



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2020 – 07:58 am BST

PDB ID : 4P70
Title : Crystal Structure of Unmodified tRNA Proline (CGG) Bound to Codon CCG on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2014-03-25
Resolution : 3.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

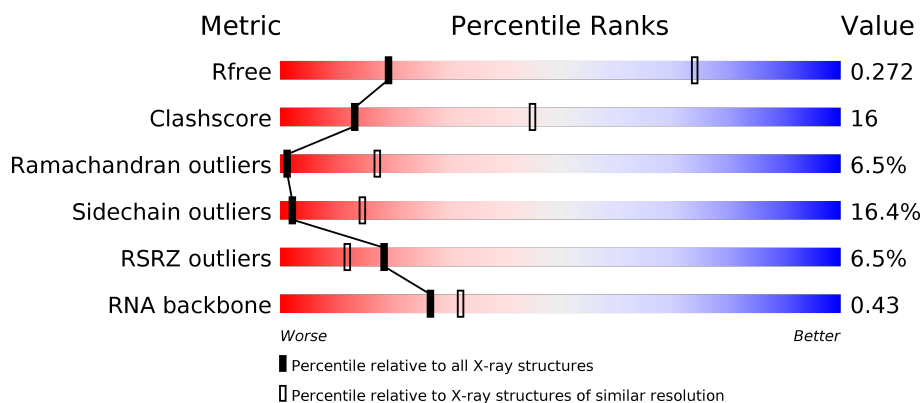
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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	1013 (3.84-3.52)
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RSRZ outliers	127900	1471 (3.86-3.50)
RNA backbone	3102	1024 (4.30-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div>5%</div> <div>35% 47% 14% ..</div> </div>
1	XA	1522	<div> <div>5%</div> <div>33% 48% 15% ..</div> </div>
2	QB	256	<div> <div>4%</div> <div>49% 36% 7% • 7%</div> </div>
2	XB	256	<div> <div></div> <div>46% 36% 9% • 7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	% 64% 27% 8% .
16	QP	88	% 65% 24% 7% 5%
16	XP	88	23% 52% 39% 5% 5%
17	QQ	105	13% 59% 32% . . 5%
17	XQ	105	13% 70% 21% 5% 5%
18	QR	88	% 52% 22% . . 20%
18	XR	88	3% 43% 33% . 20%
19	QS	93	34% 42% 32% 15% . 10%
19	XS	93	9% 31% 45% 11% . 10%
20	QT	106	8% 56% 33% 5% 7%
20	XT	106	32% 45% 39% 9% 7%
21	QU	27	74% 44% 44% . 7%
21	XU	27	56% 59% 30% . 7%
22	RA	2916	5% 35% 43% 18% . .
22	YA	2916	4% 34% 44% 18% . .
23	RB	122	% 40% 42% 15% . .
23	YB	122	% 34% 43% 17% . .
24	RD	276	% 52% 38% 9% .
24	YD	276	2% 55% 35% 8% .
25	RE	206	3% 47% 39% 11% .
25	YE	206	% 52% 36% 10% .
26	RF	210	47% 38% 11% .
26	YF	210	60% 26% 9% .
27	RG	182	5% 54% 37% 7% . .
27	YG	182	2% 53% 36% 9% . .


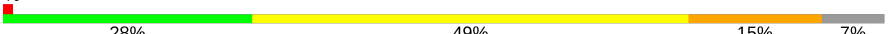
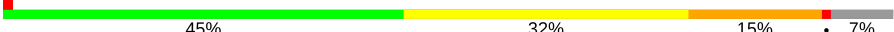
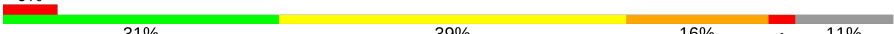
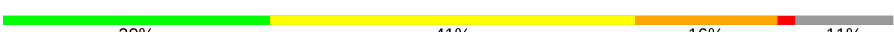
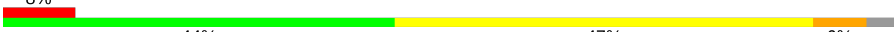
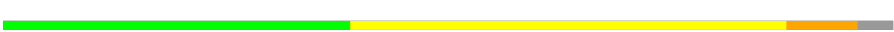




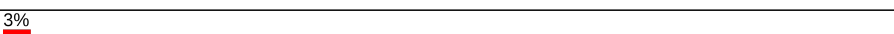


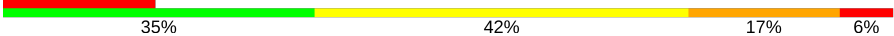
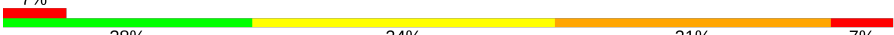







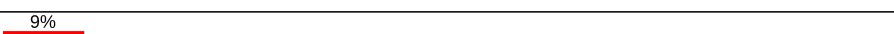
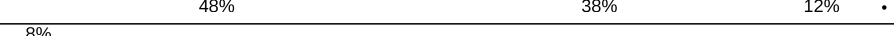
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Mol	Chain	Length	Quality of chain
28	RH	180	
28	YH	180	
29	RI	148	
29	YI	148	
30	RN	140	
30	YN	140	
31	RO	122	
31	YO	122	
32	RP	150	
32	YP	150	
33	RQ	141	
33	YQ	141	
34	RR	118	
34	YR	118	
35	RS	112	
35	YS	112	
36	RT	146	
36	YT	146	
37	RU	118	
37	YU	118	
38	RV	101	
38	YV	101	
39	RW	113	
39	YW	113	
40	RX	96	

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Mol	Chain	Length	Quality of chain
40	YX	96	
41	RY	110	
41	YY	110	
42	RZ	206	
42	YZ	206	
43	R0	85	
43	Y0	85	
44	R1	98	
44	Y1	98	
45	R2	72	
45	Y2	72	
46	R3	60	
46	Y3	60	
47	R4	71	
47	Y4	71	
48	R5	60	
48	Y5	60	
49	R6	54	
49	Y6	54	
50	R7	49	
50	Y7	49	
51	R8	65	
51	Y8	65	
52	R9	37	
52	Y9	37	

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Mol	Chain	Length	Quality of chain
53	QV	77	
53	XV	77	
54	QX	25	
54	XX	25	
55	QY	17	
55	XY	17	
56	Z6	3	
56	Z8	3	

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
58	MG	RA	3002	-	-	-	X
58	MG	RA	3067	-	-	-	X
58	MG	RA	3212	-	-	-	X
58	MG	RA	3227	-	-	-	X
58	MG	Y0	101	-	-	-	X
58	MG	YA	3018	-	-	-	X
58	MG	YA	3214	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291730 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called 23S rRNA.

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

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

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

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

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

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L31.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a RNA chain called P-site tRNA fMET.

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

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	8	Total 173	C 77	N 33	O 55	P 8	0	0	0
54	XX	8	Total 173	C 77	N 33	O 55	P 8	0	0	0

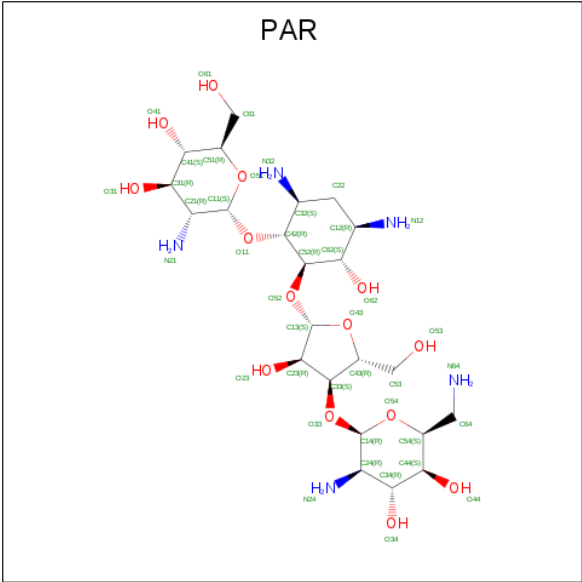
- Molecule 55 is a RNA chain called A site ASL of tRNA-Proline CGG (unmodified).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	QY	8	Total 174	C 77	N 33	O 56	P 8	0	0	0
55	XY	8	Total 174	C 77	N 33	O 56	P 8	0	0	0

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

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

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



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

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QA	76	Total	Mg	0	0
			76	76		
58	RP	2	Total	Mg	0	0
			2	2		
58	YA	265	Total	Mg	0	0
			265	265		
58	QM	1	Total	Mg	0	0
			1	1		
58	YD	2	Total	Mg	0	0
			2	2		
58	QV	1	Total	Mg	0	0
			1	1		
58	XA	82	Total	Mg	0	0
			82	82		
58	R0	1	Total	Mg	0	0
			1	1		
58	Y0	1	Total	Mg	0	0
			1	1		
58	YQ	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	R8	2	Total 2	Mg 2	0	0
58	YX	1	Total 1	Mg 1	0	0
58	RD	1	Total 1	Mg 1	0	0
58	XB	1	Total 1	Mg 1	0	0
58	QF	1	Total 1	Mg 1	0	0
58	R5	1	Total 1	Mg 1	0	0
58	RA	247	Total 247	Mg 247	0	0
58	YP	2	Total 2	Mg 2	0	0
58	Y5	1	Total 1	Mg 1	0	0
58	RE	2	Total 2	Mg 2	0	0
58	YB	3	Total 3	Mg 3	0	0
58	XV	2	Total 2	Mg 2	0	0
58	RB	2	Total 2	Mg 2	0	0
58	RF	1	Total 1	Mg 1	0	0
58	XM	1	Total 1	Mg 1	0	0

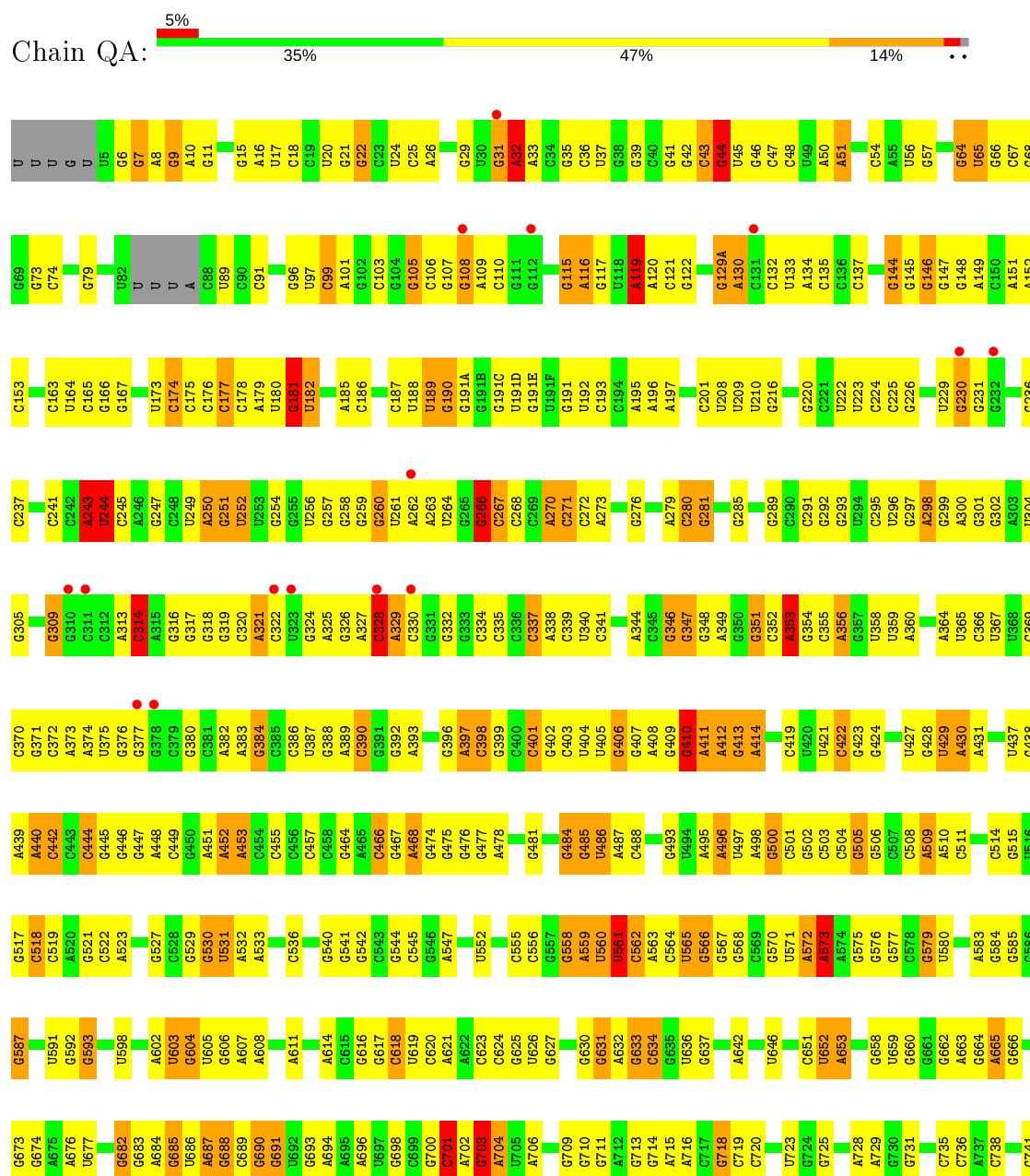
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

