wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 02:11 AM EDT

PDB ID	:	4TUA
Title	:	Crystal structure of ASL-Thr bound to Codon ACC-A on the Ribosome
Authors	:	Fagan, C.E.; Dunham, C.M.
Deposited on	:	2014-06-24
Resolution	:	3.60 Å(reported)

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

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

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

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

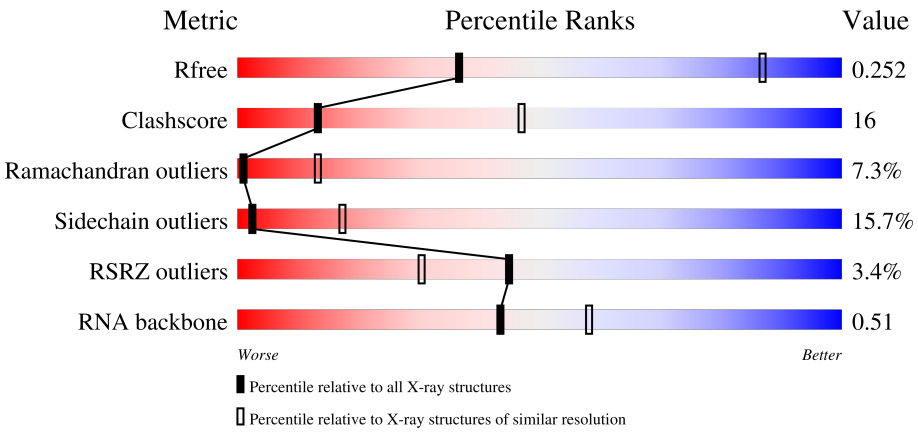
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

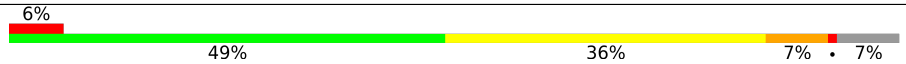
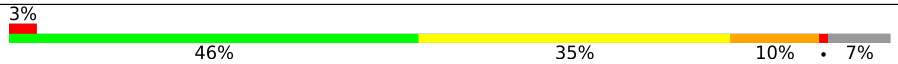
The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	

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Mol	Chain	Length	Quality of chain
3	QC	239	%, 54%, 29%, •, 14%
3	XC	239	54%, 29%, •, 14%
4	QD	209	69%, 25%, 5%
4	XD	209	67%, 27%, 5%, •
5	QE	162	%, 57%, 30%, 6%, 7%
5	XE	162	52%, 36%, 6%, 7%
6	QF	101	68%, 27%, 5%
6	XF	101	%, 65%, 32%, •
7	QG	156	8%, 67%, 29%, •, •
7	XG	156	4%, 73%, 23%, •, •
8	QH	138	59%, 37%, •
8	XH	138	64%, 30%, 5%
9	QI	128	4%, 57%, 38%, •, •, •
9	XI	128	2%, 55%, 34%, 10%, •, •
10	QJ	105	4%, 42%, 43%, 9%, •, 6%
10	XJ	105	2%, 41%, 44%, 10%, 6%
11	QK	129	7%, 58%, 30%, •, 8%
11	XK	129	4%, 61%, 29%, •, 8%
12	QL	132	4%, 30%, 49%, 14%, •, 5%
12	XL	132	2%, 32%, 47%, 14%, •, 5%
13	QM	126	6%, 48%, 37%, 10%, •
13	XM	126	2%, 50%, 36%, 10%, •
14	QN	61	44%, 44%, 10%, •
14	XN	61	51%, 38%, 10%, •
15	QO	89	66%, 27%, 6%, •

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Mol	Chain	Length	Quality of chain
15	XO	89	67% 24% 8% •
16	QP	88	2% 69% 20% 6% 5%
16	XP	88	2% 56% 36% • 5%
17	QQ	105	59% 33% • • 5%
17	XQ	105	69% 22% 5% 5%
18	QR	88	2% 53% 20% • • 20%
18	XR	88	% 44% 32% • 20%
19	QS	93	4% 41% 31% 17% • 10%
19	XS	93	2% 33% 42% 12% • 10%
20	QT	106	4% 50% 38% 6% 7%
20	XT	106	8% 41% 42% 9% • 7%
21	QU	27	4% 48% 44% 7%
21	XU	27	4% 67% 26% 7%
22	QV	77	% 57% 34% 9%
22	XV	77	% 64% 27% 9%
23	QX	25	4% 36% 8% 56%
23	XX	25	4% 28% 16% 56%
24	QY	17	71% 18% 12%
24	XY	17	65% 29% 6%
25	RA	2915	4% 55% 33% 10% • •
25	YA	2915	4% 56% 33% 10% • •
26	RB	122	50% 40% 8% •
26	YB	122	57% 31% 11% •
27	RD	276	55% 35% 8% •
27	YD	276	29% 53% 15% • •

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Mol	Chain	Length	Quality of chain
28	RE	206	2% 22% 48% 25% 5%
28	YE	206	.% 23% 48% 24% 5%
29	RF	210	61% 28% 8%
29	YF	210	2% 34% 48% 12%
30	RG	182	4% 52% 38% 8%
30	YG	182	2% 54% 35% 9%
31	RH	180	22% 24% 43% 19% 8% 6%
31	YH	180	.% 23% 44% 19% 8% 6%
32	RI	148	5% 39% 44% 16%
32	YI	148	4% 43% 40% 16%
33	RN	140	.% 49% 42% 7%
33	YN	140	49% 41% 8%
34	RO	122	70% 25%
34	YO	122	69% 27%
35	RP	150	4% 54% 32% 10%
35	YP	150	2% 48% 32% 16%
36	RQ	141	4% 30% 50% 16%
36	YQ	141	.% 29% 50% 18%
37	RR	118	44% 47% 9%
37	YR	118	57% 31% 12%
38	RS	112	.% 43% 40% 15%
38	YS	112	.% 12% 62% 21%
39	RT	146	.% 45% 40% 9% 6%
39	YT	146	.% 43% 40% 10% 6%
40	RU	118	3% 67% 25% 6%

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Mol	Chain	Length	Quality of chain
40	YU	118	2% 50% 42% 8%
41	RV	101	6% 59% 30% 10%
41	YV	101	3% 44% 44% 12%
42	RW	113	2% 64% 27% 9%
42	YW	113	2% 65% 26% 9%
43	RX	96	56% 32% 7%
43	YX	96	54% 35% 6%
44	RY	110	9% 28% 48% 16% 7%
44	YY	110	5% 45% 32% 15% 7%
45	RZ	206	6% 53% 24% 9% 11%
45	YZ	206	3% 44% 38% 7% 11%
46	R0	85	65% 28%
46	Y0	85	55% 39%
47	R1	98	3% 62% 28% 7%
47	Y1	98	4% 57% 33% 7%
48	R2	72	% 58% 31% 6%
48	Y2	72	% 24% 53% 18%
49	R3	60	3% 68% 25% 5%
49	Y3	60	5% 62% 27% 10%
50	R4	71	28% 6% 44% 41% 10%
50	Y4	71	10% 28% 35% 31% 6%
51	R5	60	8% 17% 52% 23% 7%
51	Y5	60	8% 38% 42% 17%
52	R6	54	63% 17% 43% 30% 9%
52	Y6	54	54% 24% 44% 19% 9%

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Mol	Chain	Length	Quality of chain
53	R7	49	4% 67% 24% 8%
53	Y7	49	4% 63% 29% 8%
54	R8	65	2% 22% 45% 25% 8%
54	Y8	65	2% 20% 43% 29% 6%
55	R9	37	97% 68% 30%
55	Y9	37	100% 68% 30%
56	Z5	3	33% 33% 33%
56	Z6	3	33% 33% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1653	-	-	-	X
57	MG	QA	1681	-	-	-	X
57	MG	QA	1695	-	-	-	X
57	MG	RA	3002	-	-	-	X
57	MG	RA	3013	-	-	-	X
57	MG	RA	3175	-	-	-	X
57	MG	RA	3202	-	-	-	X
57	MG	RA	3244	-	-	-	X
57	MG	RA	3245	-	-	-	X
57	MG	RA	3247	-	-	-	X
57	MG	RA	3253	-	-	-	X
57	MG	RA	3255	-	-	-	X
57	MG	RA	3263	-	-	-	X
57	MG	RA	3266	-	-	-	X
57	MG	RA	3270	-	-	-	X
57	MG	RA	3276	-	-	-	X
57	MG	RA	3281	-	-	-	X
57	MG	RA	3287	-	-	-	X
57	MG	RA	3296	-	-	-	X
57	MG	RA	3305	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	XA	1605	-	-	-	X
57	MG	XA	1659	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1679	-	-	-	X
57	MG	XA	1691	-	-	-	X
57	MG	XA	1699	-	-	-	X
57	MG	XA	1705	-	-	-	X
57	MG	XA	1709	-	-	-	X
57	MG	XA	1713	-	-	-	X
57	MG	Y0	102	-	-	-	X
57	MG	YA	3104	-	-	-	X
57	MG	YA	3128	-	-	-	X
57	MG	YA	3189	-	-	-	X
57	MG	YA	3203	-	-	-	X
57	MG	YA	3206	-	-	-	X
57	MG	YA	3225	-	-	-	X
57	MG	YA	3233	-	-	-	X
57	MG	YA	3272	-	-	-	X
57	MG	YA	3275	-	-	-	X
57	MG	YA	3277	-	-	-	X
57	MG	YA	3280	-	-	-	X
57	MG	YA	3285	-	-	-	X
57	MG	YA	3289	-	-	-	X
57	MG	YA	3297	-	-	-	X
57	MG	YA	3308	-	-	-	X
57	MG	YA	3320	-	-	-	X
57	MG	YA	3330	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 292311 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
			Total	C	N	O	P			
1	QA	1500	32246	14353	5981	10413	1499	0	0	0
1	XA	1500	32249	14354	5984	10412	1499	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	QX	11	220	98	43	68	11	0	0	0
23	XX	11	220	98	43	68	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	QY	15	321	143	57	106	15	0	0	0
24	XY	16	344	153	62	113	16	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	R5	59	459	288	90	76	5	0	0	0
51	Y5	58	454	285	89	75	5	0	0	0

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called CC-Puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
56	Z5	3	74	40	13	19	2	0	0	0
56	Z6	3	74	40	13	19	2	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	QA	95	95	95	0	0
57	QE	1	1	1	0	0
57	QF	1	1	1	0	0
57	QM	1	1	1	0	0
57	QV	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	QX	2	2	2	0	0
57	QY	1	1	1	0	0
57	RA	307	307	307	0	0
57	RB	5	5	5	0	0
57	RD	1	1	1	0	0
57	RE	2	2	2	0	0
57	RF	1	1	1	0	0
57	RR	1	1	1	0	0
57	R0	1	1	1	0	0
57	R1	1	1	1	0	0
57	R5	1	1	1	0	0
57	R8	1	1	1	0	0
57	XA	114	114	114	0	0
57	XF	1	1	1	0	0
57	XV	3	3	3	0	0
57	XX	2	2	2	0	0
57	YA	337	337	337	0	0
57	YB	3	3	3	0	0
57	YD	1	1	1	0	0
57	YE	2	2	2	0	0
57	YP	2	2	2	0	0

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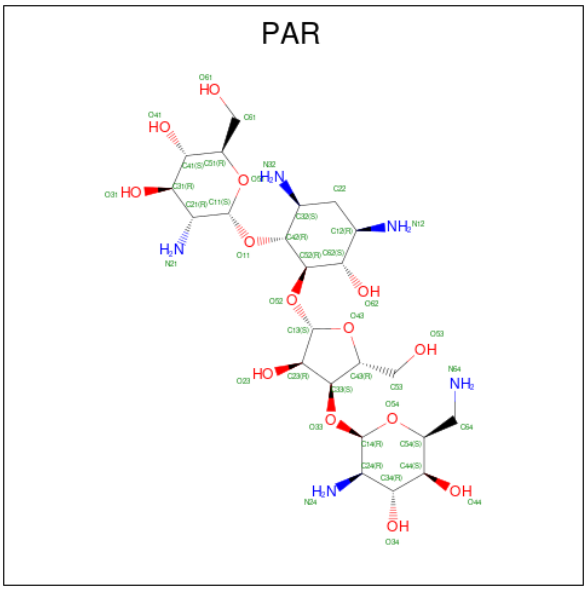
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	YQ	1	1	1	0	0
			Total	Mg		
57	Y0	3	3	3	0	0
			Total	Mg		
57	Y5	1	1	1	0	0
			Total	Mg		
57	Y7	1	1	1	0	0

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



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

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

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

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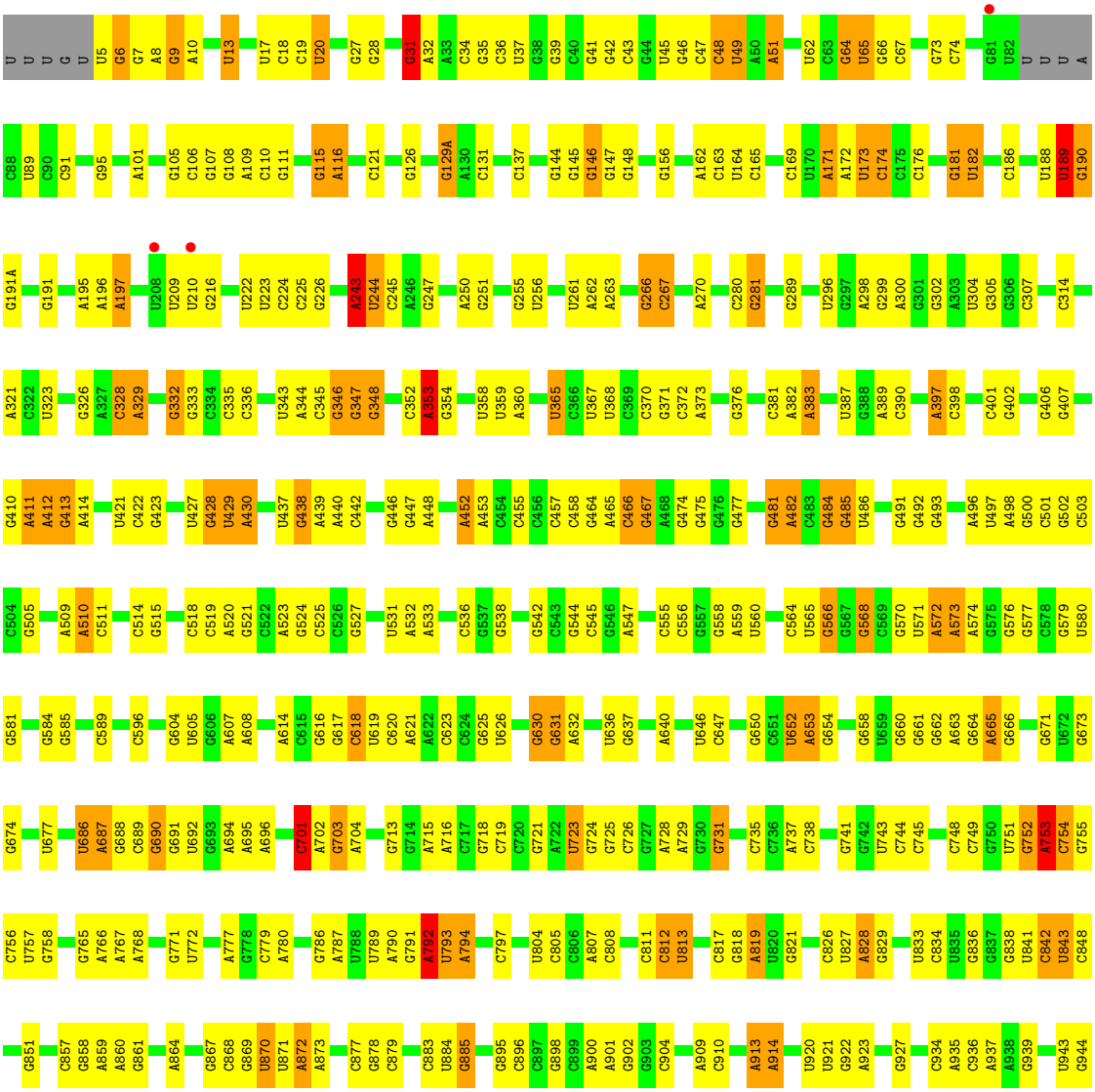
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	XN	1	1	1	0	0

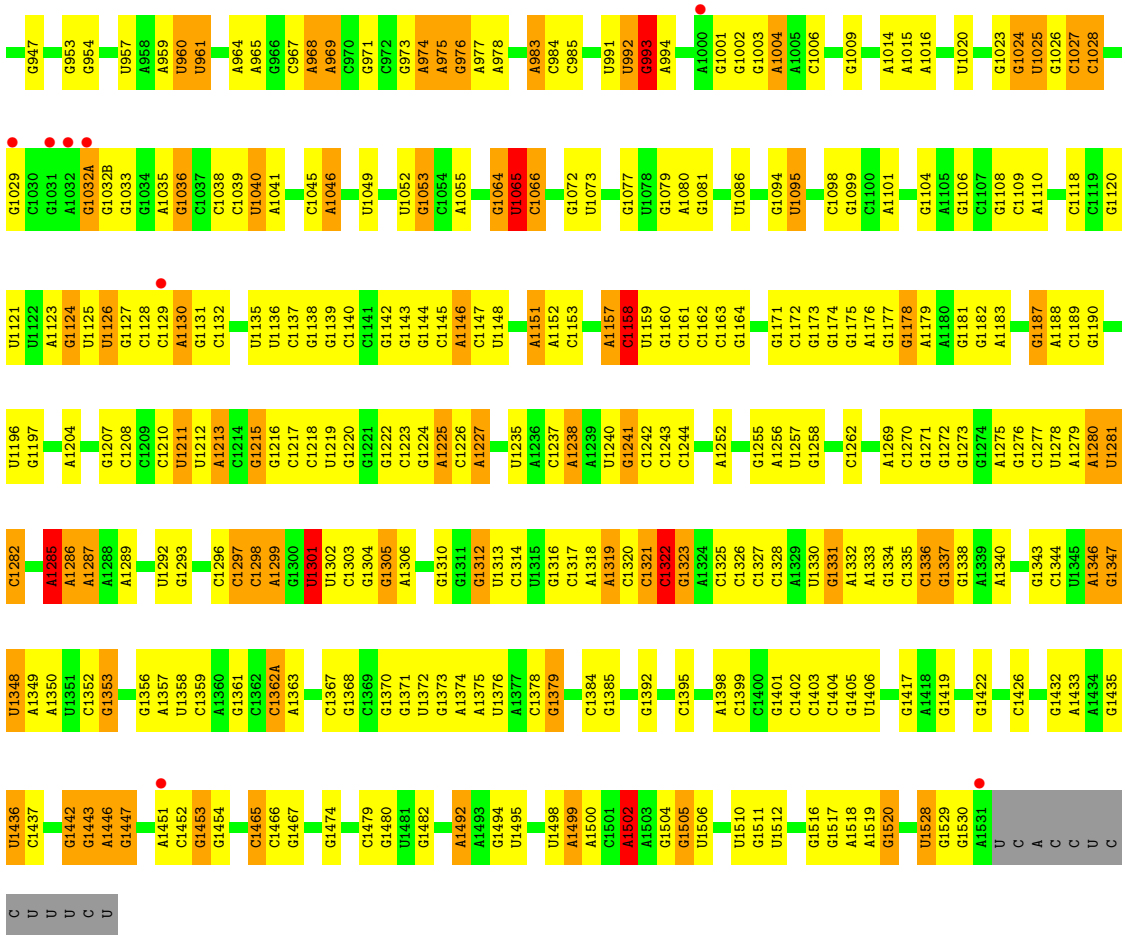
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

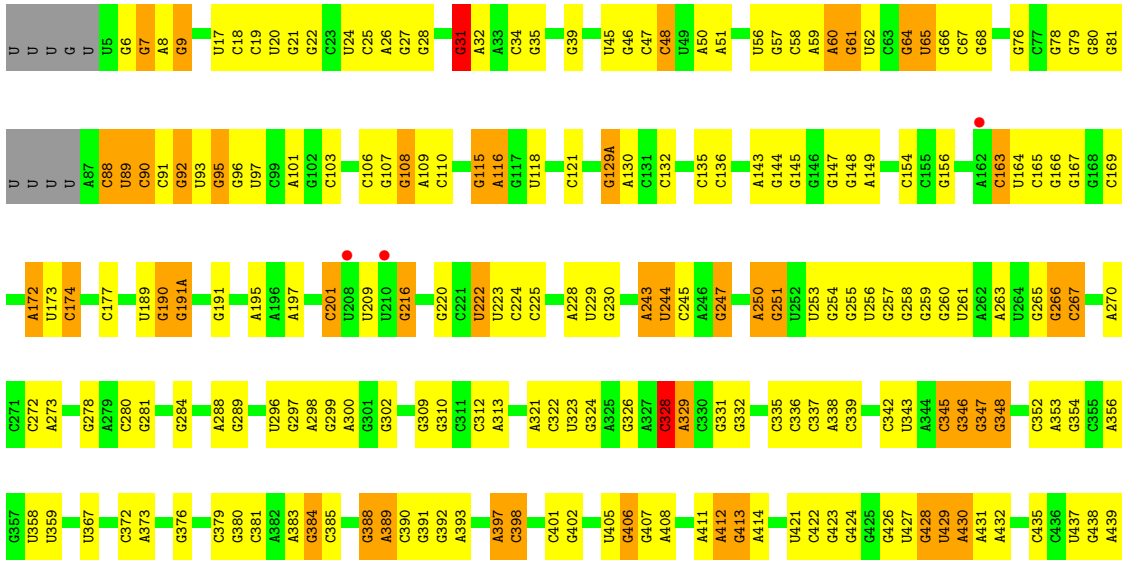
Chain QA:

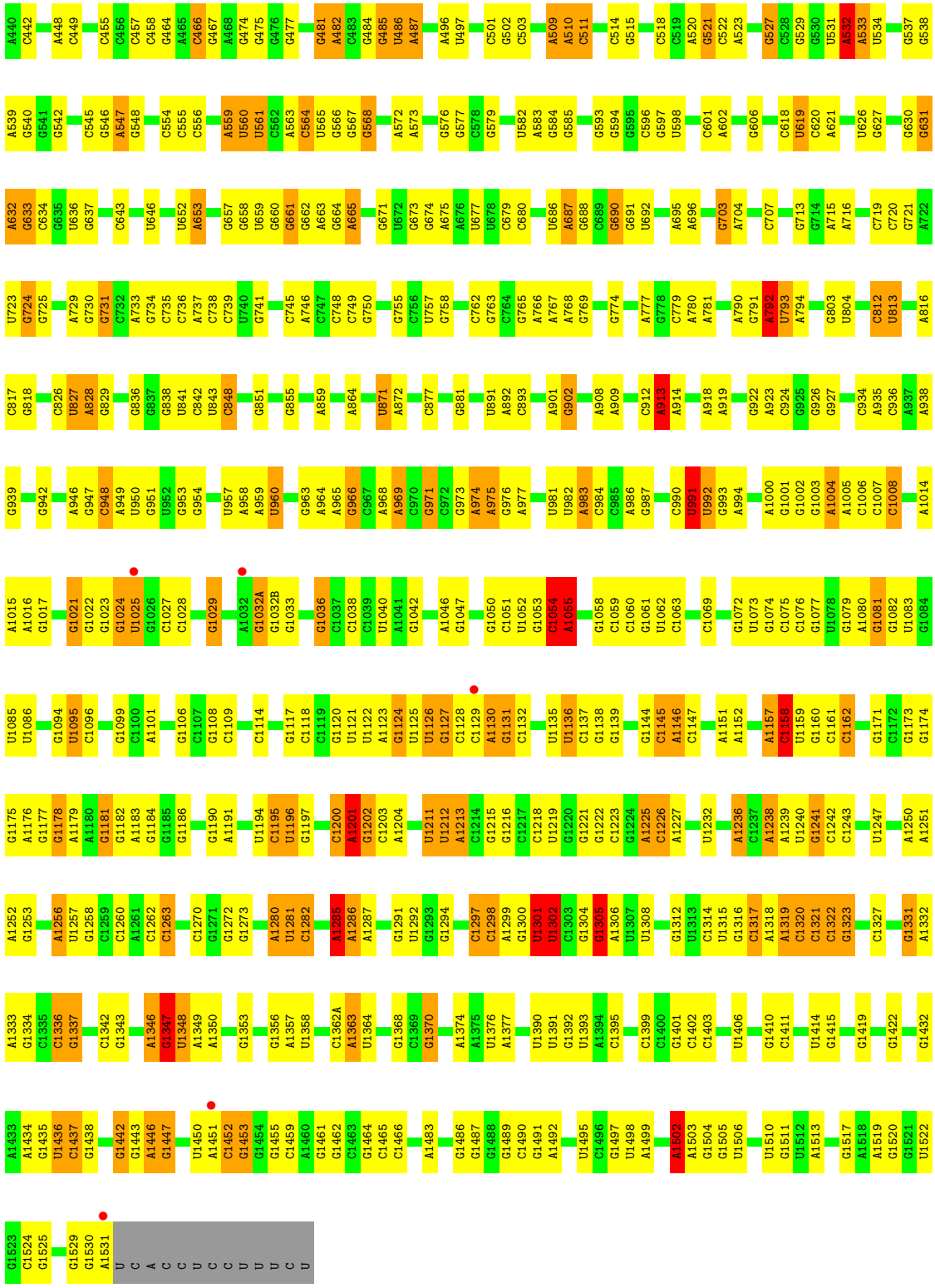




- Molecule 1: 16S rRNA

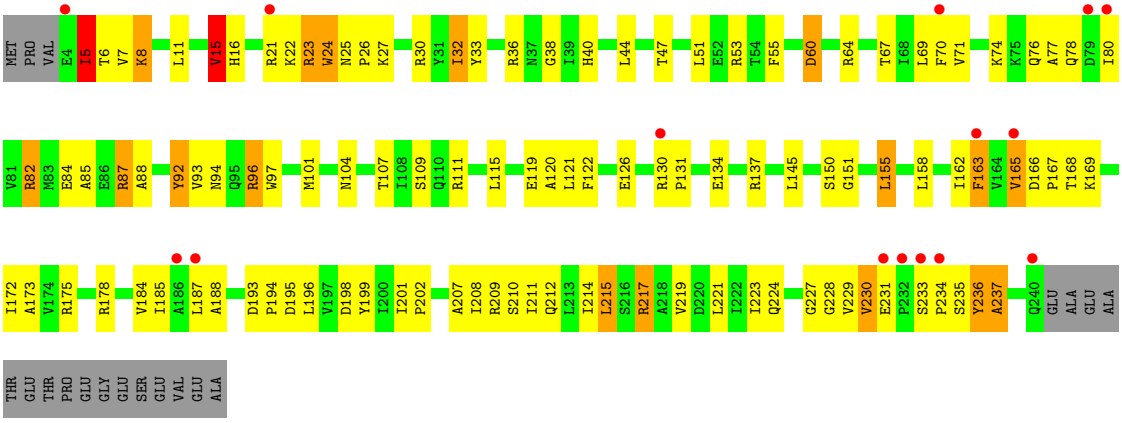
Chain XA:





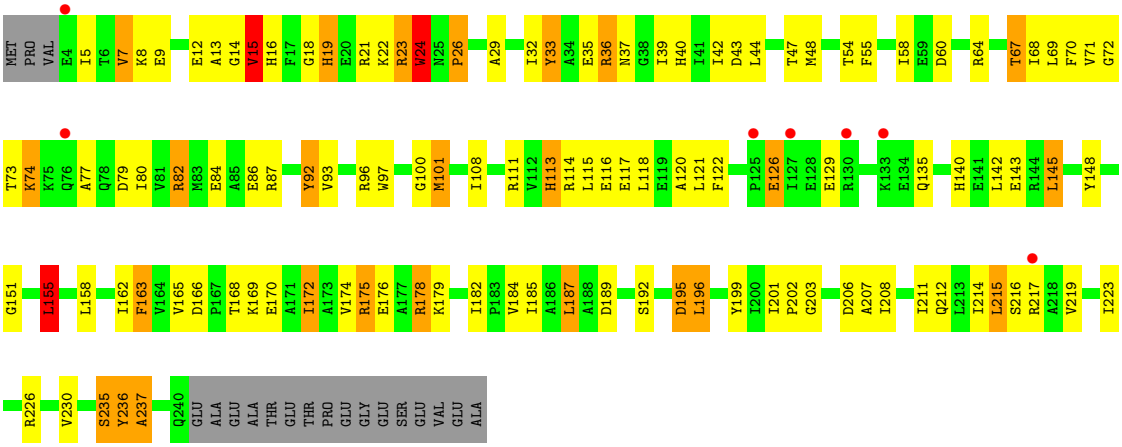
- Molecule 2: 30S ribosomal protein S2

Chain QB:



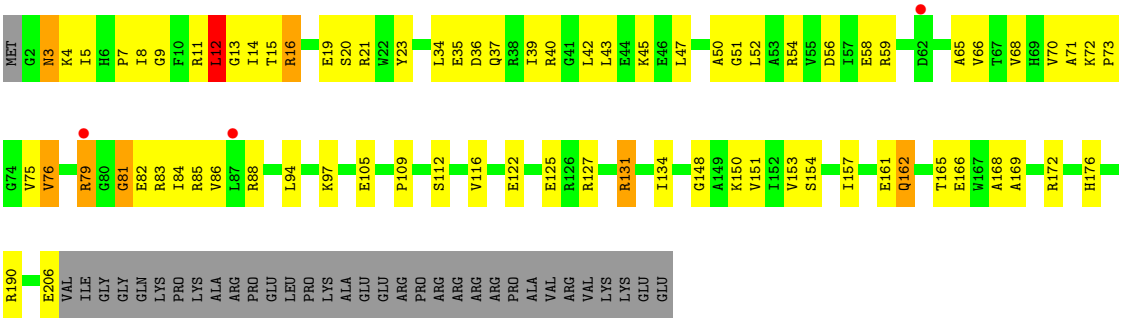
- Molecule 2: 30S ribosomal protein S2

Chain XB:



