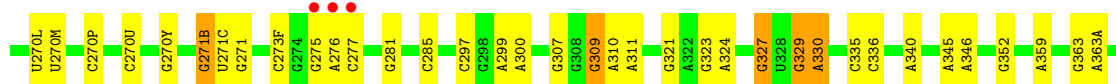
- Molecule 34: 50S ribosomal protein L36



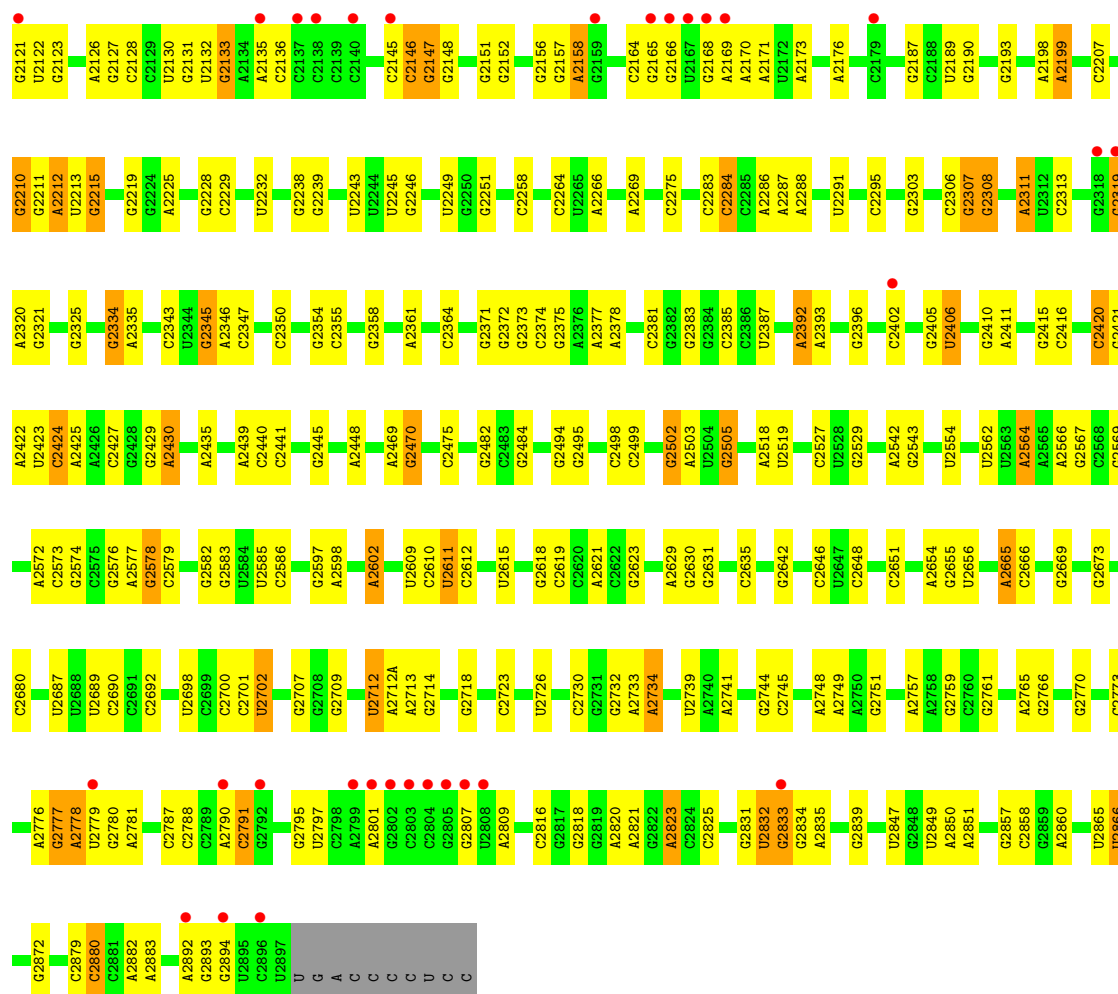
- Molecule 34: 50S ribosomal protein L36



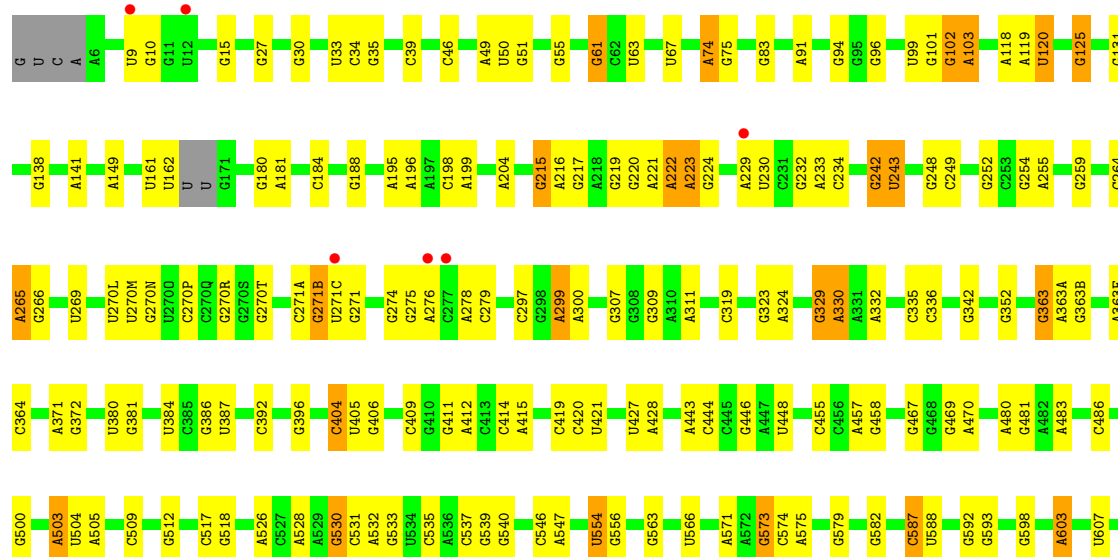
- Molecule 35: 23S rRNA



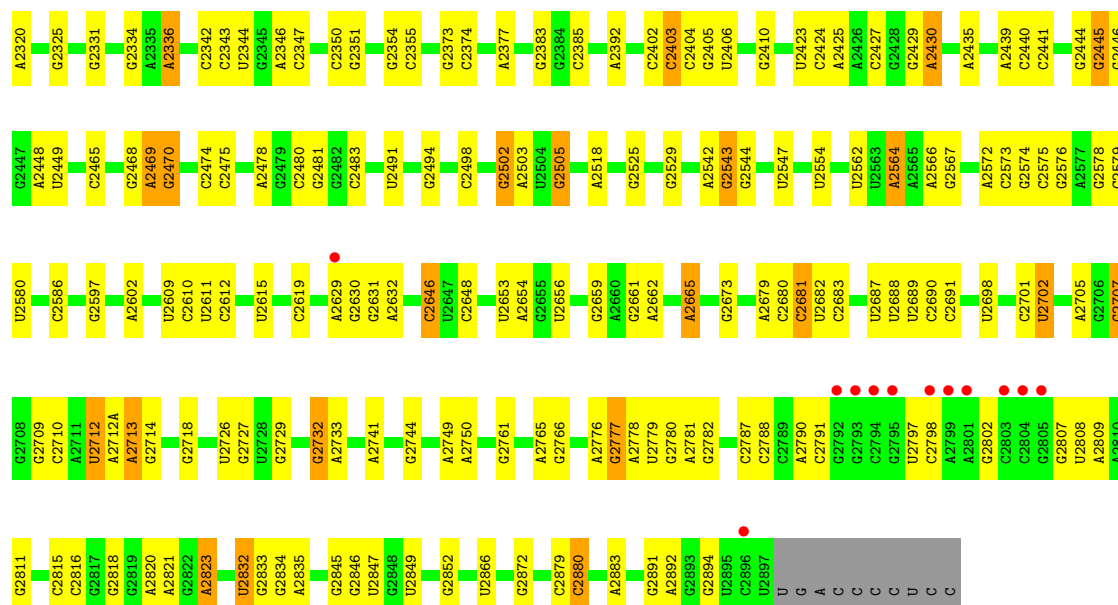
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C2007	A1872	G1725	C1598	A1471	A1342	A1204	A1096	U1026	G932	C806	C654I	U588	A462
G2008	G1878	G1599	C1599	A1479	A1349	G1206	U1097	A1027	G938	U807	U657	U594	A483
G2010	C1882	G1728	C1600	G1479	U1352	A1210	G1099	U1033	A941	C812	G666	U593	C486
G2012	G1883	U1729	A1603	G1480	A1353	U1211	U1101	C1041	G942	G818	G669	A603	G494
A2019	A1884	U1730	A1482	U1483	G1212	G1212	C1102	G1042	U943	A819	A670	G604	G500
A2020	A1885	G1731	G1483	U1484	A1365	A1213	U1103	C1043	G944	A820	G671	C605	G500
G2023	G1888	C1734	G1485	G1485	A1368	A1214	U1105	A1045	A945	U827	C672	U606	A503
A2031	A1889	G1742	A1490	A1490	G1368	C1217	G1106	A1046	G946	U828	G673	U607	U504
A2032	A1900	G1743	C1370	C1370	G1369	A1220	C1109	G1047	A953	C845	G674	A608	A505
A2033	A1901	G1756	C1493	C1493	A1378	A1252	G1110	A1048	G954	C846	A675	U614	G508
G2036	C1902	A1615	A1494	A1494	A1378	A1253	A1111	C1049	G955	U847	A676	G616	G509
G2037	G1906	C1617	A1495	A1495	A1379	A1254	G1112	A1050	A960	C856	A677	G617	C510
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G2039	G1921	A1773	U1497	U1497	G1384	G1239	G1122	A1054	A960	U858	C693	A621	G512
C2043	G1922	A1779	A1507	A1507	G1385	U1240	C1123	G1055	C961	C859	G702	G622	A514
G2052	G1929	U1779	C1508	C1508	G1388	G1244	U1130	A1056	C971	U860	G717	G627	C517
G2053	G1930	A1780	A1510	A1510	U1394	G1252	G1131	G1058	G972	U864	A722	G628	G523
G2055	U1931	G1782	G1512	G1512	A1395	A1253	C1136	U1060	C974	U868	C730	G629	A526
G2056	A1936	A1784	U1514	U1514	C1403	G1256	G1137	U1061	A980	C869	C730	G630	A526
A2059	A1937	A1784	G1525	G1525	C1404	G1256	G1138	G1063	A980	C890	G745	A634	A529
A2060	A1938	A1787	C1533	C1533	C1407	U1262	G1139	U1065	A983	C881	G746	A633	G530
A2061	U1939	A1791	G1534	G1534	C1411	G1264	C1140	U1066	A984	C884	U747	A637	C531
C2063	C1942	G1799	U1535	U1535	G1416	G1265	A1142A	A1067	C885	C885	G748	G638	A522
C2064	U1943	C1800	C1537	C1537	G1417	G1266	A1143	A1068	C886	C886	A750	U639	U534
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G2069	C1962	A1815	C1543	C1543	A1419	A1272	G1168	G1071	C989	C888	A752	A646	C537
G2070	G1963	G1816	A1544	A1544	U1420	U1273	G1169	C1072	G993	C893	G765	C650	G540
C2073	G1964	G1817	A1545	A1545	G1421	U1273	G1170	A1073	C994	C893	G765	G651	G540
U2096	C1967	A1818	A1546	A1546	A1427	A1278	G1171	C1075	C995	A896	G768	A654	A547
G2100	A1969	U1819	A1564	A1564	C1428	A1284	G1173	A1077	A996	C897	G771	G654A	C547
U2101	A1970	U1820	A1568	A1568	G1441	G1296	U1174	C1078	A1000	C899	G776	C654B	U553
U2102	A1971	G1828	G1559	G1559	G1442	U1300	U1175	C1079	G1003	A899	G776	U554	U554
C2107	A1972	A1829	A1566	A1566	A1444A	A1301	A1177	U1080	G1004	A900	G776	G	G
G1980	G1835	G1835	A1567	A1567	C1445	G1309	C1179	U1081	C1005	A901	A782	G	G
A1981	A1847	A1847	G1568	G1568	A1449	U1312	G1183	U1082	C1006	C904	A783	C	C
C1982	A1848	A1848	A1569	A1569	G1449A	U1313	G1187	A1084	U1012	U905	A784	C	A571
C1990	C1990	C1990	A1578	A1578	U1454	C1314	U1188	A1085	C1013	G906	G785	C	A572
G1991	G1858	U1859	U1578	U1578	G1455	G1319	A1189	G1087	U1014	U907	A788	C	G573
G1992	A1859	G1860	A1586	A1586	G1455	G1319	G1190	A1088	G1015	A910	A789	G	A575
G1993	G1863	U1864	A1587	A1587	G1458	C1327	G1191	G1089	U1019	C914	C790	C	G579
A1999	G1863	U1864	C1588	C1588	G1459	G1328	G1192	U1091	G915	C915	A793	G	G580
G2119	G1863	U1864	C1589	C1589	G1461	U1329	G1193	C1092	G1022	G916	A800	C	C581
G2120	G1863	U1864	C1589	C1589	G1461	U1329	A1194	U1094	G1024	A917	A800	C	G582
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• Molecule 35: 23S rRNA



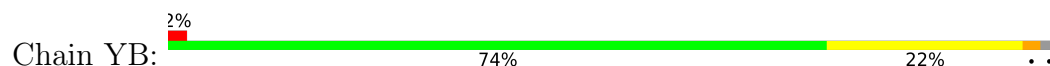
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G2210	U2113	C1996	G1858	G1567	G1449	A1301	C1140	U1060	G956	C846	G693	G614
G2114	A2114	C2006	A1859	A1569	G1449A	A1424	U1141	G1062	U957	U847	U694	A616
U2213	G2115	G2010	G1859	U1578	U1454	C1306	C1153	G1064	U958	C856	G695	G618
G2215	A2117	G2011	G1878	A1579	G1455	G1309	G1173	U1065	A959	C857	G701	A621
A2225	U2118	G2012	G1878	G1581	G1458	G1310	A1173	A960	C961	U858	G702	G622
U2233	G2120	A2013	G1878	A1730	C1458	G1327	A1174	G1068	U961	G859	G717	U626
G2234	U2121	A2014	C1881	A1732	G1459	G1328	U1175	A1069	A973	U860	A722	A627
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G2243	G2125	C2021	G1888	C1598	A1471	U1341	G1187	C1075	A984	U868	C730	A633
U2249	A2126	U2022	A1889	G1607	A1755	A1342	U1188	G1076	C985	G869	A734	C634
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C2283	G2132	G2035	G1769	G1622	A1490	U1354	U1205	A1085	A996	C884	A752	A646
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G2288	G2147	G2043	U1779	G1638	U1497	A1366	A1210	A1088	G1003	C886	G765	G648
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U2312	U2172	G2073	G1967	A1689	C1537	C1407	A1253	U1113	A1027	A917	A793	C
G2315	A2173	U2076	G1968	U1693	G1538	C1408	G1271	G1122	U1033	A918	A800	G
G2318	G2176	G2080	A1969	C1675	G1540	C1411	G1266	C1124	G1033	G919	G805	C
G2319	C2177	A2311	A1970	G1674	U1541	G1416	G1264	G1125	A1045	G832	C806	C
G2319	G2179	G2090	A1972	G1682	G1542	A1419	A1265	A1126	A1046	U907	U807	C
G2319	U2312	G2093	G1980	A1689	A1543	U1420	G1266	A1129	G1047	C912	C912	G654S
G2319	G2187	U2099	A1981	U1693	C1544	G1421	G1271	U1130	A1050	A819	A819	A655
G2319	G2188	G2100	C1982	G1694	A1545	A1428	A1272	G1131	A1054	A820	A820	A655
G2319	U2189	G2100	G1982	U1694	A1558	A1427	C1290	C1135	G1055	U827	U827	G662
G2319	G2190	G2101	G1991	G1695	G1559	C1428	C1291	G1136	A1057	G947	G947	G662
G2319	G2191	G2101	U1991	G1695	G1559	C1428	C1291	G1137	A1057	G948	G948	A676



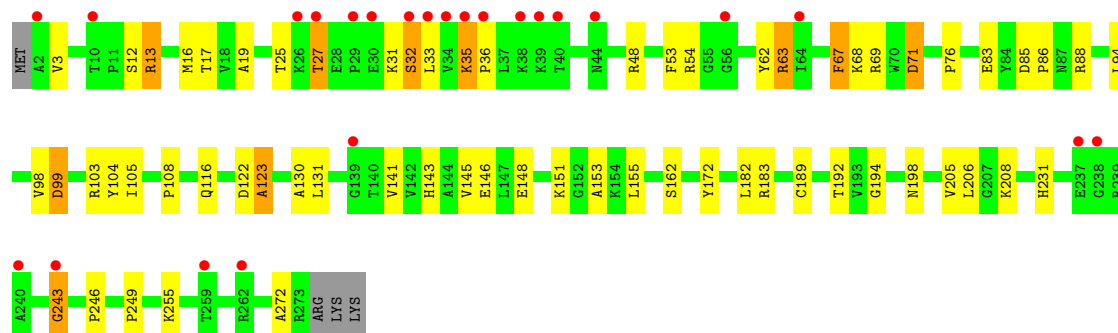
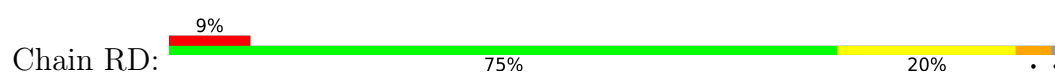
• Molecule 36: 5S rRNA