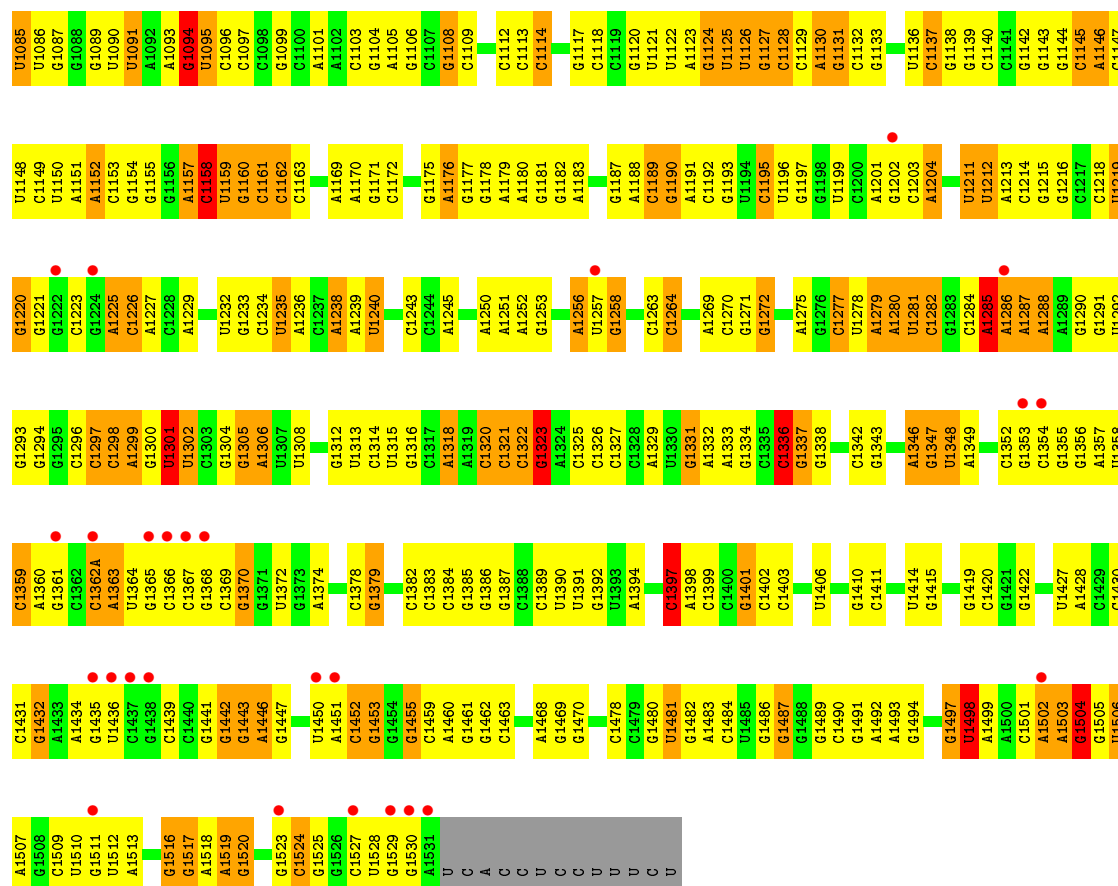
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

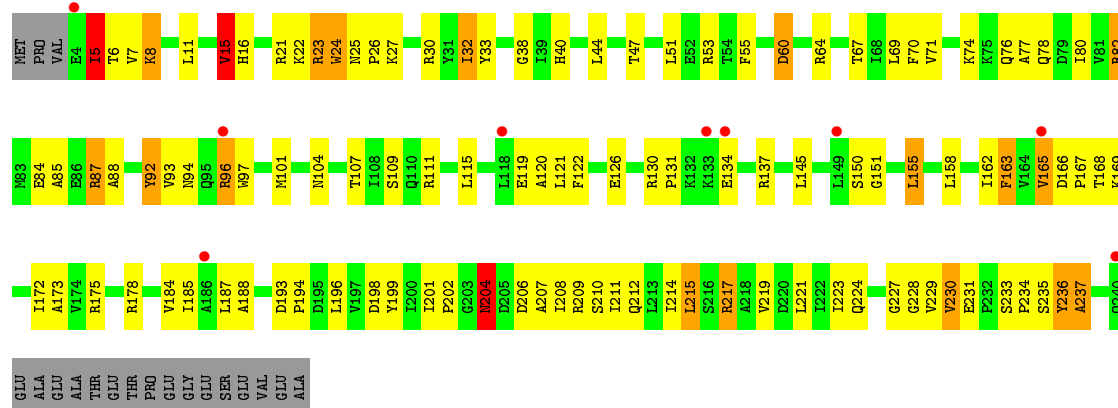
• Molecule 1: 16S rRNA



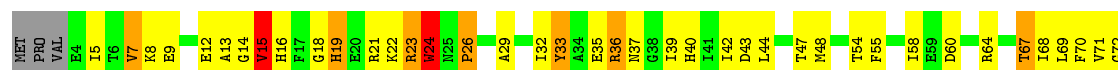


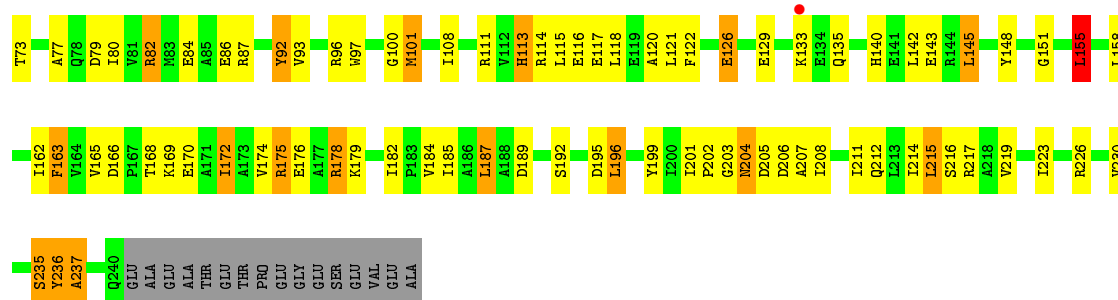


• Molecule 2: 30S ribosomal protein S2

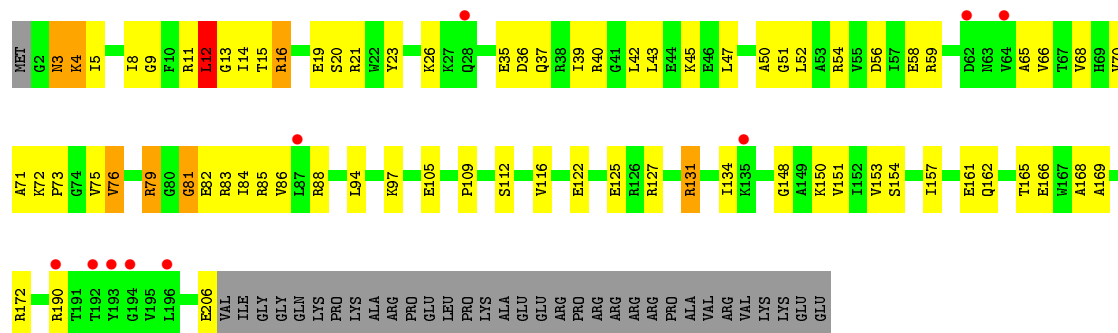


• Molecule 2: 30S ribosomal protein S2

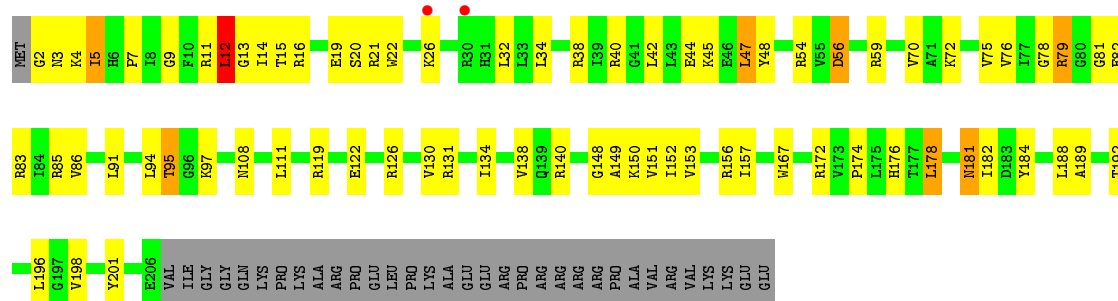




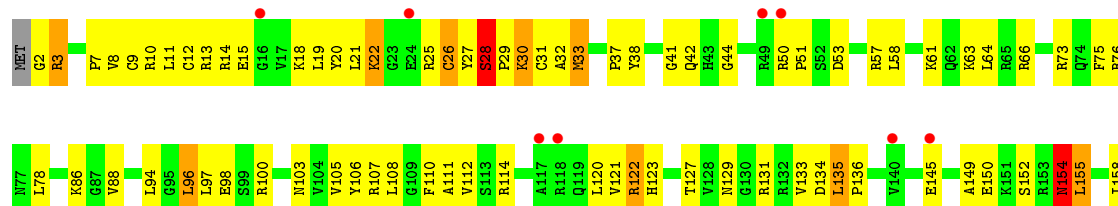
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