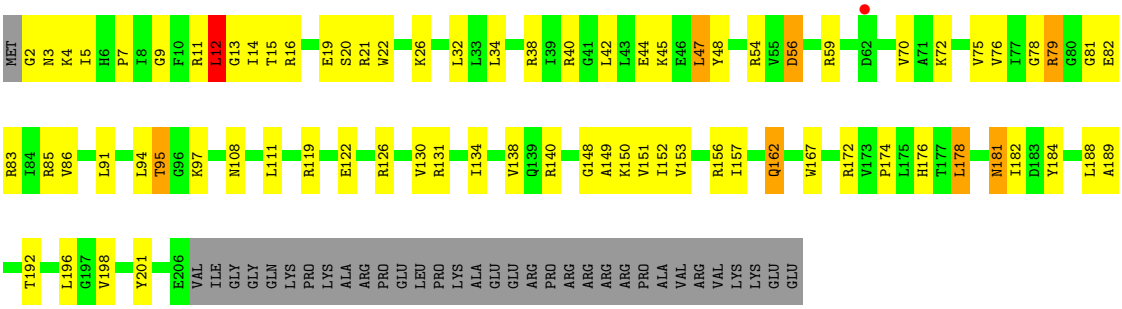
- Molecule 3: 30S ribosomal protein S3

Chain QC:



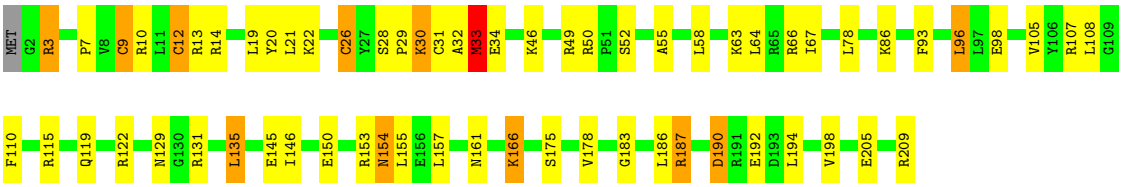
- Molecule 3: 30S ribosomal protein S3

Chain XC:



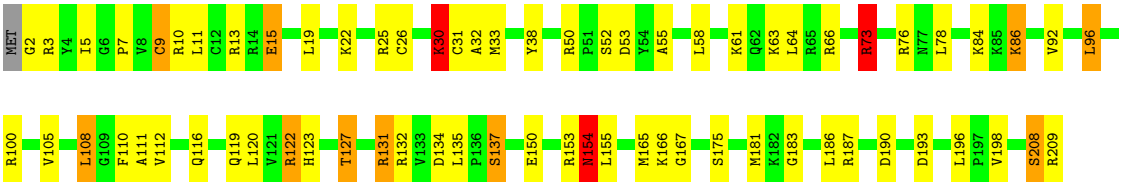
- Molecule 4: 30S ribosomal protein S4

Chain QD: 69% 25% 5%



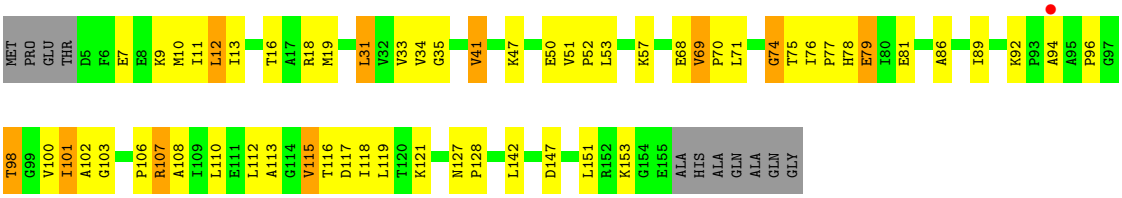
- Molecule 4: 30S ribosomal protein S4

Chain XD: 67% 27% 5%



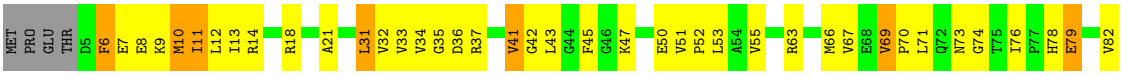
- Molecule 5: 30S ribosomal protein S5

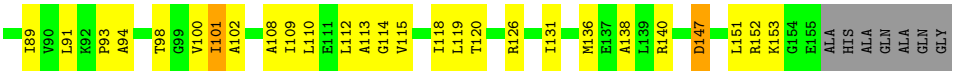
Chain QE: % 57% 30% 6% 7%



- Molecule 5: 30S ribosomal protein S5

Chain XE: 52% 36% 6% 7%



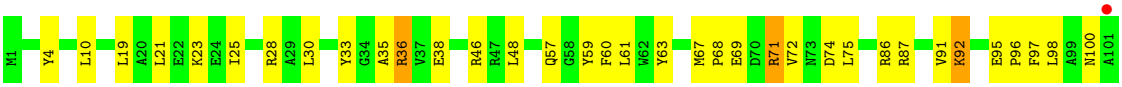


• Molecule 6: 30S ribosomal protein S6

Chain QF:

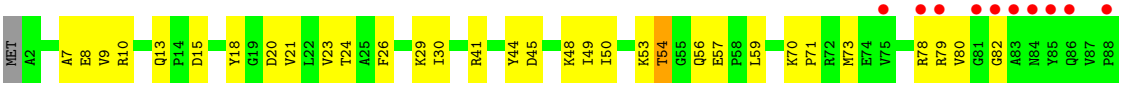
• Molecule 6: 30S ribosomal protein S6

Chain XF:



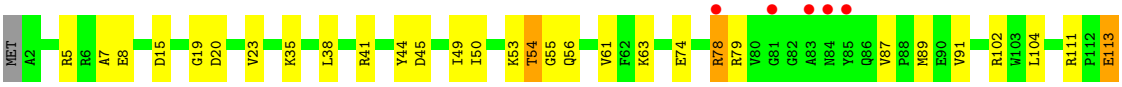
• Molecule 7: 30S ribosomal protein S7

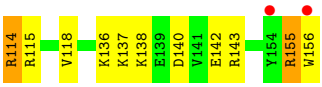
Chain QG:



• Molecule 7: 30S ribosomal protein S7

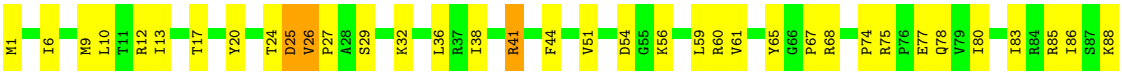
Chain XG:





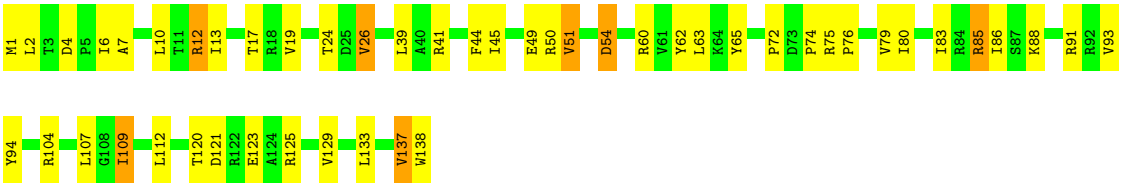
• Molecule 8: 30S ribosomal protein S8

Chain QH:



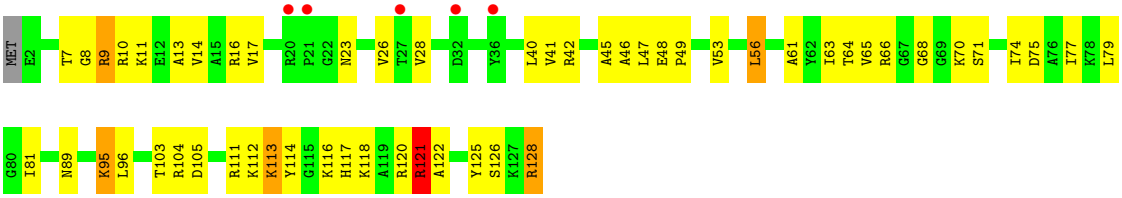
- Molecule 8: 30S ribosomal protein S8

Chain XH:



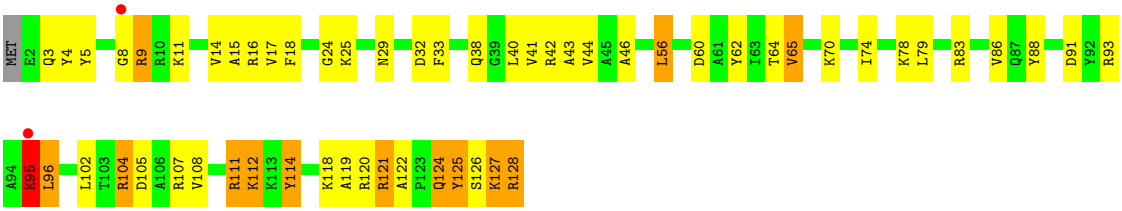
- Molecule 9: 30S ribosomal protein S9

Chain QI:



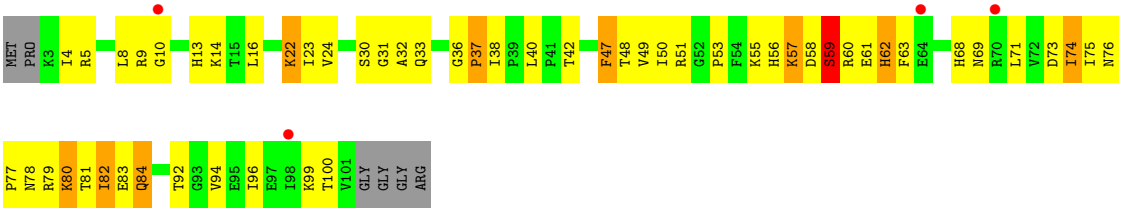
- Molecule 9: 30S ribosomal protein S9

Chain XI:



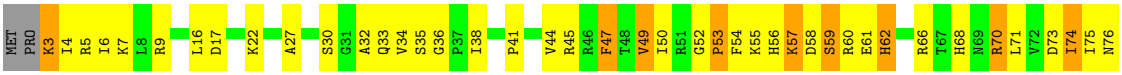
- Molecule 10: 30S ribosomal protein S10

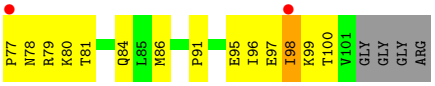
Chain QJ:



- Molecule 10: 30S ribosomal protein S10

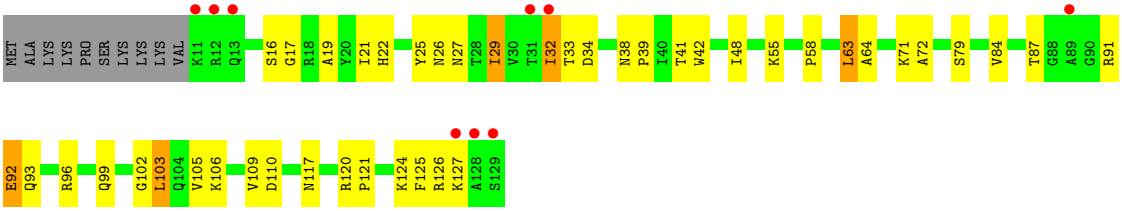
Chain XJ:





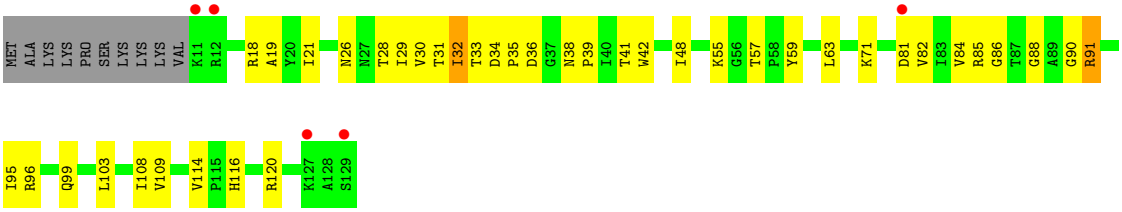
• Molecule 11: 30S ribosomal protein S11

Chain QK:



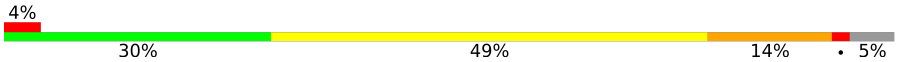
• Molecule 11: 30S ribosomal protein S11

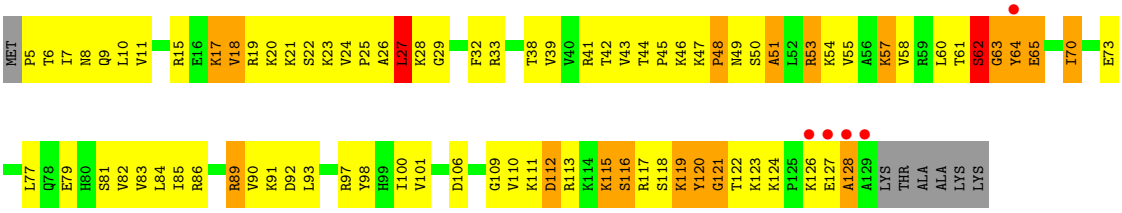
Chain XK:



• Molecule 12: 30S ribosomal protein S12

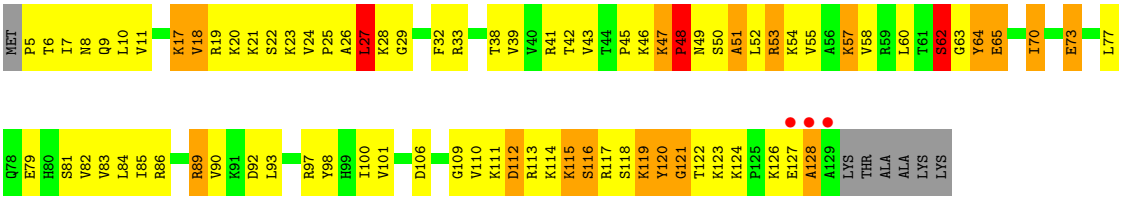
Chain QL:





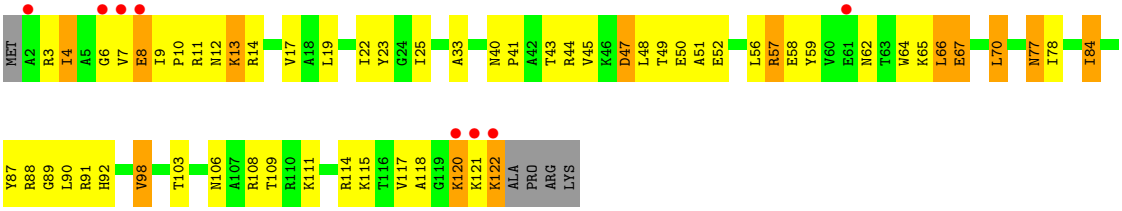
• Molecule 12: 30S ribosomal protein S12

Chain XL:



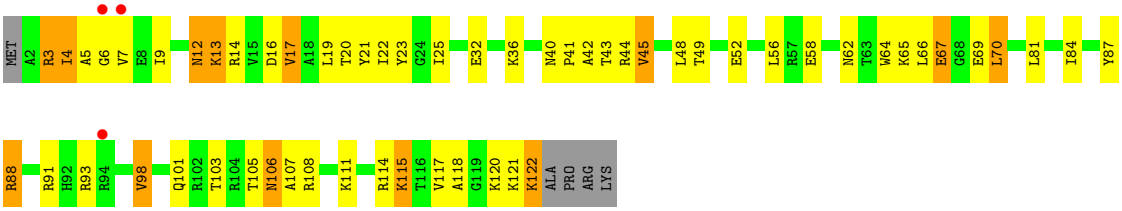
• Molecule 13: 30S ribosomal protein S13

Chain QM:



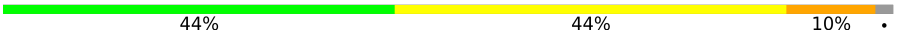
- Molecule 13: 30S ribosomal protein S13

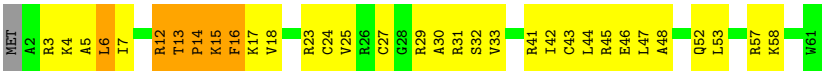
Chain XM:



- Molecule 14: 30S ribosomal protein S14 type Z

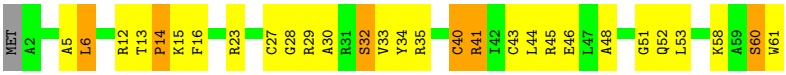
Chain QN:





- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:

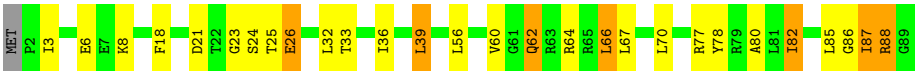


- Molecule 15: 30S ribosomal protein S15

Chain QO:

- Molecule 15: 30S ribosomal protein S15

Chain XO:

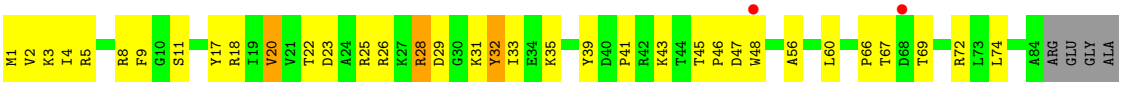


- Molecule 16: 30S ribosomal protein S16

Chain QP:

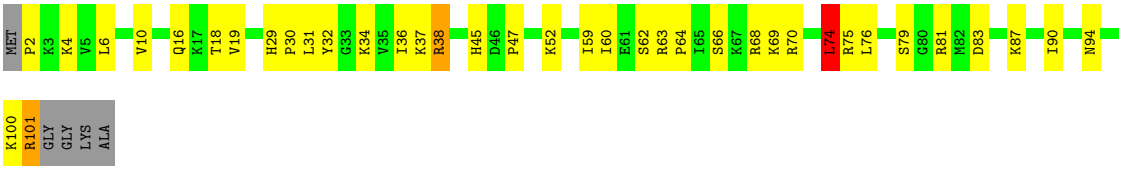
• Molecule 16: 30S ribosomal protein S16

Chain XP:



• Molecule 17: 30S ribosomal protein S17

Chain QQ:



• Molecule 17: 30S ribosomal protein S17

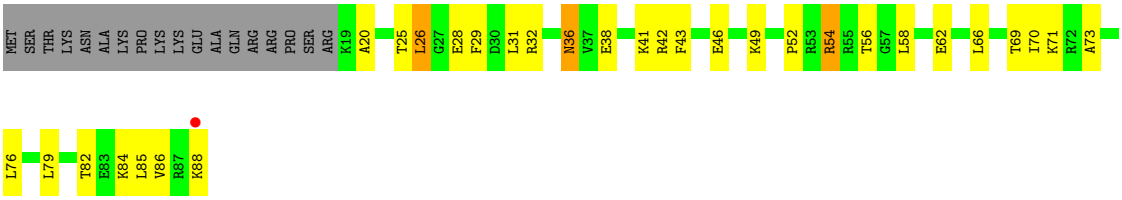
Chain XQ:

• Molecule 18: 30S ribosomal protein S18

Chain QR:

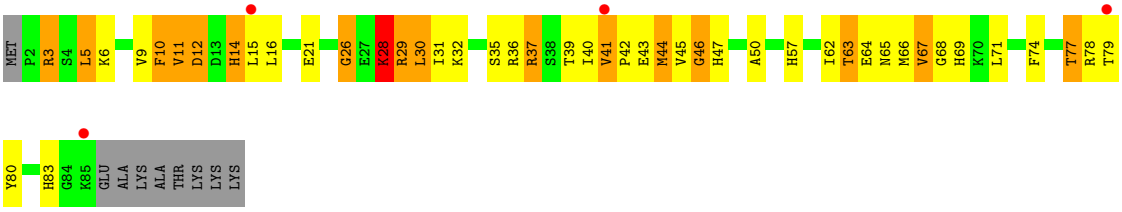
• Molecule 18: 30S ribosomal protein S18

Chain XR:



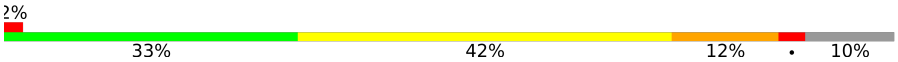
• Molecule 19: 30S ribosomal protein S19

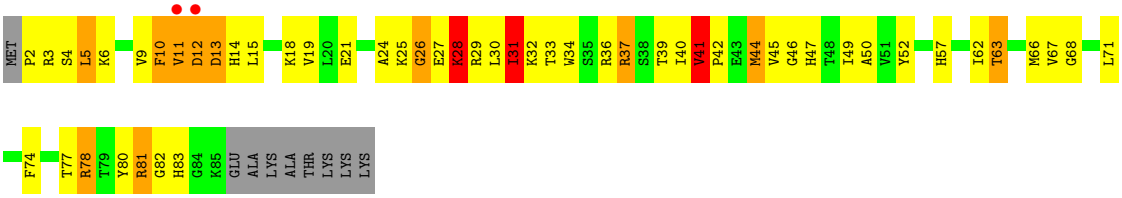
Chain QS:



• Molecule 19: 30S ribosomal protein S19

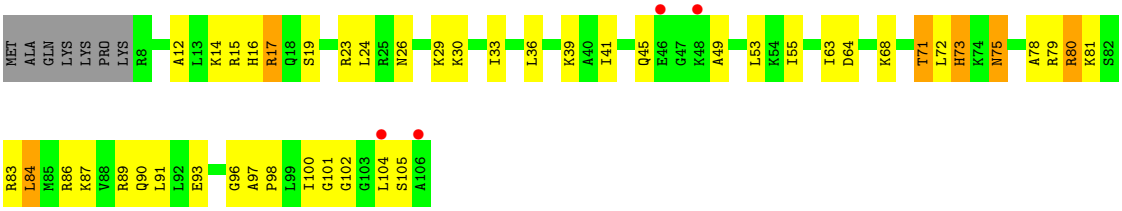
Chain XS:





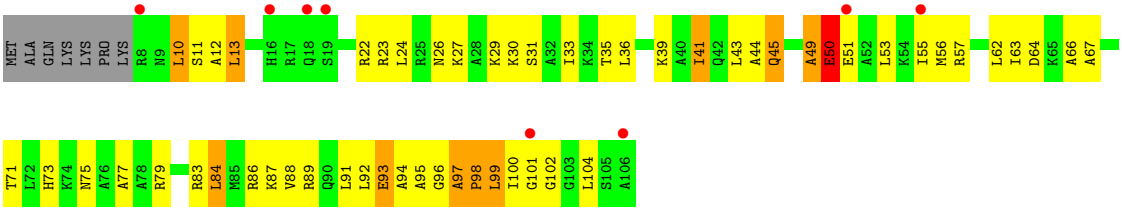
• Molecule 20: 30S ribosomal protein S20

Chain QT:



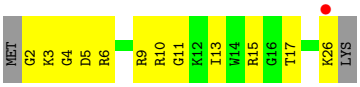
• Molecule 20: 30S ribosomal protein S20

Chain XT:



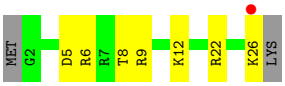
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



• Molecule 21: 30S ribosomal protein Thx

Chain XU:

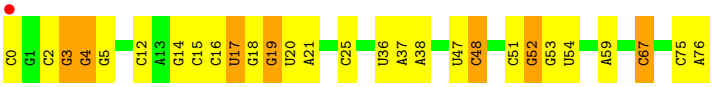


• Molecule 22: P-site tRNA-fMet

Chain QV:

• Molecule 22: P-site tRNA-fMet

Chain XV:



• Molecule 23: messenger RNA

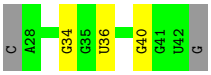
Chain QX:

• Molecule 23: messenger RNA

Chain XX:

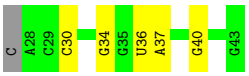
• Molecule 24: A-site ASL-Thr

Chain QY:



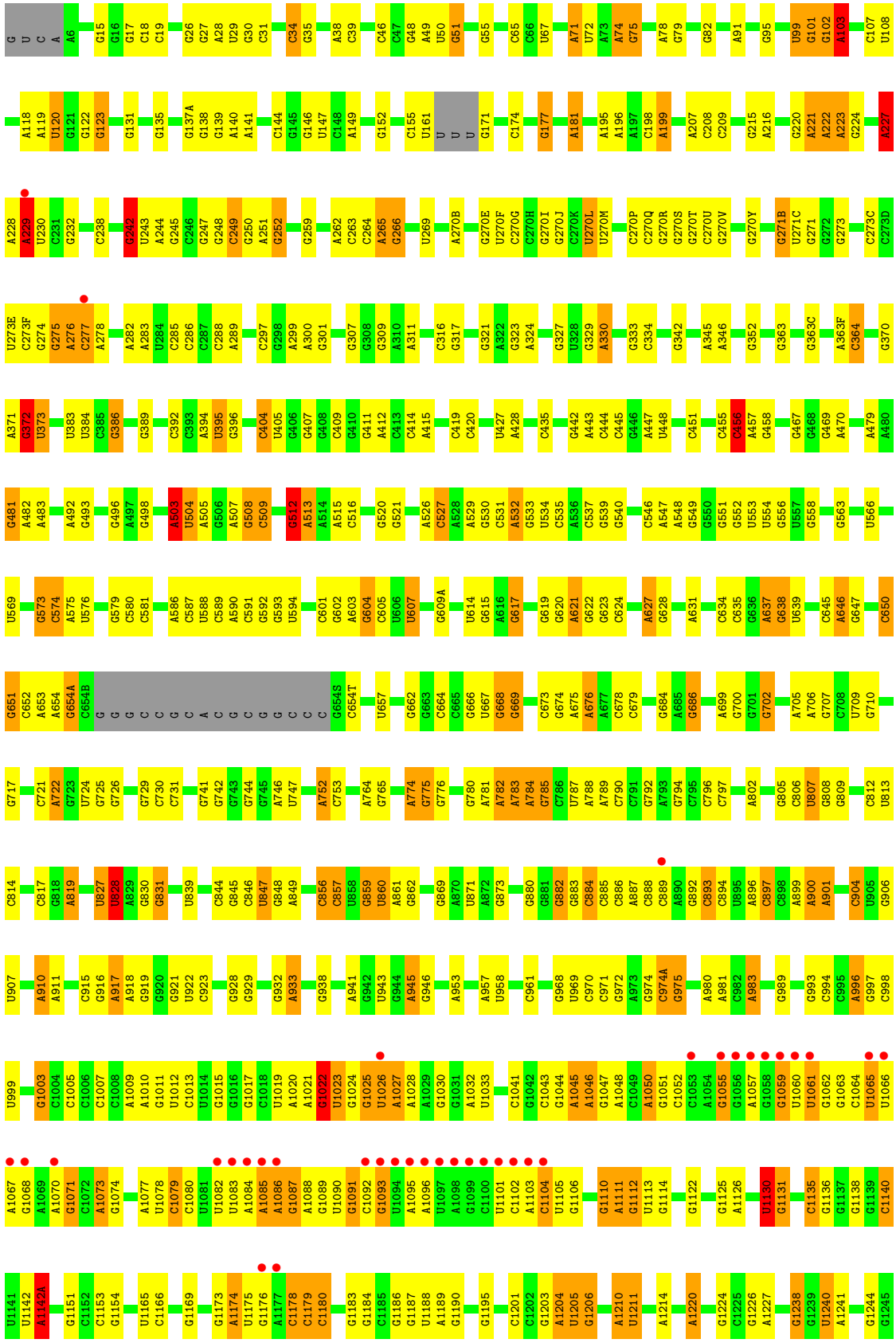
• Molecule 24: A-site ASL-Thr

Chain XY:



• Molecule 25: 23S rRNA

Chain RA: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A228 A229 U230 C231 G232 C238 G242 U243 A244 G245 C246 G247 G248 C249 G250 A251 G252 G259 A262 C263 C264 A265 A266 U269 A270B G270E U270F C270G C270H G270I G270J C270K U270L U270M C270P C270Q G270R G270S G270T C270U G270V G270Y G271B U271C G271 G272 G273 C273C C273D
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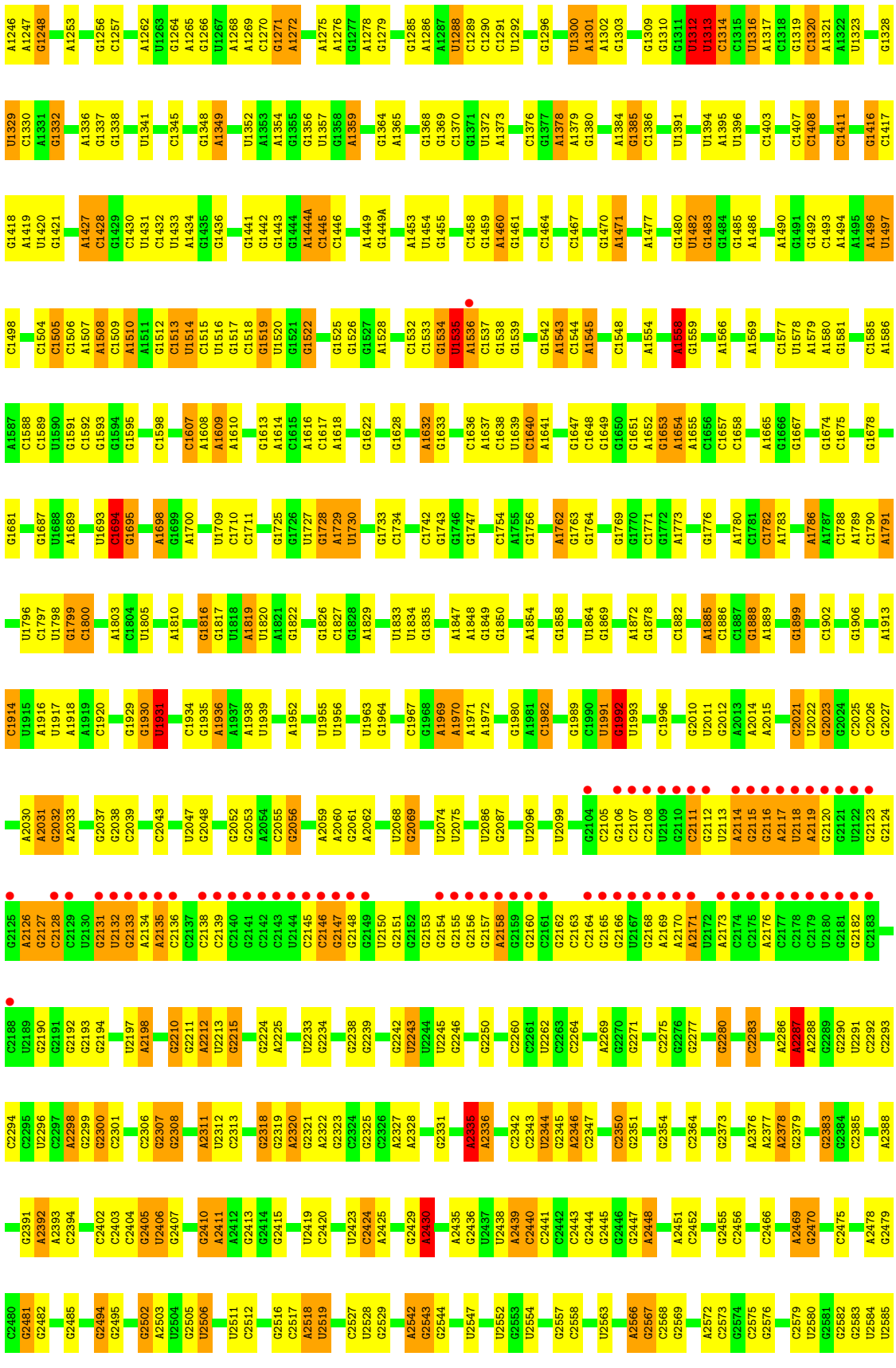
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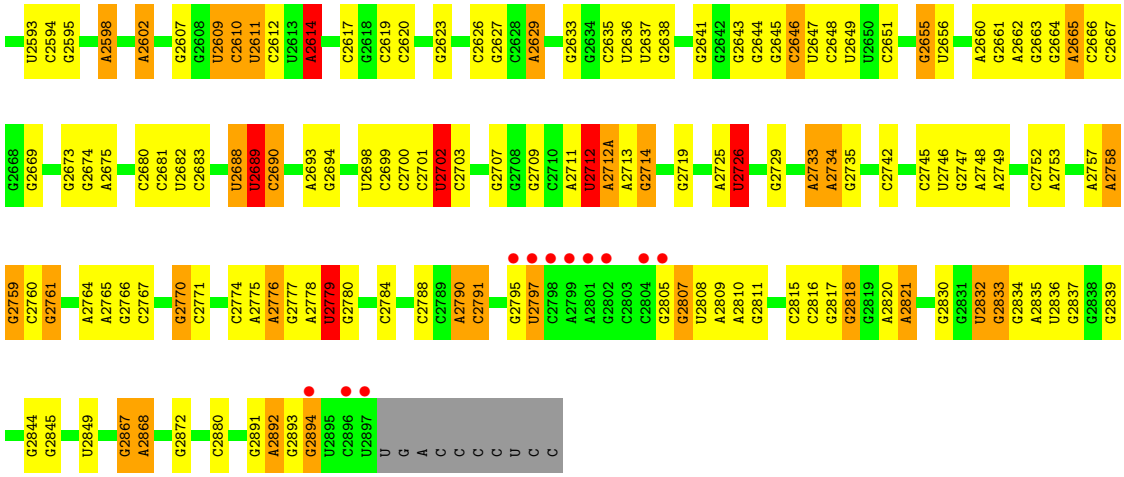
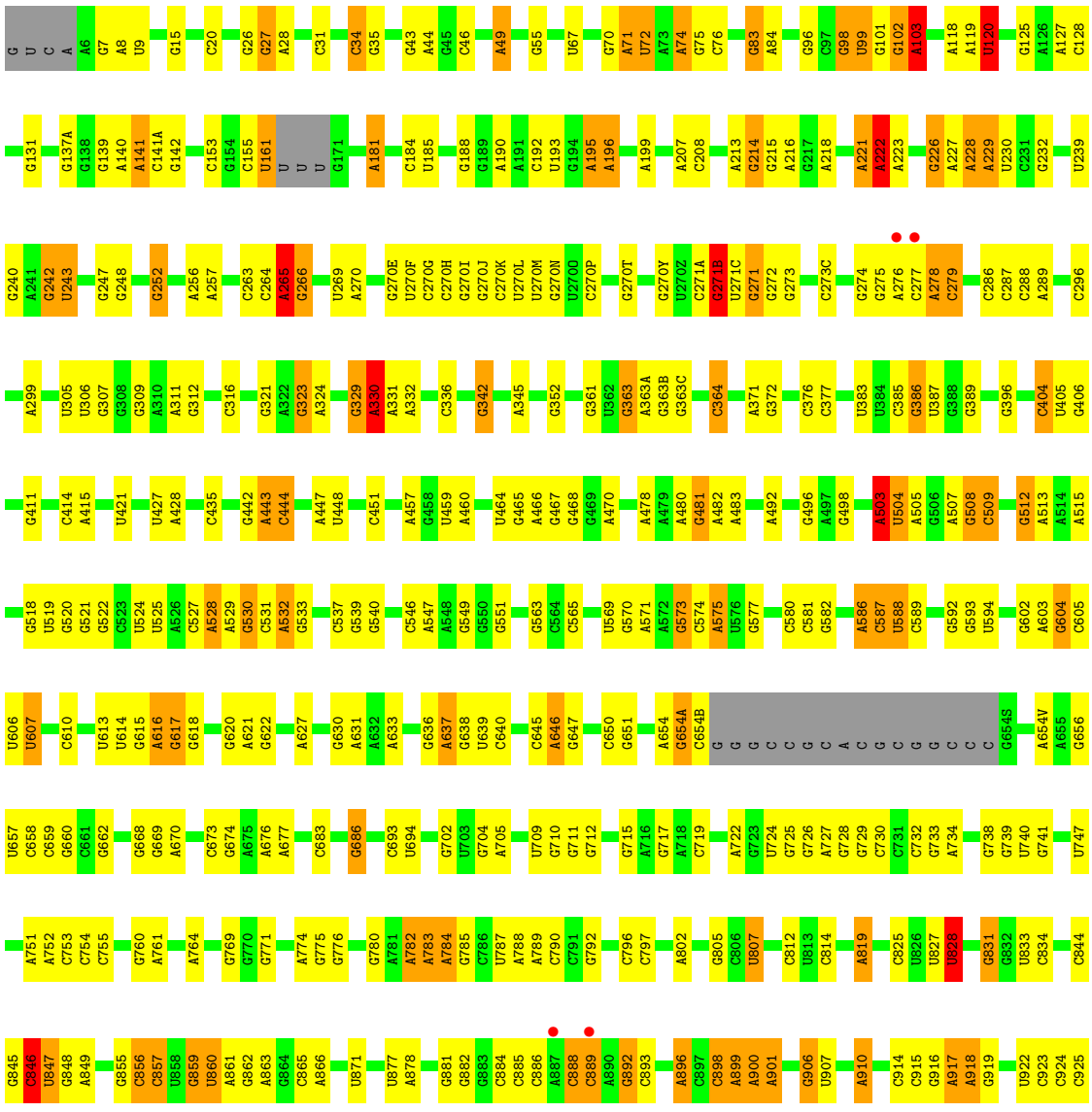
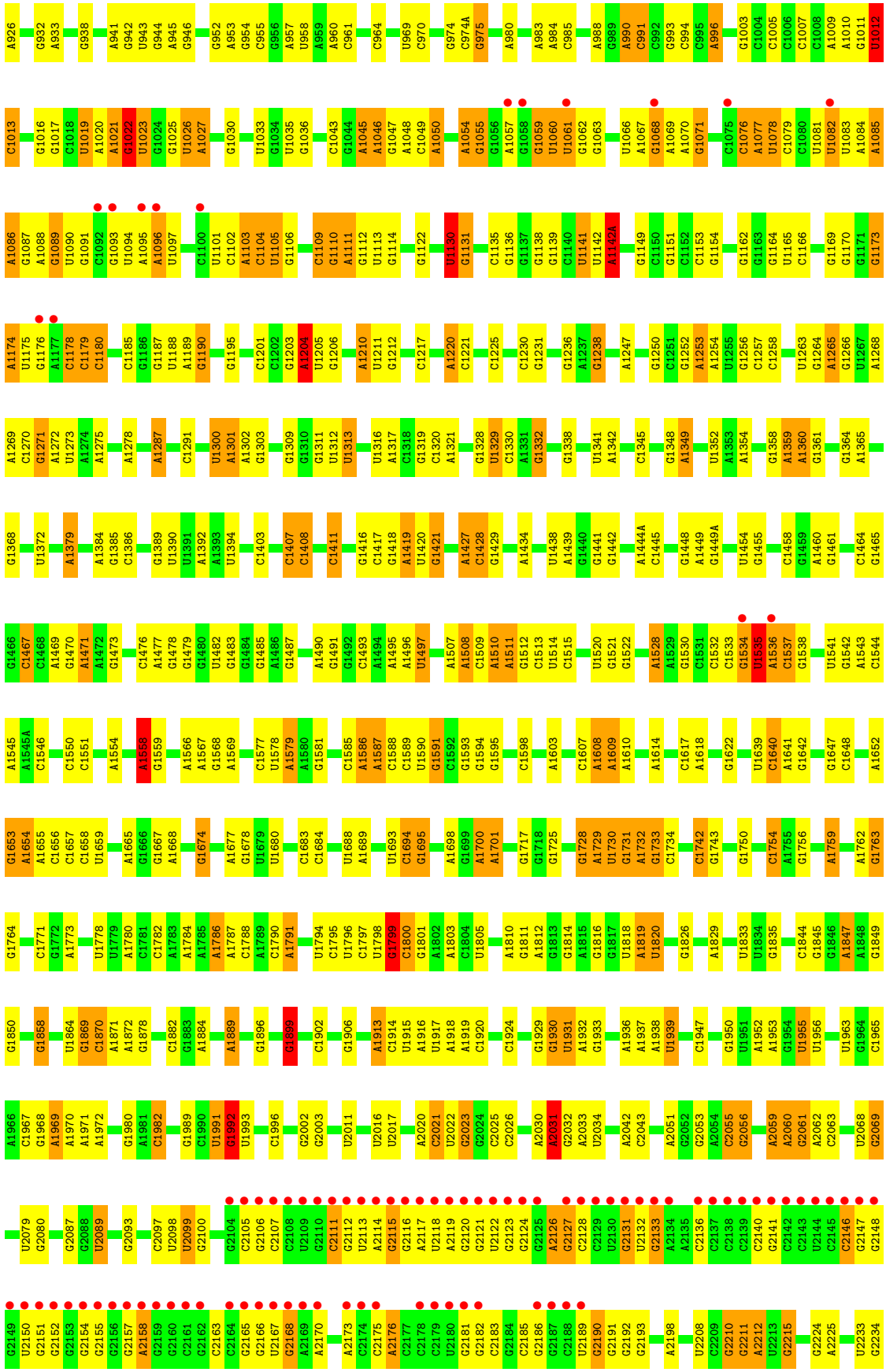


• Molecule 25: 23S rRNA

Chain YA:

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A1174 U1175 G1176 A1177 C1178 G1179 C1180 C1185 G1186 G1187 U1188 A1189 G1190 G1195 C1201 C1202 G1203 A1204 U1205 G1206 A1210 U1211 G1212 C1217 A1220 C1221 C1225 C1230 G1231 G1236 A1237 G1238 A1247 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 U1263 G1264 A1265 G1266 U1267 A1268
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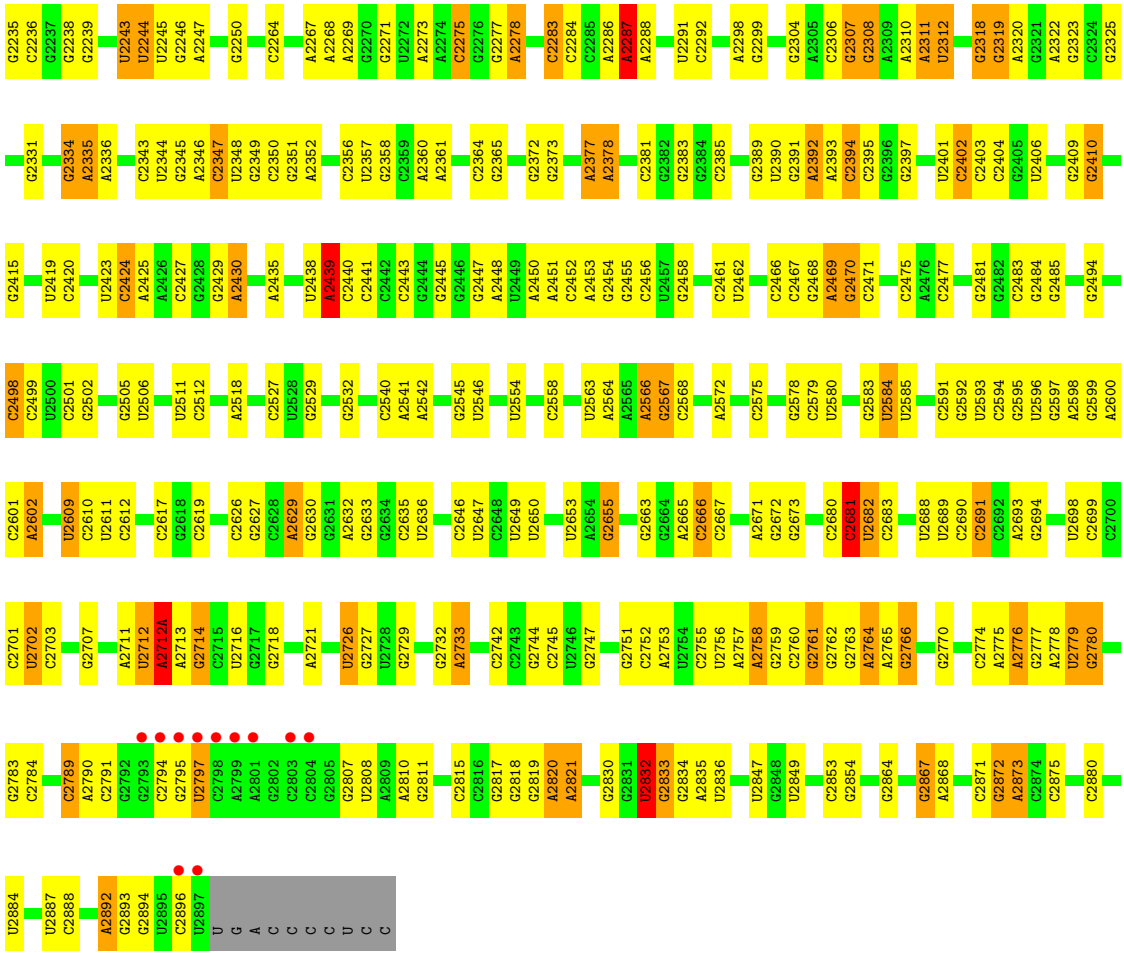
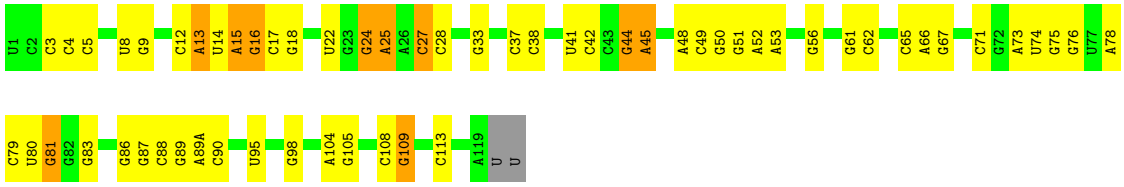
G1368 U1372 A1379 A1384 G1385 C1386 G1389 U1390 U1391 A1392 A1393 U1394 C1403 C1407 C1408 C1411 G1416 C1417 G1418 A1419 U1420 G1421 A1427 C1428 G1429 A1434 U1438 A1439 G1440 G1441 G1442 A1444A C1445 G1448 A1449 G1449A U1454 G1455 C1458 G1459 A1460 G1461 C1464 G1465
G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1473 C1476 A1477 G1478 G1479 G1480 U1482 G1483 G1484 G1485 A1486 G1487 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 C1515 U1520 G1521 G1522 A1528 A1529 G1530 C1531 C1532 C1533 G1534 U1535 A1536 C1537 G1538 U1541 G1542 A1543 C1544
A1545 A1545A C1546 C1550 C1551 A1554 A1558 G1559 A1566 A1567 G1568 A1569 C1577 U1578 A1579 A1580 G1581 C1585 A1586 A1587 C1588 C1589 U1590 G1591 C1592 G1593 G1594 G1595 C1598 A1603 C1607 A1608 A1609 A1610 A1614 C1617 A1618 G1622 U1639 C1640 A1641 G1642 G1647 C1648 A1652
G1653 A1654 A1655 C1656 C1657 C1658 U1659 A1665 G1666 G1667 A1668 G1674 A1677 G1678 U1679 U1680 C1683 C1684 U1688 A1689 U1693 C1694 G1695 A1698 G1699 A1700 A1701 G1717 G1718 G1725 G1728 A1729 U1730 G1731 A1732 G1733 C1734 C1742 G1743 G1750 C1754 A1755 G1756 A1759 A1762 G1763
G1764 C1771 G1772 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 A1810 G1811 A1812 G1813 G1814 A1815 G1816 G1817 U1818 A1819 U1820 G1826 A1829 U1833 U1834 G1835 C1844 G1845 G1846 A1847 A1848 G1849
G1850 G1858 U1864 G1869 C1870 A1871 A1872 G1878 C1882 G1883 A1884 A1889 G1896 G1899 C1902 G1906 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 C1924 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 C1947 G1950 U1951 A1952 A1953 G1954 U1955 U1956 U1963 G1964 C1965
A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1980 A1981 C1982 G1989 C1990 U1991 G1992 U1993 C1996 G2002 G2003 U2011 U2016 U2017 A2020 C2021 U2022 G2023 G2024 C2025 C2026 A2030 A2031 G2032 A2033 U2034 A2042 C2043 A2051 G2052 G2053 A2054 C2055 G2056 A2059 A2060 G2061 A2062 C2063 U2068 G2069
U2079 G2080 G2087 G2088 U2089 G2093 C2097 U2098 U2099 G2100 G2104 C2105 C2106 C2107 C2108 U2109 G2110 C2111 C2112 U2113 A2114 C2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148
G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 A2198 U2208 C2209 G2210 G2211 A2212 U2213 G2215 G2224 A2225 U2233 G2234



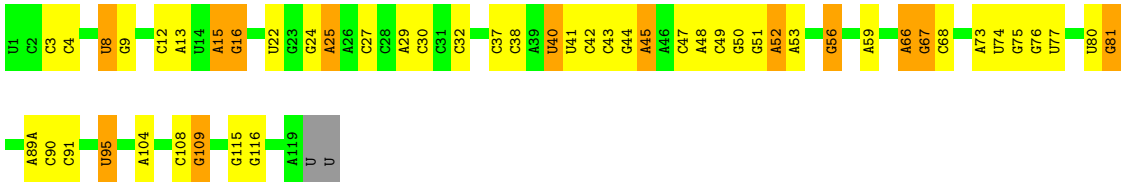
- Molecule 26: 5S rRNA

Chain RB:



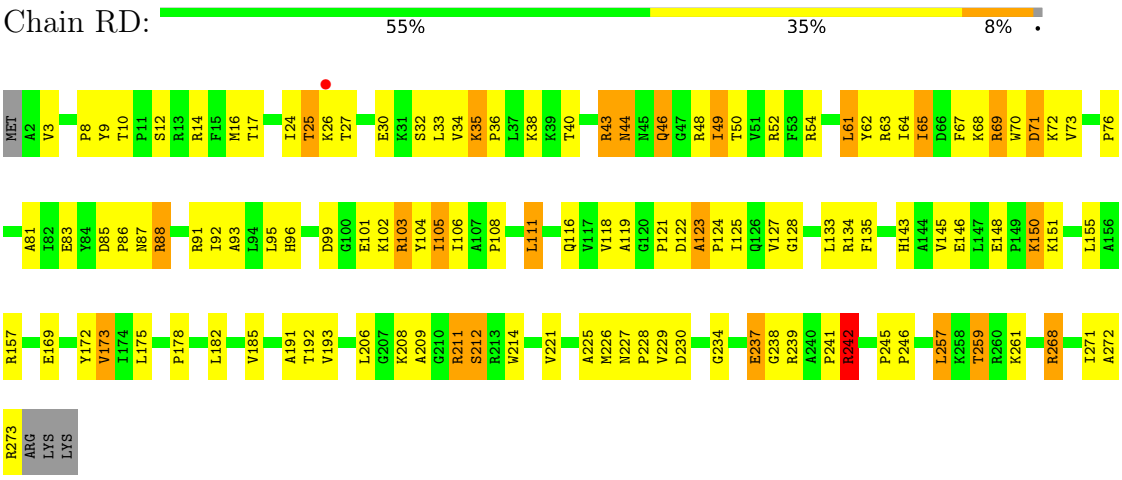
- Molecule 26: 5S rRNA

Chain YB:



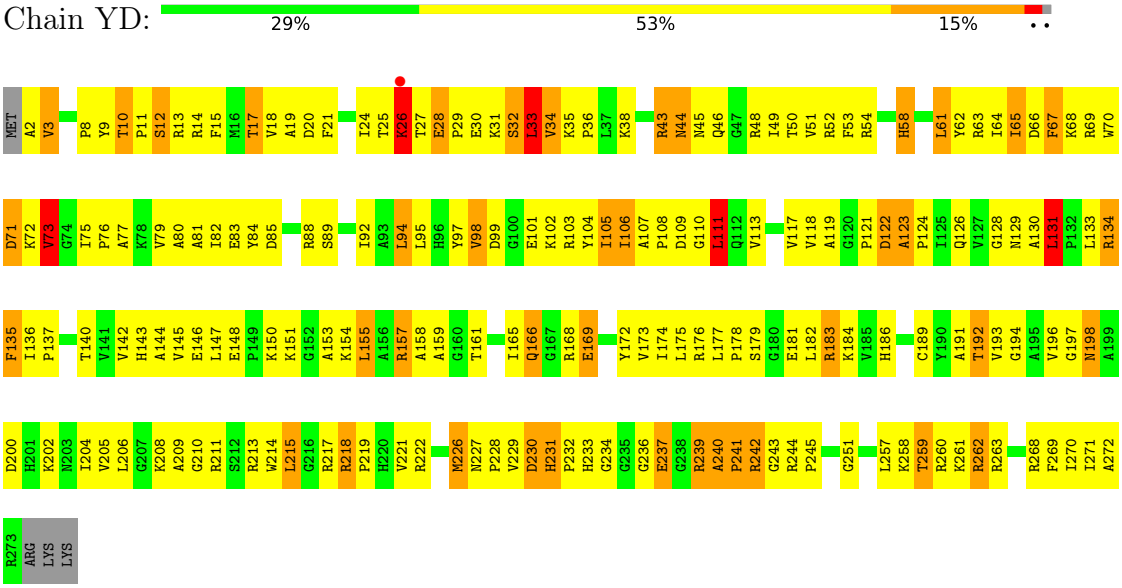
- Molecule 27: 50S ribosomal protein L2

Chain RD:



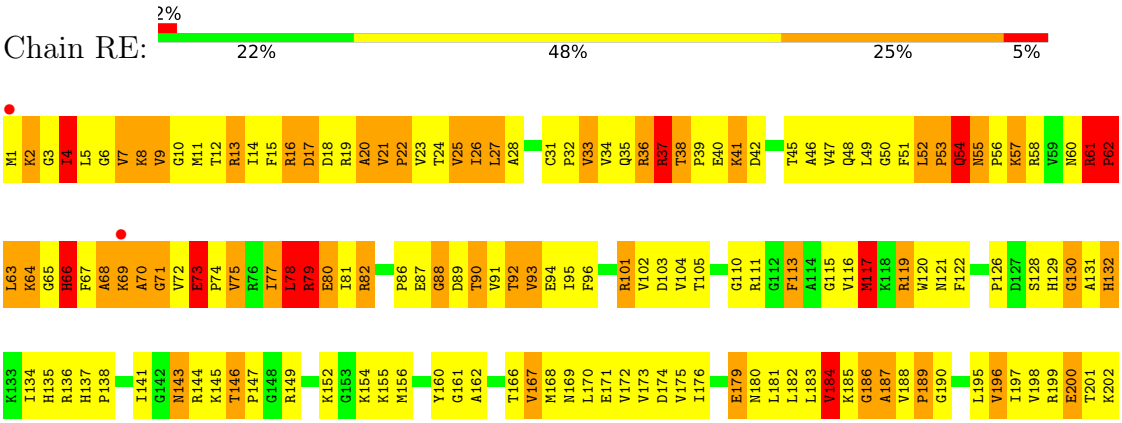
- Molecule 27: 50S ribosomal protein L2

Chain YD:



- Molecule 28: 50S ribosomal protein L3

Chain RE:



K203 A204 A205 LYS

• Molecule 28: 50S ribosomal protein L3

Chain YE: %
23% 48% 24% 5%

M1 K2 G3 I4 L5 G6 V7 K8 V9 G10 M11 T12 R13 I14 F15 R16 D17 D18 R19 A20 V21 P22 V23 T24 V25 I26 L27 A28 C31 P32 V33 V34 Q35 R36 R37 T38 P39 E40 K41 D42 T45 A46 V47 Q48 L49 G50 F51 L52 P53 Q54 N55 P56 K57 R58 V59 N60 R61 P62

L63 K64 G65 H66 F67 A68 K69 A70 G71 V72 E73 P74 V75 R76 I77 L78 R79 E80 I81 R82 P86 E87 G88 D89 T90 V91 T92 V93 E94 I95 F96 R101 V102 D103 V104 T105 K109 G110 R111 G112 F113 A114 G115 V116 M117 K118 R119 W120 N121 F122 P126 D127 S128 H129 G130 A131

H132 K133 I134 H135 R136 H137 P138 G139 S140 N143 R144 K145 T146 P147 K154 K155 M156 Y160 G161 A162 T166 V167 M168 N169 L170 E171 V172 V173 D174 V175 I176 E179 N180 L181 L182 L183 V184 K185 G186 A187 V188 P189 G190 L195 V196 I197 V198 R199 E200 T201 K202 K203 A204 A205

LYS

• Molecule 29: 50S ribosomal protein L4

Chain RF:
61% 28% 8%

MET LYS GLU VAL ALA V6 Y7 Q8 I9 P10 V11 L12 S13 L20 A21 L24 I28 L32 L33 V36 V37 R38 W39 Q40 R45 T48 T51 S60 G61 W65 P66 Q67 K68 H69 T70 A73 R74 I78 F83 V84 V89 P92 R95

L101 P102 K103 K104 V105 R106 K107 K108 G109 L110 A111 M112 A113 V114 A115 D116 R117 L125 N133 G134 K135 T136 K137 E138 A143 L148 D149 G150 V157 N160 V163 A167 W172 V173 V174 P178 L181 N182 V183 Y184 D185 I186 V187 R188 L192 V193 M194

D197 V201 I206 G207 GLY GLU ALA

• Molecule 29: 50S ribosomal protein L4

Chain YF: 2%
34% 48% 12%

MET LYS GLU VAL ALA V6 Y7 Q8 I9 P10 V11 L12 S13 P14 R17 R18 E19 L20 A21 L24 P25 A26 E27 I28 N29 P30 H31 L32 L33 W34 E35 V36 V37 R38 W39 Q40 L41 A42 K43 R44 R45 R46 G47 T51 K52 T53 R54 G55 E56 Y59 S60 G61 R62 K63 I64 W65

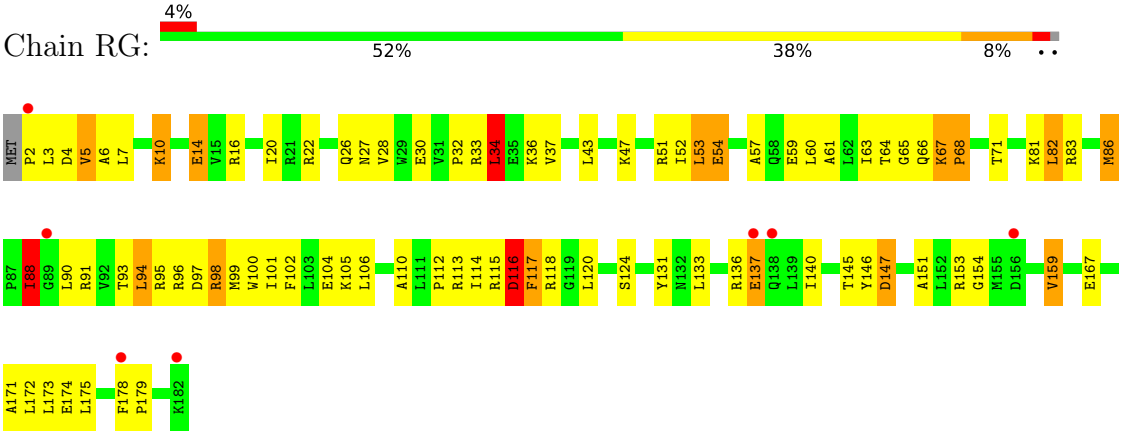
P66 Q67 K68 H69 T70 G71 R72 A73 R74 A80 F81 I82 F83 V84 V89 F90 K93 L101 P102 K103 K104 V105 R106 K107 K108 G109 L110 A111 M112 A115 D116 R117 A118 R119 E120 G121 K122 L123 L124 L125 V126 E127 A128 F129 A130 G131 V132 N133 G134 K135 T136 K137 E138 F139 L140

A141 W142 A143 K144 E145 A146 G147 L148 D149 G150 S151 E152 L155 L156 V157 N160 E161 L162 V163 R164 R165 A166 A167 R168 N169 V173 V174 T175 L176 A177 P178 E179 G180 L181 N182 V183 Y184 D185 I186 V187 R188 T189 L192 V193 M194 D195 L196 D197 A198 W199 E200 V201 F202 I206 G207