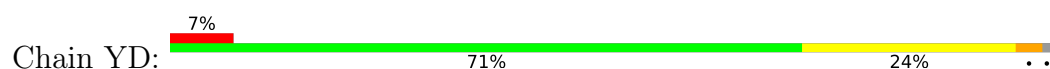
• Molecule 36: 5S rRNA

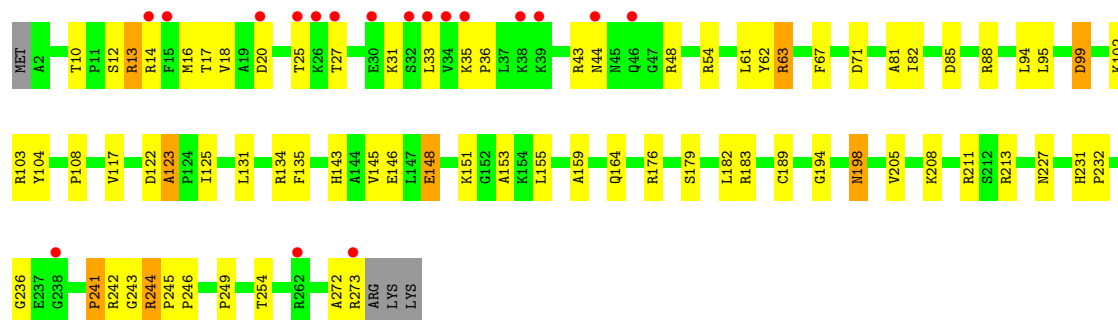


• Molecule 37: 50S ribosomal protein L2

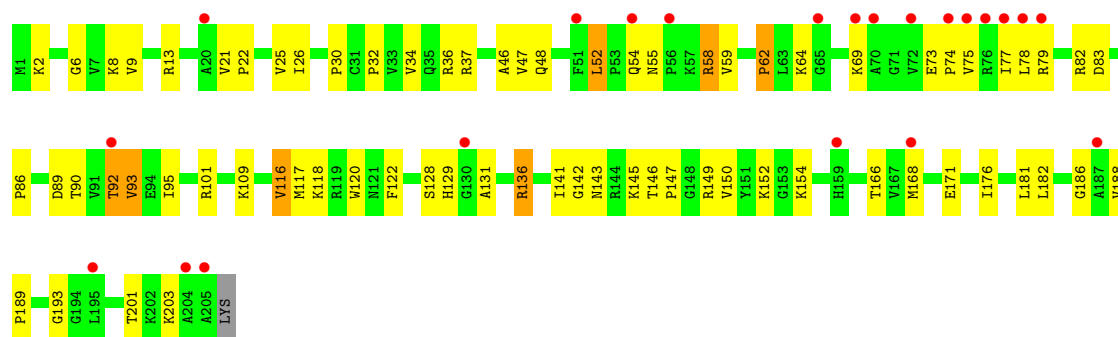


• Molecule 37: 50S ribosomal protein L2

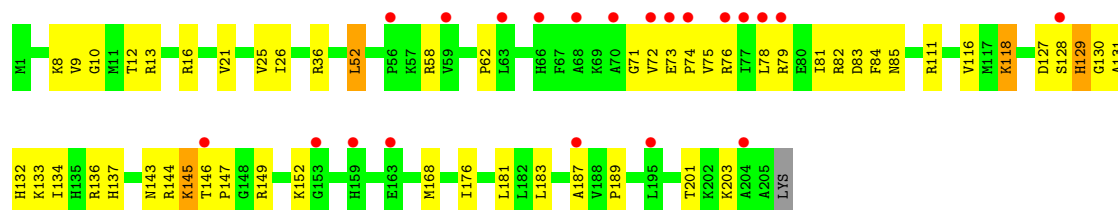
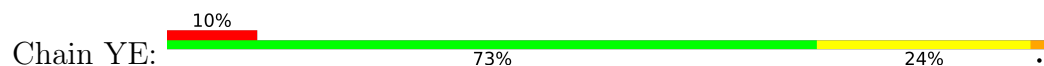




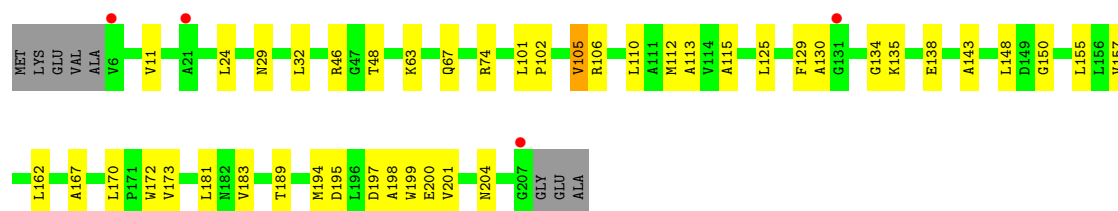
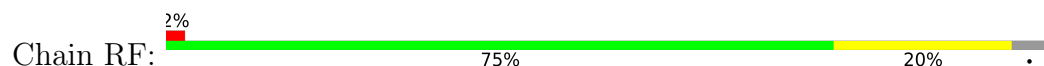
• Molecule 38: 50S ribosomal protein L3



• Molecule 38: 50S ribosomal protein L3

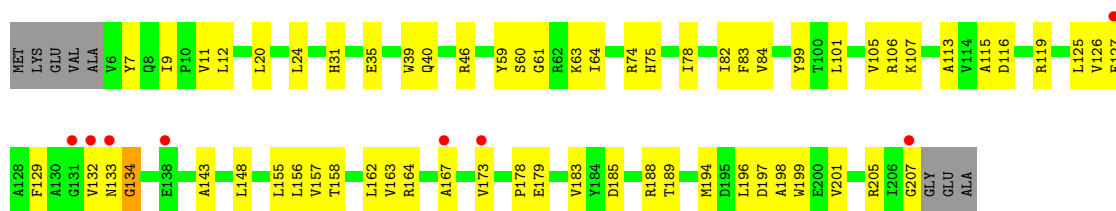


• Molecule 39: 50S ribosomal protein L4

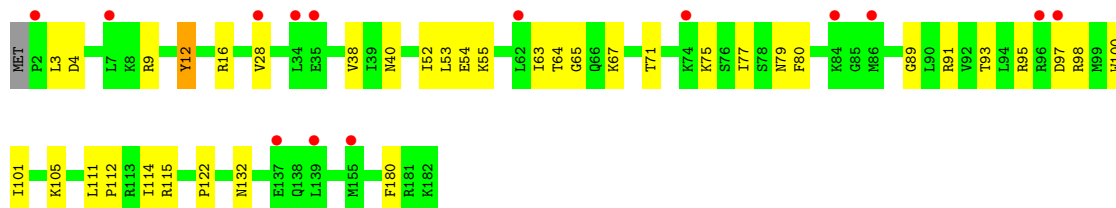
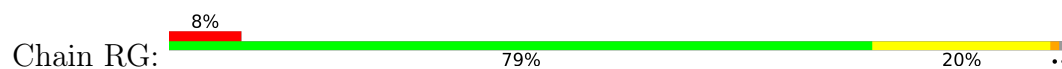


• Molecule 39: 50S ribosomal protein L4

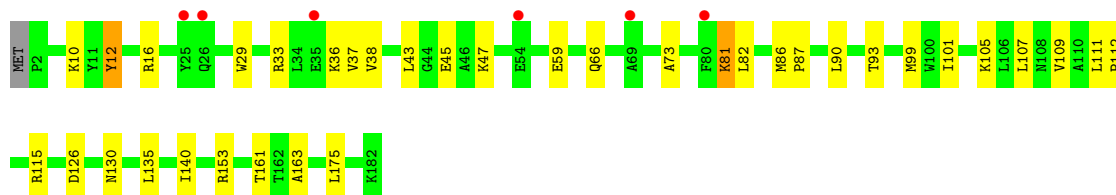
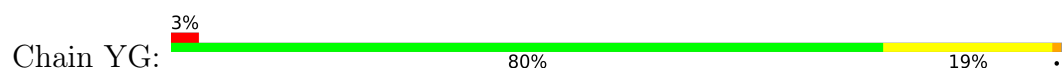




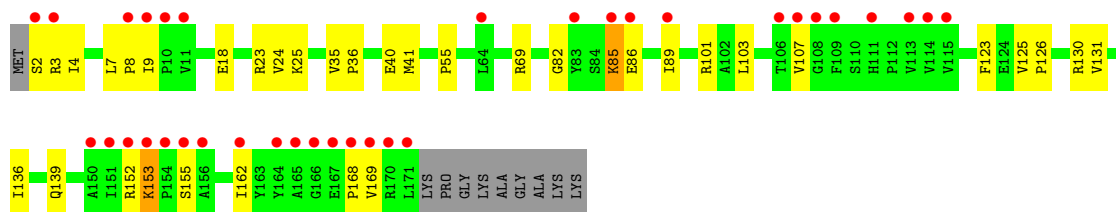
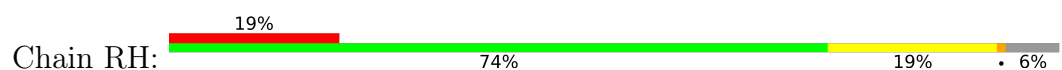
• Molecule 40: 50S ribosomal protein L5



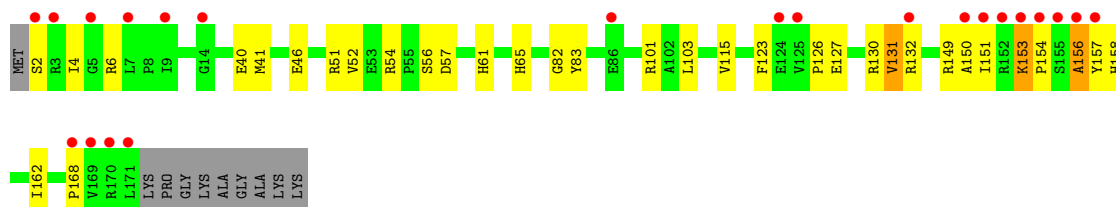
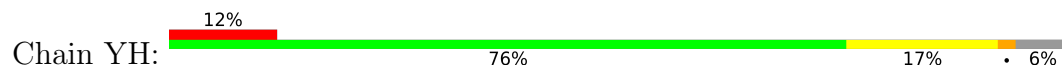
• Molecule 40: 50S ribosomal protein L5



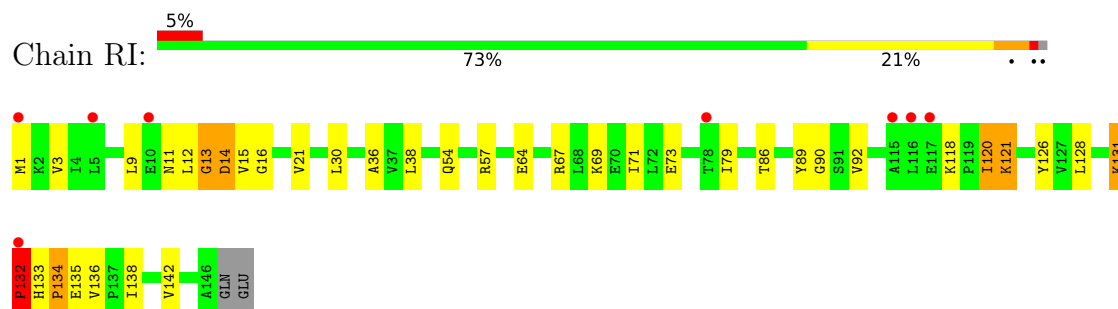
• Molecule 41: 50S ribosomal protein L6



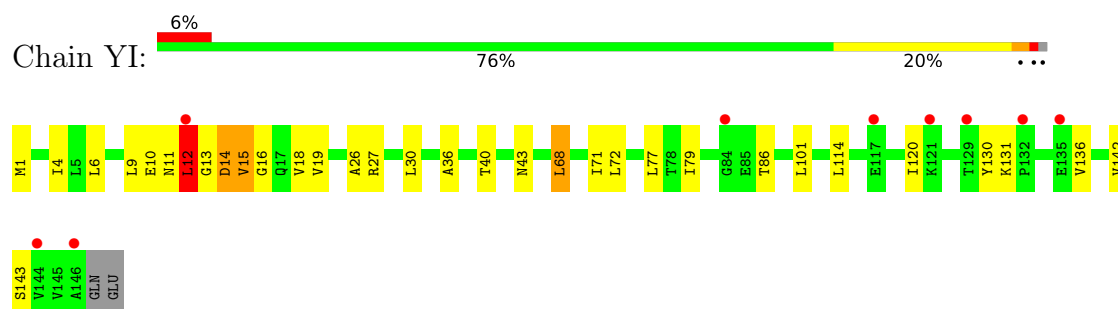
• Molecule 41: 50S ribosomal protein L6



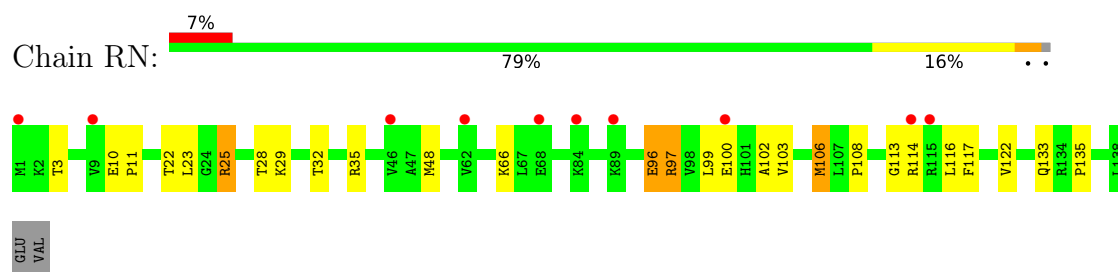
- Molecule 42: 50S ribosomal protein L9



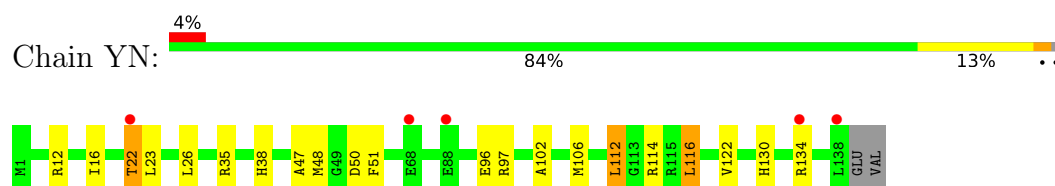
- Molecule 42: 50S ribosomal protein L9



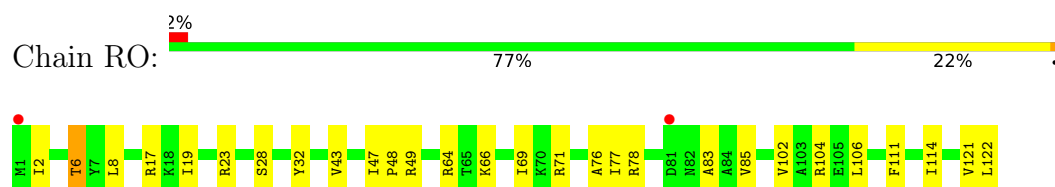
- Molecule 43: 50S ribosomal protein L13



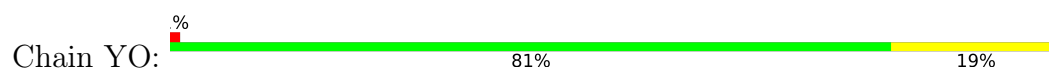
- Molecule 43: 50S ribosomal protein L13



- Molecule 44: 50S ribosomal protein L14

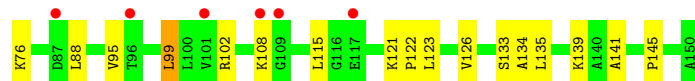
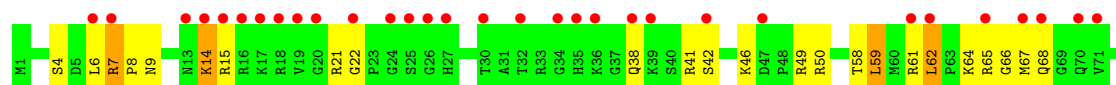
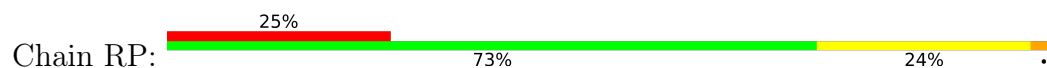


- Molecule 44: 50S ribosomal protein L14

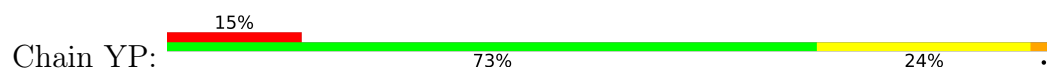




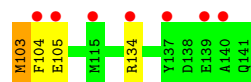
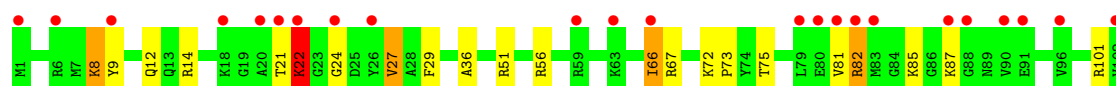
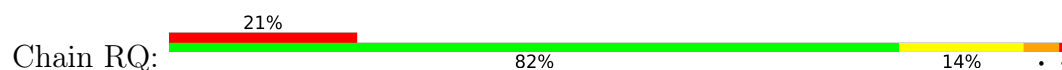
- Molecule 45: 50S ribosomal protein L15



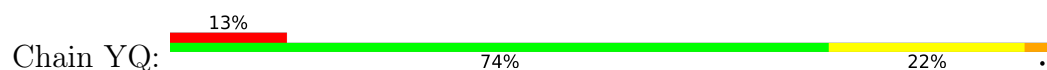
- Molecule 45: 50S ribosomal protein L15



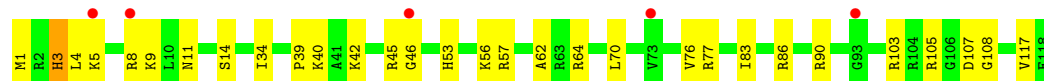
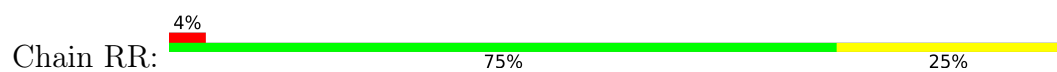
- Molecule 46: 50S ribosomal protein L16



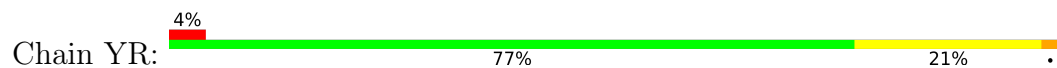
- Molecule 46: 50S ribosomal protein L16



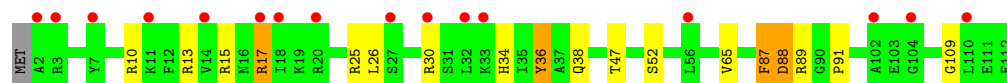
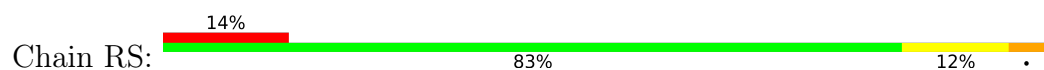
- Molecule 47: 50S ribosomal protein L17



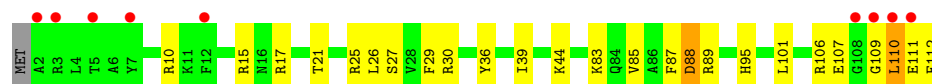
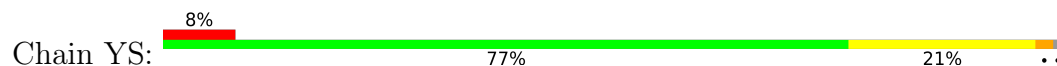
- Molecule 47: 50S ribosomal protein L17



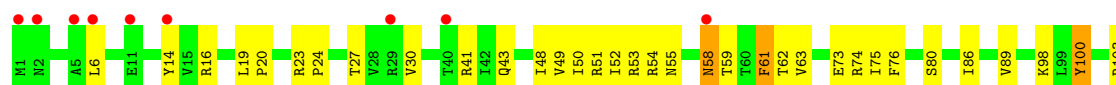
- Molecule 48: 50S ribosomal protein L18



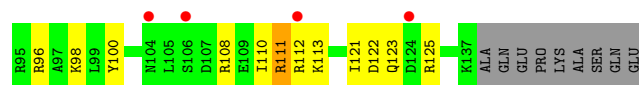
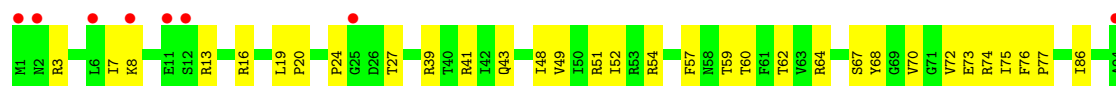
- Molecule 48: 50S ribosomal protein L18