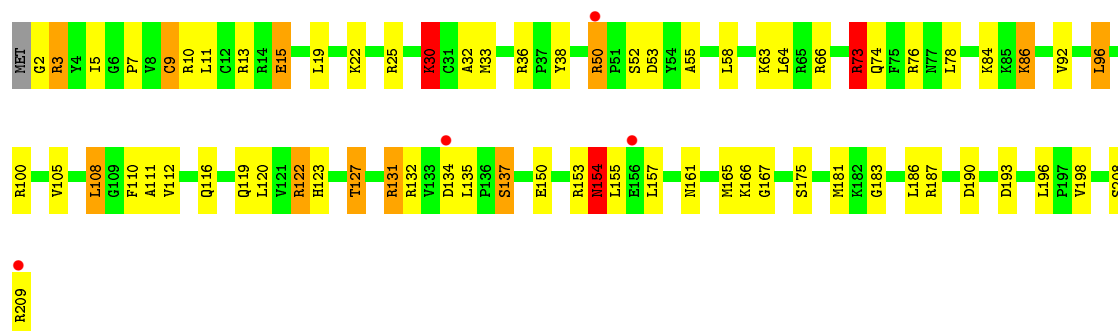


• Molecule 4: 30S ribosomal protein S4

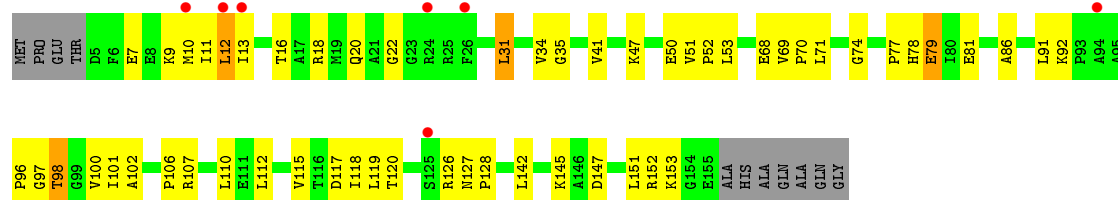




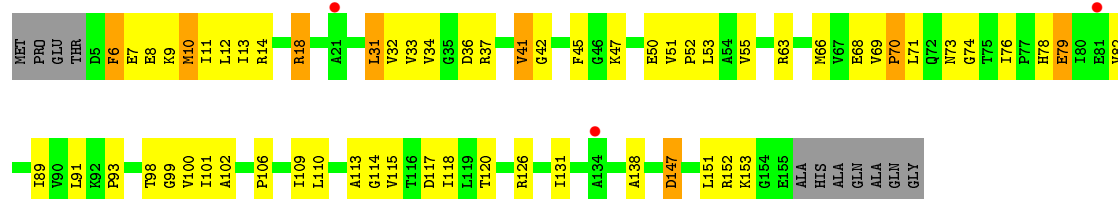
- Molecule 4: 30S ribosomal protein S4



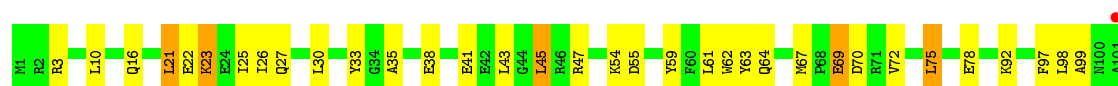
- Molecule 5: 30S ribosomal protein S5



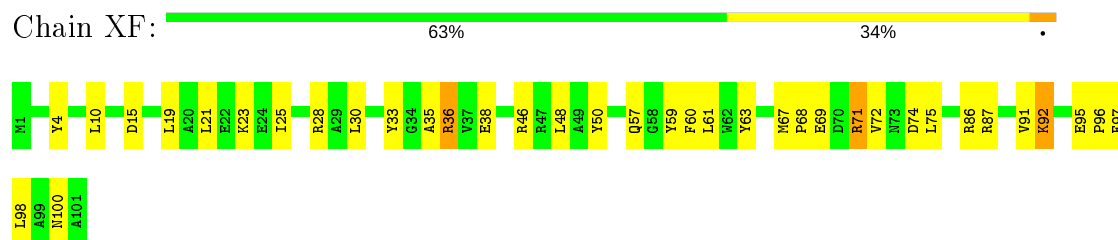
- Molecule 5: 30S ribosomal protein S5



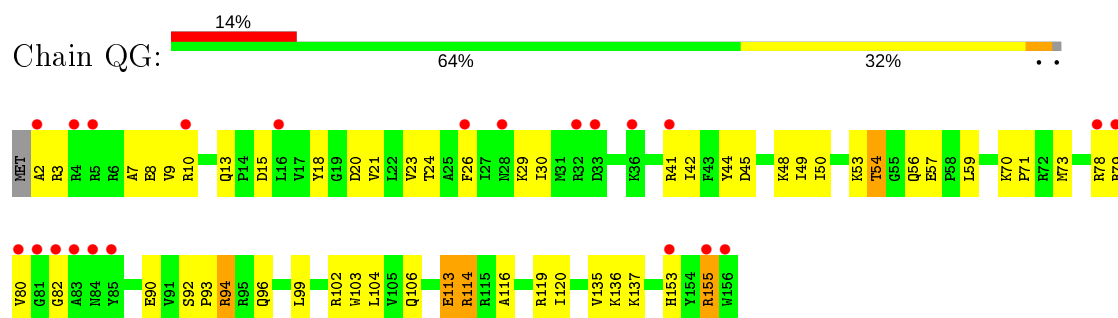
- Molecule 6: 30S ribosomal protein S6



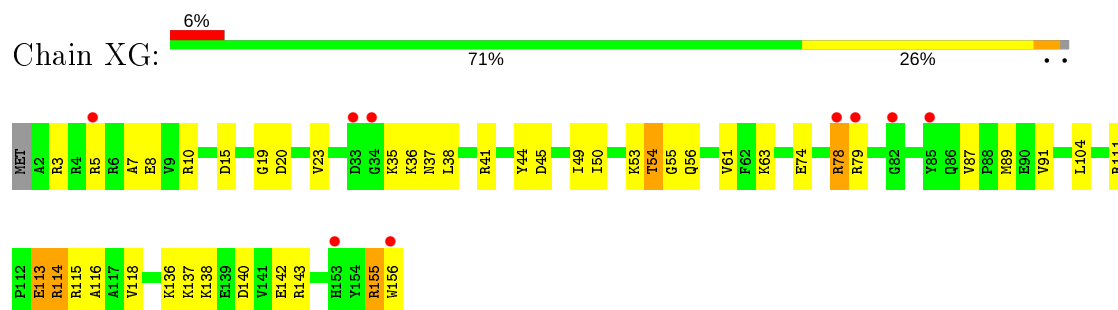
- Molecule 6: 30S ribosomal protein S6



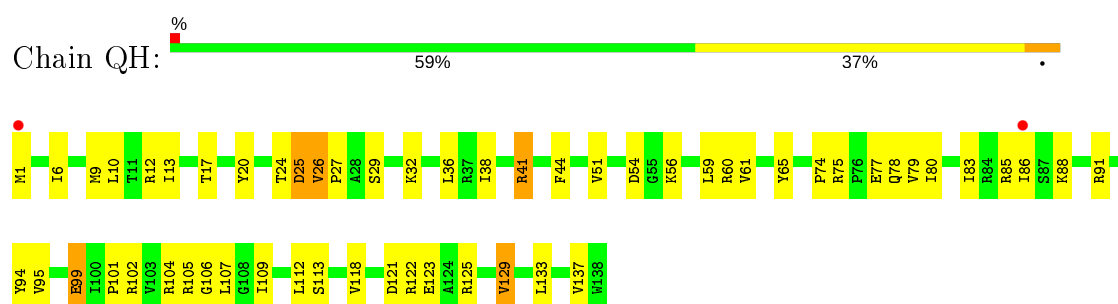
- Molecule 7: 30S ribosomal protein S7



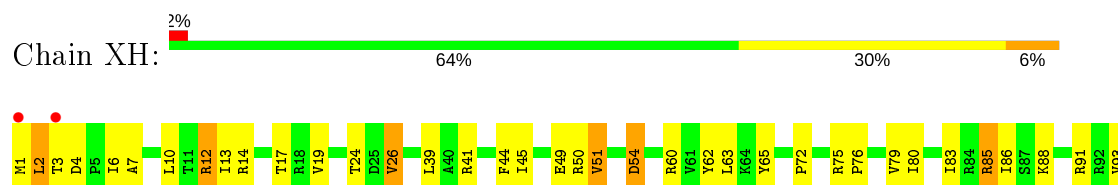
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

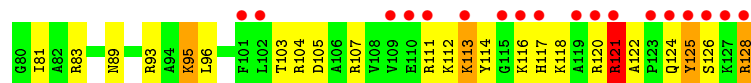
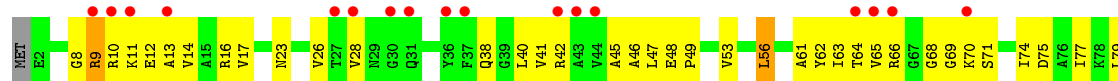


- Molecule 8: 30S ribosomal protein S8

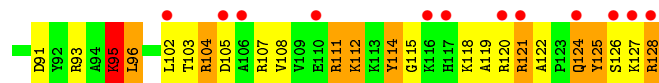
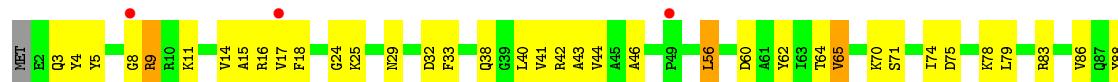




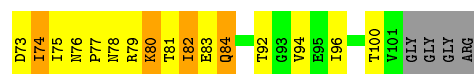
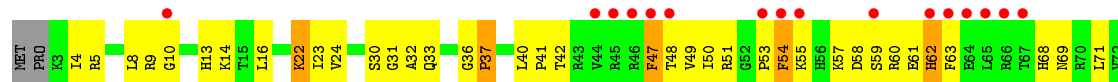
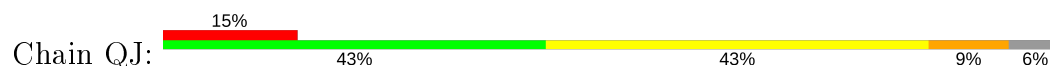
- Molecule 9: 30S ribosomal protein S9



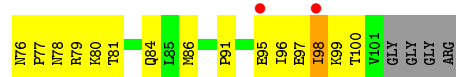
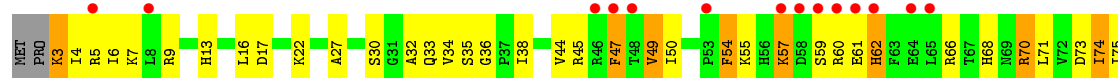
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

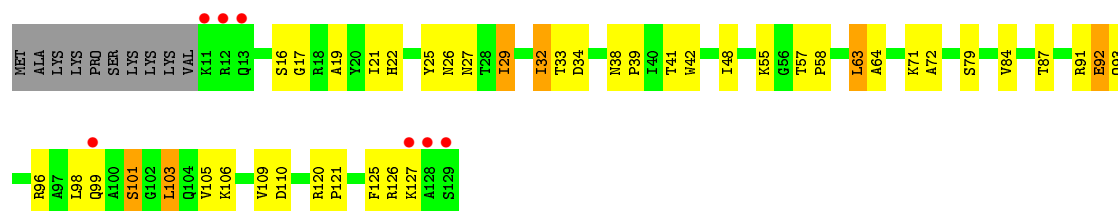


- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

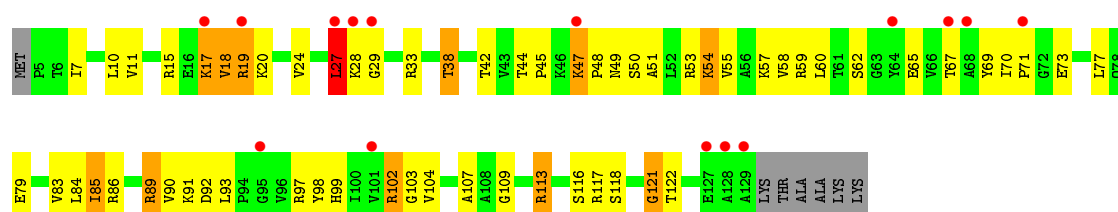




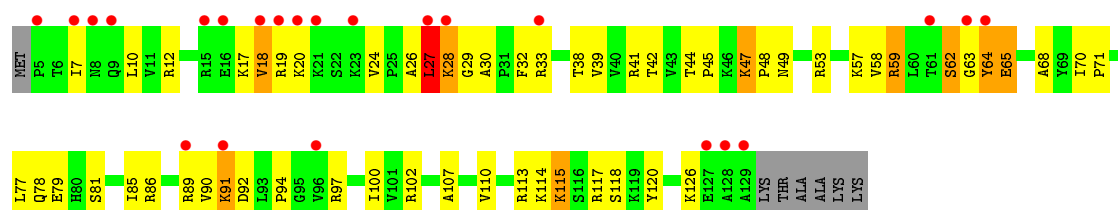
- Molecule 11: 30S ribosomal protein S11



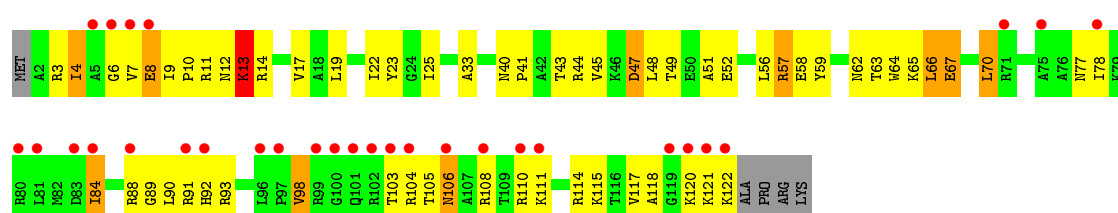
- Molecule 12: 30S ribosomal protein S12