GLY GLU ALA

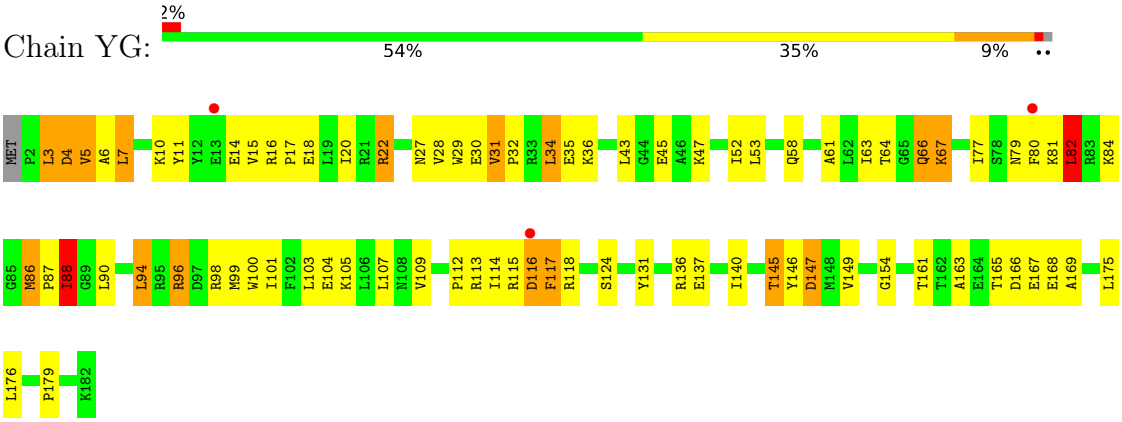
• Molecule 30: 50S ribosomal protein L5

Chain RG:



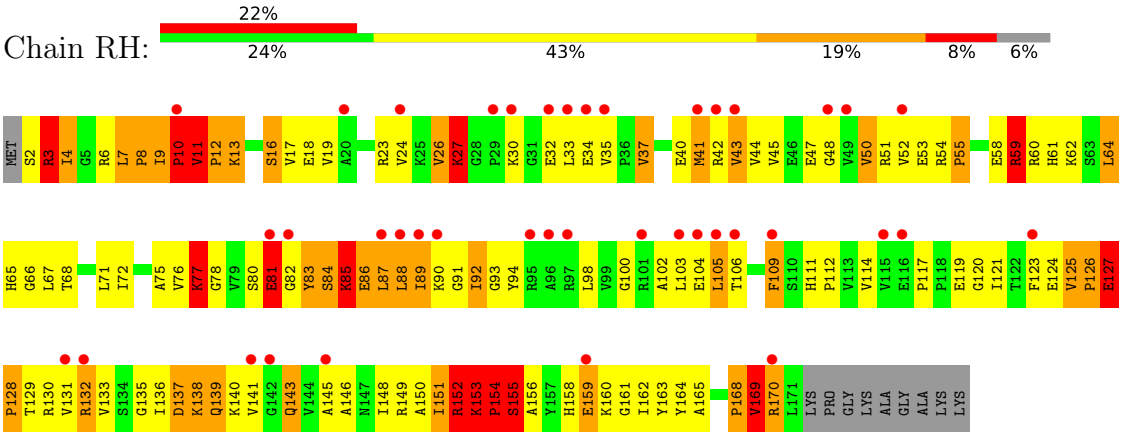
• Molecule 30: 50S ribosomal protein L5

Chain YG:



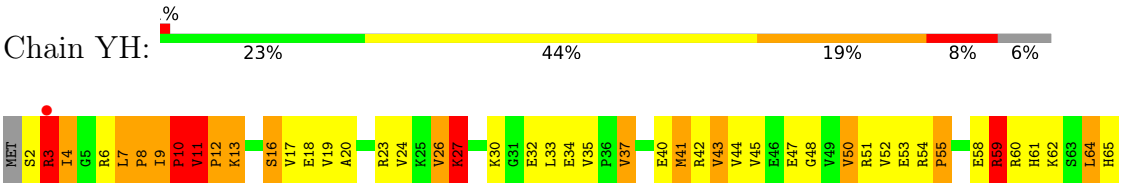
• Molecule 31: 50S ribosomal protein L6

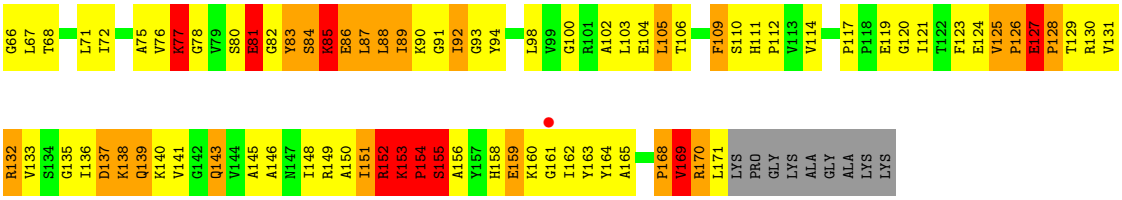
Chain RH:



• Molecule 31: 50S ribosomal protein L6

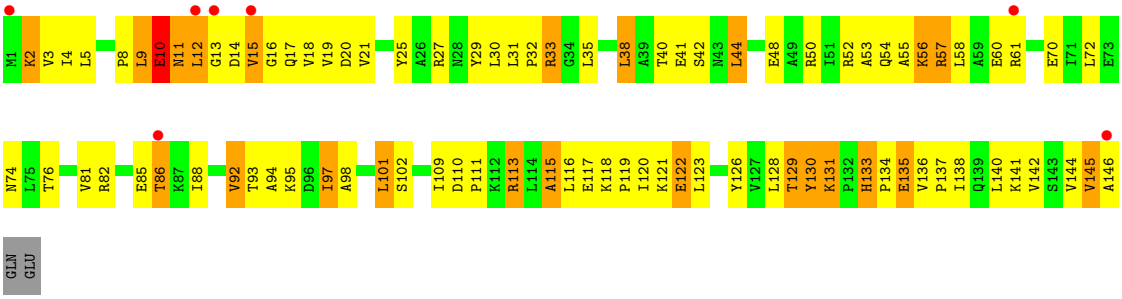
Chain YH:





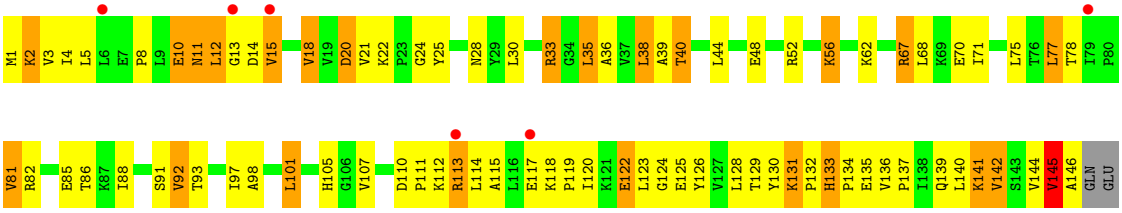
• Molecule 32: 50S ribosomal protein L9

Chain RI:



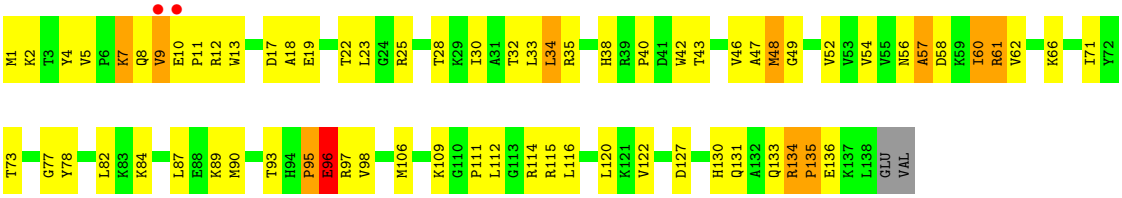
• Molecule 32: 50S ribosomal protein L9

Chain YI:



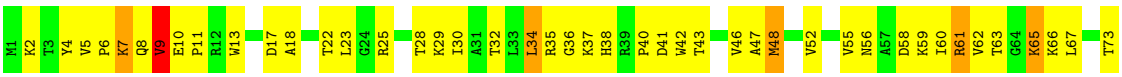
• Molecule 33: 50S ribosomal protein L13

Chain RN:



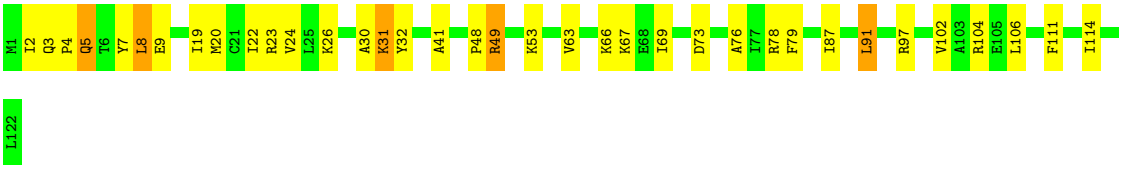
• Molecule 33: 50S ribosomal protein L13

Chain YN:



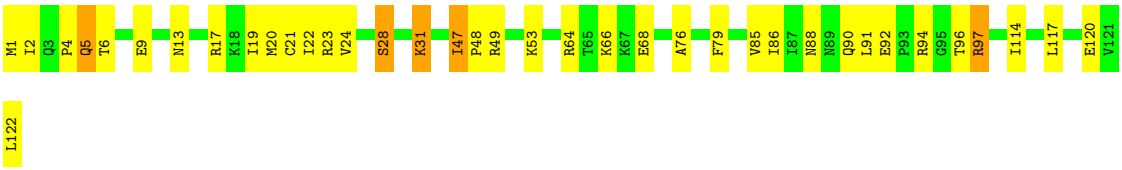
• Molecule 34: 50S ribosomal protein L14

Chain RO:



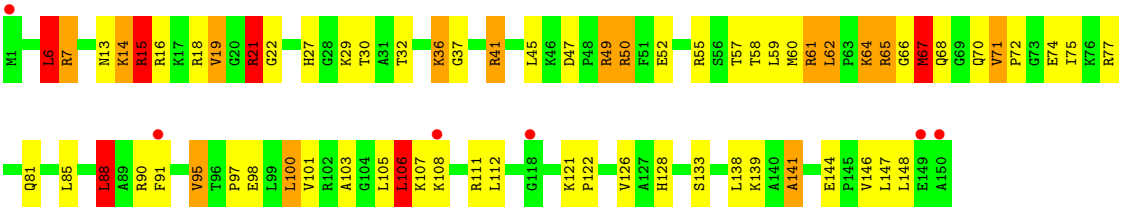
• Molecule 34: 50S ribosomal protein L14

Chain YO:



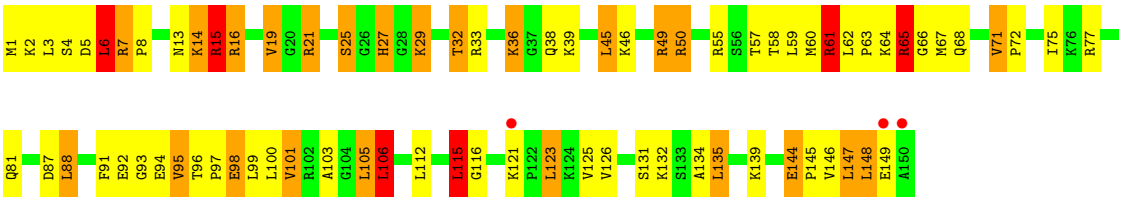
• Molecule 35: 50S ribosomal protein L15

Chain RP:



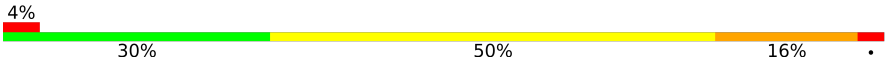
• Molecule 35: 50S ribosomal protein L15

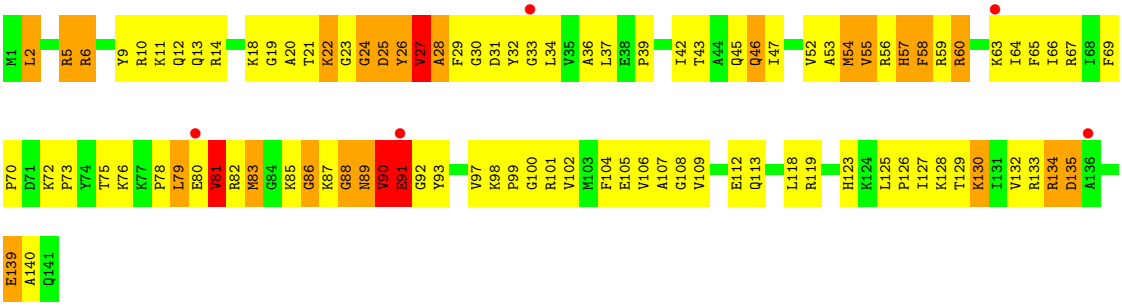
Chain YP:



• Molecule 36: 50S ribosomal protein L16

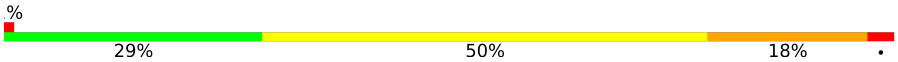
Chain RQ:

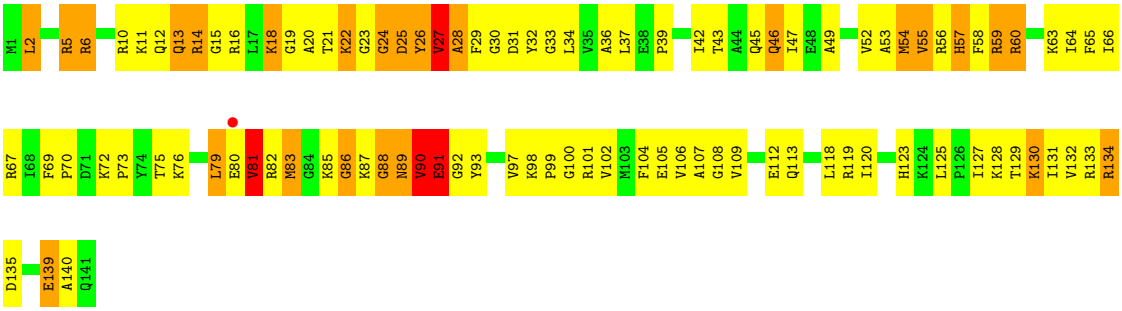




- Molecule 36: 50S ribosomal protein L16

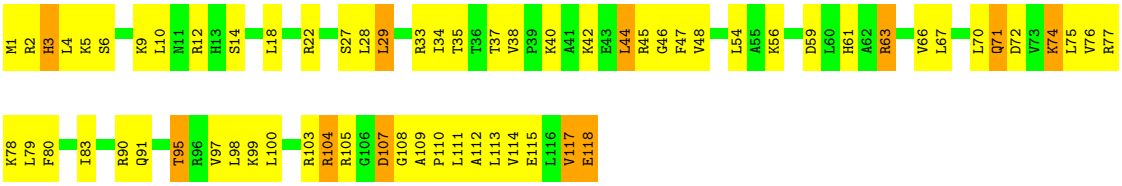
Chain YQ:





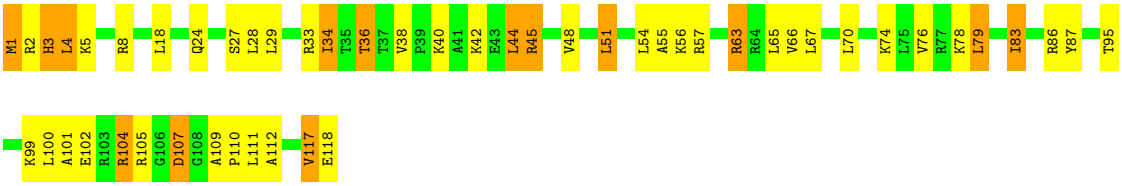
- Molecule 37: 50S ribosomal protein L17

Chain RR:



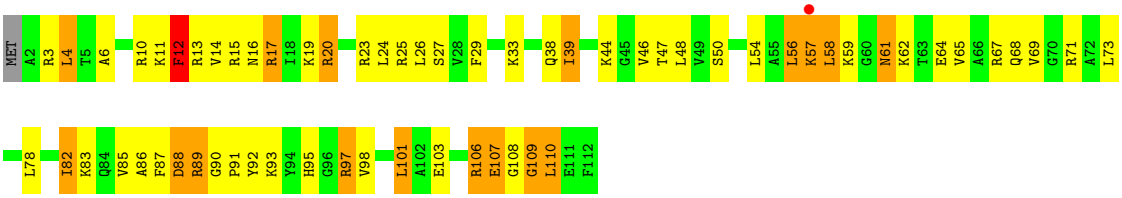
- Molecule 37: 50S ribosomal protein L17

Chain YR:



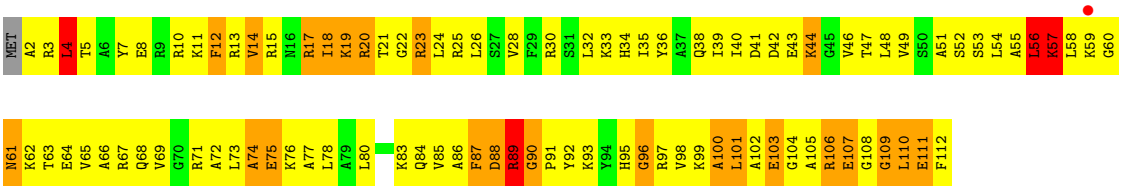
- Molecule 38: 50S ribosomal protein L18

Chain RS:



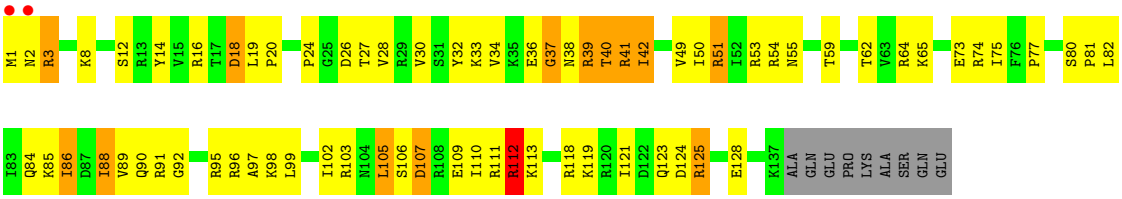
• Molecule 38: 50S ribosomal protein L18

Chain YS:



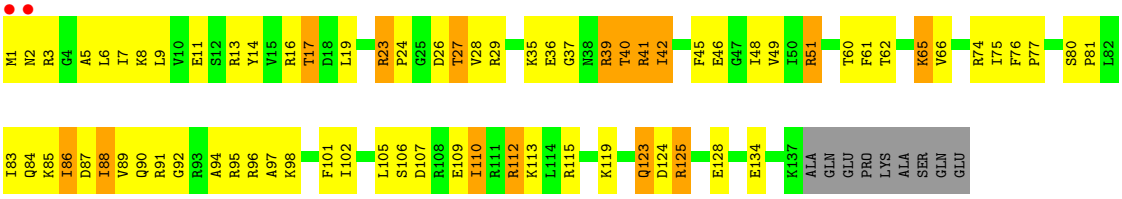
• Molecule 39: 50S ribosomal protein L19

Chain RT:



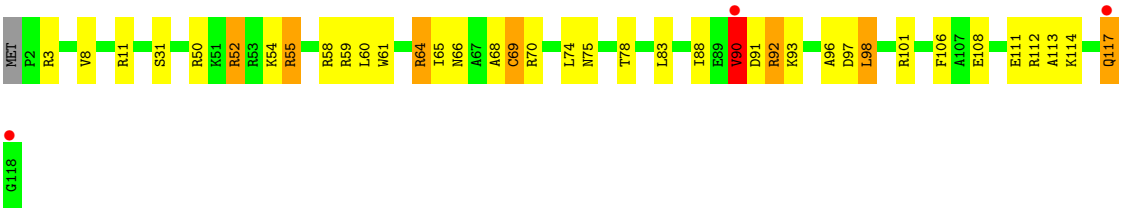
• Molecule 39: 50S ribosomal protein L19

Chain YT:



• Molecule 40: 50S ribosomal protein L20

Chain RU:



• Molecule 40: 50S ribosomal protein L20

Chain YU: 2% 50% 42% 8%

MET P2 K5 V8 R11 R12 K15 K16 I17 L18 K19 K22 L27 K30 L39 R50 K51 R52 R53 K54 R55 R58 R59 L60 W61 R64 I65 N66 A67 A68 C69 R70 Q71 L74 N75 Y76 S77 T78 E79 I80 L83 I88 E89 V90 D91 R92

K93 N94 L95 A96 D97 L98 A99 V100 R101 E102 P103 Q104 V105 F106 A107 E108 L109 V110 E111 R112 A113 K114 Q117 G118

- Molecule 41: 50S ribosomal protein L21

Chain RV: 6% 59% 30% 10%

M1 T7 R13 V14 E15 P16 K19 L20 R21 V22 E23 K24 L25 D26 E34 L35 P36 V37 L38 L39 L40 K44 T45 V46 V47 G48 T49 P50 V51 V52 E53 G54 A55 S56 V57 E60 V61 L62 G63 H64 V72 K76 A77 K78 V79 Q80 Y81 K84 K85 T92

K97 E98 I99 R100 G101

- Molecule 41: 50S ribosomal protein L21

Chain YV: 3% 44% 44% 12%

M1 F2 A3 I4 T7 K10 Q11 Y12 R13 V14 E15 P16 G17 L18 K19 L20 R21 V22 E23 K24 L25 A31 E34 L35 P36 V37 L38 L39 L40 K44 T45 V46 V47 G48 T49 P50 V51 V52 E53 G54 A55 S56 A59 E60 V61 L62 G63 H64 G65 R66 V72 S73

K76 A77 K78 V79 Q80 Y81 K85 R88 Q89 P90 Y91 T92 E93 L94 L95 I96 I99 R100 G101

- Molecule 42: 50S ribosomal protein L22

Chain RW: 2% 64% 27% 9%

M1 R11 R15 K16 V17 R18 L19 V20 L23 I24 R25 G26 K27 S28 L29 E30 R33 Y38 T39 N40 K41 R42 V47 L51 N60 D63 D67 R68 L69 Y70 V71 A74 Y75 V76 L82 L86 P87 G91 R92 A93 D94 I95 I96 K97 K98 R99

T100 T104 V105 I106 L107 K110 H111 G112 K113

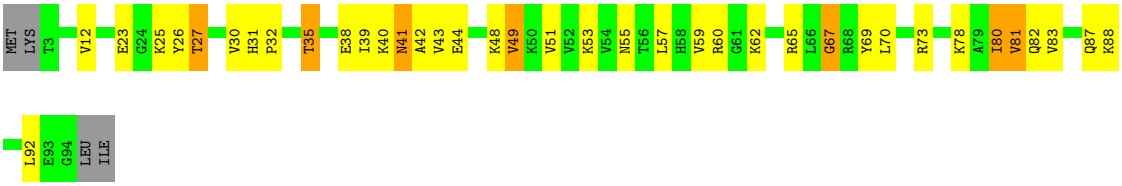
- Molecule 42: 50S ribosomal protein L22

Chain YW: 2% 65% 26% 9%

M1 R11 P14 R15 K16 V17 R18 L23 R33 R37 N40 K41 R42 Y45 K49 V50 L51 E52 N57 N61 D67 R68 L69 Y70 V71 K72 A73 V76 L86 P87 R88 A89 R90 G91 R92 I95 I96 K97 K98 R99 T100 V105 I106 L107

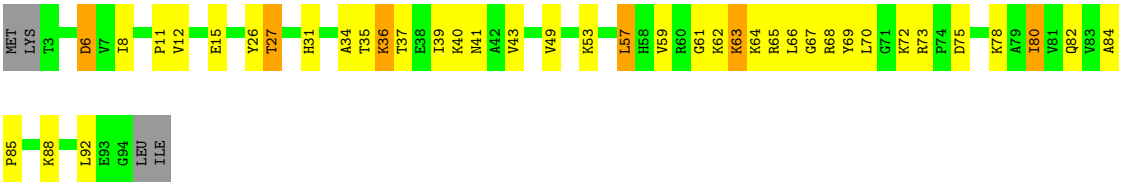
• Molecule 43: 50S ribosomal protein L23

Chain RX:



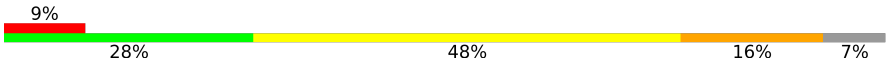
• Molecule 43: 50S ribosomal protein L23

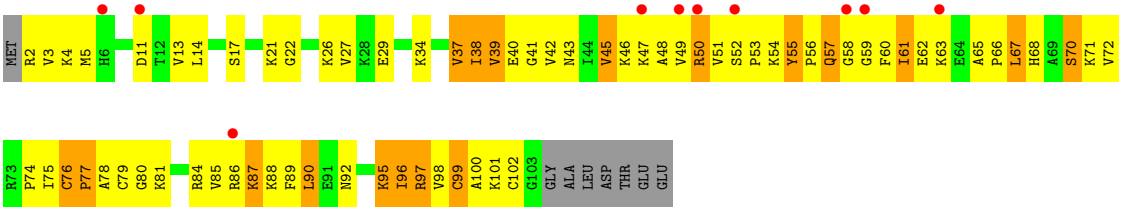
Chain YX:



• Molecule 44: 50S ribosomal protein L24

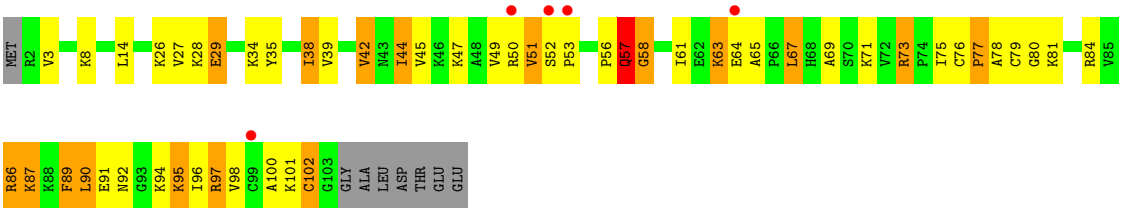
Chain RY:





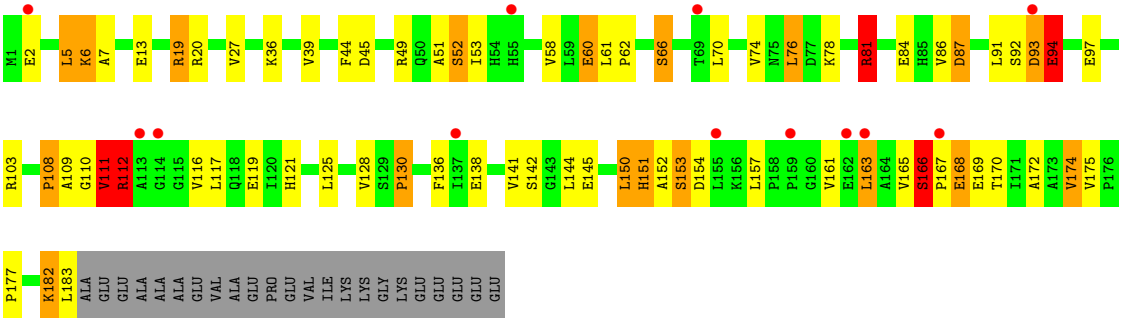
• Molecule 44: 50S ribosomal protein L24

Chain YY:



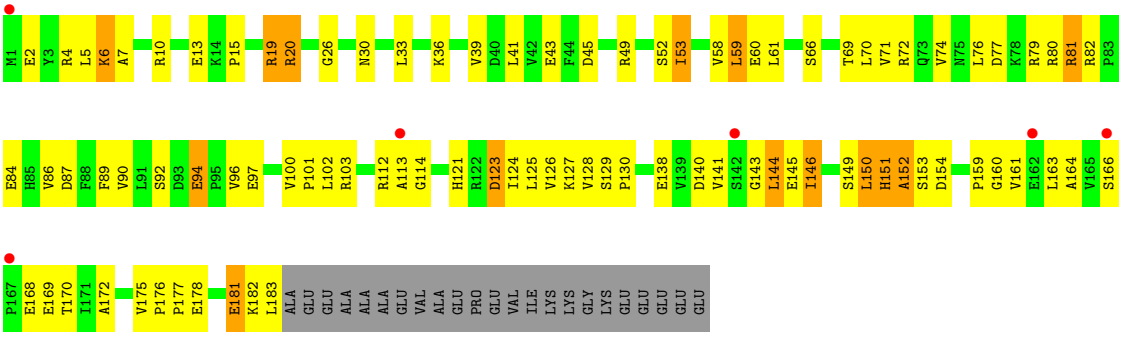
• Molecule 45: 50S ribosomal protein L25

Chain RZ:



- Molecule 45: 50S ribosomal protein L25

Chain YZ:



- Molecule 46: 50S ribosomal protein L27

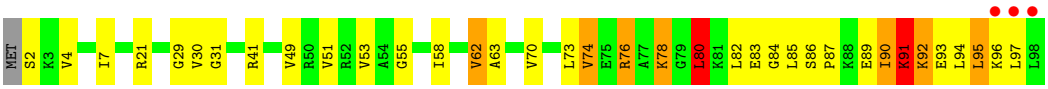
Chain R0:

- Molecule 46: 50S ribosomal protein L27

Chain Y0:

- Molecule 47: 50S ribosomal protein L28

Chain R1:

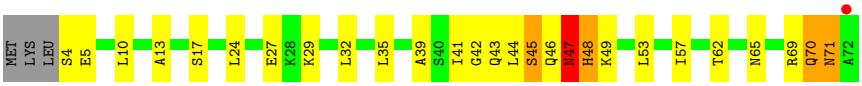


- Molecule 47: 50S ribosomal protein L28

Chain Y1:

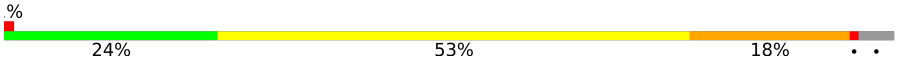
• Molecule 48: 50S ribosomal protein L29