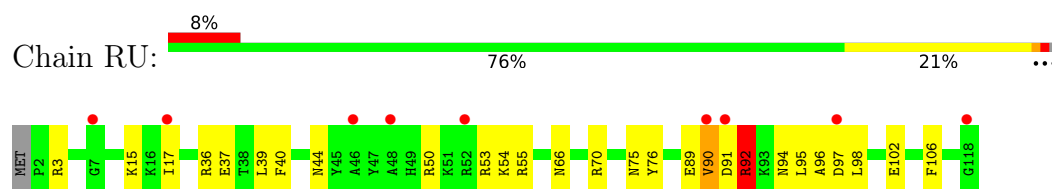
- Molecule 49: 50S ribosomal protein L19



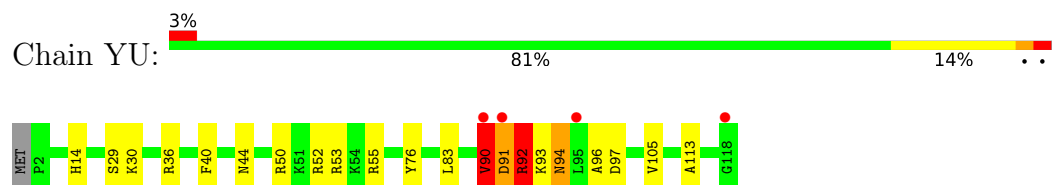
- Molecule 49: 50S ribosomal protein L19



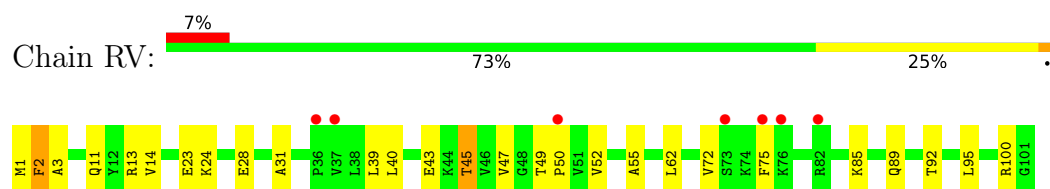
- Molecule 50: 50S ribosomal protein L20



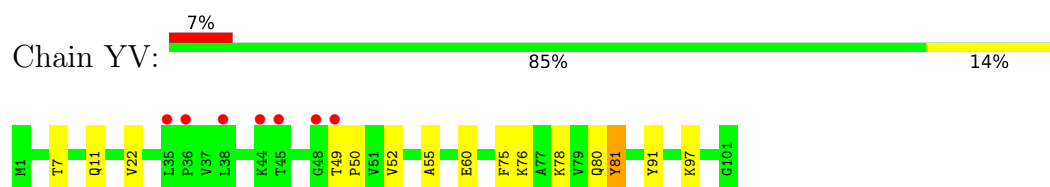
- Molecule 50: 50S ribosomal protein L20



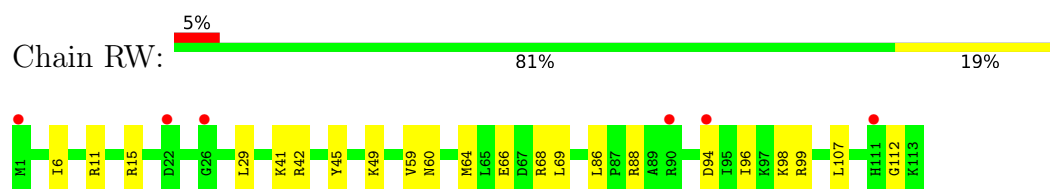
- Molecule 51: 50S ribosomal protein L21



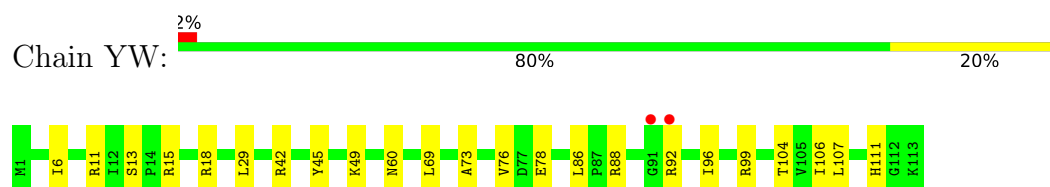
- Molecule 51: 50S ribosomal protein L21



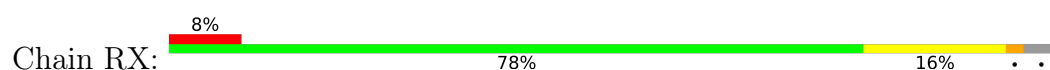
- Molecule 52: 50S ribosomal protein L22



- Molecule 52: 50S ribosomal protein L22

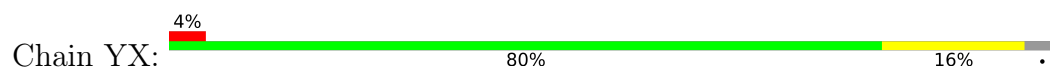


- Molecule 53: 50S ribosomal protein L23

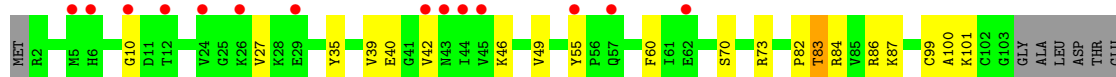
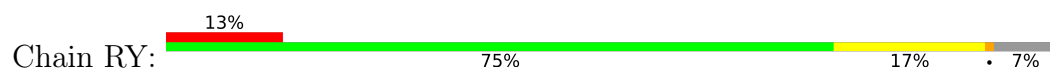




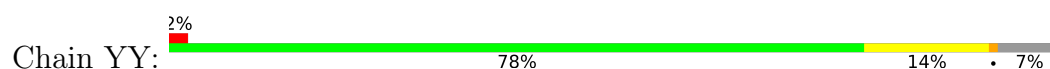
- Molecule 53: 50S ribosomal protein L23



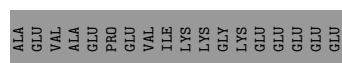
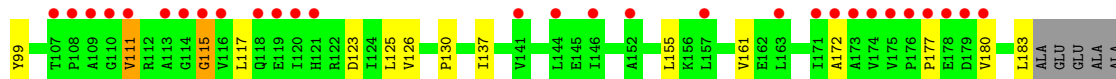
- Molecule 54: 50S ribosomal protein L24



- Molecule 54: 50S ribosomal protein L24



- Molecule 55: 50S ribosomal protein L25



- Molecule 55: 50S ribosomal protein L25





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.38Å 449.76Å 619.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.10 49.74 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.74-3.10) 97.1 (49.74-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.225 , 0.266 0.225 , 0.266	Depositor DCC
R_{free} test set	52649 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	294981	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, PAR, MG, ZN

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	0.53	0/36098	0.49	7/56341 (0.0%)
1	XA	0.57	0/36101	0.50	6/56346 (0.0%)
2	QB	0.44	0/1959	0.96	9/2642 (0.3%)
2	XB	0.49	0/1959	0.94	3/2642 (0.1%)
3	QC	0.45	0/1629	0.89	4/2195 (0.2%)
3	XC	0.48	0/1629	0.83	3/2195 (0.1%)
4	QD	0.54	0/1704	0.87	5/2284 (0.2%)
4	XD	0.55	0/1704	0.90	9/2284 (0.4%)
5	QE	0.50	0/1171	0.91	3/1576 (0.2%)
5	XE	0.52	0/1171	0.84	2/1576 (0.1%)
6	QF	0.53	0/856	0.81	0/1154
6	XF	0.52	0/856	0.83	1/1154 (0.1%)
7	QG	0.45	0/1276	0.96	7/1709 (0.4%)
7	XG	0.47	0/1276	0.93	4/1709 (0.2%)
8	QH	0.46	0/1136	0.89	3/1527 (0.2%)
8	XH	0.53	0/1136	0.86	3/1527 (0.2%)
9	QI	0.50	0/1029	1.14	10/1379 (0.7%)
9	XI	0.49	0/1029	1.03	6/1379 (0.4%)
10	QJ	0.43	0/814	0.98	3/1095 (0.3%)
10	XJ	0.50	0/814	0.87	1/1095 (0.1%)
11	QK	0.51	0/900	0.86	1/1213 (0.1%)
11	XK	0.52	0/900	0.90	4/1213 (0.3%)
12	QL	0.54	0/991	1.05	12/1327 (0.9%)
12	XL	0.59	0/991	1.02	9/1327 (0.7%)
13	QM	0.50	0/974	1.10	6/1303 (0.5%)
13	XM	0.47	0/974	1.07	7/1303 (0.5%)
14	QN	0.49	0/501	0.90	0/664
14	XN	0.55	0/501	1.05	4/664 (0.6%)
15	QO	0.53	0/745	0.81	0/992
15	XO	0.49	0/745	0.81	0/992
16	QP	0.54	0/721	0.95	3/970 (0.3%)
16	XP	0.51	0/721	1.01	2/970 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.53	0/847	0.91	3/1131 (0.3%)
17	XQ	0.51	0/847	0.86	3/1131 (0.3%)
18	QR	0.57	0/579	1.05	2/768 (0.3%)
18	XR	0.56	0/579	0.95	3/768 (0.4%)
19	QS	0.46	0/689	1.06	5/926 (0.5%)
19	XS	0.56	0/689	1.25	12/926 (1.3%)
20	QT	0.52	0/765	0.99	3/1007 (0.3%)
20	XT	0.47	0/765	1.06	4/1007 (0.4%)
21	QU	0.52	0/221	0.82	0/288
21	XU	0.60	0/221	0.93	1/288 (0.3%)
22	QV	0.48	0/1832	0.46	0/2855
22	XV	0.55	0/1832	0.43	0/2855
23	QX	0.41	0/446	0.54	0/695
23	XX	0.45	0/446	0.55	0/695
24	QY	0.38	0/1790	0.47	0/2789
24	XY	0.39	0/1790	0.46	0/2789
25	R0	0.58	0/657	0.89	2/874 (0.2%)
25	Y0	0.64	0/657	0.94	2/874 (0.2%)
26	R1	0.61	0/770	1.06	4/1022 (0.4%)
26	Y1	0.64	0/770	0.98	3/1022 (0.3%)
27	R2	0.56	0/583	0.98	2/771 (0.3%)
27	Y2	0.58	0/583	1.04	4/771 (0.5%)
28	R3	0.45	0/474	0.81	0/635
28	Y3	0.56	0/474	0.82	0/635
29	R4	0.57	0/594	1.44	10/795 (1.3%)
29	Y4	0.50	0/594	1.55	14/795 (1.8%)
30	R5	0.60	0/473	1.25	6/639 (0.9%)
30	Y5	0.68	0/473	1.01	2/639 (0.3%)
31	R6	0.68	0/431	1.60	7/575 (1.2%)
31	Y6	0.67	0/431	1.57	9/575 (1.6%)
32	R7	0.68	0/438	0.86	0/575
32	Y7	0.71	0/438	0.98	3/575 (0.5%)
33	R8	0.66	0/525	1.21	9/691 (1.3%)
33	Y8	0.80	1/525 (0.2%)	1.22	8/691 (1.2%)
34	R9	0.57	0/310	0.71	0/407
34	Y9	0.62	0/310	0.81	0/407
35	RA	0.62	0/69521	0.52	15/108529 (0.0%)
35	YA	0.70	0/69543	0.54	17/108563 (0.0%)
36	RB	0.50	0/2878	0.49	0/4490
36	YB	0.62	0/2878	0.51	0/4490
37	RD	0.67	0/2165	1.03	12/2919 (0.4%)
37	YD	0.74	0/2165	1.03	12/2919 (0.4%)
38	RE	0.62	1/1601 (0.1%)	1.14	16/2160 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YE	0.69	0/1601	1.17	12/2160 (0.6%)
39	RF	0.59	0/1620	0.95	4/2194 (0.2%)
39	YF	0.65	0/1620	0.98	7/2194 (0.3%)
40	RG	0.49	0/1499	1.02	10/2016 (0.5%)
40	YG	0.55	0/1499	0.97	4/2016 (0.2%)
41	RH	0.45	0/1332	1.13	9/1802 (0.5%)
41	YH	0.59	0/1332	1.12	14/1802 (0.8%)
42	RI	0.57	2/1151 (0.2%)	1.32	21/1558 (1.3%)
42	YI	0.50	0/1151	1.16	14/1558 (0.9%)
43	RN	0.57	0/1131	1.05	7/1525 (0.5%)
43	YN	0.62	0/1131	1.02	8/1525 (0.5%)
44	RO	0.60	0/943	0.86	1/1269 (0.1%)
44	YO	0.67	0/943	0.98	1/1269 (0.1%)
45	RP	0.59	0/1162	1.20	7/1544 (0.5%)
45	YP	0.65	0/1162	1.18	12/1544 (0.8%)
46	RQ	0.59	0/1143	1.14	9/1527 (0.6%)
46	YQ	0.65	0/1143	1.18	10/1527 (0.7%)
47	RR	0.63	0/982	0.95	4/1312 (0.3%)
47	YR	0.65	0/982	1.02	5/1312 (0.4%)
48	RS	0.54	0/892	1.21	10/1187 (0.8%)
48	YS	0.58	0/892	1.12	6/1187 (0.5%)
49	RT	0.60	0/1155	1.06	13/1542 (0.8%)
49	YT	0.62	0/1155	1.14	11/1542 (0.7%)
50	RU	0.59	0/982	1.11	10/1306 (0.8%)
50	YU	0.66	0/982	1.05	8/1306 (0.6%)
51	RV	0.54	0/790	1.04	3/1057 (0.3%)
51	YV	0.67	0/790	1.10	4/1057 (0.4%)
52	RW	0.62	0/911	0.92	1/1220 (0.1%)
52	YW	0.63	0/911	0.88	1/1220 (0.1%)
53	RX	0.59	0/739	0.96	4/993 (0.4%)
53	YX	0.65	0/739	0.91	2/993 (0.2%)
54	RY	0.53	0/798	0.97	3/1064 (0.3%)
54	YY	0.63	0/798	1.02	4/1064 (0.4%)
55	RZ	0.46	0/1493	1.07	12/2026 (0.6%)
55	YZ	0.53	0/1493	1.08	8/2026 (0.4%)
All	All	0.61	4/319657 (0.0%)	0.69	589/478147 (0.1%)

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
48	RS	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	RI	133	HIS	C-N	5.84	1.47	1.33
38	RE	136	ARG	C-N	-5.40	1.23	1.33
42	RI	134	PRO	N-CD	-5.12	1.40	1.47
33	Y8	23	VAL	CB-CG1	-5.00	1.36	1.52

The worst 5 of 589 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y4	39	CYS	N-CA-C	-12.70	95.90	112.41
13	XM	7	VAL	N-CA-C	-12.60	101.18	113.53
26	R1	75	GLU	N-CA-C	-11.51	100.25	114.75
39	RF	199	TRP	N-CA-C	-11.32	99.96	113.88
35	RA	1992	G	C2'-C3'-O3'	11.15	126.23	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	RS	17	ARG	Sidechain

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	16277	208	0
1	XA	32249	0	16279	180	0
2	QB	1924	0	1975	28	0
2	XB	1924	0	1975	29	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	19	0
4	QD	1674	0	1718	29	0
4	XD	1674	0	1718	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	11	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	8	0
8	QH	1116	0	1177	13	0
8	XH	1116	0	1177	20	0
9	QI	1010	0	1037	23	0
9	XI	1010	0	1037	24	0
10	QJ	801	0	849	19	0
10	XJ	801	0	849	15	0
11	QK	885	0	904	17	0
11	XK	885	0	904	9	0
12	QL	975	0	1062	17	0
12	XL	975	0	1062	16	0
13	QM	964	0	1034	35	0
13	XM	964	0	1034	16	0
14	QN	492	0	529	14	0
14	XN	492	0	529	5	0
15	QO	734	0	771	7	0
15	XO	734	0	771	4	0
16	QP	705	0	725	14	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	10	0
18	QR	574	0	644	13	0
18	XR	574	0	644	8	0
19	QS	674	0	699	21	0
19	XS	674	0	699	14	0
20	QT	763	0	860	6	0
20	XT	763	0	861	17	0
21	QU	217	0	234	5	0
21	XU	217	0	234	1	0
22	QV	1640	0	837	5	0
22	XV	1640	0	837	4	0
23	QX	396	0	197	1	0
23	XX	396	0	197	3	0
24	QY	1602	0	811	23	0
24	XY	1602	0	811	10	0
25	R0	648	0	672	15	0
25	Y0	648	0	672	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	R1	763	0	848	12	0
26	Y1	763	0	848	11	0
27	R2	581	0	629	14	0
27	Y2	581	0	629	11	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	4	0
29	R4	581	0	577	17	0
29	Y4	581	0	577	17	0
30	R5	459	0	480	9	0
30	Y5	459	0	480	11	0
31	R6	424	0	450	11	0
31	Y6	424	0	450	9	0
32	R7	430	0	480	7	0
32	Y7	430	0	480	7	0
33	R8	517	0	582	18	0
33	Y8	517	0	582	33	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	6	0
35	RA	62071	0	31280	358	0
35	YA	62091	0	31290	306	0
36	RB	2573	0	1306	16	0
36	YB	2573	0	1306	13	0
37	RD	2115	0	2195	43	0
37	YD	2115	0	2195	53	0
38	RE	1568	0	1634	46	0
38	YE	1568	0	1634	32	0
39	RF	1585	0	1632	24	0
39	YF	1585	0	1632	32	0
40	RG	1474	0	1535	21	0
40	YG	1474	0	1535	19	0
41	RH	1307	0	1382	22	0
41	YH	1307	0	1382	20	0
42	RI	1136	0	1223	12	0
42	YI	1136	0	1223	12	0
43	RN	1104	0	1180	24	0
43	YN	1104	0	1180	9	0
44	RO	933	0	996	23	0
44	YO	933	0	996	19	0
45	RP	1145	0	1227	30	0
45	YP	1145	0	1227	28	0
46	RQ	1122	0	1179	25	0
46	YQ	1122	0	1177	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	RR	968	0	1033	19	0
47	YR	968	0	1033	17	0
48	RS	882	0	943	9	0
48	YS	882	0	943	16	0
49	RT	1141	0	1202	29	0
49	YT	1141	0	1202	24	0
50	RU	964	0	1022	22	0
50	YU	964	0	1022	20	0
51	RV	779	0	852	18	0
51	YV	779	0	852	12	0
52	RW	900	0	964	15	0
52	YW	900	0	964	18	0
53	RX	725	0	778	9	0
53	YX	725	0	778	9	0
54	RY	785	0	878	14	0
54	YY	785	0	878	9	0
55	RZ	1461	0	1493	28	0
55	YZ	1461	0	1493	32	0
56	QA	73	0	0	0	0
56	QF	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	1	0	0	0	0
56	QX	2	0	0	0	0
56	R0	1	0	0	0	0
56	R5	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	281	0	0	0	0
56	RB	4	0	0	0	0
56	RD	1	0	0	0	0
56	RE	4	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RR	1	0	0	0	0
56	RU	1	0	0	0	0
56	XA	91	0	0	0	0
56	XF	1	0	0	0	0
56	XM	1	0	0	0	0
56	XV	2	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Y2	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	2	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	347	0	0	0	0
56	YB	6	0	0	0	0
56	YE	3	0	0	0	0
56	YN	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	0	0
57	XA	42	0	45	4	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	294981	0	199667	2249	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 2249 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)
55:YZ:94:GLU:CG	55:YZ:95:PRO:HD3	1.74	1.18
35:RA:1138:G:H21	43:RN:106:MET:HE1	1.05	1.09
35:RA:2055:C:H5'	35:RA:2056:G:H5''	1.35	1.07
55:YZ:94:GLU:HB3	55:YZ:95:PRO:CD	1.85	1.07
19:QS:10:PHE:HB2	19:QS:16:LEU:HD11	1.34	1.06