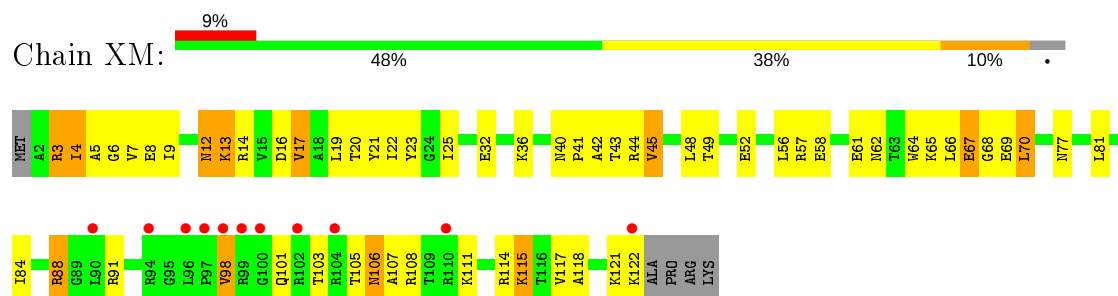
- Molecule 13: 30S ribosomal protein S13



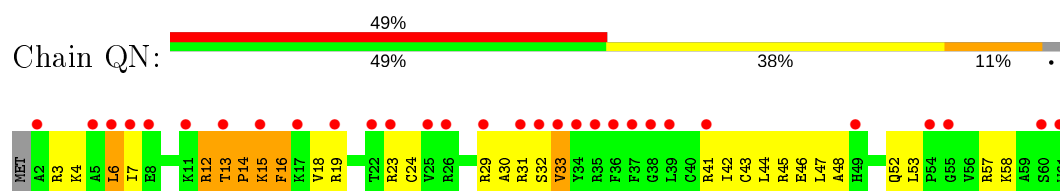
- Molecule 13: 30S ribosomal protein S13



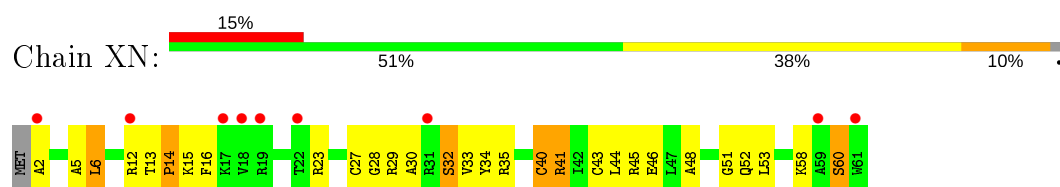
- Molecule 13: 30S ribosomal protein S13



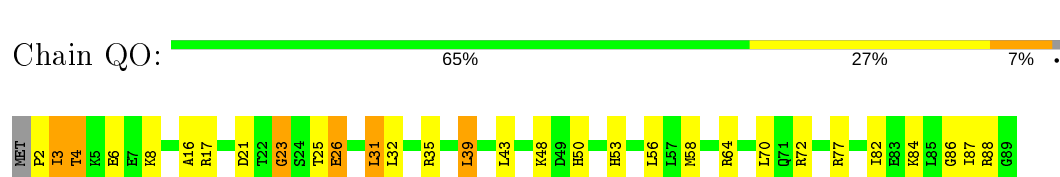
- Molecule 14: 30S ribosomal protein S14 type Z



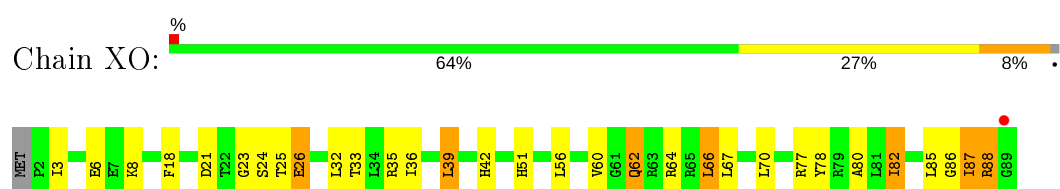
- Molecule 14: 30S ribosomal protein S14 type Z



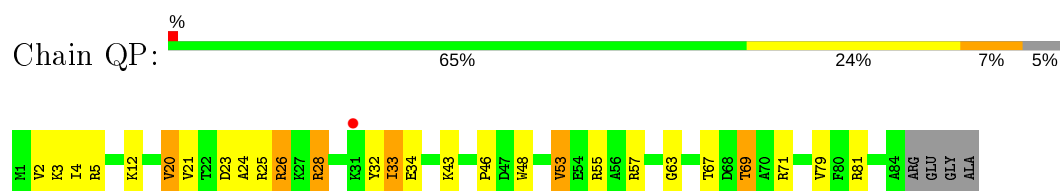
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

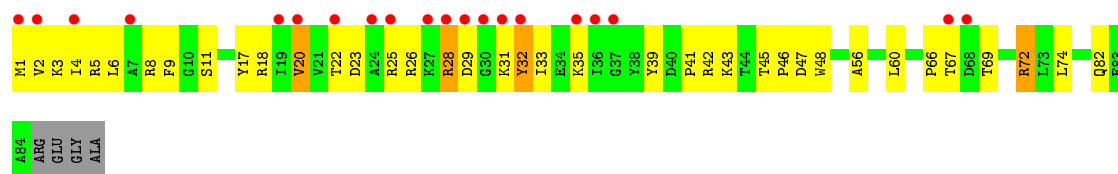


- Molecule 16: 30S ribosomal protein S16



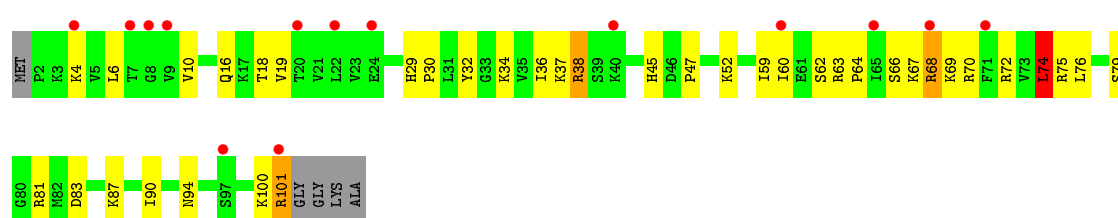
- Molecule 16: 30S ribosomal protein S16

Chain XP:



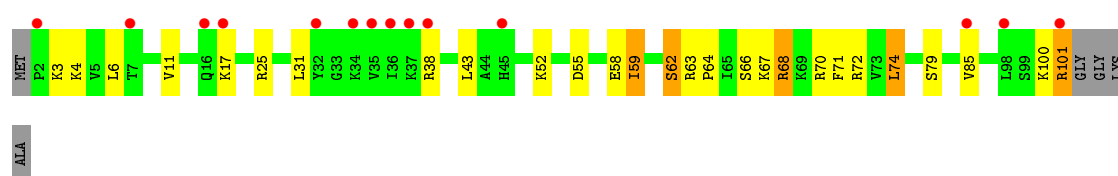
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



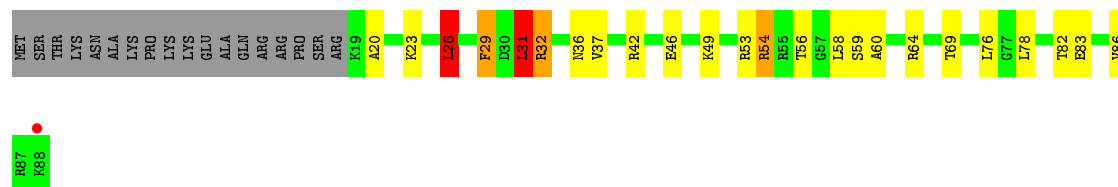
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



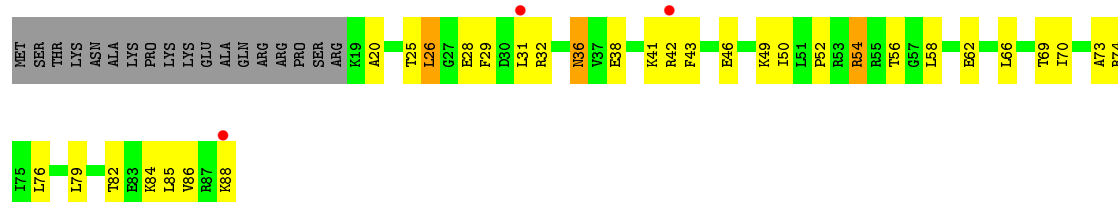
- Molecule 18: 30S ribosomal protein S18

Chain QR:

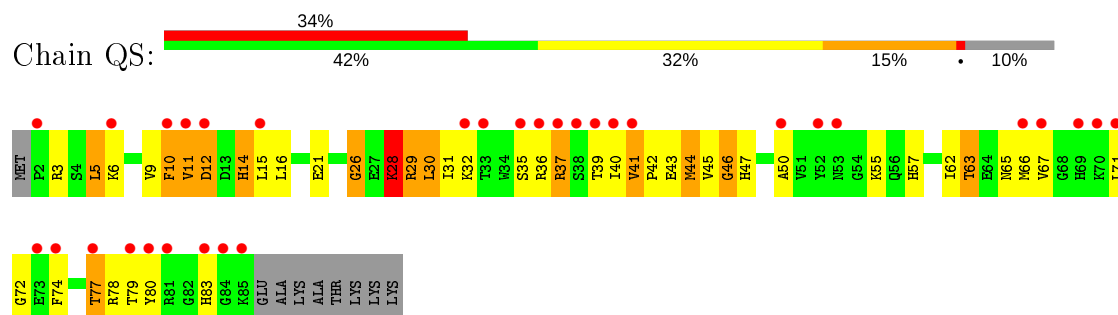


- Molecule 18: 30S ribosomal protein S18

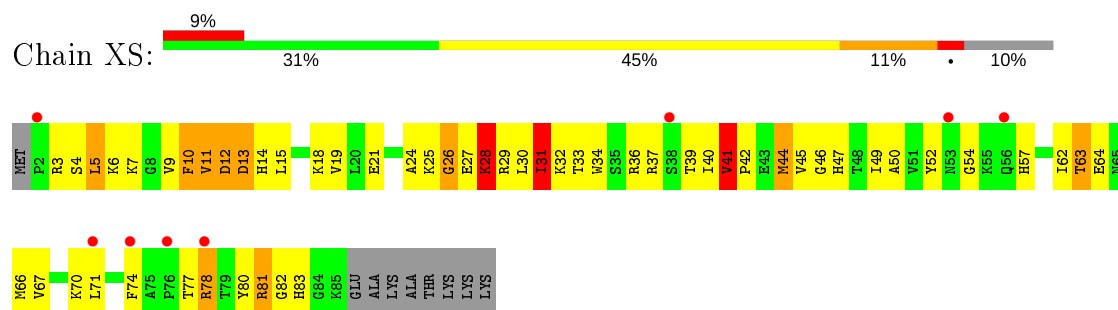
Chain XR:



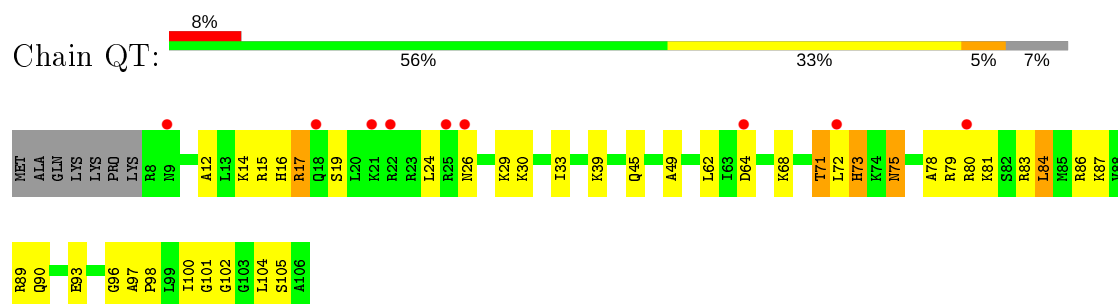
- Molecule 19: 30S ribosomal protein S19