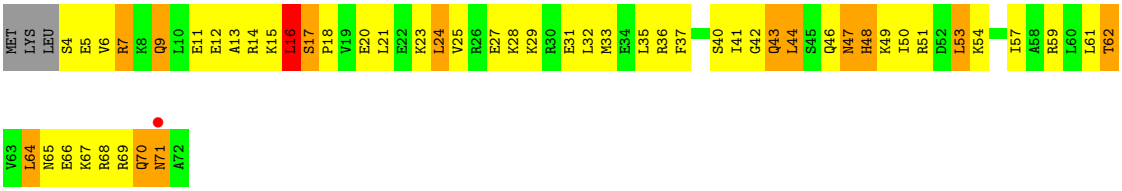
Chain R2:



• Molecule 48: 50S ribosomal protein L29

Chain Y2:





• Molecule 49: 50S ribosomal protein L30

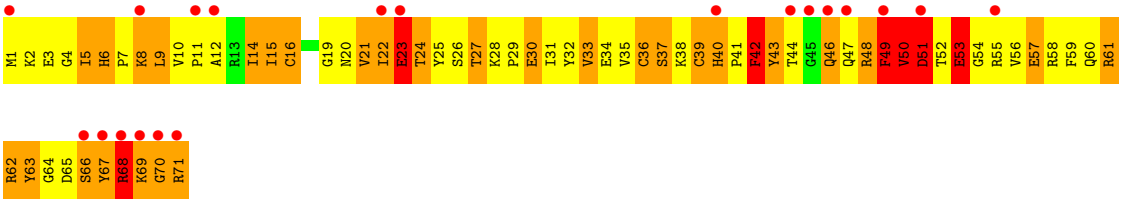
Chain R3:

• Molecule 49: 50S ribosomal protein L30

Chain Y3:

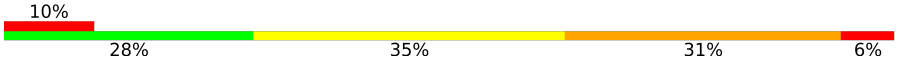
• Molecule 50: 50S ribosomal protein L31

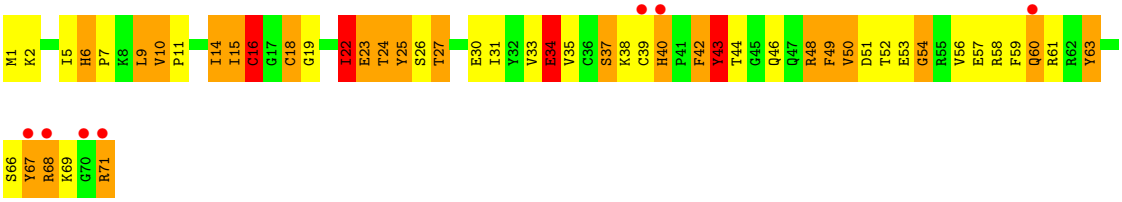
Chain R4:



• Molecule 50: 50S ribosomal protein L31

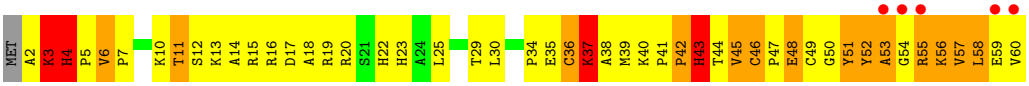
Chain Y4:





• Molecule 51: 50S ribosomal protein L32

Chain R5:

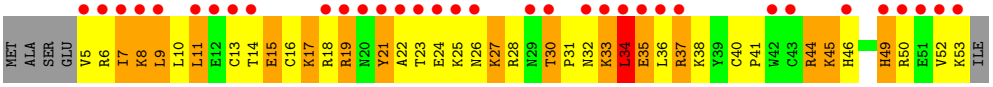


• Molecule 51: 50S ribosomal protein L32

Chain Y5:

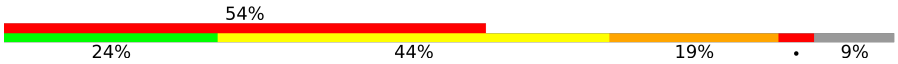
• Molecule 52: 50S ribosomal protein L33

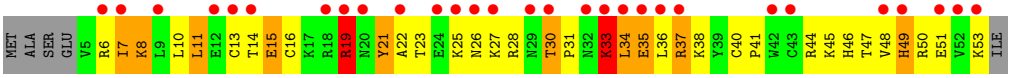
Chain R6:



• Molecule 52: 50S ribosomal protein L33

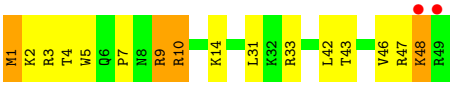
Chain Y6:





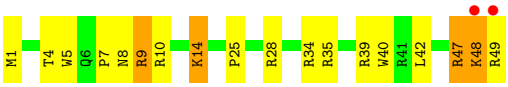
• Molecule 53: 50S ribosomal protein L34

Chain R7:



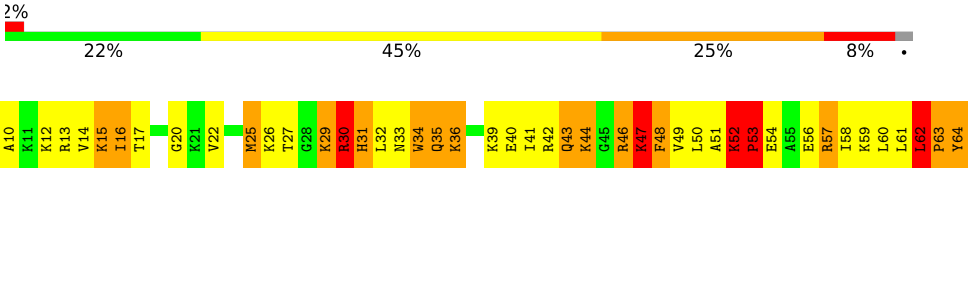
• Molecule 53: 50S ribosomal protein L34

Chain Y7:



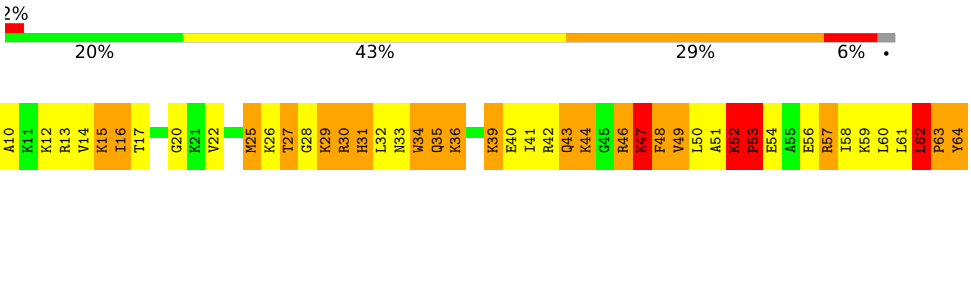
• Molecule 54: 50S ribosomal protein L35

Chain R8:



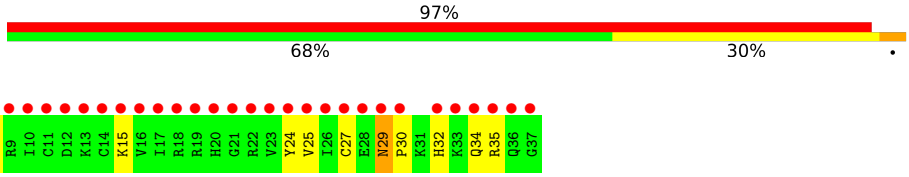
• Molecule 54: 50S ribosomal protein L35

Chain Y8:



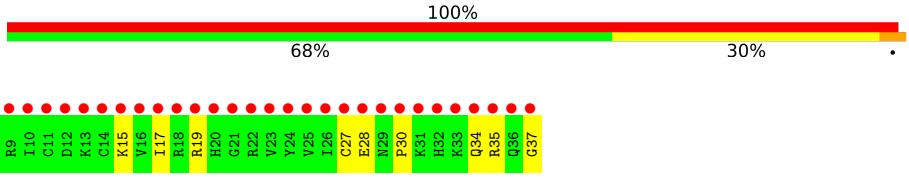
• Molecule 55: 50S ribosomal protein L36

Chain R9:



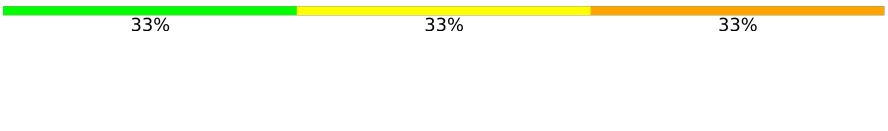
• Molecule 55: 50S ribosomal protein L36

Chain Y9:



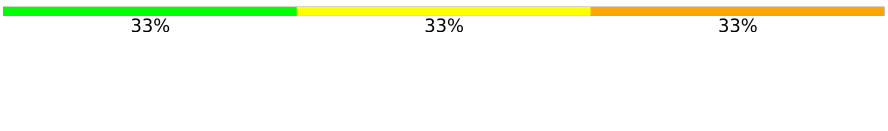
• Molecule 56: CC-Puro

Chain Z5:



• Molecule 56: CC-Puro

Chain Z6:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.98Å 448.71Å 621.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.59 – 3.60 68.59 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (68.59-3.60) 98.4 (68.59-3.40)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.207 , 0.252 0.209 , 0.252	Depositor DCC
R_{free} test set	35866 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 82.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	292311	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	QA	0.42	0/36097	0.97	58/56339 (0.1%)
1	XA	0.45	0/36101	0.99	55/56346 (0.1%)
2	QB	0.31	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.54	0/2195
3	XC	0.36	0/1629	0.56	0/2195
4	QD	0.26	0/1733	0.45	0/2318
4	XD	0.40	0/1733	0.59	0/2318
5	QE	0.39	1/1171 (0.1%)	0.61	1/1576 (0.1%)
5	XE	0.42	1/1171 (0.1%)	0.61	1/1576 (0.1%)
6	QF	0.38	0/856	0.55	0/1154
6	XF	0.39	0/856	0.58	0/1154
7	QG	0.33	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.51	0/1709
8	QH	0.34	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.36	0/814	0.63	2/1095 (0.2%)
10	XJ	0.39	1/814 (0.1%)	0.63	1/1095 (0.1%)
11	QK	0.38	0/900	0.59	1/1213 (0.1%)
11	XK	0.39	0/900	0.58	0/1213
12	QL	0.49	1/991 (0.1%)	0.80	1/1327 (0.1%)
12	XL	0.49	0/991	0.83	3/1327 (0.2%)
13	QM	0.32	0/974	0.58	0/1303
13	XM	0.36	0/974	0.62	0/1303
14	QN	0.37	0/501	0.62	0/664
14	XN	0.42	0/501	0.66	0/664
15	QO	0.35	0/745	0.54	0/992
15	XO	0.39	0/745	0.54	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.35	0/847	0.54	0/1131
18	QR	0.35	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.33	0/689	0.61	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.36	0/765	0.64	0/1007
20	XT	0.37	1/765 (0.1%)	0.62	0/1007
21	QU	0.30	0/221	0.54	0/288
21	XU	0.31	0/221	0.61	0/288
22	QV	0.39	1/1836 (0.1%)	0.83	0/2859
22	XV	0.40	1/1836 (0.1%)	0.83	0/2859
23	QX	0.46	0/246	0.98	0/381
23	XX	0.81	0/246	1.23	2/381 (0.5%)
24	QY	0.35	0/358	0.83	0/556
24	XY	0.59	0/384	1.00	0/597
25	RA	0.39	0/69521	0.91	73/108529 (0.1%)
25	YA	0.42	4/69521 (0.0%)	0.93	99/108529 (0.1%)
26	RB	0.38	0/2878	0.98	9/4490 (0.2%)
26	YB	0.41	0/2878	1.03	15/4490 (0.3%)
27	RD	0.51	0/2165	0.70	0/2919
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.30	0/1620	0.48	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.31	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	3/1802 (0.2%)
32	RI	0.27	0/1151	0.55	0/1558
32	YI	0.33	1/1151 (0.1%)	0.56	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.43	0/1131	0.63	0/1525
34	RO	0.41	0/943	0.62	1/1269 (0.1%)
34	YO	0.49	0/943	0.65	0/1269
35	RP	0.28	0/1162	0.60	1/1544 (0.1%)
35	YP	0.32	0/1162	0.64	0/1544
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.42	0/982	0.69	0/1312
37	YR	0.44	0/982	0.73	0/1312
38	RS	0.36	0/892	0.64	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YS	0.46	0/892	0.83	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.43	0/1155	0.66	0/1542
40	RU	0.39	0/982	0.65	0/1306
40	YU	0.51	0/982	0.70	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.45	0/790	0.73	1/1057 (0.1%)
42	RW	0.49	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.48	0/739	0.65	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.46	0/798	0.69	0/1064
45	RZ	0.29	0/1493	0.52	0/2026
45	YZ	0.29	0/1493	0.55	0/2026
46	R0	0.46	0/657	0.67	0/874
46	Y0	0.48	0/657	0.69	0/874
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.38	0/583	0.63	0/771
48	Y2	0.50	0/583	0.89	2/771 (0.3%)
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.41	0/474	0.59	0/635
50	R4	0.39	0/594	0.78	1/795 (0.1%)
50	Y4	0.37	0/594	0.68	0/795
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.49	0/468	0.72	0/632
52	R6	0.35	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.67	0/575
53	Y7	0.56	0/438	0.71	0/575
54	R8	0.63	0/525	0.94	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.26	0/310	0.45	0/407
55	Y9	0.32	0/310	0.48	0/407
56	Z5	0.78	0/40	1.81	1/60 (1.7%)
56	Z6	0.78	0/40	1.79	1/60 (1.7%)
All	All	0.41	12/316537 (0.0%)	0.88	356/473247 (0.1%)

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.57	1.48	1.61
22	XV	0	C	OP3-P	-10.53	1.48	1.61
32	YI	145	VAL	C-N	5.83	1.47	1.34
25	YA	1142(A)	A	N9-C4	-5.66	1.34	1.37
25	YA	1021	A	N9-C4	-5.60	1.34	1.37

The worst 5 of 356 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	1495	U	N1-C2-O2	10.26	129.99	122.80
28	YE	21	VAL	C-N-CD	-10.10	98.38	120.60
28	RE	21	VAL	C-N-CD	-10.08	98.42	120.60
26	YB	81	G	C5-C6-O6	-9.56	122.86	128.60
1	XA	1495	U	N1-C2-O2	9.41	129.39	122.80

There are no chirality outliers.

There are no planarity outliers.

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	32246	0	16278	532	0
1	XA	32249	0	16279	521	0
2	QB	1924	0	1975	62	0
2	XB	1924	0	1975	83	0
3	QC	1605	0	1668	51	0
3	XC	1605	0	1668	61	0
4	QD	1703	0	1764	57	0
4	XD	1703	0	1764	49	0
5	QE	1155	0	1213	61	0
5	XE	1155	0	1213	58	0
6	QF	843	0	857	17	0
6	XF	843	0	857	21	0
7	QG	1257	0	1296	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	23	0
8	QH	1116	0	1177	40	0
8	XH	1116	0	1177	30	0
9	QI	1010	0	1037	33	0
9	XI	1010	0	1037	49	0
10	QJ	801	0	849	66	0
10	XJ	801	0	849	62	0
11	QK	885	0	904	26	0
11	XK	885	0	904	28	0
12	QL	975	0	1062	97	0
12	XL	975	0	1062	96	0
13	QM	964	0	1034	51	0
13	XM	964	0	1034	42	0
14	QN	492	0	529	23	0
14	XN	492	0	529	22	0
15	QO	734	0	771	20	0
15	XO	734	0	771	17	0
16	QP	705	0	725	14	0
16	XP	705	0	725	23	0
17	QQ	834	0	904	26	0
17	XQ	834	0	904	20	0
18	QR	574	0	644	10	0
18	XR	574	0	644	20	0
19	QS	674	0	699	68	0
19	XS	674	0	699	43	0
20	QT	763	0	860	34	0
20	XT	763	0	861	52	0
21	QU	217	0	234	10	0
21	XU	217	0	234	5	0
22	QV	1644	0	836	20	0
22	XV	1644	0	836	17	0
23	QX	220	0	109	1	0
23	XX	220	0	109	3	0
24	QY	321	0	162	2	0
24	XY	344	0	173	7	0
25	RA	62071	0	31291	907	0
25	YA	62071	0	31291	922	0
26	RB	2573	0	1306	41	0
26	YB	2573	0	1306	47	0
27	RD	2115	0	2195	97	0
27	YD	2115	0	2195	333	0
28	RE	1568	0	1634	291	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	288	0
29	RF	1585	0	1632	53	0
29	YF	1585	0	1632	182	0
30	RG	1474	0	1535	110	0
30	YG	1474	0	1535	62	0
31	RH	1307	0	1382	227	0
31	YH	1307	0	1382	229	0
32	RI	1136	0	1223	73	0
32	YI	1136	0	1223	47	0
33	RN	1104	0	1180	42	0
33	YN	1104	0	1180	57	0
34	RO	933	0	996	21	0
34	YO	933	0	996	26	0
35	RP	1145	0	1228	69	0
35	YP	1145	0	1228	83	0
36	RQ	1122	0	1179	169	0
36	YQ	1122	0	1179	180	0
37	RR	968	0	1033	45	0
37	YR	968	0	1033	34	0
38	RS	882	0	943	47	0
38	YS	882	0	943	165	0
39	RT	1141	0	1202	64	0
39	YT	1141	0	1202	58	0
40	RU	964	0	1022	30	0
40	YU	964	0	1022	55	0
41	RV	779	0	852	19	0
41	YV	779	0	852	48	0
42	RW	900	0	964	23	0
42	YW	900	0	964	24	0
43	RX	725	0	778	28	0
43	YX	725	0	778	20	0
44	RY	785	0	878	53	0
44	YY	785	0	878	40	0
45	RZ	1461	0	1493	43	0
45	YZ	1461	0	1493	61	0
46	R0	648	0	672	29	0
46	Y0	648	0	672	40	0
47	R1	763	0	848	25	0
47	Y1	763	0	848	31	0
48	R2	581	0	629	16	0
48	Y2	581	0	629	75	0
49	R3	469	0	518	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	13	0
50	R4	581	0	575	200	0
50	Y4	581	0	577	62	0
51	R5	459	0	480	92	0
51	Y5	454	0	475	39	0
52	R6	424	0	450	32	0
52	Y6	424	0	450	33	0
53	R7	430	0	480	18	0
53	Y7	430	0	480	19	0
54	R8	517	0	582	121	0
54	Y8	517	0	582	123	0
55	R9	307	0	338	10	0
55	Y9	307	0	338	10	0
56	Z5	74	0	51	8	0
56	Z6	74	0	51	11	0
57	QA	95	0	0	0	0
57	QE	1	0	0	0	0
57	QF	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	3	0	0	0	0
57	QX	2	0	0	0	0
57	QY	1	0	0	0	0
57	R0	1	0	0	0	0
57	R1	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	307	0	0	0	0
57	RB	5	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	114	0	0	0	0
57	XF	1	0	0	0	0
57	XV	3	0	0	0	0
57	XX	2	0	0	0	0
57	Y0	3	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	337	0	0	0	0
57	YB	3	0	0	0	0
57	YD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YE	2	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	1	0	0	0	0
58	QA	42	0	45	3	0
58	XA	42	0	45	1	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	292311	0	198412	7880	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 16.

The worst 5 of 7880 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)
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
30:RG:3:LEU:HD11	50:R4:25:TYR:CE1	1.65	1.29
51:Y5:49:CYS:SG	51:Y5:60:VAL:HG12	1.75	1.26
32:RI:144:VAL:O	32:RI:145:VAL:HG12	1.31	1.24

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	QB	235/256 (92%)	173 (74%)	46 (20%)	16 (7%)	1 15
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	4	33
3	XC	203/239 (85%)	172 (85%)	28 (14%)	3 (2%)	10	47
4	QD	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	10	47
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	6	37
5	QE	149/162 (92%)	137 (92%)	8 (5%)	4 (3%)	5	35
5	XE	149/162 (92%)	134 (90%)	12 (8%)	3 (2%)	7	41
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	12	50
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	50
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	22	61
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4	33
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	26
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	4	31
10	QJ	97/105 (92%)	77 (79%)	16 (16%)	4 (4%)	3	26
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	20
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	45
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	45
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	12
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	12
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	14
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	7
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	51
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	38
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	13	51
16	XP	82/88 (93%)	72 (88%)	9 (11%)	1 (1%)	13	51
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7	41
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10	47
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	4
19	XS	82/93 (88%)	54 (66%)	18 (22%)	10 (12%)	0	5
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	17
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	1	17
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	24
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	24
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	23
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	14
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	181 (90%)	13 (6%)	6 (3%)	4	33
29	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	8
30	RG	179/182 (98%)	139 (78%)	25 (14%)	15 (8%)	1	10
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	15
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	109 (76%)	24 (17%)	11 (8%)	1	12
32	YI	144/148 (97%)	108 (75%)	23 (16%)	13 (9%)	1	9
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	9
33	YN	136/140 (97%)	107 (79%)	16 (12%)	13 (10%)	0	8
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	45
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	9	45
35	RP	148/150 (99%)	109 (74%)	26 (18%)	13 (9%)	1	9
35	YP	148/150 (99%)	101 (68%)	35 (24%)	12 (8%)	1	11
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	7
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	7
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	24
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	20
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	7
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1	9
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	13
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	30
40	YU	115/118 (98%)	102 (89%)	11 (10%)	2 (2%)	9	45
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	17
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	11
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3	29
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	8	43
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	39
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6	39
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	3
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	5
45	RZ	181/206 (88%)	127 (70%)	34 (19%)	20 (11%)	0	6
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	0	8
46	R0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	12	50
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	8
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	17
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	1	17
48	Y2	67/72 (93%)	46 (69%)	13 (19%)	8 (12%)	0	5
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	30
49	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	43
50	R4	69/71 (97%)	22 (32%)	21 (30%)	26 (38%)	0	0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	3	29
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	0
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	2
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	40
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	40
54	R8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0 2
55	R9	35/37 (95%)	35 (100%)	0	0	100 100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
All	All	11469/12128 (95%)	9024 (79%)	1612 (14%)	833 (7%)	1 13

5 of 833 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	33	MET
12	QL	18	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	QB	205/220 (93%)	172 (84%)	33 (16%)	2 16
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5 26
3	QC	159/188 (85%)	144 (91%)	15 (9%)	8 38
3	XC	159/188 (85%)	145 (91%)	14 (9%)	10 40
4	QD	180/181 (99%)	161 (89%)	19 (11%)	6 32
4	XD	180/181 (99%)	154 (86%)	26 (14%)	3 20
5	QE	116/123 (94%)	103 (89%)	13 (11%)	6 30
5	XE	116/123 (94%)	104 (90%)	12 (10%)	7 34
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4 23
6	XF	90/90 (100%)	82 (91%)	8 (9%)	9 40
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8 37
7	XG	126/127 (99%)	114 (90%)	12 (10%)	8 37
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	32
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2	12
9	XI	98/99 (99%)	80 (82%)	18 (18%)	1	10
10	QJ	89/92 (97%)	79 (89%)	10 (11%)	6	30
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	2	17
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	35
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	35
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	23
12	XL	104/109 (95%)	89 (86%)	15 (14%)	3	20
13	QM	97/101 (96%)	73 (75%)	24 (25%)	0	4
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	8
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	21
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	40
15	XO	79/80 (99%)	69 (87%)	10 (13%)	4	24
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	25
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6	31
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	11	42
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	53
18	QR	61/77 (79%)	50 (82%)	11 (18%)	1	11
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	19
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	9
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	6
20	QT	76/82 (93%)	67 (88%)	9 (12%)	5	28
20	XT	76/82 (93%)	67 (88%)	9 (12%)	5	28
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	59
27	RD	214/218 (98%)	175 (82%)	39 (18%)	1	10
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	12
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	5
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	RF	161/166 (97%)	142 (88%)	19 (12%)	5	28
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	24
30	RG	155/156 (99%)	134 (86%)	21 (14%)	4	23
30	YG	155/156 (99%)	133 (86%)	22 (14%)	3	21
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	8
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	8
32	RI	122/124 (98%)	100 (82%)	22 (18%)	1	11
32	YI	122/124 (98%)	97 (80%)	25 (20%)	1	7
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	13
33	YN	117/119 (98%)	95 (81%)	22 (19%)	1	9
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	35
34	YO	100/100 (100%)	88 (88%)	12 (12%)	5	27
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0	4
35	YP	116/116 (100%)	79 (68%)	37 (32%)	0	2
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	15
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	13
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	11
37	YR	101/101 (100%)	81 (80%)	20 (20%)	1	8
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	7
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	19
39	RT	120/127 (94%)	102 (85%)	18 (15%)	3	19
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	12
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	19
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2	13
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	9
41	YV	82/82 (100%)	67 (82%)	15 (18%)	1	10
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	7
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	12
43	RX	74/78 (95%)	64 (86%)	10 (14%)	4	23
43	YX	74/78 (95%)	60 (81%)	14 (19%)	1	9
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	YY	85/91 (93%)	64 (75%)	21 (25%)	0	4
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	3	19
45	YZ	162/179 (90%)	145 (90%)	17 (10%)	7	33
46	R0	65/67 (97%)	60 (92%)	5 (8%)	13	45
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	9	39
47	R1	82/83 (99%)	73 (89%)	9 (11%)	6	31
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	20
48	R2	64/67 (96%)	55 (86%)	9 (14%)	3	21
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	32
49	R3	51/52 (98%)	45 (88%)	6 (12%)	5	28
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	17
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0	3
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	5
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	3
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
53	R7	42/42 (100%)	34 (81%)	8 (19%)	1	9
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	14
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	38 (70%)	16 (30%)	0	2
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	55
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	55
All	All	9702/10066 (96%)	8183 (84%)	1519 (16%)	2	17

5 of 1519 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	XM	45	VAL
31	YH	152	ARG
15	XO	64	ARG
13	XM	32	GLU
27	YD	261	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	XB	212	GLN
12	XL	9	GLN
31	YH	147	ASN
10	XJ	78	ASN
27	YD	44	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	277 (18%)	43 (2%)
1	XA	1498/1522 (98%)	293 (19%)	37 (2%)
22	QV	76/77 (98%)	19 (25%)	1 (1%)
22	XV	76/77 (98%)	14 (18%)	1 (1%)
23	QX	9/25 (36%)	1 (11%)	0
23	XX	9/25 (36%)	0	0
24	QY	14/17 (82%)	2 (14%)	0
24	XY	15/17 (88%)	1 (6%)	0
25	RA	2879/2915 (98%)	587 (20%)	58 (2%)
25	YA	2879/2915 (98%)	596 (20%)	52 (1%)
26	RB	119/122 (97%)	15 (12%)	2 (1%)
26	YB	119/122 (97%)	21 (17%)	1 (0%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9193/9362 (98%)	1826 (19%)	195 (2%)

5 of 1826 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 195 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	345	C
25	YA	102	G
1	XA	429	U

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Mol	Chain	Res	Type
1	XA	991	U
25	YA	271(B)	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	PPU	Z6	101	56,25	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z5	101	56,25	32,40,41	2.56	6 (18%)	33,57,60	2.15	5 (15%)

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
56	PPU	Z6	101	56,25	-	2/21/43/44	0/4/4/4
56	PPU	Z5	101	56,25	-	2/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z5	101	PPU	O-C	9.32	1.41	1.23
56	Z6	101	PPU	O-C	9.28	1.41	1.23
56	Z5	101	PPU	C9-N6	-5.92	1.32	1.45
56	Z6	101	PPU	C9-N6	-5.90	1.32	1.45
56	Z5	101	PPU	C-N3'	5.70	1.46	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z5	101	PPU	C3'-N3'-C	-8.61	110.22	123.21
56	Z6	101	PPU	C3'-N3'-C	-8.60	110.24	123.21
56	Z5	101	PPU	N3-C2-N1	-4.63	121.45	128.68
56	Z6	101	PPU	N3-C2-N1	-4.61	121.48	128.68
56	Z5	101	PPU	CA-C-N3'	4.02	121.72	116.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z5	101	PPU	O-C-CA-N
56	Z6	101	PPU	O-C-CA-N
56	Z5	101	PPU	N3'-C-CA-N
56	Z6	101	PPU	N3'-C-CA-N

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	101	PPU	11	0
56	Z5	101	PPU	8	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 902 ligands modelled in this entry, 900 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	PAR	XA	1715	-	45,45,45	1.61	7 (15%)	64,67,67	1.25	5 (7%)
58	PAR	QA	1696	-	45,45,45	1.60	9 (20%)	64,67,67	1.30	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	XA	1715	-	-	6/18/94/94	0/4/4/4
58	PAR	QA	1696	-	-	4/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	XA	1715	PAR	C64-C54	5.38	1.59	1.52
58	QA	1696	PAR	C64-C54	5.27	1.59	1.52
58	QA	1696	PAR	C52-C42	3.30	1.59	1.52
58	XA	1715	PAR	C52-C42	3.12	1.58	1.52
58	XA	1715	PAR	O54-C14	3.09	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	QA	1696	PAR	C14-O54-C54	5.02	123.55	113.69
58	XA	1715	PAR	O33-C14-C24	4.55	116.06	108.22
58	XA	1715	PAR	C14-O54-C54	3.93	121.40	113.69
58	XA	1715	PAR	O52-C13-C23	3.40	115.01	107.96
58	QA	1696	PAR	O54-C54-C64	3.28	112.11	106.01

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	QA	1696	PAR	O43-C43-C53-O53
58	XA	1715	PAR	O43-C43-C53-O53
58	QA	1696	PAR	C33-C43-C53-O53
58	XA	1715	PAR	C33-C43-C53-O53
58	XA	1715	PAR	O51-C51-C61-O61

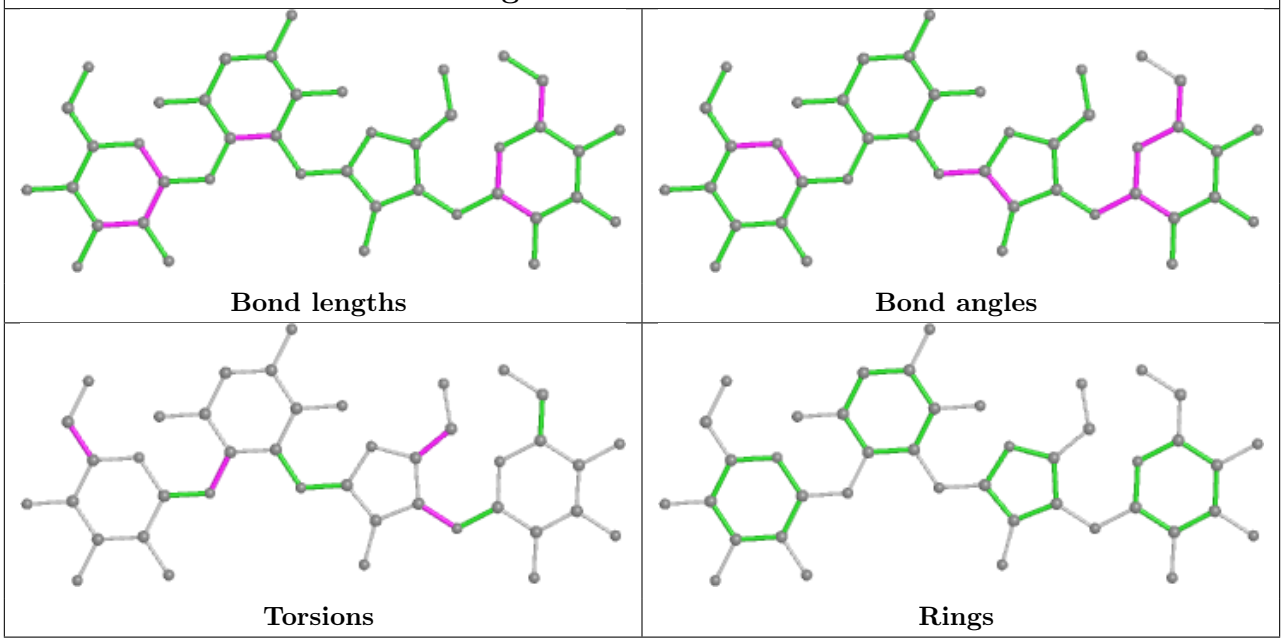
There are no ring outliers.