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	206 (88%)	27 (12%)	2 (1%)	14	44
2	XB	235/256 (92%)	207 (88%)	28 (12%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	QD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	57
4	XD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	57
5	QE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	18	49
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	18	49
8	QH	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	47
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
12	QL	123/131 (94%)	107 (87%)	15 (12%)	1 (1%)	16	47
12	XL	123/131 (94%)	108 (88%)	10 (8%)	5 (4%)	2	13
13	QM	119/126 (94%)	99 (83%)	19 (16%)	1 (1%)	16	47
13	XM	119/126 (94%)	102 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	30
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	8 (10%)	3 (4%)	2	15
20	QT	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	3	18
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
25	R0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
26	R1	95/98 (97%)	80 (84%)	12 (13%)	3 (3%)	3	18
26	Y1	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	5	25
27	R2	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	8	32
27	Y2	67/72 (93%)	60 (90%)	7 (10%)	0	100	100
28	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	R4	69/71 (97%)	44 (64%)	18 (26%)	7 (10%)	0	3
29	Y4	69/71 (97%)	41 (59%)	26 (38%)	2 (3%)	3	19
30	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
30	Y5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
31	R6	47/54 (87%)	31 (66%)	13 (28%)	3 (6%)	1	6
31	Y6	47/54 (87%)	32 (68%)	12 (26%)	3 (6%)	1	6
32	R7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
32	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	R8	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	3	18
33	Y8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	7	30
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	270/276 (98%)	244 (90%)	21 (8%)	5 (2%)	6	27
37	YD	270/276 (98%)	243 (90%)	26 (10%)	1 (0%)	30	61
38	RE	203/206 (98%)	165 (81%)	35 (17%)	3 (2%)	8	32
38	YE	203/206 (98%)	168 (83%)	30 (15%)	5 (2%)	4	21
39	RF	200/210 (95%)	184 (92%)	13 (6%)	3 (2%)	8	32
39	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	12	41
40	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
40	YG	179/182 (98%)	156 (87%)	22 (12%)	1 (1%)	21	52
41	RH	168/180 (93%)	134 (80%)	30 (18%)	4 (2%)	4	22
41	YH	168/180 (93%)	140 (83%)	26 (16%)	2 (1%)	10	37
42	RI	144/148 (97%)	115 (80%)	21 (15%)	8 (6%)	1	8
42	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	2	13
43	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	49
43	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	18	49
44	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
44	YO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	47
45	RP	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	4	20
45	YP	148/150 (99%)	118 (80%)	28 (19%)	2 (1%)	9	34
46	RQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	18	49
46	YQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	3	19
47	RR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	30
47	YR	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	7	30
48	RS	109/112 (97%)	91 (84%)	15 (14%)	3 (3%)	4	20
48	YS	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	14	44
49	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	YT	135/146 (92%)	117 (87%)	17 (13%)	1 (1%)	18	49
50	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	YU	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	4	21
51	RV	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	6	25
51	YV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	12	41
52	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
53	RX	90/96 (94%)	81 (90%)	9 (10%)	0	100	100
53	YX	90/96 (94%)	82 (91%)	7 (8%)	1 (1%)	11	39
54	RY	100/110 (91%)	91 (91%)	9 (9%)	0	100	100
54	YY	100/110 (91%)	94 (94%)	6 (6%)	0	100	100
55	RZ	181/206 (88%)	152 (84%)	24 (13%)	5 (3%)	4	20
55	YZ	181/206 (88%)	158 (87%)	19 (10%)	4 (2%)	5	24
All	All	11470/12126 (95%)	10176 (89%)	1168 (10%)	126 (1%)	11	39

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
26	R1	92	LYS
29	R4	24	THR
29	R4	43	TYR
31	R6	8	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	205 (100%)	0	100	100
2	XB	205/220 (93%)	205 (100%)	0	100	100
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	173/181 (96%)	173 (100%)	0	100	100
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	98/99 (99%)	98 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	89 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	90/99 (91%)	90 (100%)	0	100	100
12	QL	104/108 (96%)	104 (100%)	0	100	100
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	96 (99%)	1 (1%)	68	79
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	71 (97%)	2 (3%)	39	67
19	XS	73/80 (91%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
25	R0	65/67 (97%)	65 (100%)	0	100	100
25	Y0	65/67 (97%)	65 (100%)	0	100	100
26	R1	82/83 (99%)	82 (100%)	0	100	100
26	Y1	82/83 (99%)	82 (100%)	0	100	100
27	R2	64/67 (96%)	64 (100%)	0	100	100
27	Y2	64/67 (96%)	64 (100%)	0	100	100
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	63/63 (100%)	63 (100%)	0	100	100
29	Y4	63/63 (100%)	63 (100%)	0	100	100
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	51 (100%)	0	100	100
31	R6	48/52 (92%)	48 (100%)	0	100	100
31	Y6	48/52 (92%)	48 (100%)	0	100	100
32	R7	42/42 (100%)	42 (100%)	0	100	100
32	Y7	42/42 (100%)	42 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	30	61
34	R9	34/34 (100%)	34 (100%)	0	100	100
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	214 (100%)	0	100	100
37	YD	214/218 (98%)	214 (100%)	0	100	100
38	RE	165/166 (99%)	165 (100%)	0	100	100
38	YE	165/166 (99%)	165 (100%)	0	100	100
39	RF	161/166 (97%)	161 (100%)	0	100	100
39	YF	161/166 (97%)	161 (100%)	0	100	100
40	RG	155/156 (99%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YG	155/156 (99%)	155 (100%)	0	100	100
41	RH	142/148 (96%)	142 (100%)	0	100	100
41	YH	142/148 (96%)	142 (100%)	0	100	100
42	RI	122/124 (98%)	122 (100%)	0	100	100
42	YI	122/124 (98%)	122 (100%)	0	100	100
43	RN	117/119 (98%)	116 (99%)	1 (1%)	70	80
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	99 (99%)	1 (1%)	68	79
44	YO	100/100 (100%)	100 (100%)	0	100	100
45	RP	116/116 (100%)	116 (100%)	0	100	100
45	YP	116/116 (100%)	116 (100%)	0	100	100
46	RQ	111/111 (100%)	111 (100%)	0	100	100
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	101 (100%)	0	100	100
48	RS	87/88 (99%)	87 (100%)	0	100	100
48	YS	87/88 (99%)	87 (100%)	0	100	100
49	RT	120/127 (94%)	120 (100%)	0	100	100
49	YT	120/127 (94%)	120 (100%)	0	100	100
50	RU	93/94 (99%)	93 (100%)	0	100	100
50	YU	93/94 (99%)	93 (100%)	0	100	100
51	RV	82/82 (100%)	82 (100%)	0	100	100
51	YV	82/82 (100%)	82 (100%)	0	100	100
52	RW	92/92 (100%)	92 (100%)	0	100	100
52	YW	92/92 (100%)	92 (100%)	0	100	100
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	74 (100%)	0	100	100
54	RY	85/91 (93%)	85 (100%)	0	100	100
54	YY	85/91 (93%)	85 (100%)	0	100	100
55	RZ	162/179 (90%)	162 (100%)	0	100	100
55	YZ	162/179 (90%)	162 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9688/10064 (96%)	9681 (100%)	7 (0%)	88 90

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	RN	106	MET
44	RO	6	THR
33	Y8	65	GLU
33	Y8	62	LEU
19	QS	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
8	XH	78	GLN
25	Y0	12	ASN
9	XI	31	GLN
13	XM	62	ASN
29	Y4	47	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	271 (18%)	29 (1%)
1	XA	1498/1522 (98%)	282 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	14 (18%)	0
23	QX	17/19 (89%)	8 (47%)	1 (5%)
23	XX	17/19 (89%)	8 (47%)	1 (5%)
24	QY	74/76 (97%)	28 (37%)	0
24	XY	74/76 (97%)	25 (33%)	0
35	RA	2879/2915 (98%)	591 (20%)	47 (1%)
35	YA	2880/2915 (98%)	589 (20%)	44 (1%)
36	RB	119/122 (97%)	21 (17%)	1 (0%)
36	YB	119/122 (97%)	18 (15%)	0
All	All	9327/9462 (98%)	1870 (20%)	150 (1%)

5 of 1870 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	YA	503	A
35	YA	2566	A
35	YA	752	A
35	YA	1210	A
35	RA	752	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 855 ligands modelled in this entry, 851 are monoatomic - leaving 4 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	SF4	QD	501	-	0,12,12	-	-	-		
57	PAR	QA	1663	-	44,45,45	0.81	0	63,67,67	1.26	7 (11%)
58	SF4	XD	501	4	0,12,12	-	-	-		
57	PAR	XA	1670	-	44,45,45	0.86	1 (2%)	63,67,67	1.27	6 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	501	-	-	-	0/6/5/5
57	PAR	QA	1663	-	-	3/18/94/94	0/4/4/4
58	SF4	XD	501	4	-	-	0/6/5/5
57	PAR	XA	1670	-	-	4/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1670	PAR	C24-N24	-2.02	1.44	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1663	PAR	C13-O52-C52	-3.35	110.03	117.98
57	XA	1670	PAR	C13-O52-C52	-3.01	110.85	117.98
57	XA	1670	PAR	O11-C42-C32	-2.97	102.08	109.18
57	QA	1663	PAR	O62-C62-C12	-2.58	105.08	109.90
57	QA	1663	PAR	O33-C33-C23	-2.57	103.05	111.32

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1663	PAR	O54-C54-C64-N64
57	XA	1670	PAR	O54-C14-O33-C33
57	QA	1663	PAR	O51-C51-C61-O61
57	QA	1663	PAR	C23-C33-O33-C14
57	XA	1670	PAR	C43-C33-O33-C14

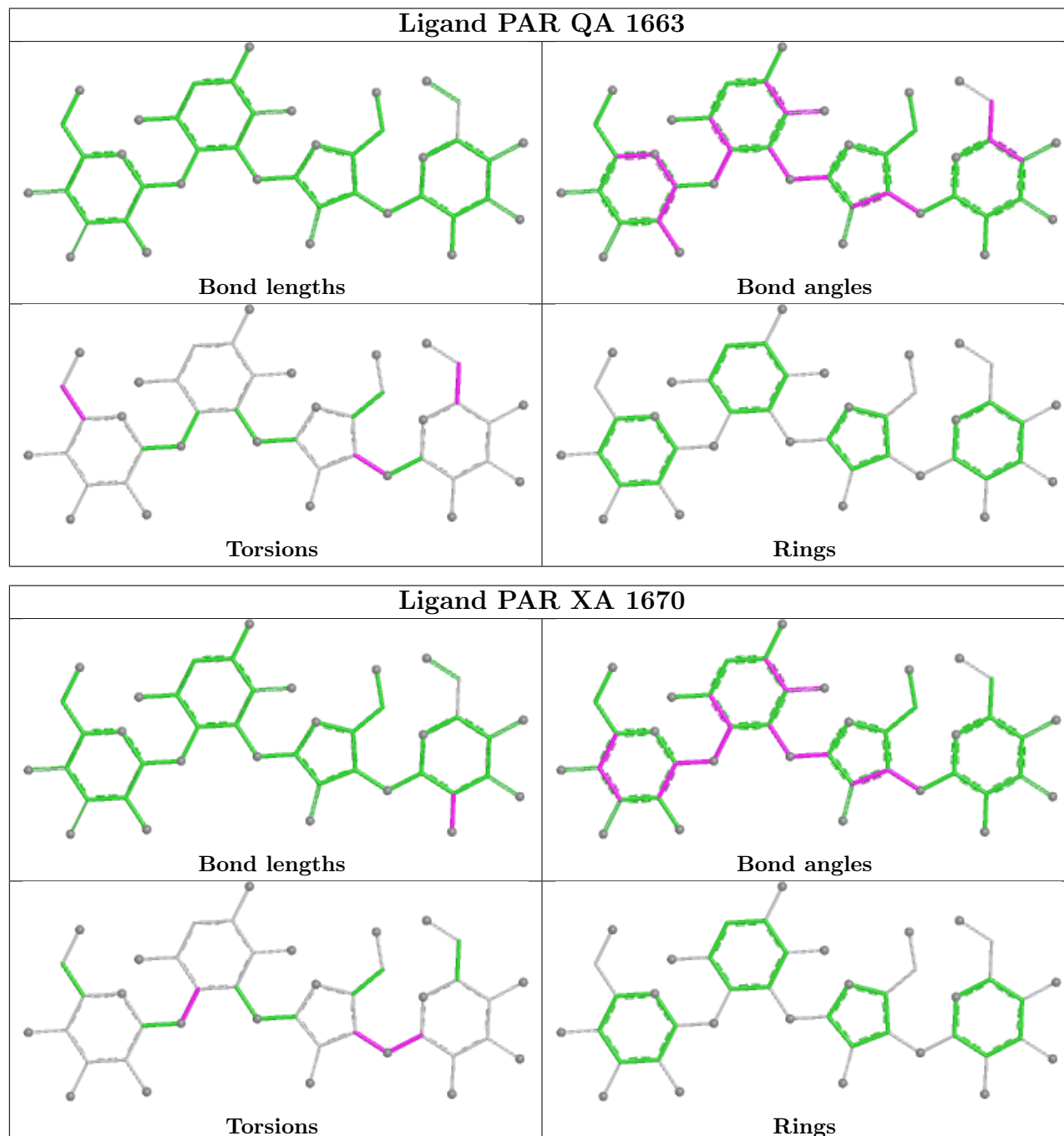
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1670	PAR	4	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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.19	31 (2%) 63 42	53, 93, 175, 270	0
1	XA	1500/1522 (98%)	0.08	20 (1%) 75 56	48, 82, 158, 266	0
2	QB	237/256 (92%)	0.78	20 (8%) 17 9	86, 128, 167, 198	0
2	XB	237/256 (92%)	0.57	11 (4%) 37 20	72, 111, 154, 176	0
3	QC	205/239 (85%)	0.72	18 (8%) 15 9	90, 129, 158, 170	0
3	XC	205/239 (85%)	0.49	13 (6%) 26 14	68, 101, 144, 170	0
4	QD	208/209 (99%)	0.52	11 (5%) 32 17	62, 89, 113, 137	0
4	XD	208/209 (99%)	0.76	21 (10%) 12 6	64, 94, 123, 150	0
5	QE	151/162 (93%)	0.53	9 (5%) 27 15	78, 105, 133, 152	0
5	XE	151/162 (93%)	0.26	6 (3%) 42 23	55, 82, 115, 150	0
6	QF	101/101 (100%)	0.30	2 (1%) 65 44	55, 85, 114, 173	0
6	XF	101/101 (100%)	0.26	2 (1%) 65 44	64, 90, 115, 138	0
7	QG	155/156 (99%)	0.79	11 (7%) 22 12	92, 115, 160, 177	0
7	XG	155/156 (99%)	0.48	6 (3%) 43 24	72, 98, 135, 156	0
8	QH	138/138 (100%)	0.85	14 (10%) 12 6	72, 102, 128, 145	0
8	XH	138/138 (100%)	0.58	6 (4%) 40 22	58, 88, 117, 138	0
9	QI	127/128 (99%)	1.42	30 (23%) 2 1	101, 129, 153, 172	0
9	XI	127/128 (99%)	1.05	19 (14%) 5 3	64, 111, 147, 159	0
10	QJ	99/105 (94%)	1.52	29 (29%) 1 1	111, 138, 174, 179	0
10	XJ	99/105 (94%)	1.12	12 (12%) 8 5	66, 119, 157, 170	0
11	QK	119/129 (92%)	0.81	8 (6%) 24 13	62, 97, 132, 163	0
11	XK	119/129 (92%)	0.75	8 (6%) 24 13	59, 85, 126, 147	0
12	QL	125/131 (95%)	1.15	20 (16%) 5 2	62, 90, 129, 179	0
12	XL	125/131 (95%)	0.79	17 (13%) 7 4	49, 70, 116, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	1.16	22 (18%)	3	1	88, 126, 155, 176	0
13	XM	121/126 (96%)	1.22	18 (14%)	5	3	72, 104, 143, 188	0
14	QN	60/61 (98%)	1.74	19 (31%)	1	1	98, 129, 156, 196	0
14	XN	60/61 (98%)	1.29	14 (23%)	2	1	66, 90, 123, 139	0
15	QO	88/89 (98%)	0.66	4 (4%)	38	20	62, 90, 125, 137	0
15	XO	88/89 (98%)	0.56	4 (4%)	38	20	56, 77, 114, 123	0
16	QP	84/88 (95%)	0.75	6 (7%)	22	12	63, 86, 115, 144	0
16	XP	84/88 (95%)	0.76	4 (4%)	35	19	70, 90, 127, 147	0
17	QQ	100/105 (95%)	0.76	8 (8%)	18	10	66, 91, 123, 149	0
17	XQ	100/105 (95%)	0.67	9 (9%)	15	8	63, 88, 116, 133	0
18	QR	70/88 (79%)	0.41	1 (1%)	73	53	63, 90, 126, 161	0
18	XR	70/88 (79%)	0.43	2 (2%)	53	32	60, 93, 118, 160	0
19	QS	84/93 (90%)	1.38	19 (22%)	2	1	101, 139, 176, 223	0
19	XS	84/93 (90%)	0.79	12 (14%)	6	3	77, 107, 139, 154	0
20	QT	99/106 (93%)	1.20	19 (19%)	3	1	63, 93, 138, 181	0
20	XT	99/106 (93%)	1.38	27 (27%)	1	1	70, 97, 127, 161	0
21	QU	25/27 (92%)	1.89	10 (40%)	1	0	95, 116, 129, 131	0
21	XU	25/27 (92%)	1.49	6 (24%)	2	1	75, 99, 123, 131	0
22	QV	77/77 (100%)	0.48	3 (3%)	43	24	71, 114, 165, 197	0
22	XV	77/77 (100%)	0.37	4 (5%)	33	17	57, 94, 129, 182	0
23	QX	18/19 (94%)	1.55	6 (33%)	1	0	77, 133, 218, 227	0
23	XX	18/19 (94%)	1.71	8 (44%)	0	0	63, 135, 222, 242	0
24	QY	75/76 (98%)	1.52	21 (28%)	1	1	79, 187, 255, 279	0
24	XY	75/76 (98%)	1.06	14 (18%)	3	1	70, 166, 221, 268	0
25	R0	82/85 (96%)	0.93	9 (10%)	10	5	60, 84, 110, 154	0
25	Y0	82/85 (96%)	0.66	5 (6%)	27	15	42, 60, 91, 131	0
26	R1	97/98 (98%)	0.96	10 (10%)	12	6	49, 69, 132, 183	0
26	Y1	97/98 (98%)	0.69	14 (14%)	6	3	34, 58, 127, 176	0
27	R2	69/72 (95%)	0.79	5 (7%)	21	11	59, 90, 130, 181	0
27	Y2	69/72 (95%)	0.71	6 (8%)	16	9	47, 66, 114, 172	0
28	R3	59/60 (98%)	0.71	2 (3%)	48	28	62, 84, 113, 156	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	Y3	59/60 (98%)	0.30	0	100	100	39, 59, 105, 133	0
29	R4	71/71 (100%)	1.31	13 (18%)	3	1	104, 148, 198, 223	0
29	Y4	71/71 (100%)	1.41	15 (21%)	2	1	80, 130, 196, 204	0
30	R5	59/60 (98%)	1.03	10 (16%)	4	2	47, 68, 154, 192	0
30	Y5	59/60 (98%)	1.08	13 (22%)	2	1	32, 60, 158, 166	0
31	R6	49/54 (90%)	2.53	29 (59%)	0	0	54, 98, 149, 190	0
31	Y6	49/54 (90%)	2.08	21 (42%)	0	0	46, 76, 135, 187	0
32	R7	49/49 (100%)	0.70	4 (8%)	17	10	45, 61, 101, 150	0
32	Y7	49/49 (100%)	0.53	4 (8%)	17	10	32, 43, 95, 165	0
33	R8	64/65 (98%)	1.26	16 (25%)	2	1	50, 73, 120, 176	0
33	Y8	64/65 (98%)	1.42	16 (25%)	2	1	41, 57, 93, 204	0
34	R9	37/37 (100%)	0.79	2 (5%)	31	17	68, 89, 125, 166	0
34	Y9	37/37 (100%)	0.28	0	100	100	44, 58, 84, 87	0
35	RA	2882/2915 (98%)	0.05	94 (3%)	49	29	43, 71, 193, 277	0
35	YA	2883/2915 (98%)	-0.11	43 (1%)	72	52	35, 54, 162, 262	0
36	RB	120/122 (98%)	0.22	1 (0%)	82	65	85, 107, 133, 149	0
36	YB	120/122 (98%)	-0.02	2 (1%)	69	48	61, 74, 95, 129	0
37	RD	272/276 (98%)	0.69	24 (8%)	15	9	41, 62, 101, 150	0
37	YD	272/276 (98%)	0.43	18 (6%)	24	13	31, 53, 83, 154	0
38	RE	205/206 (99%)	0.78	22 (10%)	11	6	45, 75, 130, 185	0
38	YE	205/206 (99%)	0.64	21 (10%)	12	6	28, 59, 118, 150	0
39	RF	202/210 (96%)	0.49	4 (1%)	65	44	46, 80, 128, 155	0
39	YF	202/210 (96%)	0.39	8 (3%)	42	23	36, 58, 122, 170	0
40	RG	181/182 (99%)	0.78	14 (7%)	19	10	76, 118, 152, 165	0
40	YG	181/182 (99%)	0.53	6 (3%)	49	29	65, 87, 128, 186	0
41	RH	170/180 (94%)	1.26	35 (20%)	2	1	88, 128, 160, 194	0
41	YH	170/180 (94%)	0.80	22 (12%)	7	4	48, 74, 113, 176	0
42	RI	146/148 (98%)	0.69	8 (5%)	30	16	63, 103, 140, 152	0
42	YI	146/148 (98%)	0.71	9 (6%)	26	14	56, 100, 139, 178	0
43	RN	138/140 (98%)	0.65	10 (7%)	21	11	52, 82, 113, 159	0
43	YN	138/140 (98%)	0.49	5 (3%)	46	26	36, 57, 104, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RO	122/122 (100%)	0.39	2 (1%) 70 49	45, 71, 97, 116	0
44	YO	122/122 (100%)	0.20	1 (0%) 82 65	34, 57, 82, 100	0
45	RP	150/150 (100%)	1.38	37 (24%) 2 1	53, 93, 141, 205	0
45	YP	150/150 (100%)	0.98	22 (14%) 6 3	29, 70, 117, 168	0
46	RQ	141/141 (100%)	1.31	30 (21%) 2 1	55, 89, 135, 178	0
46	YQ	141/141 (100%)	0.94	19 (13%) 7 4	40, 63, 116, 144	0
47	RR	118/118 (100%)	0.59	5 (4%) 40 22	48, 66, 90, 130	0
47	YR	118/118 (100%)	0.56	5 (4%) 40 22	37, 55, 82, 115	0
48	RS	111/112 (99%)	0.93	16 (14%) 6 3	73, 103, 141, 187	0
48	YS	111/112 (99%)	0.59	9 (8%) 18 10	53, 76, 127, 186	0
49	RT	137/146 (93%)	0.70	13 (9%) 14 7	54, 77, 137, 165	0
49	YT	137/146 (93%)	0.65	12 (8%) 15 9	45, 68, 129, 164	0
50	RU	117/118 (99%)	0.72	9 (7%) 19 10	49, 79, 122, 169	0
50	YU	117/118 (99%)	0.40	4 (3%) 48 28	24, 53, 91, 157	0
51	RV	101/101 (100%)	0.50	7 (6%) 23 12	53, 89, 135, 184	0
51	YV	101/101 (100%)	0.41	7 (6%) 23 12	32, 65, 113, 158	0
52	RW	113/113 (100%)	0.46	6 (5%) 32 17	45, 64, 96, 171	0
52	YW	113/113 (100%)	0.19	2 (1%) 67 47	33, 49, 88, 158	0
53	RX	92/96 (95%)	0.68	8 (8%) 16 9	53, 74, 99, 105	0
53	YX	92/96 (95%)	0.31	4 (4%) 40 22	39, 55, 86, 133	0
54	RY	102/110 (92%)	1.12	14 (13%) 6 4	71, 97, 134, 158	0
54	YY	102/110 (92%)	0.49	2 (1%) 65 44	44, 70, 106, 139	0
55	RZ	183/206 (88%)	1.23	34 (18%) 3 1	93, 135, 195, 224	0
55	YZ	183/206 (88%)	1.07	30 (16%) 4 2	56, 104, 184, 226	0
All	All	21011/21588 (97%)	0.46	1442 (6%) 23 12	24, 81, 157, 279	0