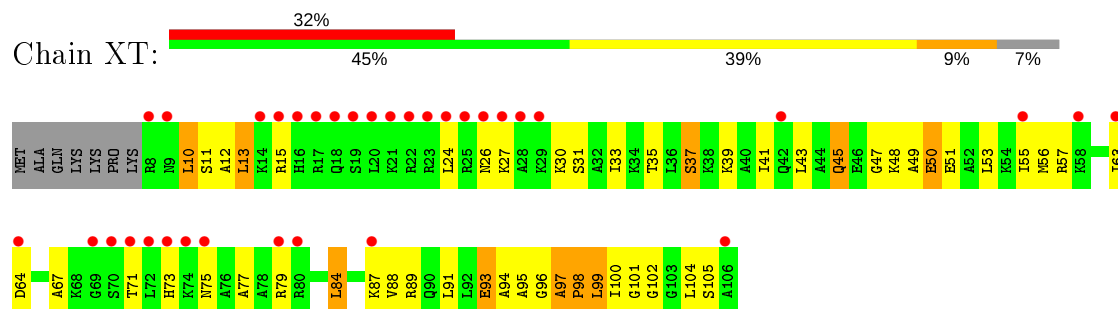
- Molecule 19: 30S ribosomal protein S19



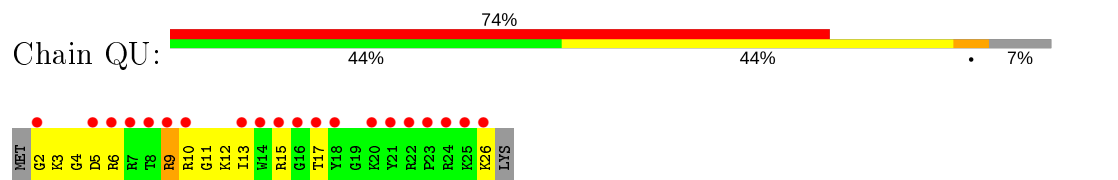
- Molecule 20: 30S ribosomal protein S20



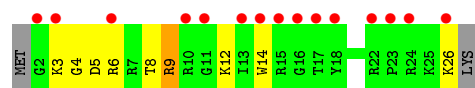
- Molecule 20: 30S ribosomal protein S20



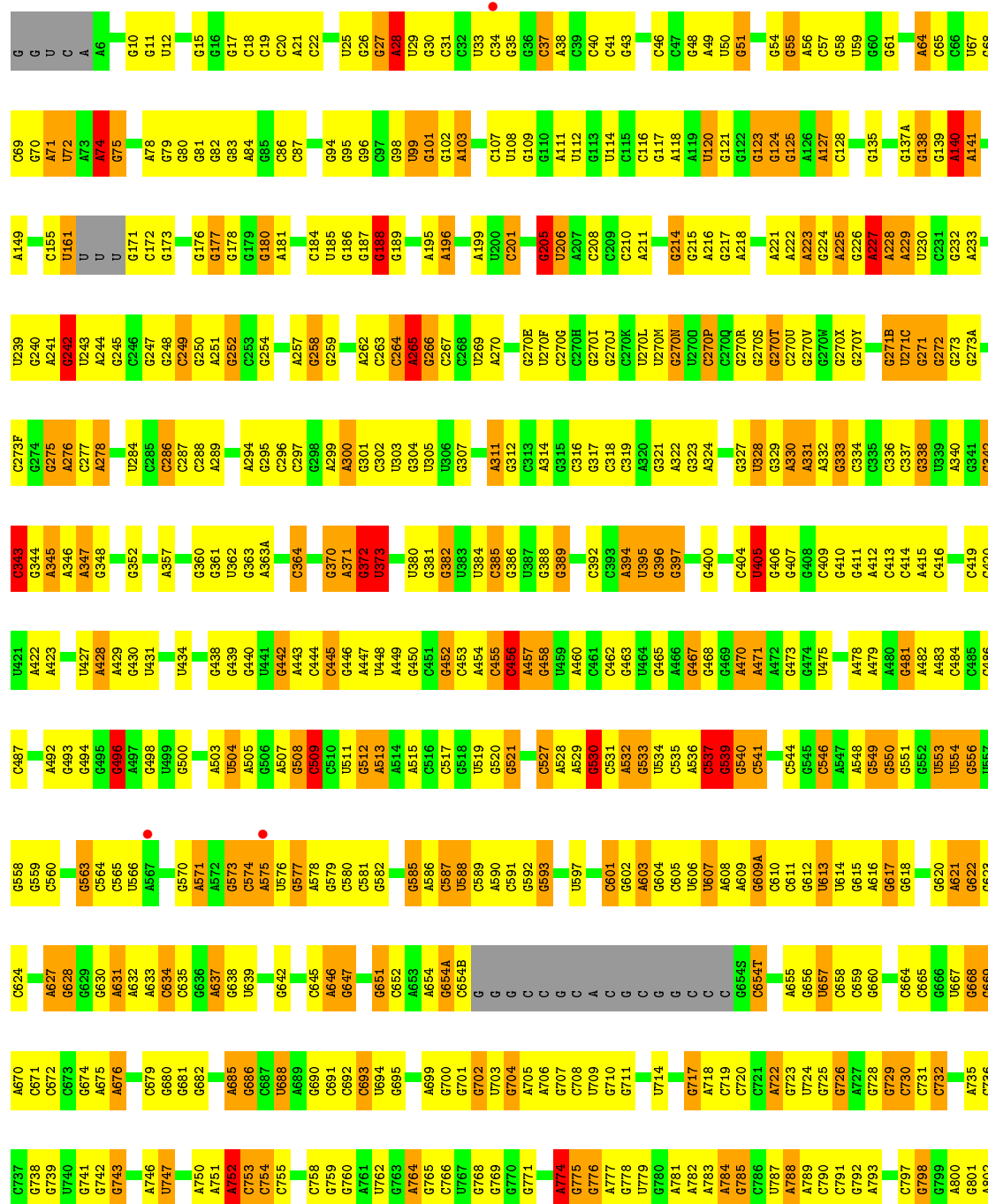
- Molecule 21: 30S ribosomal protein Thx



• Molecule 21: 30S ribosomal protein Thx



• Molecule 22: 23S rRNA



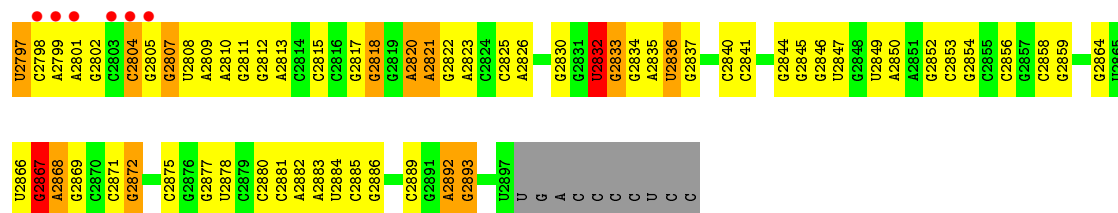
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U1730	G1643	A1507	U1578	A1508	C1432	A1359	G1284	A1210	G1136	A1069	C1007	U943	A873	G805
G1731	G1645	A1509	U1433	A1510	U1433	A1360	G1285	G1212	G1137	G1071	A1010	A945	U874	C806
A1732	C1646	A1580	U1433	A1511	U1433	A1361	G1286	G1213	G1138	G1072	U1011	A946	G875	G808
G1733	G1647	G1581	U1434	C1513	G1440	A1365	A1287	A1213	G1139	A1073	U1012	G947	G876	G809
C1734	C1648	A1582	G1441	C1514	G1441	A1366	U1288	A1214	C1140	G1074	U1013	G948	U810	U810
G1735	G1649	A1583	G1442	C1515	G1442	A1367	C1290	G1215	U1141	C1075	U1014	G949	U811	U811
C1741	C1650	C1585	A1444A	C1516	A1444A	C1370	C1291	G1216	U1142	C1076	G1015	A953	C883	C812
G1742	G1651	G1581	C1445	C1517	C1445	G1370	U1292	A1220	A1142A	C1077	G1016	A954	C884	U813
G1743	G1652	A1587	G1446	C1518	G1446	G1371	U1293	C1221	A1143	U1078	C1018	C955	C885	C814
G1746	C1653	U1520	G1448	G1519	G1448	U1372	C1293	C1222	A1148	C1079	U1019	G956	C886	C815
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G1753	C1656	U1523	G1450	U1523	G1450	A1379	C1299	C1224	G1150	U1082	A1022	U958	C888	C818
C1754	C1657	G1524	C1451	G1524	C1451	A1380	U1300	C1225	G1151	U1083	U1023	A959	A890	A819
A1755	G1658	G1525	A1453	G1525	A1453	G1381	U1301	G1226	C1152	A1084	G1024	A960	C892	U822
G1756	C1659	G1526	U1454	G1526	U1454	G1382	A1302	G1227	G1153	A1085	G1025	C961	C893	G823
U1757	A1664	U1527	G1455	G1527	G1455	G1383	G1303	G1228	G1154	A1086	G1026	G962	C894	G824
C1762	C1667	A1529	G1460	A1529	G1460	A1384	C1306	G1229A	C1155	A1087	U1027	C963	A896	A824
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C1765	C1670	C1533	G1463	C1533	G1463	G1389	G1310	G1238	G1167	G1090	U1030	C966	A899	U827
U1766	C1671	G1534	C1464	G1534	C1464	U1390	G1311	G1239	U1167	G1091	U1033	C967	U828	U828
G1769	G1672	U1535	G1465	U1535	G1465	U1391	U1312	U1240	G1168	G1093	G1034	U969	A901	A829
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G1771	A1676	A1537	C1467	A1537	C1467	A1393	G1314	G1245	G1170	A1096	U1036	C971	C903	G831
C1772	G1677	G1538	G1468	G1538	G1468	U1394	C1315	G1246	G1171	U1097	G1037	G972	U905	G832
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C1800														A866

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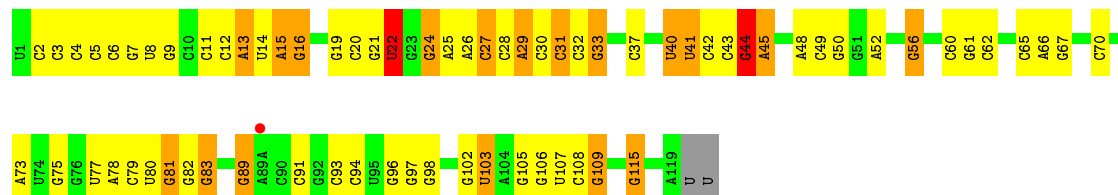


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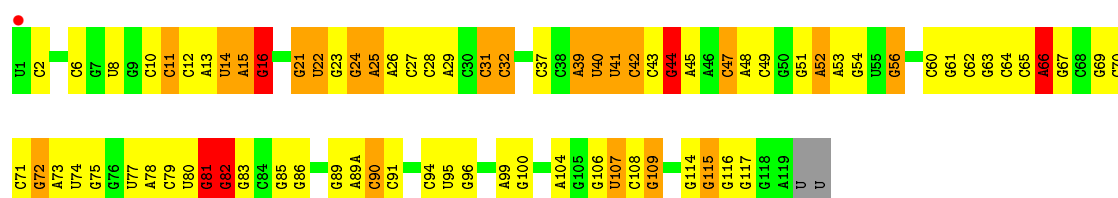
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A2779			G2583	G2507	A2439	G2370	G2305	A2241	G2106		C2036	G1965	
A2780			C2584	C2440	C2440	G2371	C2306	G2242	C2107		G2037	A1966	G1896
A2781			U2585	G2441	G2441	G2372	G2307	U2243	C2108		G2038	C1967	
A2782			C2586	G2442		G2373	G2308	U2244	U2109		C2039	G1968	G1899
A2783			A2587	C2443	C2443		A2309	G2245	A2170		C2040	G1969	A1900
A2784				G2444	G2445	A2377	A2310	A2246	A2171		C2041	A1970	A1901
A2785			C2591	G2446	G2446	G2378	A2311	A2247	U2172		A2042	A1971	G1902
A2786			G2592	G2447	G2447	G2379	U2312	A2248	C2173		C2043	A1972	G1903
A2787			U2593	G2448	G2448	G2380	C2314	U2249	C2174		G2044	G1973	G1904
A2788			C2594	A2448	A2448	C2381	C2315	G2250	C2175		G2045	C1974	G1905
A2789			U2595	U2449	U2449	G2382	G2316	G2251	A2176		G2046	G1975	G1906
A2790			G2596	A2450	A2450	G2383	C2317	G2252	C2177		G2047	U1976	
A2791			C2597	A2451	A2451	G2384		G2253	C2178		G2048		