2 monomers are involved in 4 short contacts:

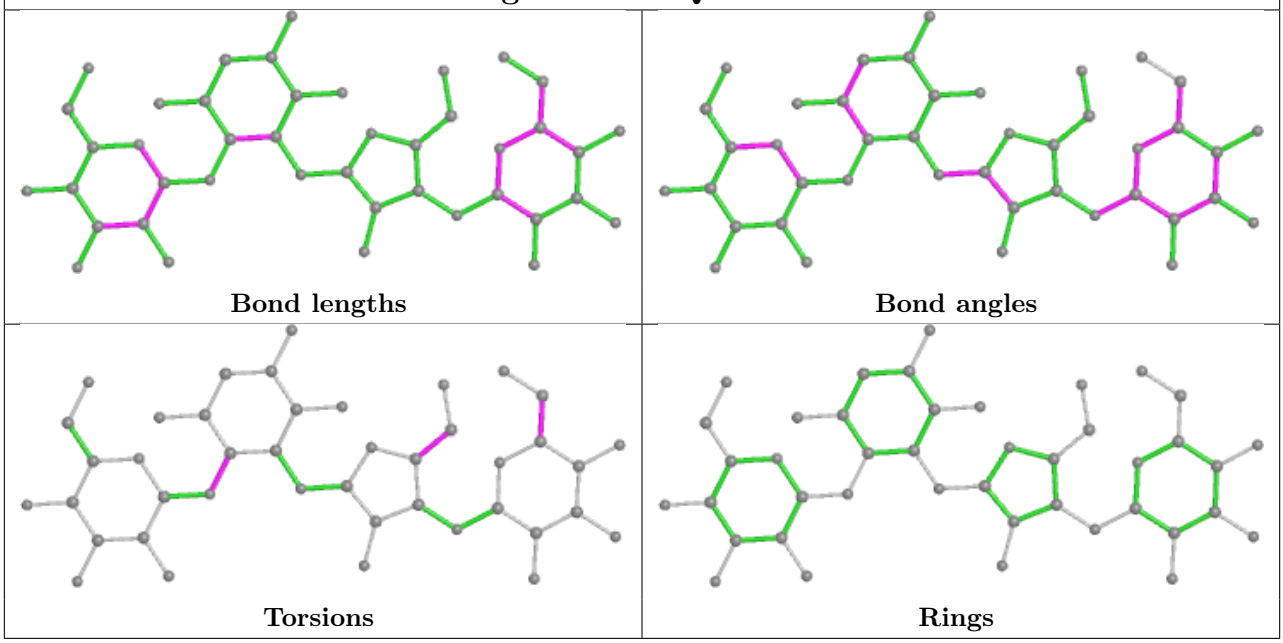
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1715	PAR	1	0
58	QA	1696	PAR	3	0

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

Ligand PAR XA 1715



Ligand PAR QA 1696



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.04	11 (0%)	87	78	37, 82, 166, 360	0
1	XA	1500/1522 (98%)	-0.01	8 (0%)	91	83	27, 73, 170, 298	0
2	QB	237/256 (92%)	0.48	15 (6%)	20	11	55, 128, 200, 260	0
2	XB	237/256 (92%)	0.34	7 (2%)	50	34	51, 115, 181, 270	0
3	QC	205/239 (85%)	0.20	3 (1%)	73	60	64, 119, 182, 242	0
3	XC	205/239 (85%)	-0.10	1 (0%)	91	83	45, 87, 134, 188	0
4	QD	208/209 (99%)	-0.15	0	100	100	39, 90, 141, 165	0
4	XD	208/209 (99%)	-0.14	0	100	100	34, 83, 139, 183	0
5	QE	151/162 (93%)	0.02	1 (0%)	87	78	49, 94, 145, 200	0
5	XE	151/162 (93%)	-0.18	0	100	100	39, 76, 128, 177	0
6	QF	101/101 (100%)	-0.25	0	100	100	34, 75, 114, 156	0
6	XF	101/101 (100%)	-0.18	1 (0%)	82	70	30, 77, 132, 236	0
7	QG	155/156 (99%)	0.55	13 (8%)	11	7	55, 111, 167, 291	0
7	XG	155/156 (99%)	0.20	7 (4%)	33	21	52, 101, 154, 205	0
8	QH	138/138 (100%)	-0.01	0	100	100	57, 93, 145, 158	0
8	XH	138/138 (100%)	0.01	0	100	100	44, 83, 126, 144	0
9	QI	127/128 (99%)	0.53	5 (3%)	39	25	62, 122, 183, 230	0
9	XI	127/128 (99%)	0.20	2 (1%)	72	57	39, 114, 166, 213	0
10	QJ	99/105 (94%)	0.67	4 (4%)	38	25	56, 133, 221, 251	0
10	XJ	99/105 (94%)	0.45	2 (2%)	65	49	43, 113, 174, 209	0
11	QK	119/129 (92%)	0.52	9 (7%)	13	8	46, 83, 150, 237	0
11	XK	119/129 (92%)	0.53	5 (4%)	36	23	33, 76, 147, 227	0
12	QL	125/132 (94%)	0.36	5 (4%)	38	25	42, 80, 142, 248	0
12	XL	125/132 (94%)	0.17	3 (2%)	59	42	32, 68, 126, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	0.39	8 (6%)	18	10	45, 118, 179, 283	0
13	XM	121/126 (96%)	0.14	3 (2%)	57	41	41, 99, 165, 284	0
14	QN	60/61 (98%)	0.28	0	100	100	52, 104, 144, 159	0
14	XN	60/61 (98%)	-0.18	0	100	100	37, 76, 109, 126	0
15	QO	88/89 (98%)	-0.03	0	100	100	36, 84, 136, 178	0
15	XO	88/89 (98%)	-0.08	0	100	100	41, 76, 120, 130	0
16	QP	84/88 (95%)	0.24	2 (2%)	59	42	43, 78, 129, 174	0
16	XP	84/88 (95%)	0.39	2 (2%)	59	42	53, 89, 138, 202	0
17	QQ	100/105 (95%)	0.16	0	100	100	51, 90, 130, 190	0
17	XQ	100/105 (95%)	0.12	0	100	100	48, 85, 127, 173	0
18	QR	70/88 (79%)	0.11	2 (2%)	51	35	43, 82, 138, 172	0
18	XR	70/88 (79%)	0.17	1 (1%)	75	61	35, 79, 124, 157	0
19	QS	84/93 (90%)	0.61	4 (4%)	30	19	70, 127, 178, 246	0
19	XS	84/93 (90%)	0.55	2 (2%)	59	42	63, 106, 161, 228	0
20	QT	99/106 (93%)	0.44	4 (4%)	38	25	56, 98, 150, 177	0
20	XT	99/106 (93%)	0.60	8 (8%)	12	7	61, 110, 169, 201	0
21	QU	25/27 (92%)	0.41	1 (4%)	38	25	62, 110, 148, 166	0
21	XU	25/27 (92%)	0.28	1 (4%)	38	25	54, 90, 124, 164	0
22	QV	77/77 (100%)	0.24	1 (1%)	77	63	41, 95, 162, 189	0
22	XV	77/77 (100%)	0.22	1 (1%)	77	63	34, 87, 125, 169	0
23	QX	11/25 (44%)	0.48	1 (9%)	9	5	55, 79, 176, 213	0
23	XX	11/25 (44%)	0.53	1 (9%)	9	5	41, 59, 161, 175	0
24	QY	15/17 (88%)	0.39	0	100	100	62, 89, 153, 156	0
24	XY	16/17 (94%)	0.31	0	100	100	57, 85, 152, 154	0
25	RA	2882/2915 (98%)	0.09	116 (4%)	38	25	24, 60, 218, 384	0
25	YA	2882/2915 (98%)	0.03	106 (3%)	41	27	19, 51, 215, 471	0
26	RB	120/122 (98%)	-0.09	0	100	100	69, 96, 130, 160	0
26	YB	120/122 (98%)	-0.24	0	100	100	50, 73, 106, 142	0
27	RD	272/276 (98%)	-0.24	1 (0%)	92	86	22, 49, 98, 171	0
27	YD	272/276 (98%)	-0.20	1 (0%)	92	86	11, 45, 84, 223	0
28	RE	205/206 (99%)	0.07	4 (1%)	65	49	22, 70, 140, 321	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	YE	205/206 (99%)	-0.01	3 (1%)	73	60	22, 68, 139, 246	0
29	RF	202/210 (96%)	0.07	1 (0%)	91	83	20, 71, 132, 203	0
29	YF	202/210 (96%)	0.02	4 (1%)	65	49	14, 63, 129, 185	0
30	RG	181/182 (99%)	0.50	7 (3%)	39	25	64, 114, 167, 218	0
30	YG	181/182 (99%)	0.11	3 (1%)	70	55	50, 83, 136, 272	0
31	RH	170/180 (94%)	1.36	40 (23%)	0	0	77, 169, 247, 338	0
31	YH	170/180 (94%)	0.38	2 (1%)	79	66	36, 90, 147, 208	0
32	RI	146/148 (98%)	0.39	7 (4%)	30	19	37, 104, 161, 269	0
32	YI	146/148 (98%)	0.36	6 (4%)	37	24	26, 102, 156, 181	0
33	RN	138/140 (98%)	0.14	2 (1%)	75	61	38, 75, 133, 194	0
33	YN	138/140 (98%)	-0.03	0	100	100	36, 70, 124, 180	0
34	RO	122/122 (100%)	0.05	0	100	100	28, 65, 109, 146	0
34	YO	122/122 (100%)	-0.02	0	100	100	17, 51, 86, 108	0
35	RP	150/150 (100%)	0.35	6 (4%)	38	25	19, 79, 151, 264	0
35	YP	150/150 (100%)	0.09	3 (2%)	65	49	15, 68, 135, 202	0
36	RQ	141/141 (100%)	0.44	5 (3%)	44	29	43, 88, 145, 228	0
36	YQ	141/141 (100%)	0.04	1 (0%)	87	78	18, 63, 121, 227	0
37	RR	118/118 (100%)	-0.06	0	100	100	26, 57, 91, 135	0
37	YR	118/118 (100%)	-0.14	0	100	100	34, 65, 112, 156	0
38	RS	111/112 (99%)	0.23	1 (0%)	84	73	60, 96, 158, 199	0
38	YS	111/112 (99%)	0.12	1 (0%)	84	73	36, 84, 137, 172	0
39	RT	137/146 (93%)	-0.08	2 (1%)	73	60	39, 74, 168, 287	0
39	YT	137/146 (93%)	-0.13	2 (1%)	73	60	29, 71, 152, 217	0
40	RU	117/118 (99%)	0.03	3 (2%)	56	40	23, 68, 138, 196	0
40	YU	117/118 (99%)	-0.09	2 (1%)	70	55	23, 57, 136, 223	0
41	RV	101/101 (100%)	0.49	6 (5%)	22	13	37, 89, 166, 286	0
41	YV	101/101 (100%)	0.14	3 (2%)	50	34	31, 84, 143, 275	0
42	RW	113/113 (100%)	0.14	2 (1%)	68	53	22, 52, 109, 206	0
42	YW	113/113 (100%)	0.02	2 (1%)	68	53	24, 53, 119, 205	0
43	RX	92/96 (95%)	0.05	0	100	100	22, 65, 110, 134	0
43	YX	92/96 (95%)	0.06	0	100	100	15, 53, 95, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	RY	102/110 (92%)	0.78	10 (9%)	7	4	48, 95, 183, 309	0
44	YY	102/110 (92%)	0.20	5 (4%)	29	18	30, 79, 135, 264	0
45	RZ	183/206 (88%)	0.68	12 (6%)	18	10	65, 123, 209, 310	0
45	YZ	183/206 (88%)	0.46	6 (3%)	46	31	49, 101, 195, 273	0
46	R0	82/85 (96%)	0.15	0	100	100	33, 71, 100, 128	0
46	Y0	82/85 (96%)	0.10	0	100	100	29, 55, 90, 119	0
47	R1	97/98 (98%)	0.29	3 (3%)	49	33	25, 62, 140, 257	0
47	Y1	97/98 (98%)	0.35	4 (4%)	37	24	17, 56, 154, 232	0
48	R2	69/72 (95%)	0.36	1 (1%)	75	61	42, 81, 158, 197	0
48	Y2	69/72 (95%)	0.04	1 (1%)	75	61	30, 64, 139, 181	0
49	R3	59/60 (98%)	0.53	2 (3%)	45	30	45, 86, 134, 177	0
49	Y3	59/60 (98%)	0.36	3 (5%)	28	17	27, 60, 128, 185	0
50	R4	71/71 (100%)	1.36	20 (28%)	0	0	110, 208, 323, 389	0
50	Y4	71/71 (100%)	0.53	7 (9%)	7	4	66, 140, 233, 334	0
51	R5	59/60 (98%)	0.37	5 (8%)	10	6	23, 64, 219, 249	0
51	Y5	58/60 (96%)	0.28	5 (8%)	10	6	27, 71, 208, 261	0
52	R6	49/54 (90%)	2.99	34 (69%)	0	0	110, 164, 240, 272	0
52	Y6	49/54 (90%)	2.60	29 (59%)	0	0	95, 147, 224, 286	0
53	R7	49/49 (100%)	-0.21	2 (4%)	37	24	24, 44, 95, 172	0
53	Y7	49/49 (100%)	-0.31	2 (4%)	37	24	18, 37, 95, 166	0
54	R8	64/65 (98%)	0.19	1 (1%)	72	57	26, 68, 121, 209	0
54	Y8	64/65 (98%)	-0.06	1 (1%)	72	57	27, 58, 128, 223	0
55	R9	37/37 (100%)	5.24	36 (97%)	0	0	96, 171, 236, 316	0
55	Y9	37/37 (100%)	4.42	37 (100%)	0	0	99, 151, 210, 312	0
56	Z5	2/3 (66%)	-0.16	0	100	100	35, 35, 35, 59	0
56	Z6	2/3 (66%)	0.37	0	100	100	32, 32, 32, 42	0
All	All	20880/21490 (97%)	0.15	712 (3%)	45	30	11, 75, 176, 471	0

The worst 5 of 712 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	RP	149	GLU	14.8
55	R9	11	CYS	12.5

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Mol	Chain	Res	Type	RSRZ
55	R9	34	GLN	11.1
55	R9	14	CYS	10.8
25	YA	2165	G	9.8