The worst 5 of 1442 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	12.8
11	QK	128	ALA	12.1
11	XK	129	SER	12.1
45	RP	13	ASN	10.6
13	XM	101	GLN	8.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3218	1/1	0.08	1.15	161,161,161,161	0
56	MG	YA	3172	1/1	0.09	0.41	115,115,115,115	0
56	MG	RA	3148	1/1	0.11	0.52	156,156,156,156	0
56	MG	YA	3346	1/1	0.13	0.54	112,112,112,112	0
56	MG	XA	1692	1/1	0.16	0.53	126,126,126,126	0
56	MG	YA	3340	1/1	0.19	0.64	117,117,117,117	0
56	MG	QA	1625	1/1	0.22	0.47	105,105,105,105	0
56	MG	QA	1653	1/1	0.22	0.25	144,144,144,144	0
56	MG	QX	102	1/1	0.23	0.55	137,137,137,137	0
56	MG	XA	1661	1/1	0.24	0.34	139,139,139,139	0
56	MG	RA	3170	1/1	0.24	0.58	159,159,159,159	0
56	MG	QA	1659	1/1	0.24	0.24	154,154,154,154	0
56	MG	RA	3236	1/1	0.24	0.89	182,182,182,182	0
56	MG	RA	3259	1/1	0.24	0.33	105,105,105,105	0
56	MG	RA	3012	1/1	0.25	0.47	120,120,120,120	0
56	MG	RA	3178	1/1	0.25	0.85	102,102,102,102	0
56	MG	RA	3217	1/1	0.26	0.49	74,74,74,74	0
56	MG	YA	3290	1/1	0.26	0.30	73,73,73,73	0
56	MG	RA	3112	1/1	0.29	0.65	131,131,131,131	0
56	MG	XA	1659	1/1	0.29	0.27	112,112,112,112	0
56	MG	YA	3233	1/1	0.32	0.44	90,90,90,90	0
56	MG	YA	3106	1/1	0.32	0.94	126,126,126,126	0
56	MG	RA	3120	1/1	0.33	0.55	106,106,106,106	0
56	MG	RA	3140	1/1	0.33	0.29	89,89,89,89	0
56	MG	RA	3164	1/1	0.34	0.83	121,121,121,121	0
56	MG	QA	1643	1/1	0.34	0.72	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1647	1/1	0.34	0.31	129,129,129,129	0
56	MG	RA	3173	1/1	0.34	0.47	109,109,109,109	0
56	MG	RA	3159	1/1	0.35	0.72	104,104,104,104	0
56	MG	YA	3118	1/1	0.37	0.29	52,52,52,52	0
56	MG	XA	1629	1/1	0.37	0.31	82,82,82,82	0
56	MG	QA	1658	1/1	0.37	0.44	108,108,108,108	0
56	MG	RA	3219	1/1	0.38	0.38	126,126,126,126	0
56	MG	RA	3166	1/1	0.38	0.50	126,126,126,126	0
56	MG	RA	3180	1/1	0.38	0.45	80,80,80,80	0
56	MG	QA	1601	1/1	0.38	0.79	134,134,134,134	0
56	MG	RA	3139	1/1	0.38	0.58	133,133,133,133	0
56	MG	YA	3163	1/1	0.39	0.55	137,137,137,137	0
56	MG	RA	3063	1/1	0.40	0.24	111,111,111,111	0
56	MG	YA	3218	1/1	0.41	0.39	99,99,99,99	0
56	MG	XA	1636	1/1	0.42	0.23	75,75,75,75	0
56	MG	XA	1655	1/1	0.42	0.85	127,127,127,127	0
56	MG	QA	1619	1/1	0.43	0.24	79,79,79,79	0
56	MG	XA	1648	1/1	0.44	0.46	101,101,101,101	0
56	MG	RA	3122	1/1	0.44	0.56	124,124,124,124	0
56	MG	YA	3164	1/1	0.44	0.22	57,57,57,57	0
56	MG	XA	1662	1/1	0.45	0.56	105,105,105,105	0
56	MG	RA	3151	1/1	0.45	0.50	95,95,95,95	0
56	MG	XX	101	1/1	0.45	0.45	104,104,104,104	0
56	MG	RA	3206	1/1	0.45	0.47	170,170,170,170	0
56	MG	YA	3202	1/1	0.45	0.55	104,104,104,104	0
56	MG	YA	3220	1/1	0.46	0.49	86,86,86,86	0
56	MG	RA	3130	1/1	0.46	0.26	68,68,68,68	0
56	MG	RA	3215	1/1	0.46	0.48	99,99,99,99	0
56	MG	QA	1656	1/1	0.46	0.23	124,124,124,124	0
56	MG	RA	3195	1/1	0.46	0.35	117,117,117,117	0
56	MG	YA	3246	1/1	0.47	0.65	82,82,82,82	0
56	MG	RA	3013	1/1	0.47	0.64	127,127,127,127	0
56	MG	YA	3155	1/1	0.48	0.54	104,104,104,104	0
56	MG	XA	1619	1/1	0.48	0.45	89,89,89,89	0
56	MG	XA	1654	1/1	0.48	0.72	108,108,108,108	0
56	MG	QA	1618	1/1	0.49	0.62	97,97,97,97	0
56	MG	RA	3102	1/1	0.49	0.23	66,66,66,66	0
56	MG	YA	3168	1/1	0.49	0.49	102,102,102,102	0
56	MG	RA	3126	1/1	0.50	0.47	77,77,77,77	0
56	MG	RA	3249	1/1	0.51	0.91	117,117,117,117	0
56	MG	RA	3057	1/1	0.51	0.57	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1607	1/1	0.51	0.40	93,93,93,93	0
56	MG	RA	3118	1/1	0.51	0.48	153,153,153,153	0
56	MG	QA	1620	1/1	0.51	0.22	113,113,113,113	0
56	MG	YA	3342	1/1	0.51	0.27	97,97,97,97	0
56	MG	RA	3051	1/1	0.51	0.52	88,88,88,88	0
56	MG	QA	1655	1/1	0.52	0.33	125,125,125,125	0
56	MG	XA	1667	1/1	0.52	0.44	107,107,107,107	0
56	MG	R9	101	1/1	0.53	0.67	140,140,140,140	0
56	MG	XA	1608	1/1	0.54	0.15	147,147,147,147	0
56	MG	RA	3202	1/1	0.54	0.44	196,196,196,196	0
56	MG	XA	1657	1/1	0.54	0.27	96,96,96,96	0
56	MG	YA	3288	1/1	0.54	0.50	106,106,106,106	0
56	MG	YA	3321	1/1	0.55	0.54	90,90,90,90	0
56	MG	QA	1637	1/1	0.55	0.29	74,74,74,74	0
56	MG	RA	3192	1/1	0.55	0.39	101,101,101,101	0
56	MG	YA	3206	1/1	0.55	0.61	103,103,103,103	0
56	MG	YQ	203	1/1	0.55	0.49	104,104,104,104	0
56	MG	RA	3245	1/1	0.56	0.36	79,79,79,79	0
56	MG	RA	3207	1/1	0.56	0.30	77,77,77,77	0
56	MG	XA	1614	1/1	0.56	0.43	114,114,114,114	0
56	MG	XA	1658	1/1	0.56	0.26	88,88,88,88	0
56	MG	QA	1644	1/1	0.56	0.14	142,142,142,142	0
56	MG	XA	1602	1/1	0.57	0.30	85,85,85,85	0
56	MG	RA	3003	1/1	0.57	0.57	172,172,172,172	0
56	MG	RA	3220	1/1	0.57	0.20	102,102,102,102	0
56	MG	YP	201	1/1	0.58	0.55	102,102,102,102	0
56	MG	QA	1612	1/1	0.58	0.62	85,85,85,85	0
56	MG	RA	3221	1/1	0.59	0.27	90,90,90,90	0
56	MG	YA	3286	1/1	0.59	0.41	83,83,83,83	0
56	MG	QA	1635	1/1	0.59	0.35	103,103,103,103	0
56	MG	RA	3191	1/1	0.59	0.19	102,102,102,102	0
56	MG	QA	1617	1/1	0.59	0.36	62,62,62,62	0
56	MG	XA	1689	1/1	0.60	0.23	65,65,65,65	0
56	MG	YA	3238	1/1	0.60	0.18	67,67,67,67	0
56	MG	YB	201	1/1	0.60	0.48	97,97,97,97	0
56	MG	XA	1690	1/1	0.60	0.20	49,49,49,49	0
56	MG	RA	3153	1/1	0.60	0.28	116,116,116,116	0
56	MG	QA	1657	1/1	0.61	0.28	102,102,102,102	0
56	MG	RA	3210	1/1	0.61	0.36	103,103,103,103	0
56	MG	RA	3263	1/1	0.61	0.34	75,75,75,75	0
56	MG	RA	3201	1/1	0.61	0.37	92,92,92,92	0
56	MG	QA	1647	1/1	0.61	0.28	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3143	1/1	0.61	0.35	102,102,102,102	0
56	MG	RA	3045	1/1	0.62	0.38	105,105,105,105	0
56	MG	QA	1642	1/1	0.62	0.20	96,96,96,96	0
56	MG	QA	1626	1/1	0.62	0.13	71,71,71,71	0
56	MG	QA	1632	1/1	0.62	0.76	113,113,113,113	0
56	MG	XA	1620	1/1	0.62	0.22	83,83,83,83	0
56	MG	RA	3223	1/1	0.63	0.58	120,120,120,120	0
56	MG	RA	3133	1/1	0.63	0.35	113,113,113,113	0
56	MG	RA	3113	1/1	0.63	0.34	72,72,72,72	0
56	MG	QA	1672	1/1	0.63	0.36	82,82,82,82	0
56	MG	QA	1614	1/1	0.63	0.35	67,67,67,67	0
56	MG	YA	3234	1/1	0.63	0.35	129,129,129,129	0
56	MG	RA	3073	1/1	0.64	0.52	92,92,92,92	0
56	MG	YA	3326	1/1	0.64	0.33	78,78,78,78	0
56	MG	RA	3121	1/1	0.64	0.35	89,89,89,89	0
56	MG	YA	3241	1/1	0.64	0.34	128,128,128,128	0
56	MG	RA	3155	1/1	0.64	0.19	69,69,69,69	0
56	MG	XA	1611	1/1	0.64	0.30	73,73,73,73	0
56	MG	YA	3222	1/1	0.64	0.28	64,64,64,64	0
56	MG	RA	3264	1/1	0.64	0.18	66,66,66,66	0
56	MG	XA	1663	1/1	0.65	0.27	109,109,109,109	0
56	MG	YA	3333	1/1	0.65	0.45	74,74,74,74	0
56	MG	XA	1646	1/1	0.65	0.41	122,122,122,122	0
56	MG	RA	3181	1/1	0.65	0.32	78,78,78,78	0
56	MG	XA	1634	1/1	0.66	0.21	72,72,72,72	0
56	MG	RA	3044	1/1	0.66	0.36	78,78,78,78	0
56	MG	YA	3205	1/1	0.66	0.40	66,66,66,66	0
56	MG	QA	1638	1/1	0.66	0.41	97,97,97,97	0
56	MG	YA	3217	1/1	0.66	0.29	126,126,126,126	0
56	MG	YA	3252	1/1	0.66	0.20	37,37,37,37	0
56	MG	RA	3277	1/1	0.66	0.44	71,71,71,71	0
56	MG	YB	203	1/1	0.66	0.23	77,77,77,77	0
56	MG	RA	3279	1/1	0.66	0.86	105,105,105,105	0
56	MG	XA	1632	1/1	0.66	0.49	92,92,92,92	0
56	MG	RA	3150	1/1	0.67	0.19	86,86,86,86	0
56	MG	XA	1633	1/1	0.67	0.36	95,95,95,95	0
56	MG	RA	3271	1/1	0.67	0.29	86,86,86,86	0
56	MG	XA	1691	1/1	0.67	0.57	98,98,98,98	0
56	MG	XA	1650	1/1	0.67	0.11	106,106,106,106	0
56	MG	RA	3011	1/1	0.67	0.54	108,108,108,108	0
56	MG	YA	3187	1/1	0.67	0.12	57,57,57,57	0
56	MG	XA	1644	1/1	0.67	0.22	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3323	1/1	0.67	0.48	77,77,77,77	0
56	MG	RP	203	1/1	0.68	0.30	79,79,79,79	0
56	MG	RA	3001	1/1	0.68	0.23	64,64,64,64	0
56	MG	RA	3209	1/1	0.68	0.36	130,130,130,130	0
56	MG	RA	3142	1/1	0.68	0.42	176,176,176,176	0
56	MG	YA	3300	1/1	0.68	0.35	78,78,78,78	0
56	MG	YA	3239	1/1	0.68	0.44	133,133,133,133	0
56	MG	RA	3212	1/1	0.68	0.28	71,71,71,71	0
56	MG	YA	3193	1/1	0.68	0.67	108,108,108,108	0
56	MG	XM	201	1/1	0.69	0.16	111,111,111,111	0
56	MG	RA	3067	1/1	0.69	0.51	55,55,55,55	0
56	MG	RA	3135	1/1	0.69	0.27	52,52,52,52	0
56	MG	RA	3161	1/1	0.69	0.33	85,85,85,85	0
56	MG	YA	3182	1/1	0.69	0.49	91,91,91,91	0
56	MG	XA	1668	1/1	0.69	0.60	92,92,92,92	0
56	MG	RA	3199	1/1	0.70	0.58	93,93,93,93	0
56	MG	RA	3035	1/1	0.70	0.61	78,78,78,78	0
56	MG	YA	3337	1/1	0.70	0.58	88,88,88,88	0
56	MG	RA	3177	1/1	0.70	0.30	95,95,95,95	0
56	MG	QA	1607	1/1	0.70	0.18	76,76,76,76	0
56	MG	YA	3103	1/1	0.70	0.17	61,61,61,61	0
56	MG	RB	203	1/1	0.70	0.34	64,64,64,64	0
56	MG	RA	3262	1/1	0.70	0.45	86,86,86,86	0
56	MG	YA	3154	1/1	0.70	0.42	81,81,81,81	0
56	MG	YP	203	1/1	0.70	0.32	47,47,47,47	0
56	MG	QA	1648	1/1	0.70	0.37	97,97,97,97	0
56	MG	YA	3198	1/1	0.71	0.31	67,67,67,67	0
56	MG	YA	3162	1/1	0.71	0.42	72,72,72,72	0
56	MG	YA	3294	1/1	0.71	0.55	98,98,98,98	0
56	MG	YA	3298	1/1	0.71	0.23	89,89,89,89	0
56	MG	YA	3191	1/1	0.71	0.43	80,80,80,80	0
56	MG	RA	3247	1/1	0.71	0.21	66,66,66,66	0
56	MG	QA	1661	1/1	0.72	0.10	137,137,137,137	0
56	MG	RA	3196	1/1	0.72	0.29	90,90,90,90	0
56	MG	QA	1621	1/1	0.72	0.38	118,118,118,118	0
56	MG	YA	3061	1/1	0.72	0.25	44,44,44,44	0
56	MG	QA	1645	1/1	0.72	0.34	74,74,74,74	0
56	MG	YA	3165	1/1	0.72	0.21	77,77,77,77	0
56	MG	YA	3308	1/1	0.72	0.29	83,83,83,83	0
56	MG	QA	1649	1/1	0.72	0.38	79,79,79,79	0
56	MG	RA	3123	1/1	0.72	0.40	72,72,72,72	0
56	MG	YA	3122	1/1	0.72	0.27	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1642	1/1	0.73	0.20	81,81,81,81	0
56	MG	RA	3146	1/1	0.73	0.51	92,92,92,92	0
56	MG	YA	3329	1/1	0.73	0.23	66,66,66,66	0
56	MG	RA	3273	1/1	0.73	0.34	55,55,55,55	0
56	MG	RA	3152	1/1	0.73	0.21	48,48,48,48	0
56	MG	RA	3127	1/1	0.73	0.17	39,39,39,39	0
56	MG	XA	1664	1/1	0.73	0.36	87,87,87,87	0
56	MG	RA	3246	1/1	0.73	0.28	108,108,108,108	0
56	MG	YA	3114	1/1	0.73	0.23	43,43,43,43	0
56	MG	YA	3225	1/1	0.73	0.17	36,36,36,36	0
56	MG	QA	1602	1/1	0.73	0.26	43,43,43,43	0
56	MG	XA	1637	1/1	0.73	0.15	63,63,63,63	0
56	MG	XA	1638	1/1	0.73	0.17	66,66,66,66	0
56	MG	YA	3131	1/1	0.74	0.17	50,50,50,50	0
56	MG	RA	3275	1/1	0.74	0.36	92,92,92,92	0
56	MG	RA	3214	1/1	0.74	0.23	74,74,74,74	0
56	MG	RA	3266	1/1	0.74	0.49	80,80,80,80	0
56	MG	YQ	202	1/1	0.74	0.32	80,80,80,80	0
56	MG	XA	1680	1/1	0.74	0.36	56,56,56,56	0
56	MG	YA	3111	1/1	0.75	0.43	102,102,102,102	0
56	MG	YA	3262	1/1	0.75	0.24	70,70,70,70	0
56	MG	YA	3181	1/1	0.75	0.49	65,65,65,65	0
56	MG	RA	3083	1/1	0.75	0.25	64,64,64,64	0
56	MG	RA	3225	1/1	0.75	0.26	68,68,68,68	0
56	MG	XA	1613	1/1	0.75	0.13	52,52,52,52	0
56	MG	RA	3278	1/1	0.75	0.34	75,75,75,75	0
56	MG	RA	3233	1/1	0.75	0.48	91,91,91,91	0
56	MG	QA	1631	1/1	0.76	0.12	68,68,68,68	0
56	MG	YA	3167	1/1	0.76	0.20	35,35,35,35	0
56	MG	RA	3256	1/1	0.76	0.51	74,74,74,74	0
56	MG	RD	301	1/1	0.76	0.28	57,57,57,57	0
56	MG	QA	1670	1/1	0.76	0.32	77,77,77,77	0
56	MG	RA	3186	1/1	0.76	0.13	57,57,57,57	0
56	MG	RA	3080	1/1	0.76	0.24	49,49,49,49	0
56	MG	RA	3231	1/1	0.76	0.14	50,50,50,50	0
56	MG	XA	1684	1/1	0.77	0.30	61,61,61,61	0
56	MG	YA	3035	1/1	0.77	0.45	61,61,61,61	0
56	MG	YA	3199	1/1	0.77	0.20	53,53,53,53	0
56	MG	YA	3240	1/1	0.77	0.30	95,95,95,95	0
56	MG	RA	3244	1/1	0.77	0.44	56,56,56,56	0
56	MG	YA	3203	1/1	0.77	0.28	88,88,88,88	0
56	MG	RA	3252	1/1	0.77	0.47	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1628	1/1	0.77	0.72	96,96,96,96	0
56	MG	YA	3211	1/1	0.77	0.20	62,62,62,62	0
56	MG	YA	3179	1/1	0.77	0.26	71,71,71,71	0
56	MG	YA	3156	1/1	0.77	0.38	75,75,75,75	0
56	MG	YA	3158	1/1	0.77	0.19	43,43,43,43	0
56	MG	QA	1623	1/1	0.77	0.40	92,92,92,92	0
56	MG	YA	3190	1/1	0.77	0.21	64,64,64,64	0
56	MG	RA	3046	1/1	0.77	0.31	47,47,47,47	0
56	MG	YA	3197	1/1	0.78	0.72	82,82,82,82	0
56	MG	YA	3313	1/1	0.78	0.53	87,87,87,87	0
56	MG	RA	3099	1/1	0.78	0.40	42,42,42,42	0
56	MG	QA	1654	1/1	0.78	0.31	77,77,77,77	0
56	MG	RA	3042	1/1	0.78	0.30	46,46,46,46	0
56	MG	RB	202	1/1	0.78	0.14	75,75,75,75	0
56	MG	XA	1671	1/1	0.78	0.52	62,62,62,62	0
56	MG	YA	3144	1/1	0.78	0.10	35,35,35,35	0
56	MG	XA	1678	1/1	0.78	0.28	55,55,55,55	0
56	MG	YA	3039	1/1	0.78	0.30	44,44,44,44	0
56	MG	RA	3203	1/1	0.78	0.62	101,101,101,101	0
56	MG	YA	3189	1/1	0.78	0.28	67,67,67,67	0
56	MG	YA	3291	1/1	0.78	0.34	90,90,90,90	0
56	MG	YA	3076	1/1	0.78	0.39	54,54,54,54	0
56	MG	RA	3162	1/1	0.78	0.19	58,58,58,58	0
56	MG	RA	3183	1/1	0.78	0.22	49,49,49,49	0
56	MG	YA	3301	1/1	0.78	0.13	28,28,28,28	0
56	MG	QA	1608	1/1	0.79	0.17	79,79,79,79	0
56	MG	QA	1646	1/1	0.79	0.23	97,97,97,97	0
56	MG	YA	3338	1/1	0.79	0.74	94,94,94,94	0
56	MG	RA	3149	1/1	0.79	0.48	89,89,89,89	0
56	MG	XA	1666	1/1	0.79	0.13	145,145,145,145	0
56	MG	RA	3250	1/1	0.79	0.50	63,63,63,63	0
56	MG	YA	3145	1/1	0.79	0.23	49,49,49,49	0
56	MG	YA	3151	1/1	0.79	0.15	38,38,38,38	0
56	MG	XA	1625	1/1	0.79	0.10	45,45,45,45	0
56	MG	XA	1669	1/1	0.79	0.11	43,43,43,43	0
56	MG	YA	3228	1/1	0.79	0.23	60,60,60,60	0
56	MG	R0	101	1/1	0.79	0.26	57,57,57,57	0
56	MG	YA	3285	1/1	0.80	0.23	57,57,57,57	0
56	MG	RA	3222	1/1	0.80	0.21	86,86,86,86	0
56	MG	YA	3088	1/1	0.80	0.39	45,45,45,45	0
56	MG	RA	3235	1/1	0.80	0.35	51,51,51,51	0
56	MG	QA	1630	1/1	0.80	0.12	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3293	1/1	0.80	0.38	73,73,73,73	0
56	MG	XA	1660	1/1	0.80	0.44	72,72,72,72	0
56	MG	RA	3224	1/1	0.80	0.20	63,63,63,63	0
56	MG	QA	1660	1/1	0.80	0.09	87,87,87,87	0
56	MG	QA	1639	1/1	0.80	0.26	81,81,81,81	0
56	MG	YA	3125	1/1	0.80	0.39	51,51,51,51	0
56	MG	XA	1631	1/1	0.80	0.24	71,71,71,71	0
56	MG	XA	1687	1/1	0.80	0.50	85,85,85,85	0
56	MG	YA	3282	1/1	0.80	0.20	40,40,40,40	0
56	MG	QA	1650	1/1	0.81	0.22	68,68,68,68	0
56	MG	RA	3276	1/1	0.81	0.35	84,84,84,84	0
56	MG	RA	3132	1/1	0.81	0.31	65,65,65,65	0
56	MG	RA	3055	1/1	0.81	0.12	33,33,33,33	0
56	MG	RA	3092	1/1	0.81	0.16	57,57,57,57	0
56	MG	XA	1618	1/1	0.81	0.32	43,43,43,43	0
56	MG	YA	3046	1/1	0.81	0.24	24,24,24,24	0
56	MG	YA	3344	1/1	0.81	0.12	44,44,44,44	0
56	MG	YA	3169	1/1	0.81	0.21	58,58,58,58	0
56	MG	QF	201	1/1	0.81	0.18	87,87,87,87	0
56	MG	QA	1651	1/1	0.81	0.17	88,88,88,88	0
56	MG	RA	3125	1/1	0.81	0.21	71,71,71,71	0
56	MG	QA	1603	1/1	0.81	0.54	93,93,93,93	0
56	MG	QA	1641	1/1	0.81	0.29	72,72,72,72	0
56	MG	YA	3188	1/1	0.81	0.15	72,72,72,72	0
56	MG	YA	3157	1/1	0.82	0.10	16,16,16,16	0
56	MG	YA	3091	1/1	0.82	0.32	64,64,64,64	0
56	MG	YA	3316	1/1	0.82	0.26	47,47,47,47	0
56	MG	RA	3010	1/1	0.82	0.27	35,35,35,35	0
56	MG	RA	3198	1/1	0.82	0.10	64,64,64,64	0
56	MG	RA	3138	1/1	0.82	0.37	47,47,47,47	0
56	MG	RA	3184	1/1	0.82	0.41	140,140,140,140	0
56	MG	Y6	102	1/1	0.82	0.10	9,9,9,9	0
56	MG	Y9	101	1/1	0.82	0.40	82,82,82,82	0
56	MG	YA	3033	1/1	0.82	0.24	43,43,43,43	0
56	MG	YA	3127	1/1	0.82	0.10	34,34,34,34	0
56	MG	YA	3215	1/1	0.82	0.13	36,36,36,36	0
56	MG	RA	3009	1/1	0.82	0.26	36,36,36,36	0
56	MG	XA	1681	1/1	0.82	0.32	58,58,58,58	0
56	MG	RA	3016	1/1	0.82	0.53	82,82,82,82	0
56	MG	YA	3060	1/1	0.82	0.21	39,39,39,39	0
56	MG	RA	3248	1/1	0.82	0.24	71,71,71,71	0
56	MG	YA	3226	1/1	0.82	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3114	1/1	0.82	0.16	48,48,48,48	0
56	MG	RA	3101	1/1	0.82	0.11	32,32,32,32	0
56	MG	YA	3025	1/1	0.83	0.34	26,26,26,26	0
56	MG	RA	3238	1/1	0.83	0.28	46,46,46,46	0
56	MG	XA	1649	1/1	0.83	0.30	81,81,81,81	0
56	MG	YA	3330	1/1	0.83	0.20	84,84,84,84	0
56	MG	YA	3096	1/1	0.83	0.23	39,39,39,39	0
56	MG	YA	3140	1/1	0.83	0.27	49,49,49,49	0
56	MG	YA	3141	1/1	0.83	0.26	38,38,38,38	0
56	MG	YA	3102	1/1	0.83	0.29	48,48,48,48	0
56	MG	XA	1685	1/1	0.83	0.43	58,58,58,58	0
56	MG	YA	3147	1/1	0.83	0.30	58,58,58,58	0
56	MG	YA	3171	1/1	0.83	0.21	73,73,73,73	0
56	MG	YA	3148	1/1	0.83	0.14	36,36,36,36	0
56	MG	YA	3306	1/1	0.83	0.40	90,90,90,90	0
56	MG	YA	3045	1/1	0.83	0.17	31,31,31,31	0
56	MG	RA	3111	1/1	0.83	0.41	69,69,69,69	0
56	MG	RA	3060	1/1	0.83	0.10	26,26,26,26	0
56	MG	RA	3104	1/1	0.83	0.20	57,57,57,57	0
56	MG	YX	101	1/1	0.83	0.23	101,101,101,101	0
56	MG	YA	3263	1/1	0.84	0.68	70,70,70,70	0
56	MG	QA	1636	1/1	0.84	0.21	52,52,52,52	0
56	MG	XV	101	1/1	0.84	0.20	77,77,77,77	0
56	MG	RP	202	1/1	0.84	0.36	95,95,95,95	0
56	MG	YA	3166	1/1	0.84	0.12	27,27,27,27	0
56	MG	RA	3097	1/1	0.84	0.51	87,87,87,87	0
56	MG	YA	3071	1/1	0.84	0.18	27,27,27,27	0
56	MG	RA	3269	1/1	0.84	0.40	60,60,60,60	0
56	MG	YA	3170	1/1	0.84	0.19	79,79,79,79	0
56	MG	YA	3297	1/1	0.84	0.16	56,56,56,56	0
56	MG	QA	1652	1/1	0.84	0.13	142,142,142,142	0
56	MG	RA	3048	1/1	0.84	0.33	38,38,38,38	0
56	MG	YA	3129	1/1	0.84	0.26	45,45,45,45	0
56	MG	YA	3302	1/1	0.84	0.41	85,85,85,85	0
56	MG	RA	3160	1/1	0.84	0.27	74,74,74,74	0
56	MG	YA	3132	1/1	0.84	0.15	40,40,40,40	0
56	MG	YA	3183	1/1	0.84	0.12	48,48,48,48	0
56	MG	XA	1639	1/1	0.84	0.62	79,79,79,79	0
56	MG	YA	3317	1/1	0.84	0.20	50,50,50,50	0
56	MG	YA	3261	1/1	0.85	0.60	71,71,71,71	0
56	MG	RA	3119	1/1	0.85	0.20	98,98,98,98	0
56	MG	RA	3211	1/1	0.85	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1673	1/1	0.85	0.39	62,62,62,62	0
56	MG	RA	3145	1/1	0.85	0.23	43,43,43,43	0
56	MG	YA	3055	1/1	0.85	0.48	91,91,91,91	0
56	MG	R5	101	1/1	0.85	0.14	31,31,31,31	0
56	MG	RA	3077	1/1	0.85	0.27	41,41,41,41	0
56	MG	YA	3150	1/1	0.85	0.27	78,78,78,78	0
56	MG	XA	1621	1/1	0.85	0.29	41,41,41,41	0
56	MG	QA	1662	1/1	0.85	0.23	63,63,63,63	0
56	MG	YA	3085	1/1	0.85	0.11	23,23,23,23	0
56	MG	YA	3128	1/1	0.85	0.31	39,39,39,39	0
56	MG	RB	201	1/1	0.85	0.14	72,72,72,72	0
56	MG	YA	3242	1/1	0.85	0.27	63,63,63,63	0
56	MG	YA	3243	1/1	0.85	0.34	53,53,53,53	0
56	MG	RA	3189	1/1	0.85	0.32	69,69,69,69	0
56	MG	YA	3159	1/1	0.85	0.21	30,30,30,30	0
56	MG	YA	3259	1/1	0.85	0.33	46,46,46,46	0
56	MG	YA	3260	1/1	0.85	0.38	56,56,56,56	0
56	MG	RA	3176	1/1	0.86	0.12	51,51,51,51	0
56	MG	QA	1634	1/1	0.86	0.18	59,59,59,59	0
56	MG	YA	3196	1/1	0.86	0.29	99,99,99,99	0
56	MG	RE	301	1/1	0.86	0.24	34,34,34,34	0
56	MG	RA	3193	1/1	0.86	0.16	121,121,121,121	0
56	MG	XA	1652	1/1	0.86	0.15	46,46,46,46	0
56	MG	YA	3248	1/1	0.86	0.20	36,36,36,36	0
56	MG	RA	3134	1/1	0.86	0.31	66,66,66,66	0
56	MG	RA	3062	1/1	0.86	0.23	29,29,29,29	0
56	MG	RA	3197	1/1	0.86	0.17	75,75,75,75	0
56	MG	QA	1615	1/1	0.86	0.12	92,92,92,92	0
56	MG	XA	1683	1/1	0.86	0.50	66,66,66,66	0
56	MG	YA	3213	1/1	0.86	0.33	57,57,57,57	0
56	MG	YA	3271	1/1	0.86	0.16	60,60,60,60	0
56	MG	YA	3273	1/1	0.86	0.17	37,37,37,37	0
56	MG	YA	3175	1/1	0.86	0.08	35,35,35,35	0
56	MG	YA	3176	1/1	0.86	0.29	61,61,61,61	0
56	MG	YA	3178	1/1	0.86	0.28	44,44,44,44	0
56	MG	YA	3153	1/1	0.86	0.09	27,27,27,27	0
56	MG	YA	3347	1/1	0.86	0.40	74,74,74,74	0
56	MG	RA	3251	1/1	0.86	0.47	78,78,78,78	0
56	MG	RA	3154	1/1	0.86	0.20	57,57,57,57	0
56	MG	RA	3065	1/1	0.86	0.29	25,25,25,25	0
56	MG	QA	1668	1/1	0.86	0.53	90,90,90,90	0
56	MG	YQ	201	1/1	0.86	0.33	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3261	1/1	0.86	0.16	38,38,38,38	0