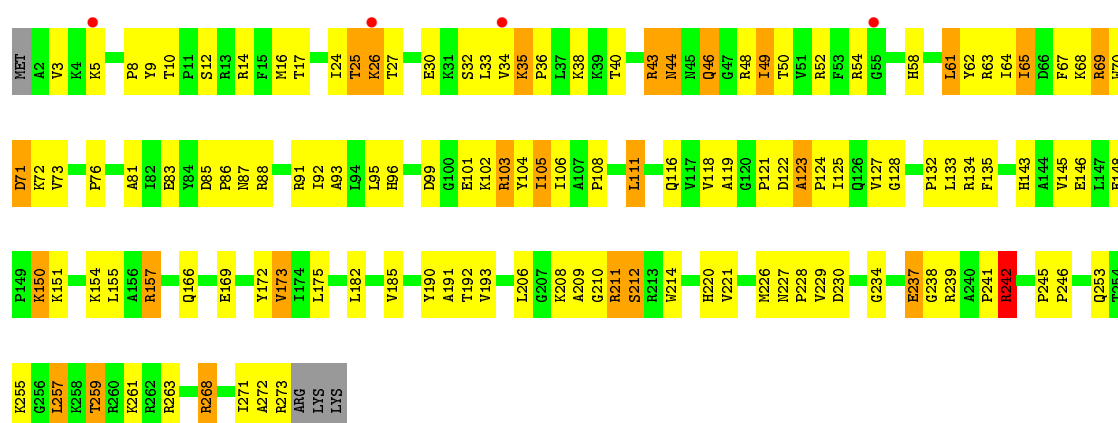
• Molecule 23: 5S rRNA



• Molecule 23: 5S rRNA

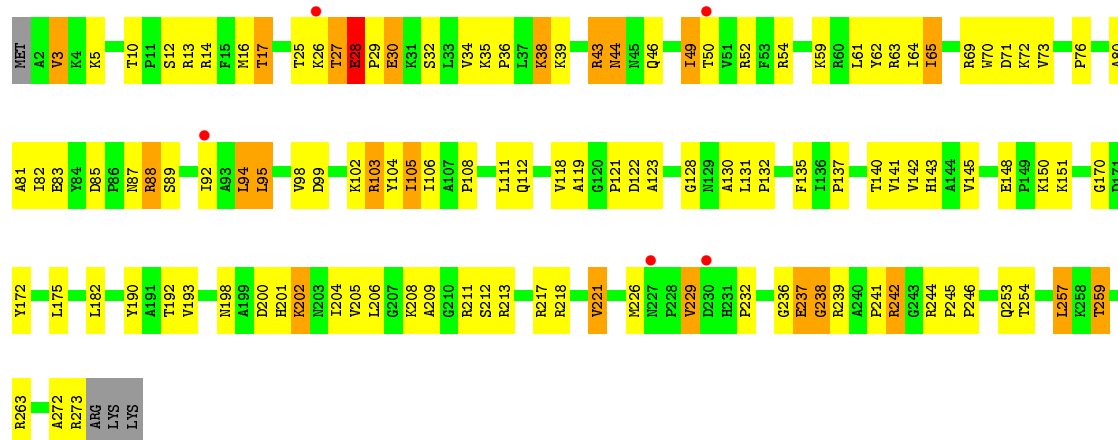


• Molecule 24: 50S ribosomal protein L2

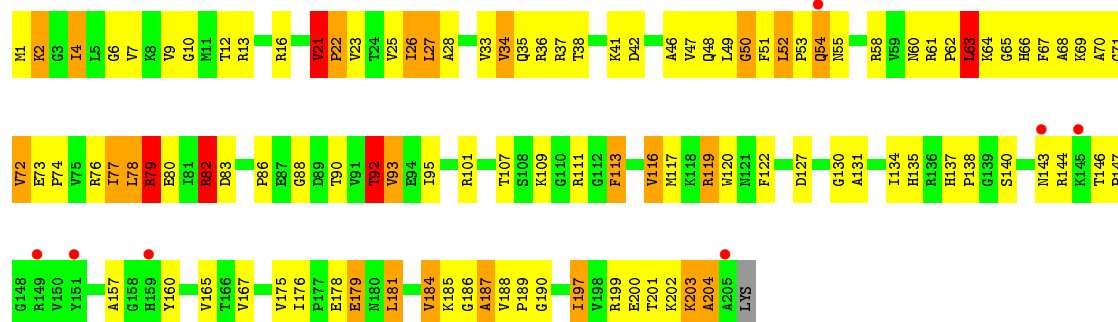


• Molecule 24: 50S ribosomal protein L2

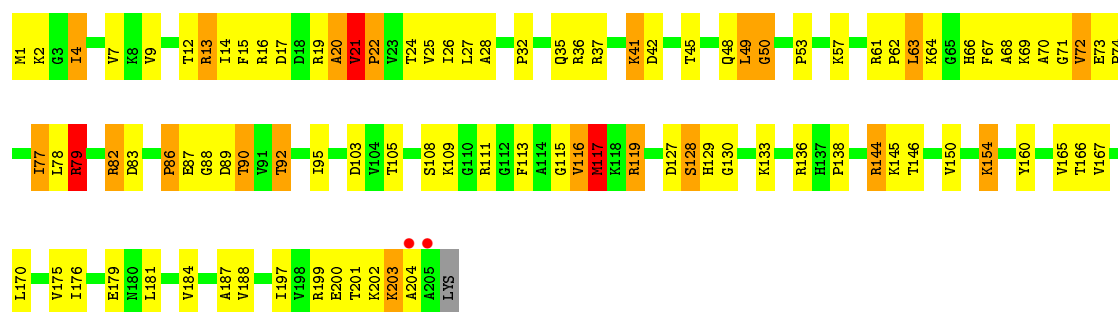




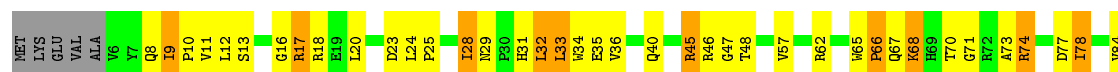
- Molecule 25: 50S ribosomal protein L3

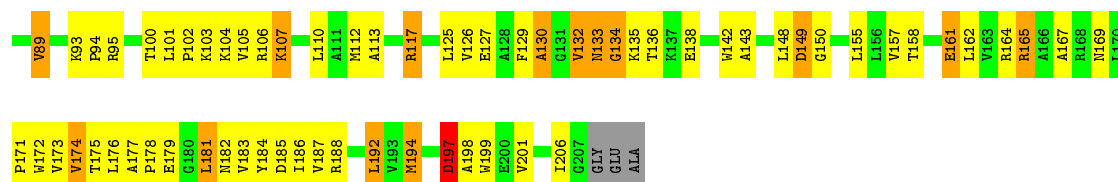


- Molecule 25: 50S ribosomal protein L3



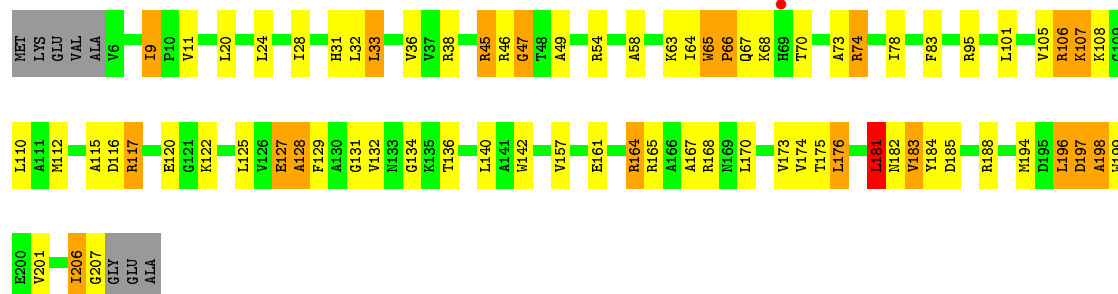
- Molecule 26: 50S ribosomal protein L4





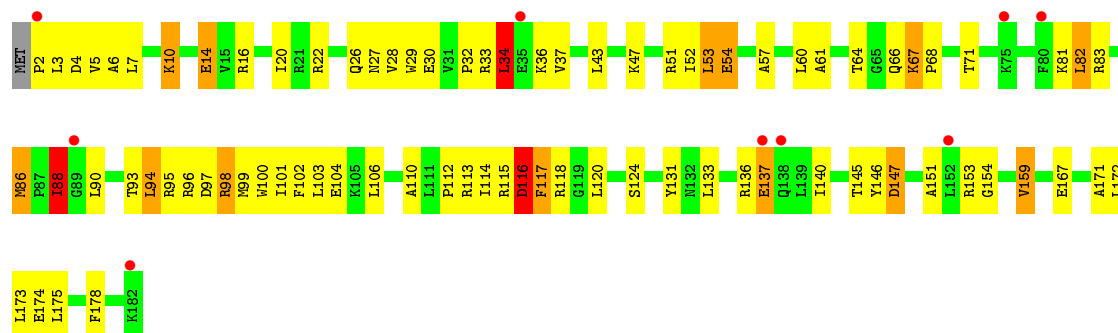
- Molecule 26: 50S ribosomal protein L4

Chain YF: 60% 26% 9% .



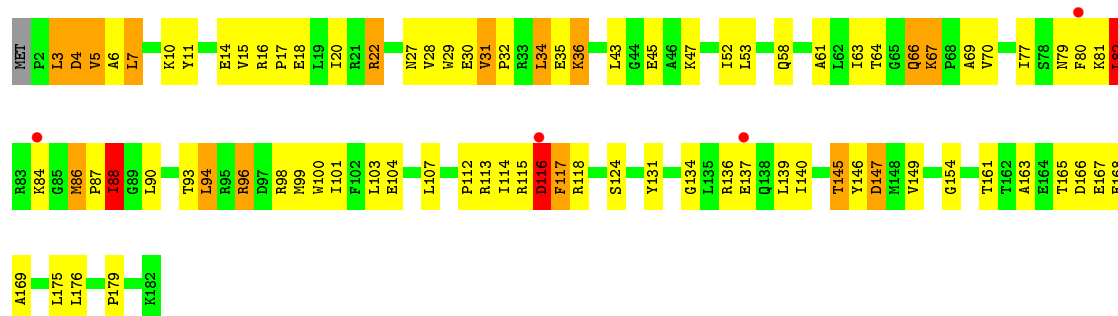
- Molecule 27: 50S ribosomal protein L5

Chain RG: 5% 54% 37% 7% ..

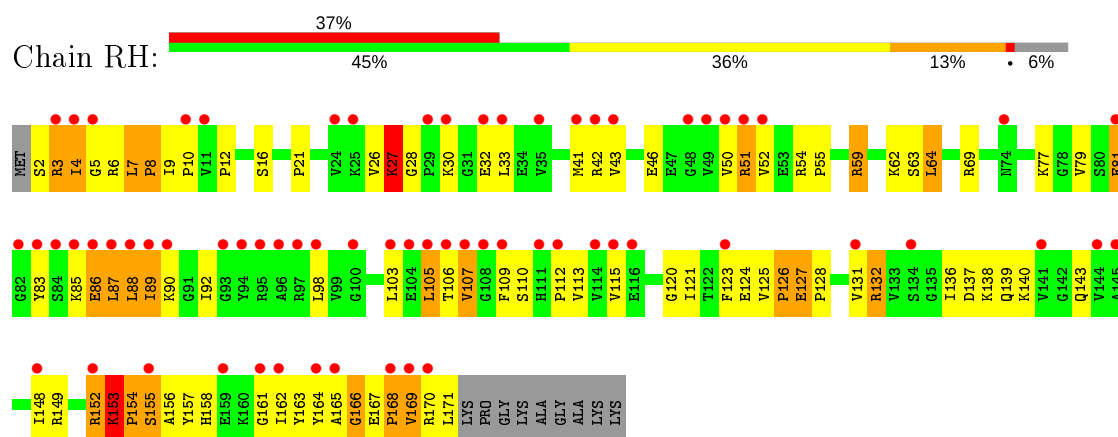


- Molecule 27: 50S ribosomal protein L5

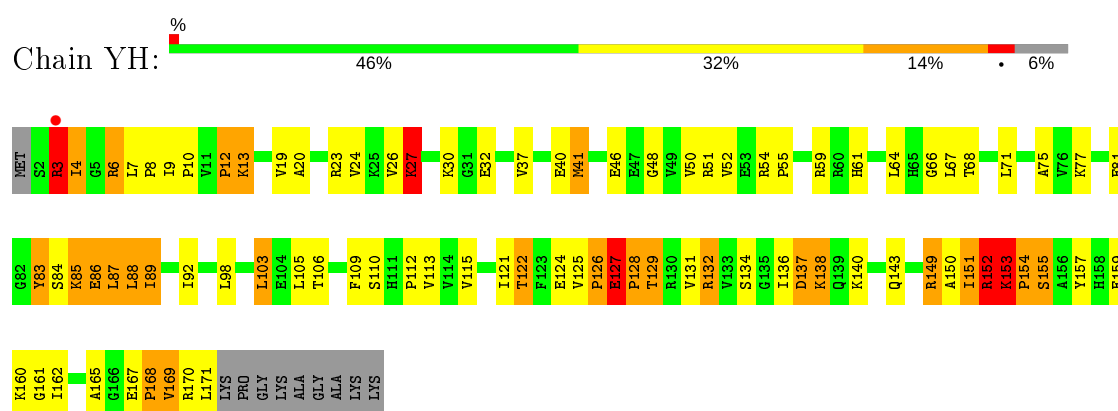
Chain YG: 2% 53% 36% 9% ..