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
56	PPU	Z5	101	37/38	0.94	0.29	44,44,45,45	0
56	PPU	Z6	101	37/38	0.94	0.26	28,28,29,29	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å^2)	Q<0.9
57	MG	YA	3128	1/1	0.23	0.48	24,24,24,24	0
57	MG	XA	1685	1/1	0.50	0.30	51,51,51,51	0
57	MG	RA	3281	1/1	0.53	0.42	57,57,57,57	0
57	MG	QY	101	1/1	0.54	0.26	51,51,51,51	0
57	MG	YA	3203	1/1	0.54	0.46	40,40,40,40	0
57	MG	RA	3287	1/1	0.56	0.46	60,60,60,60	0
57	MG	YA	3330	1/1	0.56	0.68	52,52,52,52	0
57	MG	RA	3255	1/1	0.57	2.72	76,76,76,76	0
57	MG	XA	1705	1/1	0.59	0.52	58,58,58,58	0
57	MG	YA	3142	1/1	0.61	0.32	39,39,39,39	0
57	MG	XA	1711	1/1	0.62	0.35	47,47,47,47	0
57	MG	YA	3206	1/1	0.63	0.48	55,55,55,55	0
57	MG	RA	3245	1/1	0.63	0.59	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3308	1/1	0.64	0.87	64,64,64,64	0
57	MG	RD	301	1/1	0.64	0.44	51,51,51,51	0
57	MG	RA	3214	1/1	0.65	0.26	29,29,29,29	0
57	MG	YA	3280	1/1	0.65	0.67	67,67,67,67	0
57	MG	RA	3263	1/1	0.66	0.41	49,49,49,49	0
57	MG	R0	101	1/1	0.66	0.25	31,31,31,31	0
57	MG	RA	3290	1/1	0.66	0.14	62,62,62,62	0
57	MG	YA	3285	1/1	0.68	0.60	31,31,31,31	0
57	MG	QA	1695	1/1	0.68	0.49	44,44,44,44	0
57	MG	XA	1659	1/1	0.68	0.53	35,35,35,35	0
57	MG	RA	3208	1/1	0.69	0.15	32,32,32,32	0
57	MG	QA	1628	1/1	0.69	0.27	44,44,44,44	0
57	MG	YA	3289	1/1	0.70	0.56	62,62,62,62	0
57	MG	QA	1653	1/1	0.70	0.62	61,61,61,61	0
57	MG	XA	1628	1/1	0.70	0.12	36,36,36,36	0
59	ZN	XD	301	1/1	0.70	0.32	43,43,43,43	0
57	MG	XA	1605	1/1	0.71	0.55	26,26,26,26	0
57	MG	RA	3210	1/1	0.71	0.34	29,29,29,29	0
57	MG	RA	3013	1/1	0.71	0.48	25,25,25,25	0
57	MG	RA	3276	1/1	0.71	0.52	51,51,51,51	0
57	MG	QA	1675	1/1	0.71	0.22	32,32,32,32	0
57	MG	YA	3233	1/1	0.71	0.41	32,32,32,32	0
57	MG	XA	1713	1/1	0.72	0.87	57,57,57,57	0
57	MG	RA	3171	1/1	0.72	0.20	57,57,57,57	0
57	MG	RA	3296	1/1	0.72	0.40	40,40,40,40	0
57	MG	YA	3277	1/1	0.72	0.89	30,30,30,30	0
57	MG	YA	3170	1/1	0.72	0.23	29,29,29,29	0
57	MG	XA	1679	1/1	0.73	0.57	43,43,43,43	0
57	MG	YA	3071	1/1	0.73	0.12	14,14,14,14	0
57	MG	RA	3305	1/1	0.73	0.59	41,41,41,41	0
57	MG	RA	3202	1/1	0.73	0.42	50,50,50,50	0
57	MG	Y0	101	1/1	0.73	0.30	16,16,16,16	0
57	MG	RA	3194	1/1	0.73	0.27	59,59,59,59	0
57	MG	RA	3253	1/1	0.74	0.63	77,77,77,77	0
57	MG	YA	3297	1/1	0.74	0.58	53,53,53,53	0
57	MG	YA	3225	1/1	0.74	0.41	23,23,23,23	0
57	MG	YA	3174	1/1	0.75	0.24	50,50,50,50	0
57	MG	RA	3129	1/1	0.75	0.25	38,38,38,38	0
57	MG	XA	1714	1/1	0.75	0.39	26,26,26,26	0
57	MG	RA	3211	1/1	0.75	0.32	56,56,56,56	0
57	MG	YA	3320	1/1	0.75	0.44	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1699	1/1	0.75	0.56	44,44,44,44	0
57	MG	RA	3212	1/1	0.75	0.22	55,55,55,55	0
57	MG	RA	3213	1/1	0.75	0.31	38,38,38,38	0
57	MG	RA	3113	1/1	0.76	0.19	9,9,9,9	0
57	MG	YA	3311	1/1	0.76	0.30	47,47,47,47	0
57	MG	YA	3272	1/1	0.77	0.49	37,37,37,37	0
57	MG	YA	3104	1/1	0.77	0.48	26,26,26,26	0
57	MG	XA	1687	1/1	0.77	0.13	54,54,54,54	0
57	MG	XA	1691	1/1	0.77	0.48	34,34,34,34	0
57	MG	RA	3156	1/1	0.78	0.20	29,29,29,29	0
57	MG	RA	3298	1/1	0.78	0.17	56,56,56,56	0
57	MG	QA	1625	1/1	0.78	0.16	59,59,59,59	0
57	MG	RA	3266	1/1	0.78	1.01	22,22,22,22	0
57	MG	YA	3293	1/1	0.78	0.32	40,40,40,40	0
57	MG	RA	3270	1/1	0.78	0.64	49,49,49,49	0
57	MG	YA	3180	1/1	0.78	0.19	42,42,42,42	0
57	MG	XA	1709	1/1	0.78	0.61	49,49,49,49	0
57	MG	RA	3244	1/1	0.78	0.70	60,60,60,60	0
57	MG	QA	1681	1/1	0.78	0.60	43,43,43,43	0
57	MG	RA	3247	1/1	0.78	0.69	58,58,58,58	0
57	MG	Y0	102	1/1	0.78	0.46	27,27,27,27	0
57	MG	RA	3002	1/1	0.78	0.52	24,24,24,24	0
57	MG	XA	1649	1/1	0.79	0.33	27,27,27,27	0
57	MG	QA	1647	1/1	0.79	0.28	65,65,65,65	0
57	MG	YA	3275	1/1	0.79	0.48	66,66,66,66	0
57	MG	XA	1666	1/1	0.79	0.20	48,48,48,48	0
57	MG	XA	1695	1/1	0.79	0.28	43,43,43,43	0
57	MG	YA	3337	1/1	0.79	0.39	41,41,41,41	0
57	MG	YA	3209	1/1	0.79	0.35	34,34,34,34	0
57	MG	R8	101	1/1	0.79	0.39	29,29,29,29	0
57	MG	YA	3229	1/1	0.79	0.30	50,50,50,50	0
57	MG	RA	3301	1/1	0.80	0.38	52,52,52,52	0
57	MG	YA	3162	1/1	0.80	0.25	46,46,46,46	0
57	MG	QA	1630	1/1	0.80	0.22	80,80,80,80	0
57	MG	YA	3250	1/1	0.80	0.41	50,50,50,50	0
57	MG	RA	3062	1/1	0.80	0.13	51,51,51,51	0
57	MG	XA	1652	1/1	0.80	0.14	44,44,44,44	0
57	MG	YA	3336	1/1	0.80	0.55	29,29,29,29	0
57	MG	YA	3189	1/1	0.80	0.42	27,27,27,27	0
57	MG	RA	3175	1/1	0.80	0.45	24,24,24,24	0
57	MG	XA	1660	1/1	0.80	0.21	44,44,44,44	0
57	MG	RA	3285	1/1	0.80	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3306	1/1	0.81	0.56	42,42,42,42	0
57	MG	YA	3226	1/1	0.81	0.11	44,44,44,44	0
57	MG	YA	3190	1/1	0.81	0.22	6,6,6,6	0
57	MG	YA	3282	1/1	0.81	0.57	48,48,48,48	0
57	MG	YA	3335	1/1	0.81	0.44	19,19,19,19	0
57	MG	RA	3221	1/1	0.81	0.22	36,36,36,36	0
57	MG	YA	3177	1/1	0.81	0.52	20,20,20,20	0
57	MG	RA	3268	1/1	0.81	0.35	47,47,47,47	0
57	MG	YA	3294	1/1	0.81	0.49	48,48,48,48	0
57	MG	YA	3274	1/1	0.81	0.74	45,45,45,45	0
57	MG	RA	3267	1/1	0.82	0.46	57,57,57,57	0
57	MG	YA	3235	1/1	0.82	0.47	18,18,18,18	0
57	MG	YA	3195	1/1	0.82	0.20	34,34,34,34	0
57	MG	YA	3252	1/1	0.82	0.39	23,23,23,23	0
57	MG	XF	201	1/1	0.82	0.20	49,49,49,49	0
57	MG	R1	101	1/1	0.82	0.24	32,32,32,32	0
57	MG	RA	3278	1/1	0.82	0.40	38,38,38,38	0
57	MG	YA	3213	1/1	0.82	0.42	29,29,29,29	0
57	MG	YA	3220	1/1	0.82	0.29	60,60,60,60	0
57	MG	YA	3281	1/1	0.82	0.44	44,44,44,44	0
57	MG	RA	3072	1/1	0.82	0.36	38,38,38,38	0
57	MG	YA	3187	1/1	0.82	0.24	37,37,37,37	0
57	MG	RA	3157	1/1	0.82	0.35	21,21,21,21	0
57	MG	YA	3137	1/1	0.83	0.29	12,12,12,12	0
57	MG	QA	1679	1/1	0.83	0.54	45,45,45,45	0
57	MG	QA	1631	1/1	0.83	0.10	32,32,32,32	0
57	MG	XA	1648	1/1	0.83	0.26	21,21,21,21	0
57	MG	QA	1693	1/1	0.83	0.39	49,49,49,49	0
57	MG	QA	1672	1/1	0.83	0.31	24,24,24,24	0
57	MG	XA	1654	1/1	0.83	0.35	42,42,42,42	0
57	MG	YA	3243	1/1	0.83	0.32	18,18,18,18	0
57	MG	QA	1621	1/1	0.83	0.30	50,50,50,50	0
57	MG	RA	3184	1/1	0.83	0.37	35,35,35,35	0
57	MG	RR	201	1/1	0.83	0.52	9,9,9,9	0
57	MG	RA	3289	1/1	0.83	0.55	54,54,54,54	0
57	MG	YA	3202	1/1	0.83	0.10	15,15,15,15	0
57	MG	RA	3269	1/1	0.83	0.54	35,35,35,35	0
57	MG	RA	3295	1/1	0.83	0.65	51,51,51,51	0
57	MG	YA	3130	1/1	0.83	0.09	25,25,25,25	0
57	MG	RB	203	1/1	0.84	0.37	58,58,58,58	0
57	MG	YA	3200	1/1	0.84	0.33	33,33,33,33	0
57	MG	YA	3295	1/1	0.84	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3291	1/1	0.84	0.56	30,30,30,30	0
57	MG	QA	1635	1/1	0.84	0.22	44,44,44,44	0
57	MG	RA	3162	1/1	0.84	0.14	46,46,46,46	0
57	MG	YA	3317	1/1	0.84	0.40	57,57,57,57	0
57	MG	QA	1669	1/1	0.84	0.39	38,38,38,38	0
57	MG	R5	101	1/1	0.84	0.28	12,12,12,12	0
57	MG	RA	3173	1/1	0.84	0.14	38,38,38,38	0
57	MG	RA	3303	1/1	0.84	0.77	50,50,50,50	0
57	MG	QA	1678	1/1	0.84	0.56	41,41,41,41	0
57	MG	YP	201	1/1	0.84	0.25	22,22,22,22	0
57	MG	RA	3227	1/1	0.84	0.29	14,14,14,14	0
57	MG	XA	1693	1/1	0.84	0.72	36,36,36,36	0
57	MG	YA	3234	1/1	0.84	0.69	54,54,54,54	0
57	MG	RA	3274	1/1	0.85	0.35	52,52,52,52	0
57	MG	YA	3056	1/1	0.85	0.20	5,5,5,5	0
57	MG	QA	1691	1/1	0.85	0.41	26,26,26,26	0
57	MG	YA	3074	1/1	0.85	0.47	32,32,32,32	0
57	MG	XA	1696	1/1	0.85	0.53	25,25,25,25	0
57	MG	YA	3310	1/1	0.85	0.34	32,32,32,32	0
57	MG	YA	3196	1/1	0.85	0.31	34,34,34,34	0
57	MG	RA	3164	1/1	0.85	0.10	28,28,28,28	0
57	MG	YA	3318	1/1	0.85	0.26	38,38,38,38	0
57	MG	XA	1704	1/1	0.85	0.13	47,47,47,47	0
57	MG	YA	3326	1/1	0.85	0.87	69,69,69,69	0
57	MG	RA	3204	1/1	0.85	0.18	16,16,16,16	0
57	MG	RB	204	1/1	0.85	0.36	39,39,39,39	0
57	MG	YA	3156	1/1	0.85	0.27	28,28,28,28	0
57	MG	RA	3283	1/1	0.85	0.69	42,42,42,42	0
57	MG	YA	3216	1/1	0.85	0.44	47,47,47,47	0
57	MG	XA	1712	1/1	0.85	0.28	49,49,49,49	0
57	MG	RA	3231	1/1	0.85	0.39	14,14,14,14	0
57	MG	Y0	103	1/1	0.85	0.50	50,50,50,50	0
57	MG	QA	1689	1/1	0.85	0.17	78,78,78,78	0
57	MG	RA	3265	1/1	0.86	0.81	72,72,72,72	0
57	MG	YA	3299	1/1	0.86	0.64	48,48,48,48	0
57	MG	YA	3300	1/1	0.86	0.99	69,69,69,69	0
57	MG	XA	1698	1/1	0.86	0.33	24,24,24,24	0
57	MG	QA	1677	1/1	0.86	0.48	26,26,26,26	0
57	MG	YA	3251	1/1	0.86	0.55	36,36,36,36	0
57	MG	XA	1702	1/1	0.86	0.46	38,38,38,38	0
57	MG	QA	1603	1/1	0.86	0.31	9,9,9,9	0
57	MG	RA	3299	1/1	0.86	0.25	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3207	1/1	0.86	0.44	34,34,34,34	0
57	MG	XA	1707	1/1	0.86	0.37	40,40,40,40	0
57	MG	XA	1663	1/1	0.86	0.45	37,37,37,37	0
57	MG	QA	1649	1/1	0.86	0.34	32,32,32,32	0
57	MG	RA	3161	1/1	0.86	0.67	36,36,36,36	0
57	MG	RA	3112	1/1	0.86	0.15	31,31,31,31	0
57	MG	XA	1627	1/1	0.86	0.16	4,4,4,4	0
57	MG	QA	1692	1/1	0.86	0.54	73,73,73,73	0
57	MG	RA	3117	1/1	0.86	0.12	43,43,43,43	0
57	MG	RA	3294	1/1	0.86	0.59	54,54,54,54	0
57	MG	YA	3302	1/1	0.87	0.52	41,41,41,41	0
57	MG	QA	1668	1/1	0.87	0.44	25,25,25,25	0
57	MG	RA	3251	1/1	0.87	0.34	23,23,23,23	0
57	MG	RA	3149	1/1	0.87	0.22	21,21,21,21	0
57	MG	QA	1645	1/1	0.87	0.60	41,41,41,41	0
57	MG	RA	3193	1/1	0.87	0.23	49,49,49,49	0
57	MG	QA	1670	1/1	0.87	0.43	25,25,25,25	0
57	MG	YA	3143	1/1	0.87	0.27	25,25,25,25	0
57	MG	YA	3151	1/1	0.87	0.16	10,10,10,10	0
57	MG	YA	3287	1/1	0.87	0.94	47,47,47,47	0
57	MG	RA	3104	1/1	0.87	0.18	4,4,4,4	0
57	MG	QA	1657	1/1	0.87	0.06	55,55,55,55	0
57	MG	QA	1688	1/1	0.87	0.24	58,58,58,58	0
57	MG	YA	3173	1/1	0.87	0.35	40,40,40,40	0
57	MG	QA	1666	1/1	0.87	0.55	32,32,32,32	0
57	MG	YA	3263	1/1	0.87	0.31	23,23,23,23	0
57	MG	YA	3267	1/1	0.87	0.31	41,41,41,41	0
57	MG	YA	3270	1/1	0.88	0.35	20,20,20,20	0
57	MG	RA	3151	1/1	0.88	0.16	13,13,13,13	0
57	MG	YA	3309	1/1	0.88	0.56	57,57,57,57	0
57	MG	YA	3070	1/1	0.88	0.20	5,5,5,5	0
57	MG	RA	3180	1/1	0.88	0.43	40,40,40,40	0
57	MG	YA	3314	1/1	0.88	0.45	47,47,47,47	0
57	MG	XA	1661	1/1	0.88	0.25	22,22,22,22	0
57	MG	YA	3178	1/1	0.88	0.64	40,40,40,40	0
57	MG	QA	1673	1/1	0.88	0.30	35,35,35,35	0
57	MG	YA	3322	1/1	0.88	0.41	44,44,44,44	0
57	MG	XA	1618	1/1	0.88	0.31	37,37,37,37	0
57	MG	YA	3329	1/1	0.88	0.30	51,51,51,51	0
57	MG	QF	201	1/1	0.88	0.17	41,41,41,41	0
57	MG	QA	1623	1/1	0.88	0.29	26,26,26,26	0
57	MG	XA	1637	1/1	0.88	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3080	1/1	0.88	0.48	20,20,20,20	0
57	MG	YA	3150	1/1	0.88	0.25	42,42,42,42	0
57	MG	RA	3134	1/1	0.88	0.19	22,22,22,22	0
57	MG	RA	3144	1/1	0.88	0.23	32,32,32,32	0
57	MG	QA	1690	1/1	0.88	0.27	29,29,29,29	0
57	MG	YA	3166	1/1	0.88	0.57	36,36,36,36	0
57	MG	XA	1684	1/1	0.89	0.38	26,26,26,26	0
57	MG	RA	3282	1/1	0.89	0.63	51,51,51,51	0
57	MG	YA	3284	1/1	0.89	0.31	39,39,39,39	0
57	MG	YA	3198	1/1	0.89	0.40	86,86,86,86	0
57	MG	RA	3115	1/1	0.89	0.17	16,16,16,16	0
57	MG	XA	1689	1/1	0.89	0.53	21,21,21,21	0
57	MG	YA	3292	1/1	0.89	0.39	47,47,47,47	0
57	MG	RA	3068	1/1	0.89	0.35	28,28,28,28	0
57	MG	YA	3124	1/1	0.89	0.23	32,32,32,32	0
57	MG	XA	1629	1/1	0.89	0.40	20,20,20,20	0
57	MG	YA	3296	1/1	0.89	0.58	55,55,55,55	0
57	MG	QA	1636	1/1	0.89	0.47	39,39,39,39	0
57	MG	XA	1644	1/1	0.89	0.30	27,27,27,27	0
57	MG	QA	1680	1/1	0.89	0.23	18,18,18,18	0
57	MG	RA	3170	1/1	0.89	0.22	24,24,24,24	0
57	MG	YA	3306	1/1	0.89	0.46	66,66,66,66	0
57	MG	YA	3148	1/1	0.89	0.11	55,55,55,55	0
57	MG	YA	3149	1/1	0.89	0.46	22,22,22,22	0
57	MG	RB	205	1/1	0.89	0.41	41,41,41,41	0
57	MG	RA	3091	1/1	0.89	0.22	30,30,30,30	0
57	MG	XA	1658	1/1	0.89	0.10	61,61,61,61	0
57	MG	XA	1706	1/1	0.89	0.41	47,47,47,47	0
57	MG	QA	1624	1/1	0.89	0.18	39,39,39,39	0
57	MG	YA	3246	1/1	0.89	0.75	39,39,39,39	0
57	MG	RA	3174	1/1	0.89	0.18	20,20,20,20	0
57	MG	QA	1602	1/1	0.89	0.54	18,18,18,18	0
57	MG	QA	1648	1/1	0.89	0.34	49,49,49,49	0
57	MG	YA	3175	1/1	0.89	0.41	34,34,34,34	0
57	MG	YA	3334	1/1	0.89	0.62	48,48,48,48	0
57	MG	RA	3261	1/1	0.89	0.31	135,135,135,135	0
57	MG	XA	1678	1/1	0.89	0.41	23,23,23,23	0
57	MG	RA	3300	1/1	0.89	0.82	43,43,43,43	0
57	MG	YA	3185	1/1	0.89	0.64	77,77,77,77	0
57	MG	XV	101	1/1	0.89	0.20	25,25,25,25	0
57	MG	XV	103	1/1	0.89	0.11	7,7,7,7	0
57	MG	YA	3278	1/1	0.89	0.34	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3034	1/1	0.89	0.48	10,10,10,10	0
57	MG	QA	1601	1/1	0.90	0.18	38,38,38,38	0
57	MG	YA	3194	1/1	0.90	0.15	27,27,27,27	0
57	MG	RA	3243	1/1	0.90	0.20	37,37,37,37	0
57	MG	YA	3105	1/1	0.90	0.28	5,5,5,5	0
57	MG	YA	3114	1/1	0.90	0.20	7,7,7,7	0
57	MG	YA	3115	1/1	0.90	0.37	29,29,29,29	0
57	MG	YA	3291	1/1	0.90	0.32	28,28,28,28	0
57	MG	XA	1694	1/1	0.90	0.15	13,13,13,13	0
57	MG	RA	3196	1/1	0.90	0.24	55,55,55,55	0
57	MG	XA	1645	1/1	0.90	0.44	25,25,25,25	0
57	MG	RA	3199	1/1	0.90	0.32	44,44,44,44	0
57	MG	YA	3139	1/1	0.90	0.38	46,46,46,46	0
57	MG	YA	3211	1/1	0.90	0.16	13,13,13,13	0
57	MG	RA	3280	1/1	0.90	0.40	47,47,47,47	0
57	MG	QA	1687	1/1	0.90	0.50	40,40,40,40	0
57	MG	YA	3144	1/1	0.90	0.49	44,44,44,44	0
57	MG	YA	3221	1/1	0.90	0.33	28,28,28,28	0
57	MG	RA	3250	1/1	0.90	0.27	25,25,25,25	0
57	MG	XA	1657	1/1	0.90	0.15	23,23,23,23	0
57	MG	RA	3166	1/1	0.90	0.24	9,9,9,9	0
57	MG	RA	3252	1/1	0.90	0.36	35,35,35,35	0
57	MG	YA	3152	1/1	0.90	0.14	15,15,15,15	0
57	MG	YA	3154	1/1	0.90	0.47	56,56,56,56	0
57	MG	RF	301	1/1	0.90	0.07	52,52,52,52	0
57	MG	RA	3207	1/1	0.90	0.27	43,43,43,43	0
57	MG	RA	3138	1/1	0.90	0.46	62,62,62,62	0
57	MG	QA	1620	1/1	0.90	0.32	40,40,40,40	0
57	MG	YA	3328	1/1	0.90	0.63	54,54,54,54	0
57	MG	XA	1667	1/1	0.90	0.17	25,25,25,25	0
57	MG	QA	1639	1/1	0.90	0.35	27,27,27,27	0
57	MG	QA	1626	1/1	0.90	0.17	29,29,29,29	0
57	MG	YA	3268	1/1	0.90	0.23	17,17,17,17	0
57	MG	XA	1683	1/1	0.90	0.12	20,20,20,20	0
57	MG	RA	3152	1/1	0.90	0.11	17,17,17,17	0
57	MG	YB	201	1/1	0.90	0.30	47,47,47,47	0
57	MG	YA	3051	1/1	0.90	0.31	3,3,3,3	0
57	MG	QX	101	1/1	0.90	0.14	38,38,38,38	0
57	MG	YA	3186	1/1	0.90	0.18	8,8,8,8	0
57	MG	RA	3116	1/1	0.90	0.14	33,33,33,33	0
57	MG	Y7	101	1/1	0.90	0.55	31,31,31,31	0
57	MG	RA	3075	1/1	0.90	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3210	1/1	0.91	0.29	33,33,33,33	0
57	MG	RA	3198	1/1	0.91	0.80	46,46,46,46	0
57	MG	XX	101	1/1	0.91	0.21	47,47,47,47	0
57	MG	RA	3275	1/1	0.91	0.62	50,50,50,50	0
57	MG	YA	3041	1/1	0.91	0.38	18,18,18,18	0
57	MG	YA	3044	1/1	0.91	0.28	2,2,2,2	0
57	MG	YA	3224	1/1	0.91	0.17	13,13,13,13	0
57	MG	QA	1667	1/1	0.91	0.82	44,44,44,44	0
57	MG	YA	3054	1/1	0.91	0.43	34,34,34,34	0
57	MG	YA	3228	1/1	0.91	0.19	21,21,21,21	0
57	MG	YA	3169	1/1	0.91	0.14	18,18,18,18	0
57	MG	RA	3140	1/1	0.91	0.27	20,20,20,20	0
57	MG	YA	3069	1/1	0.91	0.26	15,15,15,15	0
57	MG	RA	3168	1/1	0.91	0.30	38,38,38,38	0
57	MG	RA	3082	1/1	0.91	0.26	30,30,30,30	0
57	MG	RA	3147	1/1	0.91	0.30	28,28,28,28	0
57	MG	YA	3312	1/1	0.91	0.26	33,33,33,33	0
57	MG	YA	3248	1/1	0.91	0.28	37,37,37,37	0
57	MG	YA	3103	1/1	0.91	0.11	15,15,15,15	0
57	MG	RA	3088	1/1	0.91	0.35	12,12,12,12	0
57	MG	YA	3319	1/1	0.91	0.37	56,56,56,56	0
57	MG	RA	3150	1/1	0.91	0.12	15,15,15,15	0
57	MG	YA	3321	1/1	0.91	0.40	36,36,36,36	0
57	MG	QV	103	1/1	0.91	0.40	30,30,30,30	0
57	MG	YA	3323	1/1	0.91	0.28	52,52,52,52	0
57	MG	RA	3176	1/1	0.91	0.28	26,26,26,26	0
57	MG	YA	3188	1/1	0.91	0.22	31,31,31,31	0
57	MG	YA	3116	1/1	0.91	0.22	13,13,13,13	0
57	MG	YA	3271	1/1	0.91	0.33	35,35,35,35	0
57	MG	RA	3118	1/1	0.91	0.20	35,35,35,35	0
57	MG	RA	3119	1/1	0.91	0.46	43,43,43,43	0
57	MG	RA	3124	1/1	0.91	0.32	12,12,12,12	0
57	MG	RA	3011	1/1	0.91	0.32	11,11,11,11	0
57	MG	YA	3138	1/1	0.91	0.50	9,9,9,9	0
57	MG	YD	301	1/1	0.91	0.31	16,16,16,16	0
57	MG	XA	1669	1/1	0.91	0.39	11,11,11,11	0
57	MG	RA	3235	1/1	0.91	0.47	8,8,8,8	0
57	MG	XA	1626	1/1	0.91	0.20	23,23,23,23	0
57	MG	QA	1664	1/1	0.91	0.42	31,31,31,31	0
57	MG	RA	3271	1/1	0.91	0.36	41,41,41,41	0
57	MG	RA	3273	1/1	0.91	0.87	45,45,45,45	0
57	MG	XA	1668	1/1	0.92	0.28	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QE	201	1/1	0.92	0.57	37,37,37,37	0
57	MG	YA	3192	1/1	0.92	0.42	12,12,12,12	0
57	MG	YA	3193	1/1	0.92	0.18	18,18,18,18	0
57	MG	RA	3026	1/1	0.92	0.09	8,8,8,8	0
57	MG	YA	3078	1/1	0.92	0.26	12,12,12,12	0
57	MG	RA	3044	1/1	0.92	0.26	22,22,22,22	0
57	MG	QA	1616	1/1	0.92	0.16	7,7,7,7	0
57	MG	RA	3177	1/1	0.92	0.54	25,25,25,25	0
57	MG	QM	201	1/1	0.92	0.12	45,45,45,45	0
57	MG	RA	3183	1/1	0.92	0.07	37,37,37,37	0
57	MG	RA	3223	1/1	0.92	0.32	7,7,7,7	0
57	MG	RA	3226	1/1	0.92	0.42	32,32,32,32	0
57	MG	YA	3125	1/1	0.92	0.32	14,14,14,14	0
57	MG	QA	1651	1/1	0.92	0.16	56,56,56,56	0
57	MG	RA	3185	1/1	0.92	0.21	36,36,36,36	0
57	MG	YA	3135	1/1	0.92	0.23	30,30,30,30	0
57	MG	RA	3191	1/1	0.92	0.12	36,36,36,36	0
57	MG	YA	3218	1/1	0.92	0.21	40,40,40,40	0
57	MG	XA	1609	1/1	0.92	0.16	1,1,1,1	0
57	MG	RA	3242	1/1	0.92	0.61	46,46,46,46	0
57	MG	XA	1620	1/1	0.92	0.58	22,22,22,22	0
57	MG	XA	1624	1/1	0.92	0.14	18,18,18,18	0
57	MG	YA	3313	1/1	0.92	0.31	23,23,23,23	0
57	MG	QA	1682	1/1	0.92	0.24	20,20,20,20	0
57	MG	QX	102	1/1	0.92	0.28	45,45,45,45	0
57	MG	RA	3195	1/1	0.92	0.32	4,4,4,4	0
57	MG	YA	3230	1/1	0.92	0.23	8,8,8,8	0
57	MG	QA	1686	1/1	0.92	0.32	38,38,38,38	0
57	MG	RA	3197	1/1	0.92	0.57	26,26,26,26	0
57	MG	QA	1619	1/1	0.92	0.23	40,40,40,40	0
57	MG	RA	3167	1/1	0.92	0.35	38,38,38,38	0
57	MG	RA	3293	1/1	0.92	0.23	42,42,42,42	0
57	MG	RA	3200	1/1	0.92	0.15	31,31,31,31	0
57	MG	RA	3201	1/1	0.92	0.22	45,45,45,45	0
57	MG	XA	1653	1/1	0.92	0.34	26,26,26,26	0
57	MG	RA	3256	1/1	0.92	0.42	33,33,33,33	0
57	MG	YA	3261	1/1	0.92	0.23	11,11,11,11	0
57	MG	RA	3297	1/1	0.92	0.31	29,29,29,29	0
57	MG	YA	3016	1/1	0.92	0.09	2,2,2,2	0
57	MG	YA	3032	1/1	0.92	0.37	1,1,1,1	0
57	MG	RA	3260	1/1	0.92	0.24	49,49,49,49	0
57	MG	RA	3006	1/1	0.92	0.35	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3262	1/1	0.92	0.27	38,38,38,38	0
57	MG	RA	3007	1/1	0.92	0.63	22,22,22,22	0
57	MG	RA	3264	1/1	0.92	0.42	50,50,50,50	0
57	MG	RA	3304	1/1	0.92	0.40	29,29,29,29	0
58	PAR	QA	1696	42/42	0.92	0.27	61,61,61,62	0
59	ZN	QN	101	1/1	0.92	0.13	89,89,89,89	0
57	MG	QA	1627	1/1	0.92	0.13	37,37,37,37	0
57	MG	RA	3236	1/1	0.93	0.27	13,13,13,13	0
57	MG	YA	3264	1/1	0.93	0.18	40,40,40,40	0
57	MG	YA	3266	1/1	0.93	0.25	40,40,40,40	0
57	MG	RA	3241	1/1	0.93	0.17	51,51,51,51	0
57	MG	YA	3158	1/1	0.93	0.19	18,18,18,18	0
57	MG	YA	3269	1/1	0.93	0.29	22,22,22,22	0
57	MG	XA	1650	1/1	0.93	0.25	34,34,34,34	0
57	MG	XA	1651	1/1	0.93	0.45	50,50,50,50	0
57	MG	RA	3136	1/1	0.93	0.34	2,2,2,2	0
57	MG	RA	3097	1/1	0.93	0.48	10,10,10,10	0
57	MG	RA	3139	1/1	0.93	0.31	17,17,17,17	0
57	MG	XA	1655	1/1	0.93	0.33	21,21,21,21	0
57	MG	YA	3005	1/1	0.93	0.15	1,1,1,1	0
57	MG	RB	202	1/1	0.93	0.22	59,59,59,59	0
57	MG	QA	1661	1/1	0.93	0.24	5,5,5,5	0
57	MG	RA	3111	1/1	0.93	0.23	22,22,22,22	0
57	MG	YA	3183	1/1	0.93	0.34	21,21,21,21	0
57	MG	RA	3279	1/1	0.93	1.12	54,54,54,54	0
57	MG	QA	1643	1/1	0.93	0.14	28,28,28,28	0
57	MG	RE	302	1/1	0.93	0.26	8,8,8,8	0
57	MG	YA	3290	1/1	0.93	0.59	41,41,41,41	0
57	MG	QA	1665	1/1	0.93	0.23	18,18,18,18	0
57	MG	QA	1685	1/1	0.93	0.42	38,38,38,38	0
57	MG	QA	1633	1/1	0.93	0.12	25,25,25,25	0
57	MG	RA	3182	1/1	0.93	0.16	37,37,37,37	0
57	MG	XA	1675	1/1	0.93	0.47	35,35,35,35	0
57	MG	RA	3286	1/1	0.93	0.14	66,66,66,66	0
57	MG	YA	3077	1/1	0.93	0.29	11,11,11,11	0
57	MG	RA	3004	1/1	0.93	0.27	11,11,11,11	0
57	MG	YA	3081	1/1	0.93	0.37	14,14,14,14	0
57	MG	YA	3083	1/1	0.93	0.18	15,15,15,15	0
57	MG	YA	3086	1/1	0.93	0.36	1,1,1,1	0
57	MG	XA	1681	1/1	0.93	0.48	23,23,23,23	0
57	MG	RA	3288	1/1	0.93	0.44	34,34,34,34	0
57	MG	RA	3259	1/1	0.93	0.28	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3107	1/1	0.93	0.31	1,1,1,1	0
57	MG	RA	3154	1/1	0.93	0.28	23,23,23,23	0
57	MG	XA	1686	1/1	0.93	0.15	53,53,53,53	0
57	MG	QA	1604	1/1	0.93	0.31	5,5,5,5	0
57	MG	YA	3316	1/1	0.93	0.30	28,28,28,28	0
57	MG	YA	3119	1/1	0.93	0.42	15,15,15,15	0
57	MG	YA	3217	1/1	0.93	0.14	43,43,43,43	0
57	MG	QA	1655	1/1	0.93	0.31	24,24,24,24	0
57	MG	XA	1690	1/1	0.93	0.19	48,48,48,48	0
57	MG	XA	1625	1/1	0.93	0.45	16,16,16,16	0
57	MG	RA	3222	1/1	0.93	0.36	18,18,18,18	0
57	MG	YA	3133	1/1	0.93	0.10	0,0,0,0	0
57	MG	QA	1642	1/1	0.93	0.12	37,37,37,37	0
57	MG	RA	3089	1/1	0.93	0.30	17,17,17,17	0
57	MG	RA	3132	1/1	0.93	0.08	46,46,46,46	0
57	MG	XA	1633	1/1	0.93	0.25	28,28,28,28	0
57	MG	YA	3332	1/1	0.93	0.40	32,32,32,32	0
57	MG	YA	3231	1/1	0.93	0.30	4,4,4,4	0
57	MG	YA	3232	1/1	0.93	0.28	6,6,6,6	0
57	MG	YA	3140	1/1	0.93	0.17	47,47,47,47	0
57	MG	XA	1636	1/1	0.93	0.30	52,52,52,52	0
57	MG	RA	3229	1/1	0.93	0.44	3,3,3,3	0
57	MG	YA	3238	1/1	0.93	0.16	34,34,34,34	0
57	MG	XA	1639	1/1	0.93	0.20	6,6,6,6	0
57	MG	XA	1640	1/1	0.93	0.19	24,24,24,24	0
57	MG	QV	101	1/1	0.93	0.32	21,21,21,21	0
57	MG	RA	3135	1/1	0.93	0.12	20,20,20,20	0
57	MG	XA	1708	1/1	0.93	0.35	43,43,43,43	0
57	MG	XA	1646	1/1	0.93	0.51	36,36,36,36	0
57	MG	YA	3257	1/1	0.93	0.41	9,9,9,9	0
57	MG	YA	3153	1/1	0.93	0.20	31,31,31,31	0
57	MG	RA	3069	1/1	0.94	0.29	27,27,27,27	0
57	MG	YA	3157	1/1	0.94	0.12	9,9,9,9	0
57	MG	YA	3262	1/1	0.94	0.59	5,5,5,5	0
57	MG	RA	3071	1/1	0.94	0.28	19,19,19,19	0
57	MG	YA	3160	1/1	0.94	0.16	6,6,6,6	0
57	MG	RA	3219	1/1	0.94	0.17	31,31,31,31	0
57	MG	YA	3007	1/1	0.94	0.24	4,4,4,4	0
57	MG	RA	3307	1/1	0.94	0.87	75,75,75,75	0
57	MG	YA	3020	1/1	0.94	0.46	5,5,5,5	0
57	MG	YA	3171	1/1	0.94	0.47	13,13,13,13	0
57	MG	YA	3172	1/1	0.94	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3178	1/1	0.94	0.26	25,25,25,25	0
57	MG	RA	3179	1/1	0.94	0.16	15,15,15,15	0
57	MG	RA	3114	1/1	0.94	0.44	17,17,17,17	0
57	MG	YA	3176	1/1	0.94	0.29	41,41,41,41	0
57	MG	RA	3181	1/1	0.94	0.25	28,28,28,28	0
57	MG	RA	3272	1/1	0.94	0.64	48,48,48,48	0
57	MG	YA	3179	1/1	0.94	0.25	19,19,19,19	0
57	MG	XA	1662	1/1	0.94	0.08	20,20,20,20	0
57	MG	YA	3283	1/1	0.94	0.24	34,34,34,34	0
57	MG	YA	3181	1/1	0.94	0.36	15,15,15,15	0
57	MG	YA	3055	1/1	0.94	0.35	9,9,9,9	0
57	MG	QA	1622	1/1	0.94	0.59	42,42,42,42	0
57	MG	YA	3288	1/1	0.94	0.33	38,38,38,38	0
57	MG	RA	3010	1/1	0.94	0.34	37,37,37,37	0
57	MG	QA	1614	1/1	0.94	0.19	29,29,29,29	0
57	MG	RA	3153	1/1	0.94	0.23	19,19,19,19	0
57	MG	RA	3186	1/1	0.94	0.19	34,34,34,34	0
57	MG	RA	3240	1/1	0.94	0.43	20,20,20,20	0
57	MG	QA	1608	1/1	0.94	0.20	45,45,45,45	0
57	MG	YA	3080	1/1	0.94	0.48	9,9,9,9	0
57	MG	XA	1604	1/1	0.94	0.44	19,19,19,19	0
57	MG	RA	3083	1/1	0.94	0.26	2,2,2,2	0
57	MG	XA	1606	1/1	0.94	0.26	17,17,17,17	0
57	MG	QA	1683	1/1	0.94	0.51	37,37,37,37	0
57	MG	YA	3301	1/1	0.94	0.46	52,52,52,52	0
57	MG	XA	1610	1/1	0.94	0.21	13,13,13,13	0
57	MG	YA	3305	1/1	0.94	0.42	42,42,42,42	0
57	MG	RA	3158	1/1	0.94	0.20	52,52,52,52	0
57	MG	RA	3284	1/1	0.94	0.47	32,32,32,32	0
57	MG	YA	3205	1/1	0.94	0.09	56,56,56,56	0
57	MG	YA	3111	1/1	0.94	0.40	25,25,25,25	0
57	MG	YA	3112	1/1	0.94	0.24	1,1,1,1	0
57	MG	XA	1688	1/1	0.94	0.31	30,30,30,30	0
57	MG	XA	1621	1/1	0.94	0.17	30,30,30,30	0
57	MG	XA	1623	1/1	0.94	0.48	14,14,14,14	0
57	MG	RA	3159	1/1	0.94	0.12	28,28,28,28	0
57	MG	YA	3121	1/1	0.94	0.16	19,19,19,19	0
57	MG	RA	3128	1/1	0.94	0.18	12,12,12,12	0
57	MG	RA	3036	1/1	0.94	0.20	2,2,2,2	0
57	MG	RA	3090	1/1	0.94	0.57	9,9,9,9	0
57	MG	QA	1618	1/1	0.94	0.45	20,20,20,20	0
57	MG	YA	3222	1/1	0.94	0.41	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3223	1/1	0.94	0.14	27,27,27,27	0
57	MG	YA	3324	1/1	0.94	0.37	28,28,28,28	0
57	MG	YA	3325	1/1	0.94	0.16	47,47,47,47	0
57	MG	XA	1697	1/1	0.94	0.28	19,19,19,19	0
57	MG	RA	3093	1/1	0.94	0.47	11,11,11,11	0
57	MG	XA	1631	1/1	0.94	0.35	12,12,12,12	0
57	MG	RA	3254	1/1	0.94	0.45	60,60,60,60	0
57	MG	YA	3331	1/1	0.94	0.53	43,43,43,43	0
57	MG	XA	1635	1/1	0.94	0.33	11,11,11,11	0
57	MG	RA	3055	1/1	0.94	0.29	28,28,28,28	0
57	MG	YA	3141	1/1	0.94	0.21	29,29,29,29	0
57	MG	RA	3100	1/1	0.94	0.13	2,2,2,2	0
57	MG	RA	3257	1/1	0.94	0.36	58,58,58,58	0
57	MG	RA	3258	1/1	0.94	0.25	26,26,26,26	0
57	MG	YB	202	1/1	0.94	0.23	49,49,49,49	0
57	MG	YA	3145	1/1	0.94	0.14	2,2,2,2	0
57	MG	YE	302	1/1	0.94	0.27	4,4,4,4	0
57	MG	RA	3205	1/1	0.94	0.30	19,19,19,19	0
57	MG	QA	1637	1/1	0.94	0.14	43,43,43,43	0
57	MG	YA	3244	1/1	0.94	0.33	6,6,6,6	0
57	MG	RA	3172	1/1	0.94	0.27	26,26,26,26	0
57	MG	QV	102	1/1	0.94	0.19	11,11,11,11	0
57	MG	RA	3142	1/1	0.94	0.28	11,11,11,11	0
58	PAR	XA	1715	42/42	0.94	0.27	52,52,53,53	0
57	MG	RA	3302	1/1	0.94	0.17	51,51,51,51	0
57	MG	RA	3143	1/1	0.94	0.26	22,22,22,22	0
57	MG	RA	3110	1/1	0.95	0.37	11,11,11,11	0
57	MG	RA	3137	1/1	0.95	0.36	3,3,3,3	0
57	MG	XA	1676	1/1	0.95	0.34	15,15,15,15	0
57	MG	YA	3204	1/1	0.95	0.14	25,25,25,25	0
57	MG	XA	1677	1/1	0.95	0.36	21,21,21,21	0
57	MG	RA	3160	1/1	0.95	0.28	43,43,43,43	0
57	MG	YA	3029	1/1	0.95	0.30	6,6,6,6	0
57	MG	YA	3208	1/1	0.95	0.29	31,31,31,31	0
57	MG	RA	3209	1/1	0.95	0.28	33,33,33,33	0
57	MG	RA	3248	1/1	0.95	0.12	32,32,32,32	0
57	MG	RA	3249	1/1	0.95	0.25	44,44,44,44	0
57	MG	YA	3043	1/1	0.95	0.36	2,2,2,2	0
57	MG	YA	3215	1/1	0.95	0.25	25,25,25,25	0
57	MG	YA	3147	1/1	0.95	0.29	19,19,19,19	0
57	MG	RA	3008	1/1	0.95	0.47	16,16,16,16	0
57	MG	YA	3047	1/1	0.95	0.37	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3009	1/1	0.95	0.16	22,22,22,22	0
57	MG	RA	3050	1/1	0.95	0.44	7,7,7,7	0
57	MG	YA	3303	1/1	0.95	0.37	35,35,35,35	0
57	MG	XA	1638	1/1	0.95	0.13	46,46,46,46	0
57	MG	RA	3087	1/1	0.95	0.20	35,35,35,35	0
57	MG	YA	3059	1/1	0.95	0.26	38,38,38,38	0
57	MG	YA	3060	1/1	0.95	0.26	5,5,5,5	0
57	MG	YA	3065	1/1	0.95	0.17	8,8,8,8	0
57	MG	RA	3189	1/1	0.95	0.18	12,12,12,12	0
57	MG	YA	3159	1/1	0.95	0.23	38,38,38,38	0
57	MG	RA	3215	1/1	0.95	0.24	34,34,34,34	0
57	MG	YA	3161	1/1	0.95	0.43	32,32,32,32	0
57	MG	YA	3315	1/1	0.95	0.36	17,17,17,17	0
57	MG	RA	3218	1/1	0.95	0.54	22,22,22,22	0
57	MG	RA	3052	1/1	0.95	0.35	1,1,1,1	0
57	MG	YA	3167	1/1	0.95	0.27	57,57,57,57	0
57	MG	YA	3168	1/1	0.95	0.12	32,32,32,32	0
57	MG	RA	3220	1/1	0.95	0.34	29,29,29,29	0
57	MG	YA	3240	1/1	0.95	0.43	5,5,5,5	0
57	MG	QA	1612	1/1	0.95	0.43	22,22,22,22	0
57	MG	RA	3146	1/1	0.95	0.21	38,38,38,38	0
57	MG	QA	1694	1/1	0.95	0.26	50,50,50,50	0
57	MG	QA	1629	1/1	0.95	0.21	69,69,69,69	0
57	MG	RA	3292	1/1	0.95	0.78	45,45,45,45	0
57	MG	YA	3327	1/1	0.95	0.19	56,56,56,56	0
57	MG	YA	3089	1/1	0.95	0.27	25,25,25,25	0
57	MG	YA	3095	1/1	0.95	0.24	2,2,2,2	0
57	MG	YA	3097	1/1	0.95	0.39	8,8,8,8	0
57	MG	YA	3098	1/1	0.95	0.55	12,12,12,12	0
57	MG	XA	1700	1/1	0.95	0.18	54,54,54,54	0
57	MG	YA	3333	1/1	0.95	0.38	43,43,43,43	0
57	MG	RA	3016	1/1	0.95	0.30	11,11,11,11	0
57	MG	XA	1703	1/1	0.95	0.20	25,25,25,25	0
57	MG	XA	1607	1/1	0.95	0.07	61,61,61,61	0
57	MG	RA	3017	1/1	0.95	0.32	2,2,2,2	0
57	MG	RA	3023	1/1	0.95	0.31	2,2,2,2	0
57	MG	XA	1613	1/1	0.95	0.08	18,18,18,18	0
57	MG	YB	203	1/1	0.95	0.29	20,20,20,20	0
57	MG	RA	3102	1/1	0.95	0.19	3,3,3,3	0
57	MG	QA	1676	1/1	0.95	0.24	48,48,48,48	0
57	MG	RA	3239	1/1	0.95	0.21	37,37,37,37	0
57	MG	YP	202	1/1	0.95	0.39	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1622	1/1	0.95	0.27	33,33,33,33	0
57	MG	XA	1664	1/1	0.95	0.33	18,18,18,18	0
57	MG	XA	1665	1/1	0.95	0.08	72,72,72,72	0
57	MG	Y5	101	1/1	0.95	0.24	18,18,18,18	0
57	MG	RA	3105	1/1	0.95	0.18	14,14,14,14	0
57	MG	YA	3279	1/1	0.95	0.27	30,30,30,30	0
57	MG	RA	3203	1/1	0.95	0.12	27,27,27,27	0
57	MG	YA	3197	1/1	0.95	0.45	43,43,43,43	0
57	MG	RA	3109	1/1	0.95	0.37	23,23,23,23	0
57	MG	YA	3067	1/1	0.96	0.21	31,31,31,31	0
57	MG	YA	3068	1/1	0.96	0.26	4,4,4,4	0
57	MG	RA	3092	1/1	0.96	0.24	12,12,12,12	0
57	MG	QA	1617	1/1	0.96	0.36	15,15,15,15	0
57	MG	QA	1660	1/1	0.96	0.34	10,10,10,10	0
57	MG	YA	3073	1/1	0.96	0.19	17,17,17,17	0
57	MG	RA	3056	1/1	0.96	0.36	3,3,3,3	0
57	MG	YA	3276	1/1	0.96	0.23	7,7,7,7	0
57	MG	RA	3101	1/1	0.96	0.18	14,14,14,14	0
57	MG	RA	3059	1/1	0.96	0.22	1,1,1,1	0
57	MG	XA	1630	1/1	0.96	0.11	27,27,27,27	0
57	MG	RA	3061	1/1	0.96	0.26	1,1,1,1	0
57	MG	XA	1632	1/1	0.96	0.22	18,18,18,18	0
57	MG	YA	3084	1/1	0.96	0.24	18,18,18,18	0
57	MG	QA	1641	1/1	0.96	0.23	16,16,16,16	0
57	MG	RA	3107	1/1	0.96	0.18	18,18,18,18	0
57	MG	RA	3063	1/1	0.96	0.44	1,1,1,1	0
57	MG	RA	3064	1/1	0.96	0.34	3,3,3,3	0
57	MG	RA	3067	1/1	0.96	0.21	4,4,4,4	0
57	MG	YA	3101	1/1	0.96	0.12	25,25,25,25	0
57	MG	QA	1663	1/1	0.96	0.74	27,27,27,27	0
57	MG	QA	1684	1/1	0.96	0.19	40,40,40,40	0
57	MG	XA	1643	1/1	0.96	0.34	43,43,43,43	0
57	MG	RA	3225	1/1	0.96	0.36	28,28,28,28	0
57	MG	YA	3109	1/1	0.96	0.24	23,23,23,23	0
57	MG	XA	1701	1/1	0.96	0.43	26,26,26,26	0
57	MG	YA	3199	1/1	0.96	0.18	21,21,21,21	0
57	MG	RB	201	1/1	0.96	0.13	59,59,59,59	0
57	MG	YA	3113	1/1	0.96	0.23	4,4,4,4	0
57	MG	RA	3001	1/1	0.96	0.14	7,7,7,7	0
57	MG	XA	1647	1/1	0.96	0.18	53,53,53,53	0
57	MG	RA	3187	1/1	0.96	0.26	56,56,56,56	0
57	MG	YA	3117	1/1	0.96	0.31	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3304	1/1	0.96	0.21	31,31,31,31	0
57	MG	QA	1609	1/1	0.96	0.07	4,4,4,4	0
57	MG	RA	3230	1/1	0.96	0.30	4,4,4,4	0
57	MG	YA	3307	1/1	0.96	0.33	40,40,40,40	0
57	MG	RA	3190	1/1	0.96	0.33	53,53,53,53	0
57	MG	RA	3234	1/1	0.96	0.28	2,2,2,2	0
57	MG	RA	3155	1/1	0.96	0.22	11,11,11,11	0
57	MG	YA	3212	1/1	0.96	0.17	22,22,22,22	0
57	MG	RA	3192	1/1	0.96	0.13	21,21,21,21	0
57	MG	YA	3132	1/1	0.96	0.46	35,35,35,35	0
57	MG	RA	3277	1/1	0.96	0.54	51,51,51,51	0
57	MG	XA	1656	1/1	0.96	0.36	52,52,52,52	0
57	MG	RA	3024	1/1	0.96	0.16	4,4,4,4	0
57	MG	QA	1650	1/1	0.96	0.32	16,16,16,16	0
57	MG	RA	3030	1/1	0.96	0.38	4,4,4,4	0
57	MG	XA	1602	1/1	0.96	0.58	8,8,8,8	0
57	MG	YA	3003	1/1	0.96	0.22	3,3,3,3	0
57	MG	QA	1605	1/1	0.96	0.41	17,17,17,17	0
57	MG	RA	3086	1/1	0.96	0.28	5,5,5,5	0
57	MG	YA	3009	1/1	0.96	0.53	3,3,3,3	0
57	MG	YA	3227	1/1	0.96	0.16	19,19,19,19	0
57	MG	RA	3125	1/1	0.96	0.24	20,20,20,20	0
57	MG	RA	3126	1/1	0.96	0.20	9,9,9,9	0
57	MG	YA	3022	1/1	0.96	0.25	10,10,10,10	0
57	MG	RA	3246	1/1	0.96	0.36	48,48,48,48	0
57	MG	RA	3127	1/1	0.96	0.24	5,5,5,5	0
57	MG	YA	3033	1/1	0.96	0.37	4,4,4,4	0
57	MG	RA	3165	1/1	0.96	0.31	19,19,19,19	0
57	MG	XA	1614	1/1	0.96	0.31	4,4,4,4	0
57	MG	YA	3237	1/1	0.96	0.47	3,3,3,3	0
57	MG	RA	3039	1/1	0.96	0.23	1,1,1,1	0
57	MG	YA	3155	1/1	0.96	0.13	18,18,18,18	0
57	MG	YA	3242	1/1	0.96	0.41	1,1,1,1	0
57	MG	XA	1671	1/1	0.96	0.38	5,5,5,5	0
57	MG	XA	1672	1/1	0.96	0.41	10,10,10,10	0
57	MG	XA	1674	1/1	0.96	0.52	16,16,16,16	0
57	MG	YA	3053	1/1	0.96	0.40	3,3,3,3	0
57	MG	YA	3249	1/1	0.96	0.29	3,3,3,3	0
57	MG	XA	1619	1/1	0.96	0.21	46,46,46,46	0
57	MG	QA	1644	1/1	0.96	0.18	33,33,33,33	0
57	MG	RA	3047	1/1	0.96	0.42	6,6,6,6	0
57	MG	YA	3255	1/1	0.96	0.17	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3163	1/1	0.96	0.14	34,34,34,34	0
57	MG	YA	3260	1/1	0.96	0.33	15,15,15,15	0
57	MG	YA	3164	1/1	0.96	0.18	24,24,24,24	0
57	MG	RA	3049	1/1	0.96	0.15	3,3,3,3	0
57	MG	QA	1632	1/1	0.96	0.28	16,16,16,16	0
57	MG	YA	3061	1/1	0.96	0.30	4,4,4,4	0
57	MG	YA	3062	1/1	0.96	0.29	5,5,5,5	0
57	MG	XA	1680	1/1	0.96	0.35	29,29,29,29	0
57	MG	RA	3070	1/1	0.97	0.38	4,4,4,4	0
57	MG	YA	3254	1/1	0.97	0.20	5,5,5,5	0
57	MG	YA	3048	1/1	0.97	0.32	2,2,2,2	0
57	MG	QA	1613	1/1	0.97	0.40	26,26,26,26	0
57	MG	YA	3258	1/1	0.97	0.35	12,12,12,12	0
57	MG	YA	3259	1/1	0.97	0.16	14,14,14,14	0
57	MG	XA	1682	1/1	0.97	0.28	3,3,3,3	0
57	MG	RA	3038	1/1	0.97	0.23	7,7,7,7	0
57	MG	RA	3073	1/1	0.97	0.17	17,17,17,17	0
57	MG	QA	1671	1/1	0.97	0.18	25,25,25,25	0
57	MG	RA	3076	1/1	0.97	0.24	14,14,14,14	0
57	MG	YA	3265	1/1	0.97	0.18	23,23,23,23	0
57	MG	RA	3079	1/1	0.97	0.28	16,16,16,16	0
57	MG	XA	1634	1/1	0.97	0.67	27,27,27,27	0
57	MG	RA	3163	1/1	0.97	0.28	43,43,43,43	0
57	MG	YA	3063	1/1	0.97	0.23	4,4,4,4	0
57	MG	YA	3165	1/1	0.97	0.25	23,23,23,23	0
57	MG	YA	3064	1/1	0.97	0.26	12,12,12,12	0
57	MG	RA	3041	1/1	0.97	0.21	4,4,4,4	0
57	MG	YA	3066	1/1	0.97	0.42	29,29,29,29	0
57	MG	RA	3206	1/1	0.97	0.55	45,45,45,45	0
57	MG	XA	1692	1/1	0.97	0.30	43,43,43,43	0
57	MG	RA	3120	1/1	0.97	0.34	18,18,18,18	0
57	MG	RA	3123	1/1	0.97	0.16	34,34,34,34	0
57	MG	RA	3081	1/1	0.97	0.20	11,11,11,11	0
57	MG	RA	3014	1/1	0.97	0.52	29,29,29,29	0
57	MG	RA	3169	1/1	0.97	0.35	21,21,21,21	0
57	MG	YA	3075	1/1	0.97	0.48	4,4,4,4	0
57	MG	RA	3045	1/1	0.97	0.26	11,11,11,11	0
57	MG	RA	3084	1/1	0.97	0.29	13,13,13,13	0
57	MG	RA	3085	1/1	0.97	0.27	4,4,4,4	0
57	MG	YA	3286	1/1	0.97	0.10	46,46,46,46	0
57	MG	RA	3046	1/1	0.97	0.29	11,11,11,11	0
57	MG	RA	3130	1/1	0.97	0.32	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3131	1/1	0.97	0.39	11,11,11,11	0
57	MG	YA	3184	1/1	0.97	0.10	32,32,32,32	0
57	MG	YA	3085	1/1	0.97	0.32	6,6,6,6	0
57	MG	RA	3005	1/1	0.97	0.43	4,4,4,4	0
57	MG	QA	1659	1/1	0.97	0.32	33,33,33,33	0
57	MG	YA	3090	1/1	0.97	0.22	22,22,22,22	0
57	MG	YA	3092	1/1	0.97	0.42	9,9,9,9	0
57	MG	YA	3093	1/1	0.97	0.20	24,24,24,24	0
57	MG	YA	3094	1/1	0.97	0.27	9,9,9,9	0
57	MG	YA	3298	1/1	0.97	0.21	16,16,16,16	0
57	MG	RA	3018	1/1	0.97	0.11	9,9,9,9	0
57	MG	RA	3019	1/1	0.97	0.26	8,8,8,8	0
57	MG	RA	3224	1/1	0.97	0.24	11,11,11,11	0
57	MG	YA	3100	1/1	0.97	0.43	6,6,6,6	0
57	MG	RA	3054	1/1	0.97	0.33	5,5,5,5	0
57	MG	RA	3020	1/1	0.97	0.26	1,1,1,1	0
57	MG	QA	1654	1/1	0.97	0.31	46,46,46,46	0
57	MG	RA	3228	1/1	0.97	0.34	8,8,8,8	0
57	MG	RA	3095	1/1	0.97	0.43	7,7,7,7	0
57	MG	QA	1634	1/1	0.97	0.10	24,24,24,24	0
57	MG	YA	3110	1/1	0.97	0.12	11,11,11,11	0
57	MG	RA	3060	1/1	0.97	0.27	1,1,1,1	0
57	MG	RA	3232	1/1	0.97	0.19	1,1,1,1	0
57	MG	RA	3233	1/1	0.97	0.10	18,18,18,18	0
57	MG	QA	1662	1/1	0.97	0.30	27,27,27,27	0
57	MG	YA	3004	1/1	0.97	0.30	7,7,7,7	0
57	MG	RA	3028	1/1	0.97	0.31	2,2,2,2	0
57	MG	YA	3006	1/1	0.97	0.36	1,1,1,1	0
57	MG	YA	3118	1/1	0.97	0.30	19,19,19,19	0
57	MG	XA	1615	1/1	0.97	0.41	2,2,2,2	0
57	MG	XA	1616	1/1	0.97	0.27	7,7,7,7	0
57	MG	YA	3123	1/1	0.97	0.14	4,4,4,4	0
57	MG	YA	3010	1/1	0.97	0.29	3,3,3,3	0
57	MG	YA	3012	1/1	0.97	0.40	4,4,4,4	0
57	MG	YA	3219	1/1	0.97	0.17	37,37,37,37	0
57	MG	YA	3126	1/1	0.97	0.29	5,5,5,5	0
57	MG	YA	3127	1/1	0.97	0.10	12,12,12,12	0
57	MG	YA	3014	1/1	0.97	0.26	3,3,3,3	0
57	MG	YA	3129	1/1	0.97	0.08	16,16,16,16	0
57	MG	RA	3188	1/1	0.97	0.13	25,25,25,25	0
57	MG	YA	3131	1/1	0.97	0.16	35,35,35,35	0
57	MG	RA	3029	1/1	0.97	0.34	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1656	1/1	0.97	0.28	39,39,39,39	0
57	MG	YA	3134	1/1	0.97	0.26	17,17,17,17	0
57	MG	YA	3025	1/1	0.97	0.25	6,6,6,6	0
57	MG	YA	3136	1/1	0.97	0.18	2,2,2,2	0
57	MG	YA	3027	1/1	0.97	0.25	2,2,2,2	0
57	MG	YA	3028	1/1	0.97	0.19	3,3,3,3	0
57	MG	XA	1673	1/1	0.97	0.28	36,36,36,36	0
57	MG	YA	3030	1/1	0.97	0.32	7,7,7,7	0
57	MG	RA	3106	1/1	0.97	0.18	16,16,16,16	0
57	MG	YA	3236	1/1	0.97	0.47	6,6,6,6	0
57	MG	RA	3066	1/1	0.97	0.23	1,1,1,1	0
57	MG	RA	3108	1/1	0.97	0.13	7,7,7,7	0
57	MG	YA	3239	1/1	0.97	0.27	10,10,10,10	0
57	MG	YA	3037	1/1	0.97	0.27	3,3,3,3	0
57	MG	YQ	201	1/1	0.97	0.13	152,152,152,152	0
57	MG	YA	3038	1/1	0.97	0.20	24,24,24,24	0
57	MG	YA	3146	1/1	0.97	0.20	5,5,5,5	0
57	MG	YA	3039	1/1	0.97	0.17	2,2,2,2	0
57	MG	RA	3032	1/1	0.97	0.39	28,28,28,28	0
57	MG	YA	3247	1/1	0.97	0.48	3,3,3,3	0
57	MG	YA	3042	1/1	0.97	0.37	12,12,12,12	0
57	MG	RA	3033	1/1	0.97	0.39	4,4,4,4	0
57	MG	RA	3034	1/1	0.97	0.41	4,4,4,4	0
57	MG	YA	3046	1/1	0.97	0.36	3,3,3,3	0
57	MG	YA	3122	1/1	0.98	0.35	5,5,5,5	0
57	MG	RA	3003	1/1	0.98	0.44	3,3,3,3	0
57	MG	XA	1617	1/1	0.98	0.33	4,4,4,4	0
57	MG	RA	3040	1/1	0.98	0.26	1,1,1,1	0
57	MG	YA	3049	1/1	0.98	0.36	2,2,2,2	0
57	MG	RA	3012	1/1	0.98	0.16	2,2,2,2	0
57	MG	YA	3052	1/1	0.98	0.34	14,14,14,14	0
57	MG	RA	3065	1/1	0.98	0.19	3,3,3,3	0
57	MG	RA	3122	1/1	0.98	0.19	25,25,25,25	0
57	MG	RA	3042	1/1	0.98	0.35	23,23,23,23	0
57	MG	RA	3043	1/1	0.98	0.22	5,5,5,5	0
57	MG	YA	3057	1/1	0.98	0.37	4,4,4,4	0
57	MG	YA	3058	1/1	0.98	0.28	7,7,7,7	0
57	MG	XA	1710	1/1	0.98	0.19	29,29,29,29	0
57	MG	RA	3025	1/1	0.98	0.31	3,3,3,3	0
57	MG	RA	3094	1/1	0.98	0.26	13,13,13,13	0
57	MG	QA	1610	1/1	0.98	0.32	13,13,13,13	0
57	MG	YA	3214	1/1	0.98	0.36	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1670	1/1	0.98	0.28	14,14,14,14	0
57	MG	RA	3096	1/1	0.98	0.36	11,11,11,11	0
57	MG	RA	3027	1/1	0.98	0.32	2,2,2,2	0
57	MG	RA	3098	1/1	0.98	0.33	1,1,1,1	0
57	MG	RA	3099	1/1	0.98	0.46	9,9,9,9	0
57	MG	XX	102	1/1	0.98	0.21	14,14,14,14	0
57	MG	YA	3002	1/1	0.98	0.27	1,1,1,1	0
57	MG	QA	1611	1/1	0.98	0.34	2,2,2,2	0
57	MG	RA	3133	1/1	0.98	0.14	32,32,32,32	0
57	MG	YA	3072	1/1	0.98	0.25	2,2,2,2	0
57	MG	RA	3048	1/1	0.98	0.34	1,1,1,1	0
57	MG	RA	3237	1/1	0.98	0.23	32,32,32,32	0
57	MG	RA	3238	1/1	0.98	0.28	43,43,43,43	0
57	MG	YA	3076	1/1	0.98	0.39	14,14,14,14	0
57	MG	YA	3008	1/1	0.98	0.20	3,3,3,3	0
57	MG	RA	3015	1/1	0.98	0.12	1,1,1,1	0
57	MG	RE	301	1/1	0.98	0.23	2,2,2,2	0
57	MG	YA	3011	1/1	0.98	0.32	2,2,2,2	0
57	MG	YA	3082	1/1	0.98	0.32	7,7,7,7	0
57	MG	RA	3074	1/1	0.98	0.32	2,2,2,2	0
57	MG	QA	1674	1/1	0.98	0.24	26,26,26,26	0
57	MG	YA	3015	1/1	0.98	0.31	11,11,11,11	0
57	MG	RA	3031	1/1	0.98	0.36	5,5,5,5	0
57	MG	YA	3087	1/1	0.98	0.26	4,4,4,4	0
57	MG	YA	3088	1/1	0.98	0.35	5,5,5,5	0
57	MG	YA	3018	1/1	0.98	0.39	4,4,4,4	0
57	MG	YA	3241	1/1	0.98	0.42	3,3,3,3	0
57	MG	YA	3019	1/1	0.98	0.41	3,3,3,3	0
57	MG	YA	3091	1/1	0.98	0.33	3,3,3,3	0
57	MG	XA	1641	1/1	0.98	0.23	7,7,7,7	0
57	MG	YA	3245	1/1	0.98	0.34	11,11,11,11	0
57	MG	RA	3077	1/1	0.98	0.25	3,3,3,3	0
57	MG	YA	3023	1/1	0.98	0.48	15,15,15,15	0
57	MG	YA	3024	1/1	0.98	0.33	3,3,3,3	0
57	MG	YA	3096	1/1	0.98	0.12	13,13,13,13	0
57	MG	RA	3078	1/1	0.98	0.26	11,11,11,11	0
57	MG	YA	3026	1/1	0.98	0.47	5,5,5,5	0
57	MG	YA	3099	1/1	0.98	0.37	3,3,3,3	0
57	MG	YA	3253	1/1	0.98	0.35	7,7,7,7	0
57	MG	RA	3141	1/1	0.98	0.48	5,5,5,5	0
57	MG	RA	3053	1/1	0.98	0.31	1,1,1,1	0
57	MG	QA	1615	1/1	0.98	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1603	1/1	0.98	0.26	9,9,9,9	0
57	MG	YA	3031	1/1	0.98	0.61	15,15,15,15	0
57	MG	QA	1646	1/1	0.98	0.16	56,56,56,56	0
57	MG	RA	3145	1/1	0.98	0.23	14,14,14,14	0
57	MG	YA	3182	1/1	0.98	0.08	30,30,30,30	0
57	MG	YE	301	1/1	0.98	0.28	2,2,2,2	0
57	MG	QA	1658	1/1	0.98	0.13	78,78,78,78	0
57	MG	YA	3035	1/1	0.98	0.27	2,2,2,2	0
57	MG	RA	3058	1/1	0.98	0.28	1,1,1,1	0
57	MG	XA	1608	1/1	0.98	0.26	6,6,6,6	0
57	MG	QA	1607	1/1	0.98	0.07	22,22,22,22	0
57	MG	YA	3040	1/1	0.98	0.40	1,1,1,1	0
57	MG	RA	3216	1/1	0.98	0.35	4,4,4,4	0
57	MG	RA	3217	1/1	0.98	0.50	6,6,6,6	0
57	MG	YA	3191	1/1	0.98	0.05	34,34,34,34	0
57	MG	RA	3037	1/1	0.98	0.25	7,7,7,7	0
57	MG	RA	3022	1/1	0.98	0.34	15,15,15,15	0
59	ZN	QD	301	1/1	0.98	0.26	37,37,37,37	0
57	MG	YA	3120	1/1	0.98	0.26	12,12,12,12	0
57	MG	YA	3045	1/1	0.98	0.47	5,5,5,5	0
59	ZN	XN	101	1/1	0.98	0.16	73,73,73,73	0
57	MG	XA	1601	1/1	0.99	0.48	7,7,7,7	0
57	MG	YA	3001	1/1	0.99	0.36	3,3,3,3	0
57	MG	YA	3273	1/1	0.99	0.26	37,37,37,37	0
57	MG	YA	3021	1/1	0.99	0.35	3,3,3,3	0
57	MG	QA	1640	1/1	0.99	0.16	8,8,8,8	0
57	MG	RA	3051	1/1	0.99	0.14	3,3,3,3	0
57	MG	RA	3148	1/1	0.99	0.14	22,22,22,22	0
57	MG	QA	1638	1/1	0.99	0.12	38,38,38,38	0
57	MG	QA	1606	1/1	0.99	0.09	3,3,3,3	0
57	MG	RA	3035	1/1	0.99	0.40	3,3,3,3	0
57	MG	RA	3121	1/1	0.99	0.17	20,20,20,20	0
57	MG	YA	3050	1/1	0.99	0.31	2,2,2,2	0
57	MG	RA	3103	1/1	0.99	0.17	9,9,9,9	0
57	MG	YA	3201	1/1	0.99	0.08	43,43,43,43	0
57	MG	YA	3256	1/1	0.99	0.38	13,13,13,13	0
57	MG	QA	1652	1/1	0.99	0.07	91,91,91,91	0
57	MG	XA	1611	1/1	0.99	0.14	11,11,11,11	0
57	MG	XA	1612	1/1	0.99	0.07	2,2,2,2	0
57	MG	YA	3013	1/1	0.99	0.36	4,4,4,4	0
57	MG	RA	3021	1/1	0.99	0.38	1,1,1,1	0
57	MG	YA	3102	1/1	0.99	0.29	9,9,9,9	0