56	MG	RA	3174	1/1	0.86	0.08	52,52,52,52	0
56	MG	YA	3130	1/1	0.86	0.40	69,69,69,69	0
56	MG	RA	3074	1/1	0.87	0.20	53,53,53,53	0
56	MG	YA	3001	1/1	0.87	0.40	128,128,128,128	0
56	MG	YA	3146	1/1	0.87	0.17	48,48,48,48	0
56	MG	XA	1643	1/1	0.87	0.24	63,63,63,63	0
56	MG	YA	3257	1/1	0.87	0.23	32,32,32,32	0
56	MG	YA	3319	1/1	0.87	0.10	41,41,41,41	0
56	MG	XA	1630	1/1	0.87	0.33	68,68,68,68	0
56	MG	RA	3274	1/1	0.87	0.25	59,59,59,59	0
56	MG	QA	1610	1/1	0.87	0.17	24,24,24,24	0
56	MG	RA	3089	1/1	0.87	0.41	60,60,60,60	0
56	MG	RA	3090	1/1	0.87	0.26	51,51,51,51	0
56	MG	YA	3265	1/1	0.87	0.66	72,72,72,72	0
56	MG	YA	3334	1/1	0.87	0.74	98,98,98,98	0
56	MG	YA	3180	1/1	0.87	0.39	70,70,70,70	0
56	MG	YA	3047	1/1	0.87	0.16	19,19,19,19	0
56	MG	XA	1635	1/1	0.87	0.36	62,62,62,62	0
56	MG	XA	1651	1/1	0.87	0.28	68,68,68,68	0
56	MG	RA	3136	1/1	0.87	0.15	71,71,71,71	0
56	MG	RU	201	1/1	0.87	0.24	104,104,104,104	0
56	MG	YA	3229	1/1	0.87	0.10	38,38,38,38	0
56	MG	YA	3161	1/1	0.87	0.17	46,46,46,46	0
56	MG	RA	3165	1/1	0.87	0.20	73,73,73,73	0
56	MG	YA	3235	1/1	0.87	0.31	66,66,66,66	0
56	MG	YP	202	1/1	0.87	0.12	76,76,76,76	0
56	MG	XA	1656	1/1	0.87	0.35	60,60,60,60	0
56	MG	YA	3135	1/1	0.87	0.16	42,42,42,42	0
56	MG	YA	3136	1/1	0.87	0.10	34,34,34,34	0
56	MG	Y6	101	1/1	0.87	0.09	25,25,25,25	0
56	MG	RA	3156	1/1	0.87	0.13	46,46,46,46	0
56	MG	YA	3117	1/1	0.88	0.56	68,68,68,68	0
56	MG	RA	3006	1/1	0.88	0.42	65,65,65,65	0
56	MG	YA	3212	1/1	0.88	0.16	43,43,43,43	0
56	MG	RA	3226	1/1	0.88	0.28	80,80,80,80	0
56	MG	RA	3179	1/1	0.88	0.09	15,15,15,15	0
56	MG	YA	3216	1/1	0.88	0.12	51,51,51,51	0
56	MG	YA	3324	1/1	0.88	0.18	29,29,29,29	0
56	MG	YA	3048	1/1	0.88	0.24	26,26,26,26	0
56	MG	RA	3124	1/1	0.88	0.33	61,61,61,61	0
56	MG	YA	3219	1/1	0.88	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3015	1/1	0.88	0.16	40,40,40,40	0
56	MG	RA	3100	1/1	0.88	0.33	52,52,52,52	0
56	MG	XA	1626	1/1	0.88	0.29	71,71,71,71	0
56	MG	RA	3041	1/1	0.88	0.15	26,26,26,26	0
56	MG	RA	3258	1/1	0.88	0.31	61,61,61,61	0
56	MG	XA	1682	1/1	0.88	0.21	48,48,48,48	0
56	MG	YA	3232	1/1	0.88	0.15	65,65,65,65	0
56	MG	YA	3090	1/1	0.88	0.21	33,33,33,33	0
56	MG	RA	3239	1/1	0.88	0.44	73,73,73,73	0
56	MG	YA	3012	1/1	0.88	0.28	36,36,36,36	0
56	MG	YA	3237	1/1	0.88	0.18	58,58,58,58	0
56	MG	YB	204	1/1	0.88	0.39	58,58,58,58	0
56	MG	RA	3185	1/1	0.88	0.11	59,59,59,59	0
56	MG	YA	3029	1/1	0.88	0.15	28,28,28,28	0
56	MG	RA	3094	1/1	0.88	0.36	60,60,60,60	0
56	MG	RA	3147	1/1	0.88	0.20	67,67,67,67	0
56	MG	XA	1688	1/1	0.88	0.45	80,80,80,80	0
56	MG	YA	3173	1/1	0.88	0.38	72,72,72,72	0
56	MG	YA	3245	1/1	0.88	0.36	47,47,47,47	0
56	MG	YA	3315	1/1	0.89	0.09	30,30,30,30	0
56	MG	QA	1640	1/1	0.89	0.15	52,52,52,52	0
56	MG	RA	3232	1/1	0.89	0.45	81,81,81,81	0
56	MG	RA	3253	1/1	0.89	0.19	37,37,37,37	0
56	MG	YA	3041	1/1	0.89	0.11	9,9,9,9	0
56	MG	YA	3044	1/1	0.89	0.31	34,34,34,34	0
56	MG	QA	1629	1/1	0.89	0.15	52,52,52,52	0
56	MG	RA	3216	1/1	0.89	0.14	47,47,47,47	0
56	MG	YA	3269	1/1	0.89	0.14	14,14,14,14	0
56	MG	RA	3200	1/1	0.89	0.08	22,22,22,22	0
56	MG	YA	3331	1/1	0.89	0.21	53,53,53,53	0
56	MG	RA	3260	1/1	0.89	0.30	57,57,57,57	0
56	MG	YA	3230	1/1	0.89	0.27	60,60,60,60	0
56	MG	YA	3284	1/1	0.89	0.13	16,16,16,16	0
56	MG	RA	3076	1/1	0.89	0.14	52,52,52,52	0
56	MG	RA	3023	1/1	0.89	0.27	37,37,37,37	0
56	MG	RA	3079	1/1	0.89	0.22	33,33,33,33	0
56	MG	YA	3065	1/1	0.89	0.12	45,45,45,45	0
56	MG	RA	3024	1/1	0.89	0.18	36,36,36,36	0
56	MG	YA	3075	1/1	0.89	0.08	33,33,33,33	0
56	MG	RA	3082	1/1	0.89	0.16	39,39,39,39	0
56	MG	YA	3079	1/1	0.89	0.21	26,26,26,26	0
56	MG	YA	3081	1/1	0.89	0.21	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YE	301	1/1	0.89	0.17	17,17,17,17	0
56	MG	YA	3299	1/1	0.89	0.20	36,36,36,36	0
56	MG	XA	1675	1/1	0.89	0.27	36,36,36,36	0
56	MG	RA	3267	1/1	0.89	0.28	29,29,29,29	0
56	MG	RA	3028	1/1	0.89	0.17	47,47,47,47	0
56	MG	RA	3034	1/1	0.89	0.27	48,48,48,48	0
56	MG	RA	3163	1/1	0.89	0.17	53,53,53,53	0
56	MG	QA	1633	1/1	0.89	0.19	84,84,84,84	0
56	MG	RA	3237	1/1	0.90	0.28	50,50,50,50	0
56	MG	RA	3110	1/1	0.90	0.09	47,47,47,47	0
56	MG	RA	3020	1/1	0.90	0.20	52,52,52,52	0
56	MG	QA	1613	1/1	0.90	0.16	47,47,47,47	0
56	MG	QA	1669	1/1	0.90	0.15	49,49,49,49	0
56	MG	YA	3126	1/1	0.90	0.09	31,31,31,31	0
56	MG	RA	3182	1/1	0.90	0.15	58,58,58,58	0
56	MG	QA	1616	1/1	0.90	0.30	70,70,70,70	0
56	MG	YA	3320	1/1	0.90	0.37	67,67,67,67	0
56	MG	YA	3255	1/1	0.90	0.32	23,23,23,23	0
56	MG	YA	3207	1/1	0.90	0.06	25,25,25,25	0
56	MG	RA	3032	1/1	0.90	0.24	34,34,34,34	0
56	MG	RA	3168	1/1	0.90	0.18	45,45,45,45	0
56	MG	YA	3328	1/1	0.90	0.10	40,40,40,40	0
56	MG	QA	1604	1/1	0.90	0.22	32,32,32,32	0
56	MG	RA	3187	1/1	0.90	0.25	60,60,60,60	0
56	MG	RA	3188	1/1	0.90	0.22	92,92,92,92	0
56	MG	YA	3264	1/1	0.90	0.27	48,48,48,48	0
56	MG	RA	3172	1/1	0.90	0.10	37,37,37,37	0
56	MG	YA	3336	1/1	0.90	0.20	61,61,61,61	0
56	MG	RA	3254	1/1	0.90	0.28	63,63,63,63	0
56	MG	QA	1674	1/1	0.90	0.08	140,140,140,140	0
56	MG	YA	3143	1/1	0.90	0.09	27,27,27,27	0
56	MG	YA	3341	1/1	0.90	0.19	48,48,48,48	0
56	MG	RA	3158	1/1	0.90	0.38	76,76,76,76	0
56	MG	YA	3283	1/1	0.90	0.15	28,28,28,28	0
56	MG	XA	1674	1/1	0.90	0.12	52,52,52,52	0
56	MG	YA	3087	1/1	0.90	0.26	32,32,32,32	0
56	MG	YA	3010	1/1	0.90	0.28	36,36,36,36	0
56	MG	RA	3088	1/1	0.90	0.14	39,39,39,39	0
56	MG	YA	3013	1/1	0.90	0.16	9,9,9,9	0
56	MG	YB	206	1/1	0.90	0.13	56,56,56,56	0
56	MG	YA	3185	1/1	0.90	0.07	34,34,34,34	0
56	MG	XA	1627	1/1	0.90	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1679	1/1	0.90	0.08	50,50,50,50	0
56	MG	YA	3031	1/1	0.90	0.26	36,36,36,36	0
56	MG	YA	3236	1/1	0.90	0.26	54,54,54,54	0
56	MG	RA	3053	1/1	0.90	0.29	39,39,39,39	0
56	MG	RB	204	1/1	0.90	0.34	57,57,57,57	0
56	MG	YA	3113	1/1	0.90	0.13	41,41,41,41	0
57	PAR	XA	1670	42/42	0.90	0.13	59,64,86,122	0
56	MG	RA	3131	1/1	0.91	0.25	56,56,56,56	0
56	MG	QV	101	1/1	0.91	0.18	47,47,47,47	0
56	MG	Y0	101	1/1	0.91	0.18	33,33,33,33	0
56	MG	RA	3029	1/1	0.91	0.17	12,12,12,12	0
56	MG	YA	3089	1/1	0.91	0.16	18,18,18,18	0
56	MG	RA	3171	1/1	0.91	0.15	35,35,35,35	0
56	MG	Y8	101	1/1	0.91	0.17	31,31,31,31	0
56	MG	RF	301	1/1	0.91	0.08	59,59,59,59	0
56	MG	YA	3098	1/1	0.91	0.18	30,30,30,30	0
56	MG	YA	3303	1/1	0.91	0.14	43,43,43,43	0
56	MG	RP	201	1/1	0.91	0.49	207,207,207,207	0
56	MG	YA	3307	1/1	0.91	0.25	147,147,147,147	0
56	MG	YA	3007	1/1	0.91	0.21	26,26,26,26	0
56	MG	YA	3310	1/1	0.91	0.11	31,31,31,31	0
56	MG	RA	3190	1/1	0.91	0.07	42,42,42,42	0
56	MG	YA	3107	1/1	0.91	0.17	38,38,38,38	0
56	MG	YA	3231	1/1	0.91	0.11	49,49,49,49	0
56	MG	RA	3072	1/1	0.91	0.30	53,53,53,53	0
56	MG	RA	3093	1/1	0.91	0.14	23,23,23,23	0
56	MG	XA	1601	1/1	0.91	0.19	24,24,24,24	0
56	MG	QA	1624	1/1	0.91	0.33	79,79,79,79	0
56	MG	YA	3030	1/1	0.91	0.16	16,16,16,16	0
56	MG	YA	3120	1/1	0.91	0.31	78,78,78,78	0
56	MG	YA	3325	1/1	0.91	0.07	31,31,31,31	0
56	MG	XA	1606	1/1	0.91	0.41	57,57,57,57	0
56	MG	XA	1677	1/1	0.91	0.15	49,49,49,49	0
56	MG	RA	3194	1/1	0.91	0.12	75,75,75,75	0
56	MG	RA	3268	1/1	0.91	0.09	9,9,9,9	0
56	MG	XA	1610	1/1	0.91	0.15	37,37,37,37	0
56	MG	YA	3043	1/1	0.91	0.27	38,38,38,38	0
56	MG	QA	1671	1/1	0.91	0.13	54,54,54,54	0
56	MG	YA	3186	1/1	0.91	0.18	45,45,45,45	0
56	MG	RA	3054	1/1	0.91	0.30	29,29,29,29	0
56	MG	QA	1605	1/1	0.91	0.53	62,62,62,62	0
56	MG	RA	3141	1/1	0.91	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3022	1/1	0.91	0.17	40,40,40,40	0
56	MG	YA	3050	1/1	0.91	0.21	21,21,21,21	0
56	MG	YA	3192	1/1	0.91	0.09	45,45,45,45	0
56	MG	YA	3052	1/1	0.91	0.26	37,37,37,37	0
56	MG	YA	3195	1/1	0.91	0.23	70,70,70,70	0
56	MG	RA	3058	1/1	0.91	0.17	32,32,32,32	0
56	MG	RA	3103	1/1	0.91	0.19	35,35,35,35	0
56	MG	QA	1606	1/1	0.91	0.10	49,49,49,49	0
56	MG	YB	205	1/1	0.91	0.47	77,77,77,77	0
56	MG	QA	1609	1/1	0.91	0.13	57,57,57,57	0
56	MG	YA	3200	1/1	0.91	0.06	41,41,41,41	0
56	MG	YA	3069	1/1	0.91	0.30	42,42,42,42	0
56	MG	YA	3070	1/1	0.91	0.11	16,16,16,16	0
56	MG	YA	3204	1/1	0.91	0.09	30,30,30,30	0
56	MG	RA	3025	1/1	0.91	0.30	29,29,29,29	0
56	MG	YA	3072	1/1	0.91	0.10	41,41,41,41	0
56	MG	XA	1628	1/1	0.91	0.07	38,38,38,38	0
56	MG	XF	201	1/1	0.91	0.21	65,65,65,65	0
56	MG	RA	3257	1/1	0.91	0.22	46,46,46,46	0
56	MG	YA	3063	1/1	0.92	0.18	23,23,23,23	0
56	MG	XA	1676	1/1	0.92	0.20	60,60,60,60	0
56	MG	YA	3109	1/1	0.92	0.26	29,29,29,29	0
56	MG	RA	3265	1/1	0.92	0.25	38,38,38,38	0
56	MG	RA	3228	1/1	0.92	0.23	45,45,45,45	0
56	MG	YA	3177	1/1	0.92	0.22	53,53,53,53	0
56	MG	YA	3296	1/1	0.92	0.61	84,84,84,84	0
56	MG	YA	3335	1/1	0.92	0.29	53,53,53,53	0
56	MG	R8	101	1/1	0.92	0.11	47,47,47,47	0
56	MG	YA	3116	1/1	0.92	0.12	24,24,24,24	0
56	MG	RA	3087	1/1	0.92	0.21	28,28,28,28	0
56	MG	YA	3339	1/1	0.92	0.13	40,40,40,40	0
56	MG	YA	3073	1/1	0.92	0.27	58,58,58,58	0
56	MG	YA	3036	1/1	0.92	0.24	25,25,25,25	0
56	MG	RA	3116	1/1	0.92	0.12	24,24,24,24	0
56	MG	XA	1665	1/1	0.92	0.24	57,57,57,57	0
56	MG	YA	3305	1/1	0.92	0.22	47,47,47,47	0
56	MG	QA	1665	1/1	0.92	0.19	58,58,58,58	0
56	MG	RA	3204	1/1	0.92	0.19	72,72,72,72	0
56	MG	YB	202	1/1	0.92	0.17	34,34,34,34	0
56	MG	RA	3007	1/1	0.92	0.32	71,71,71,71	0
56	MG	YA	3160	1/1	0.92	0.15	43,43,43,43	0
56	MG	YA	3311	1/1	0.92	0.17	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1686	1/1	0.92	0.14	61,61,61,61	0
56	MG	XA	1640	1/1	0.92	0.26	45,45,45,45	0
56	MG	XA	1641	1/1	0.92	0.16	36,36,36,36	0
56	MG	QA	1611	1/1	0.92	0.19	35,35,35,35	0
56	MG	RA	3040	1/1	0.92	0.11	19,19,19,19	0
56	MG	YA	3019	1/1	0.92	0.21	18,18,18,18	0
56	MG	YA	3138	1/1	0.92	0.08	30,30,30,30	0
56	MG	YA	3139	1/1	0.92	0.20	34,34,34,34	0
56	MG	RA	3242	1/1	0.92	0.10	28,28,28,28	0
57	PAR	QA	1663	42/42	0.92	0.11	59,59,76,103	0
56	MG	YA	3026	1/1	0.92	0.15	26,26,26,26	0
56	MG	YA	3201	1/1	0.93	0.09	71,71,71,71	0
56	MG	YA	3123	1/1	0.93	0.07	16,16,16,16	0
56	MG	XA	1623	1/1	0.93	0.06	32,32,32,32	0
56	MG	XA	1624	1/1	0.93	0.20	34,34,34,34	0
56	MG	YA	3318	1/1	0.93	0.27	49,49,49,49	0
56	MG	RA	3084	1/1	0.93	0.06	15,15,15,15	0
56	MG	RA	3213	1/1	0.93	0.15	33,33,33,33	0
56	MG	YA	3016	1/1	0.93	0.28	28,28,28,28	0
56	MG	YA	3209	1/1	0.93	0.25	52,52,52,52	0
56	MG	XA	1653	1/1	0.93	0.27	70,70,70,70	0
56	MG	RA	3085	1/1	0.93	0.07	14,14,14,14	0
56	MG	RA	3070	1/1	0.93	0.14	32,32,32,32	0
56	MG	YA	3327	1/1	0.93	0.42	59,59,59,59	0
56	MG	YA	3214	1/1	0.93	0.17	47,47,47,47	0
56	MG	YA	3268	1/1	0.93	0.13	23,23,23,23	0
56	MG	YA	3133	1/1	0.93	0.15	46,46,46,46	0
56	MG	RA	3021	1/1	0.93	0.10	33,33,33,33	0
56	MG	RA	3107	1/1	0.93	0.06	35,35,35,35	0
56	MG	YA	3276	1/1	0.93	0.08	22,22,22,22	0
56	MG	YA	3278	1/1	0.93	0.12	18,18,18,18	0
56	MG	YA	3279	1/1	0.93	0.29	164,164,164,164	0
56	MG	RA	3109	1/1	0.93	0.10	43,43,43,43	0
56	MG	YA	3032	1/1	0.93	0.17	9,9,9,9	0
56	MG	RR	201	1/1	0.93	0.17	41,41,41,41	0
56	MG	RA	3031	1/1	0.93	0.17	22,22,22,22	0
56	MG	RA	3129	1/1	0.93	0.12	59,59,59,59	0
56	MG	YA	3037	1/1	0.93	0.20	39,39,39,39	0
56	MG	YA	3343	1/1	0.93	0.29	57,57,57,57	0
56	MG	YA	3227	1/1	0.93	0.07	36,36,36,36	0
56	MG	YA	3038	1/1	0.93	0.19	22,22,22,22	0
56	MG	RA	3002	1/1	0.93	0.27	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1666	1/1	0.93	0.20	29,29,29,29	0
56	MG	RA	3061	1/1	0.93	0.09	9,9,9,9	0
56	MG	RA	3169	1/1	0.93	0.22	35,35,35,35	0
56	MG	QA	1667	1/1	0.93	0.18	33,33,33,33	0
56	MG	YA	3152	1/1	0.93	0.22	63,63,63,63	0
56	MG	RA	3095	1/1	0.93	0.14	22,22,22,22	0
56	MG	RA	3227	1/1	0.93	0.14	90,90,90,90	0
56	MG	RA	3208	1/1	0.93	0.36	69,69,69,69	0
56	MG	XA	1617	1/1	0.93	0.19	46,46,46,46	0
56	MG	YA	3051	1/1	0.93	0.25	36,36,36,36	0
56	MG	RA	3229	1/1	0.93	0.11	17,17,17,17	0
56	MG	RA	3036	1/1	0.93	0.28	44,44,44,44	0
56	MG	YA	3057	1/1	0.93	0.10	9,9,9,9	0
56	MG	RA	3018	1/1	0.93	0.13	24,24,24,24	0
56	MG	QX	101	1/1	0.93	0.28	76,76,76,76	0
56	MG	YA	3312	1/1	0.93	0.23	44,44,44,44	0
56	MG	YA	3015	1/1	0.94	0.20	31,31,31,31	0
56	MG	YA	3184	1/1	0.94	0.09	36,36,36,36	0
56	MG	YA	3101	1/1	0.94	0.10	10,10,10,10	0
56	MG	YA	3067	1/1	0.94	0.20	23,23,23,23	0
56	MG	YA	3289	1/1	0.94	0.23	39,39,39,39	0
56	MG	RA	3205	1/1	0.94	0.23	53,53,53,53	0
56	MG	YA	3018	1/1	0.94	0.14	21,21,21,21	0
56	MG	YA	3332	1/1	0.94	0.10	42,42,42,42	0
56	MG	YA	3247	1/1	0.94	0.18	30,30,30,30	0
56	MG	XA	1615	1/1	0.94	0.29	36,36,36,36	0
56	MG	YA	3249	1/1	0.94	0.12	46,46,46,46	0
56	MG	YA	3251	1/1	0.94	0.26	18,18,18,18	0
56	MG	RA	3078	1/1	0.94	0.17	47,47,47,47	0
56	MG	YA	3110	1/1	0.94	0.11	29,29,29,29	0
56	MG	YA	3256	1/1	0.94	0.50	48,48,48,48	0
56	MG	RA	3069	1/1	0.94	0.15	37,37,37,37	0
56	MG	RA	3086	1/1	0.94	0.19	21,21,21,21	0
56	MG	RA	3234	1/1	0.94	0.46	65,65,65,65	0
56	MG	YA	3304	1/1	0.94	0.23	37,37,37,37	0
56	MG	RE	303	1/1	0.94	0.12	29,29,29,29	0
56	MG	YA	3002	1/1	0.94	0.17	20,20,20,20	0
56	MG	YA	3084	1/1	0.94	0.10	9,9,9,9	0
56	MG	YA	3004	1/1	0.94	0.09	9,9,9,9	0
56	MG	YA	3309	1/1	0.94	0.23	43,43,43,43	0
56	MG	YA	3121	1/1	0.94	0.07	11,11,11,11	0
56	MG	YA	3034	1/1	0.94	0.27	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1627	1/1	0.94	0.05	34,34,34,34	0
56	MG	YA	3270	1/1	0.94	0.13	22,22,22,22	0
56	MG	YA	3124	1/1	0.94	0.24	50,50,50,50	0
56	MG	RA	3071	1/1	0.94	0.20	37,37,37,37	0
56	MG	YA	3275	1/1	0.94	0.32	49,49,49,49	0
56	MG	RA	3167	1/1	0.94	0.20	62,62,62,62	0
56	MG	YA	3277	1/1	0.94	0.26	31,31,31,31	0
56	MG	YA	3062	1/1	0.94	0.18	28,28,28,28	0
56	MG	YA	3092	1/1	0.94	0.07	23,23,23,23	0
56	MG	YR	201	1/1	0.94	0.11	28,28,28,28	0
56	MG	YA	3322	1/1	0.94	0.14	35,35,35,35	0
56	MG	YA	3208	1/1	0.94	0.13	48,48,48,48	0
56	MG	RA	3068	1/1	0.94	0.17	40,40,40,40	0
56	MG	YA	3287	1/1	0.95	0.04	9,9,9,9	0
56	MG	RA	3030	1/1	0.95	0.16	30,30,30,30	0
56	MG	RA	3014	1/1	0.95	0.44	63,63,63,63	0
56	MG	RE	302	1/1	0.95	0.18	37,37,37,37	0
56	MG	RA	3056	1/1	0.95	0.08	32,32,32,32	0
56	MG	YA	3149	1/1	0.95	0.14	36,36,36,36	0
56	MG	YA	3017	1/1	0.95	0.08	16,16,16,16	0
56	MG	RA	3091	1/1	0.95	0.15	27,27,27,27	0
56	MG	YA	3253	1/1	0.95	0.12	9,9,9,9	0
56	MG	YA	3119	1/1	0.95	0.24	33,33,33,33	0
56	MG	YA	3078	1/1	0.95	0.22	31,31,31,31	0
56	MG	Y2	101	1/1	0.95	0.16	57,57,57,57	0
56	MG	YA	3020	1/1	0.95	0.14	12,12,12,12	0
56	MG	YA	3221	1/1	0.95	0.13	33,33,33,33	0
56	MG	YA	3021	1/1	0.95	0.14	11,11,11,11	0
56	MG	YA	3023	1/1	0.95	0.15	26,26,26,26	0
56	MG	Y5	101	1/1	0.95	0.09	36,36,36,36	0
56	MG	RA	3115	1/1	0.95	0.07	21,21,21,21	0
56	MG	RA	3241	1/1	0.95	0.07	33,33,33,33	0
56	MG	YA	3056	1/1	0.95	0.07	10,10,10,10	0
56	MG	RA	3108	1/1	0.95	0.13	47,47,47,47	0
56	MG	XA	1616	1/1	0.95	0.22	34,34,34,34	0
56	MG	YA	3093	1/1	0.95	0.10	13,13,13,13	0
56	MG	YA	3272	1/1	0.95	0.15	26,26,26,26	0
56	MG	RA	3117	1/1	0.95	0.05	20,20,20,20	0
56	MG	YA	3274	1/1	0.95	0.06	24,24,24,24	0
56	MG	XA	1645	1/1	0.95	0.11	37,37,37,37	0
56	MG	RA	3081	1/1	0.95	0.25	34,34,34,34	0
56	MG	YA	3064	1/1	0.95	0.17	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3137	1/1	0.95	0.09	31,31,31,31	0
56	MG	RA	3128	1/1	0.95	0.09	38,38,38,38	0
56	MG	YA	3280	1/1	0.95	0.19	31,31,31,31	0
56	MG	YA	3104	1/1	0.95	0.17	18,18,18,18	0
56	MG	YA	3066	1/1	0.95	0.07	26,26,26,26	0
56	MG	YA	3008	1/1	0.95	0.14	11,11,11,11	0
56	MG	YA	3068	1/1	0.95	0.07	22,22,22,22	0
56	MG	QA	1673	1/1	0.95	0.32	62,62,62,62	0
56	MG	XA	1603	1/1	0.96	0.25	41,41,41,41	0
56	MG	RA	3255	1/1	0.96	0.10	48,48,48,48	0
56	MG	YA	3244	1/1	0.96	0.17	56,56,56,56	0
56	MG	RA	3005	1/1	0.96	0.31	60,60,60,60	0
56	MG	YA	3077	1/1	0.96	0.18	12,12,12,12	0
56	MG	YA	3054	1/1	0.96	0.09	9,9,9,9	0
56	MG	YA	3009	1/1	0.96	0.11	21,21,21,21	0
56	MG	YA	3080	1/1	0.96	0.11	17,17,17,17	0
56	MG	RA	3064	1/1	0.96	0.29	17,17,17,17	0
56	MG	YA	3083	1/1	0.96	0.14	19,19,19,19	0
56	MG	QA	1664	1/1	0.96	0.12	43,43,43,43	0
56	MG	RA	3272	1/1	0.96	0.06	48,48,48,48	0
56	MG	YA	3086	1/1	0.96	0.17	30,30,30,30	0
56	MG	RA	3105	1/1	0.96	0.12	22,22,22,22	0
56	MG	RA	3106	1/1	0.96	0.11	22,22,22,22	0
56	MG	YA	3174	1/1	0.96	0.11	16,16,16,16	0
56	MG	RA	3026	1/1	0.96	0.14	42,42,42,42	0
56	MG	YA	3292	1/1	0.96	0.21	40,40,40,40	0
56	MG	RA	3033	1/1	0.96	0.14	28,28,28,28	0
56	MG	YE	303	1/1	0.96	0.08	15,15,15,15	0
56	MG	YN	201	1/1	0.96	0.15	32,32,32,32	0
56	MG	RA	3004	1/1	0.96	0.11	34,34,34,34	0
56	MG	RA	3157	1/1	0.96	0.17	38,38,38,38	0
56	MG	RA	3019	1/1	0.96	0.12	29,29,29,29	0
56	MG	YA	3266	1/1	0.96	0.12	26,26,26,26	0
56	MG	RA	3280	1/1	0.96	0.07	35,35,35,35	0
56	MG	YA	3024	1/1	0.96	0.12	14,14,14,14	0
56	MG	YA	3100	1/1	0.96	0.13	9,9,9,9	0
56	MG	RA	3281	1/1	0.96	0.29	146,146,146,146	0
56	MG	RA	3230	1/1	0.96	0.17	9,9,9,9	0
56	MG	YA	3049	1/1	0.96	0.14	15,15,15,15	0
59	ZN	QN	101	1/1	0.96	0.10	182,182,182,182	0
56	MG	YA	3005	1/1	0.97	0.07	9,9,9,9	0
56	MG	YA	3006	1/1	0.97	0.08	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3008	1/1	0.97	0.21	31,31,31,31	0
56	MG	YA	3250	1/1	0.97	0.26	28,28,28,28	0
56	MG	XA	1672	1/1	0.97	0.21	39,39,39,39	0
56	MG	RA	3096	1/1	0.97	0.19	23,23,23,23	0
56	MG	XA	1604	1/1	0.97	0.29	31,31,31,31	0
56	MG	YA	3254	1/1	0.97	0.14	17,17,17,17	0
56	MG	XA	1622	1/1	0.97	0.06	34,34,34,34	0
56	MG	YA	3295	1/1	0.97	0.23	31,31,31,31	0
56	MG	YA	3097	1/1	0.97	0.12	34,34,34,34	0
56	MG	RA	3047	1/1	0.97	0.11	24,24,24,24	0
56	MG	YA	3258	1/1	0.97	0.10	20,20,20,20	0
56	MG	YA	3099	1/1	0.97	0.13	11,11,11,11	0
56	MG	YA	3223	1/1	0.97	0.04	9,9,9,9	0
56	MG	YA	3224	1/1	0.97	0.07	9,9,9,9	0
56	MG	YA	3014	1/1	0.97	0.20	9,9,9,9	0
56	MG	YA	3042	1/1	0.97	0.13	9,9,9,9	0
56	MG	YA	3345	1/1	0.97	0.29	47,47,47,47	0
56	MG	RA	3098	1/1	0.97	0.07	16,16,16,16	0
56	MG	YA	3194	1/1	0.97	0.13	39,39,39,39	0
56	MG	YA	3134	1/1	0.97	0.10	10,10,10,10	0
56	MG	YA	3267	1/1	0.97	0.11	9,9,9,9	0
56	MG	RA	3017	1/1	0.97	0.11	17,17,17,17	0
56	MG	XA	1609	1/1	0.97	0.21	30,30,30,30	0
56	MG	Y1	101	1/1	0.97	0.09	49,49,49,49	0
56	MG	RA	3049	1/1	0.97	0.06	9,9,9,9	0
56	MG	YA	3108	1/1	0.97	0.06	9,9,9,9	0
56	MG	YE	302	1/1	0.97	0.10	9,9,9,9	0
56	MG	RA	3075	1/1	0.97	0.10	24,24,24,24	0
56	MG	XA	1612	1/1	0.97	0.08	20,20,20,20	0
56	MG	YA	3142	1/1	0.97	0.09	18,18,18,18	0
56	MG	RA	3027	1/1	0.97	0.12	21,21,21,21	0
56	MG	RA	3175	1/1	0.97	0.08	26,26,26,26	0
56	MG	RA	3243	1/1	0.97	0.04	31,31,31,31	0
56	MG	QA	1622	1/1	0.97	0.11	41,41,41,41	0
56	MG	YA	3028	1/1	0.97	0.05	9,9,9,9	0
56	MG	YA	3281	1/1	0.97	0.17	27,27,27,27	0
56	MG	RA	3039	1/1	0.97	0.05	9,9,9,9	0
56	MG	YA	3210	1/1	0.97	0.06	51,51,51,51	0
56	MG	YA	3003	1/1	0.97	0.10	9,9,9,9	0
58	SF4	QD	501	8/8	0.97	0.07	67,82,98,141	0
56	MG	RA	3270	1/1	0.97	0.10	25,25,25,25	0
59	ZN	Y9	102	1/1	0.97	0.04	59,59,59,59	0