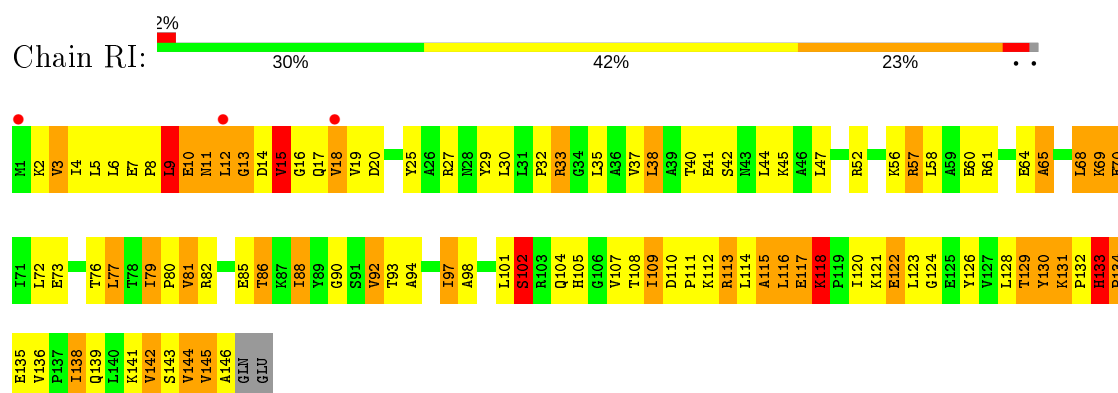
- Molecule 28: 50S ribosomal protein L6



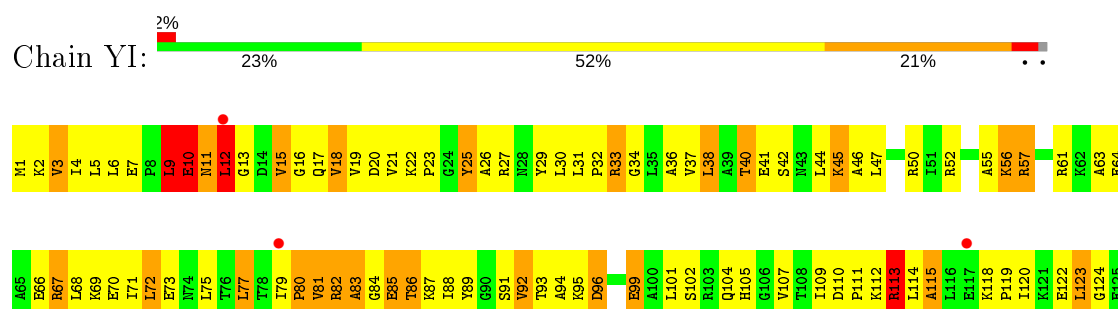
- Molecule 28: 50S ribosomal protein L6



- Molecule 29: 50S ribosomal protein L9

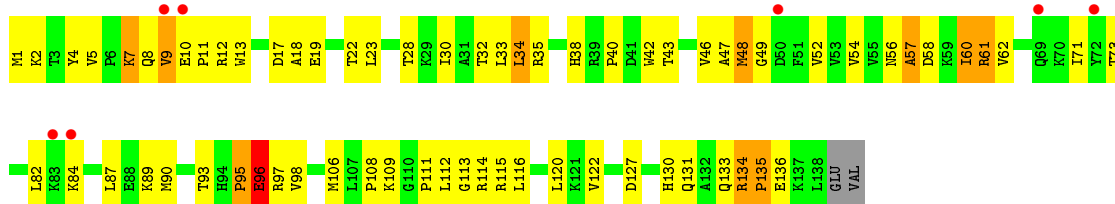


- Molecule 29: 50S ribosomal protein L9

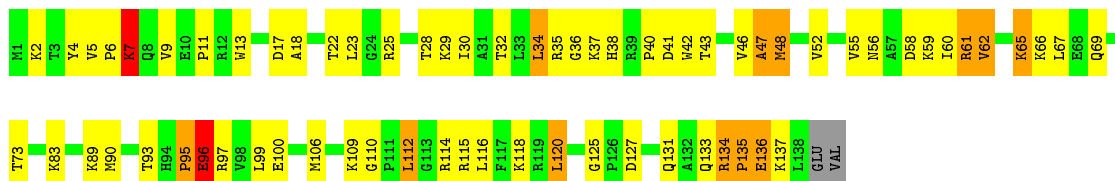




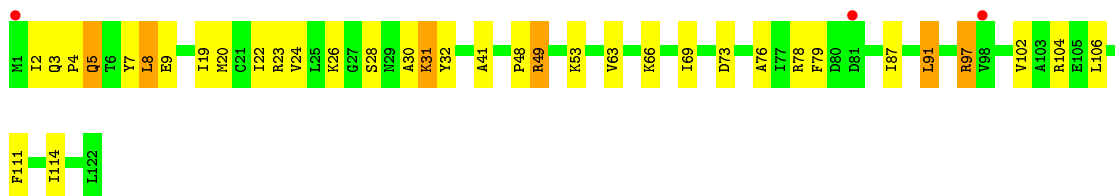
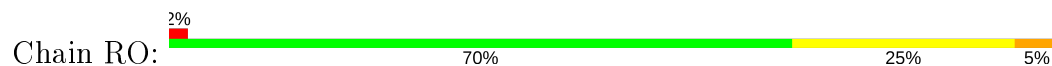
- Molecule 30: 50S ribosomal protein L13



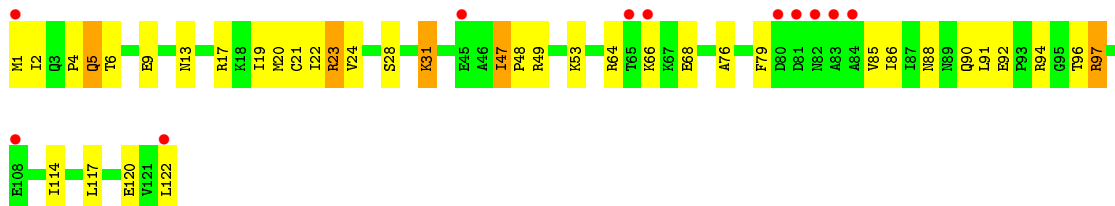
- Molecule 30: 50S ribosomal protein L13



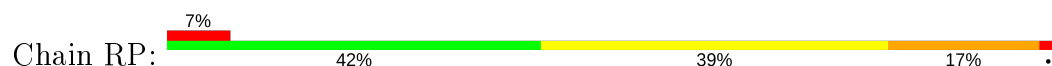
- Molecule 31: 50S ribosomal protein L14

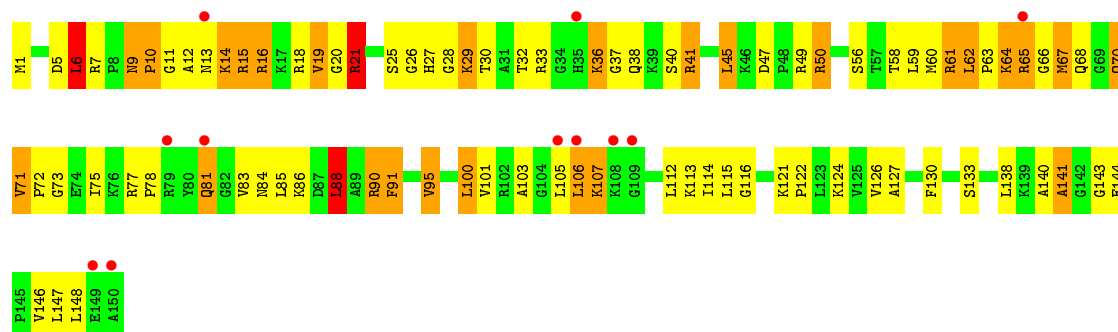


- Molecule 31: 50S ribosomal protein L14

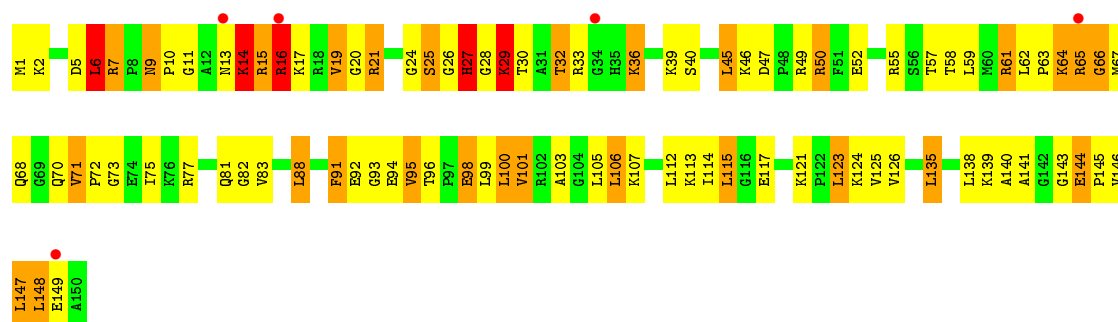


- Molecule 32: 50S ribosomal protein L15

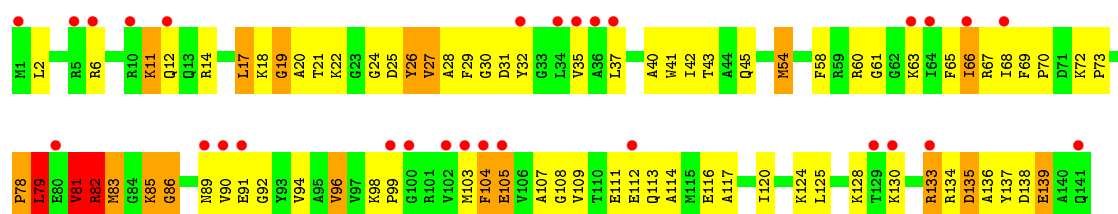




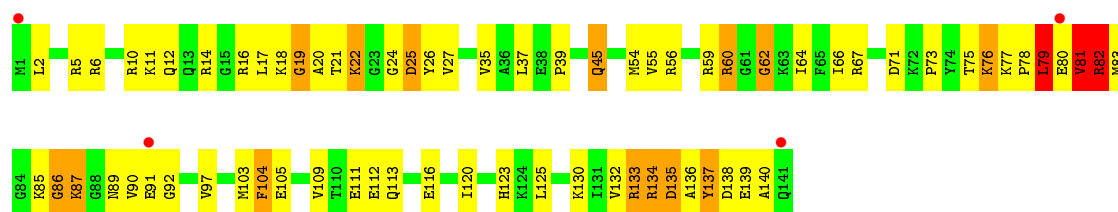
• Molecule 32: 50S ribosomal protein L15



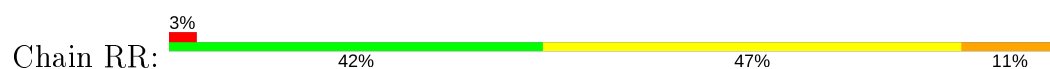
• Molecule 33: 50S ribosomal protein L16