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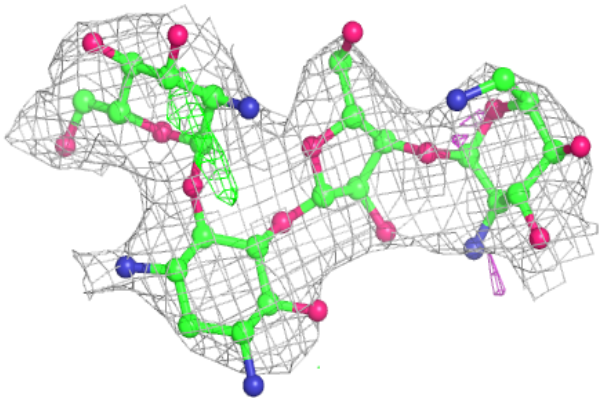
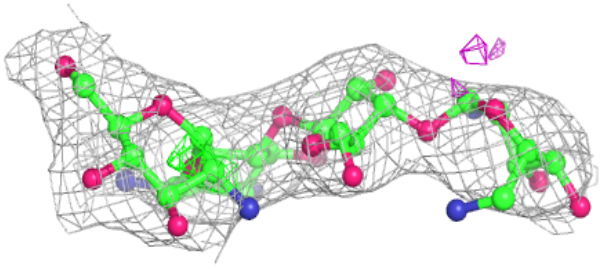
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3079	1/1	0.99	0.40	10,10,10,10	0
57	MG	XV	102	1/1	0.99	0.21	10,10,10,10	0
57	MG	YA	3036	1/1	0.99	0.14	2,2,2,2	0
57	MG	YA	3106	1/1	0.99	0.42	1,1,1,1	0
57	MG	XA	1642	1/1	0.99	0.24	9,9,9,9	0
57	MG	YA	3108	1/1	0.99	0.16	15,15,15,15	0
57	MG	YA	3017	1/1	0.99	0.25	13,13,13,13	0
57	MG	RA	3057	1/1	0.99	0.32	9,9,9,9	0

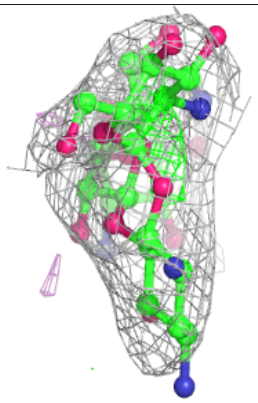
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR QA 1696:

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

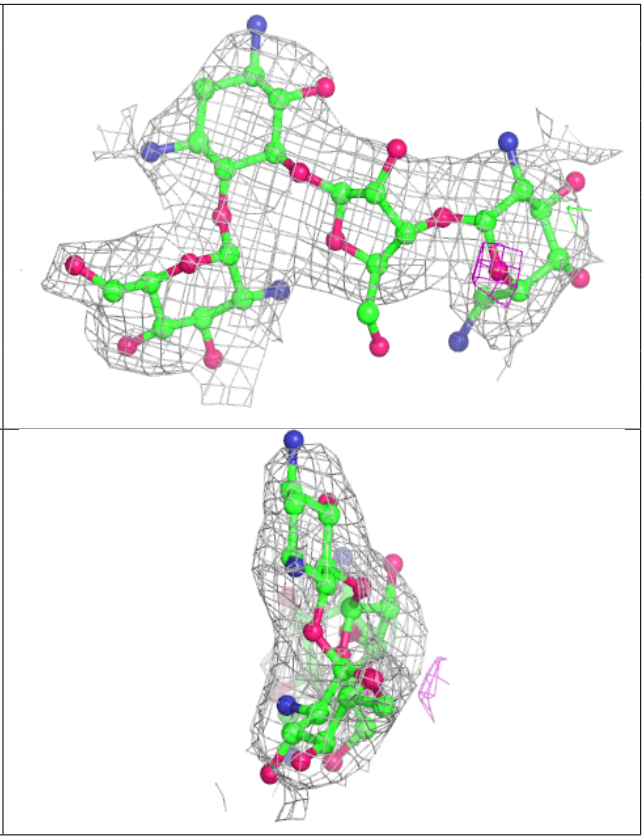






Electron density around PAR XA 1715:

$2mF_o$-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.