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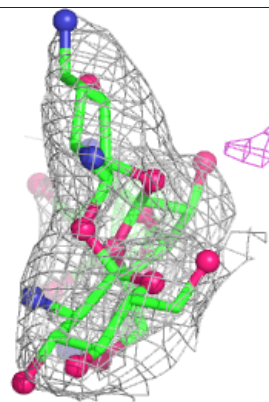
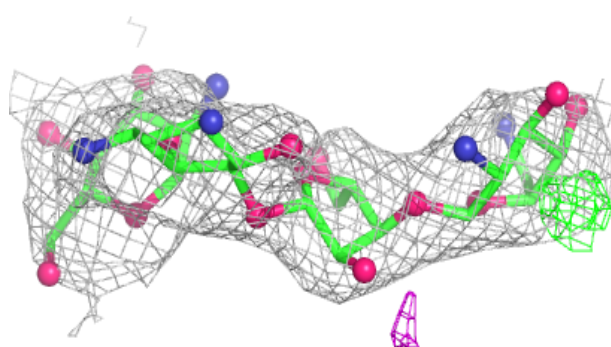
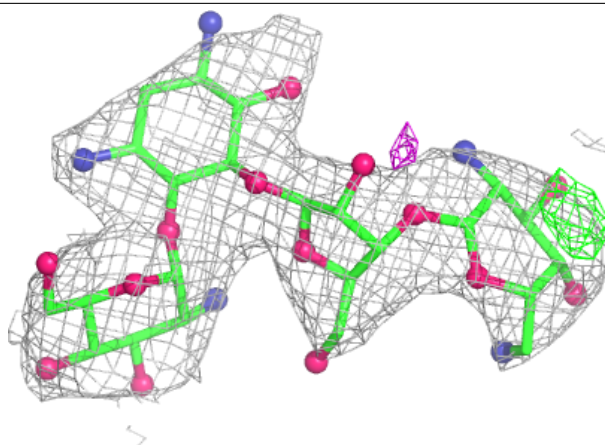
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3314	1/1	0.98	0.26	51,51,51,51	0
56	MG	RA	3052	1/1	0.98	0.04	15,15,15,15	0
56	MG	RA	3059	1/1	0.98	0.04	22,22,22,22	0
56	MG	RA	3137	1/1	0.98	0.15	13,13,13,13	0
56	MG	YA	3082	1/1	0.98	0.12	12,12,12,12	0
56	MG	YA	3040	1/1	0.98	0.06	9,9,9,9	0
56	MG	YA	3053	1/1	0.98	0.05	9,9,9,9	0
56	MG	RA	3038	1/1	0.98	0.08	15,15,15,15	0
56	MG	RA	3240	1/1	0.98	0.10	23,23,23,23	0
56	MG	RE	304	1/1	0.98	0.20	37,37,37,37	0
56	MG	YA	3105	1/1	0.98	0.04	9,9,9,9	0
56	MG	RA	3144	1/1	0.98	0.18	16,16,16,16	0
56	MG	YA	3058	1/1	0.98	0.35	38,38,38,38	0
56	MG	QM	201	1/1	0.98	0.04	61,61,61,61	0
56	MG	YA	3022	1/1	0.98	0.11	9,9,9,9	0
56	MG	XV	102	1/1	0.98	0.11	24,24,24,24	0
56	MG	XA	1605	1/1	0.98	0.29	39,39,39,39	0
58	SF4	XD	501	8/8	0.98	0.06	59,74,81,83	0
56	MG	YA	3094	1/1	0.98	0.08	9,9,9,9	0
59	ZN	R9	102	1/1	0.98	0.04	97,97,97,97	0
59	ZN	XN	101	1/1	0.98	0.07	97,97,97,97	0
56	MG	YA	3095	1/1	0.98	0.07	11,11,11,11	0
56	MG	YA	3059	1/1	0.99	0.05	9,9,9,9	0
56	MG	YA	3115	1/1	0.99	0.07	9,9,9,9	0
56	MG	YA	3074	1/1	0.99	0.16	16,16,16,16	0
56	MG	RA	3043	1/1	0.99	0.06	11,11,11,11	0
56	MG	RA	3050	1/1	0.99	0.04	14,14,14,14	0
56	MG	RA	3066	1/1	0.99	0.04	9,9,9,9	0
56	MG	YA	3011	1/1	0.99	0.05	9,9,9,9	0
56	MG	YA	3027	1/1	0.99	0.23	9,9,9,9	0
56	MG	YA	3112	1/1	0.99	0.03	11,11,11,11	0
56	MG	RA	3037	1/1	0.99	0.04	9,9,9,9	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.

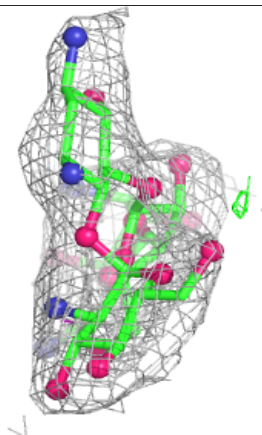
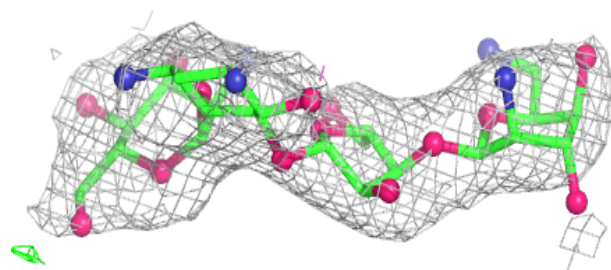
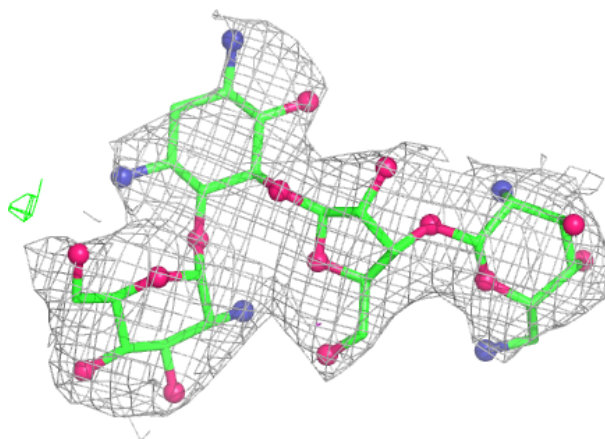
Electron density around PAR XA 1670:

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



Electron density around PAR QA 1663:

$2mF_o-DF_c$ (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.