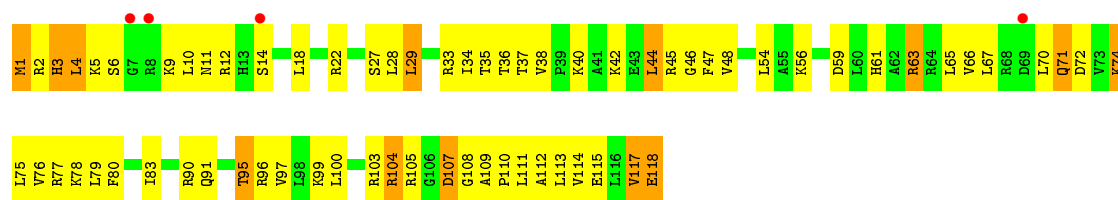


• Molecule 33: 50S ribosomal protein L16

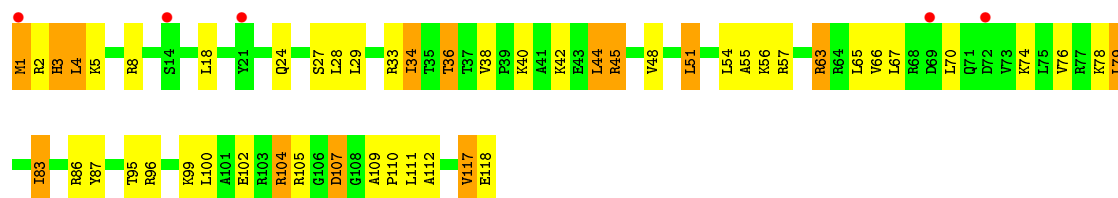


• Molecule 34: 50S ribosomal protein L17

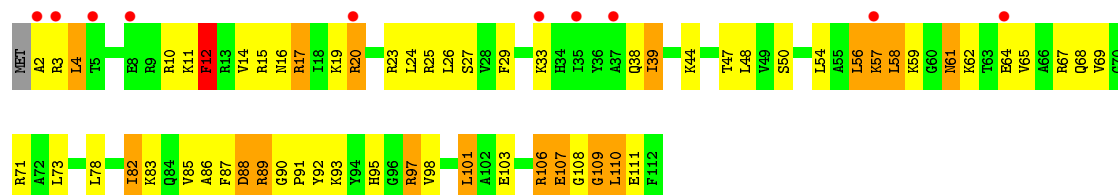
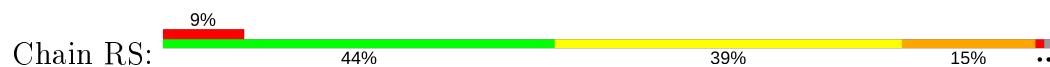




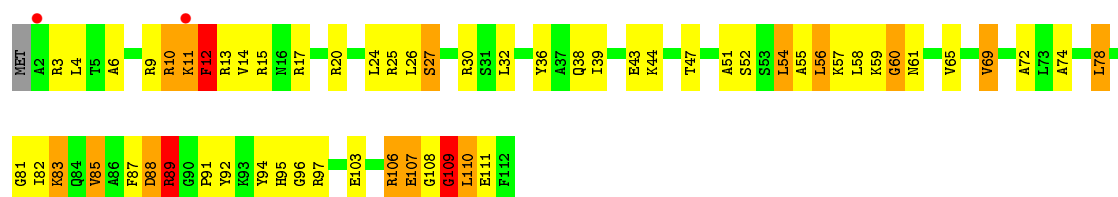
• Molecule 34: 50S ribosomal protein L17



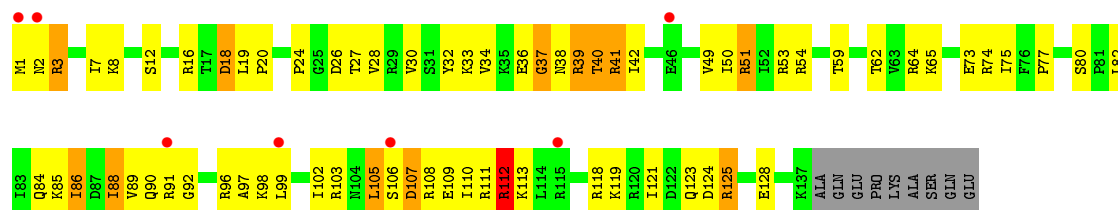
• Molecule 35: 50S ribosomal protein L18



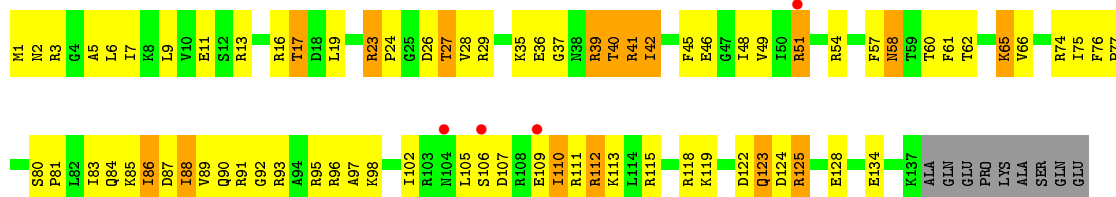
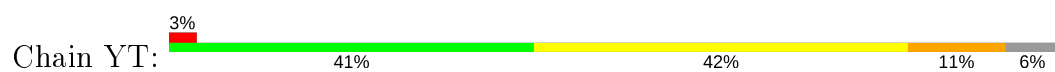
• Molecule 35: 50S ribosomal protein L18



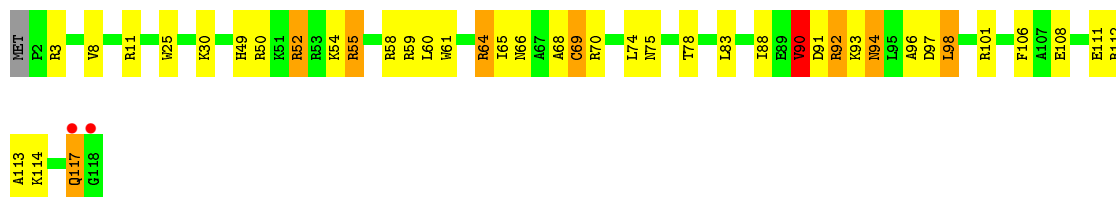
• Molecule 36: 50S ribosomal protein L19



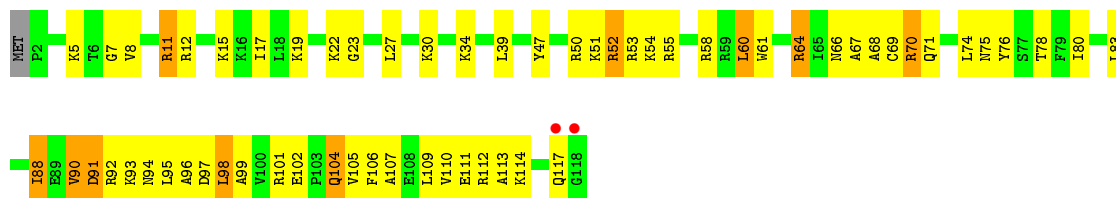
• Molecule 36: 50S ribosomal protein L19



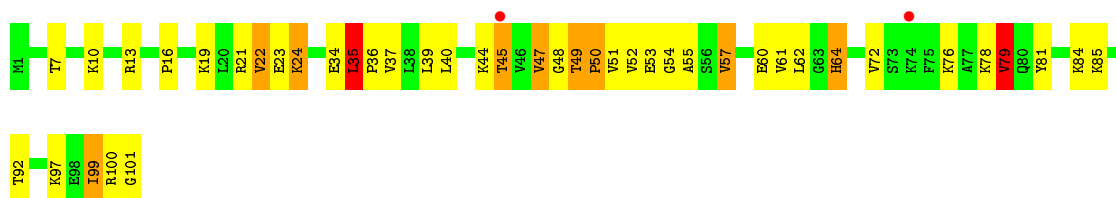
- Molecule 37: 50S ribosomal protein L20



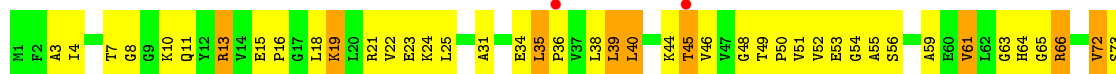
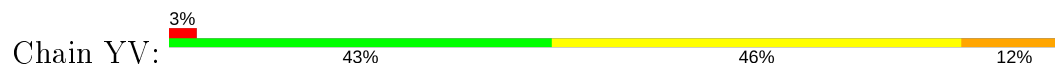
- Molecule 37: 50S ribosomal protein L20



- Molecule 38: 50S ribosomal protein L21



- Molecule 38: 50S ribosomal protein L21





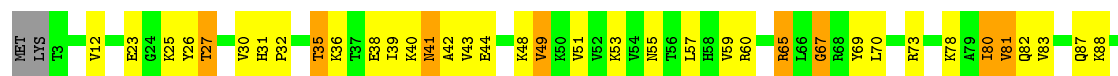
- Molecule 39: 50S ribosomal protein L22



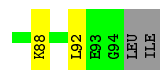
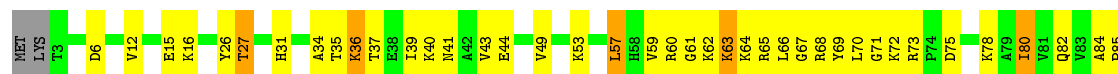
- Molecule 39: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L23

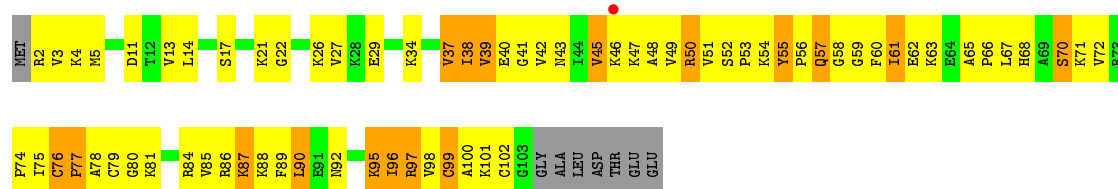


- Molecule 40: 50S ribosomal protein L23

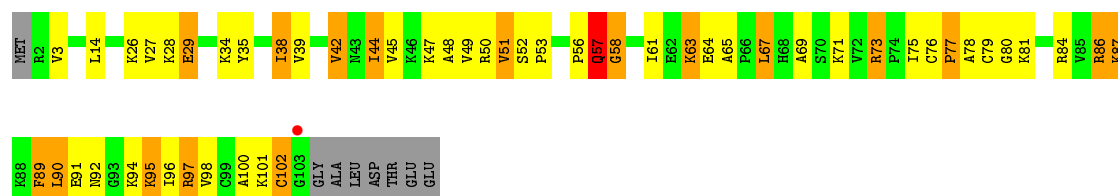


- Molecule 41: 50S ribosomal protein L24

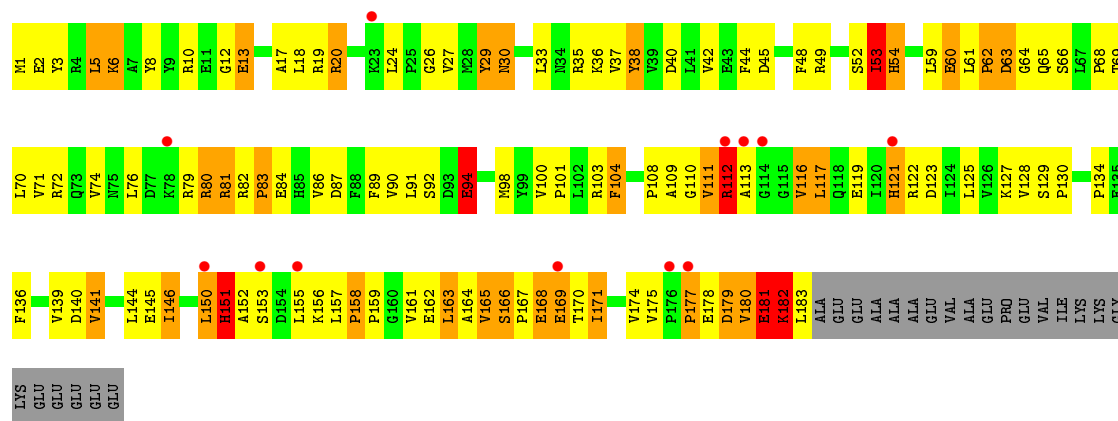




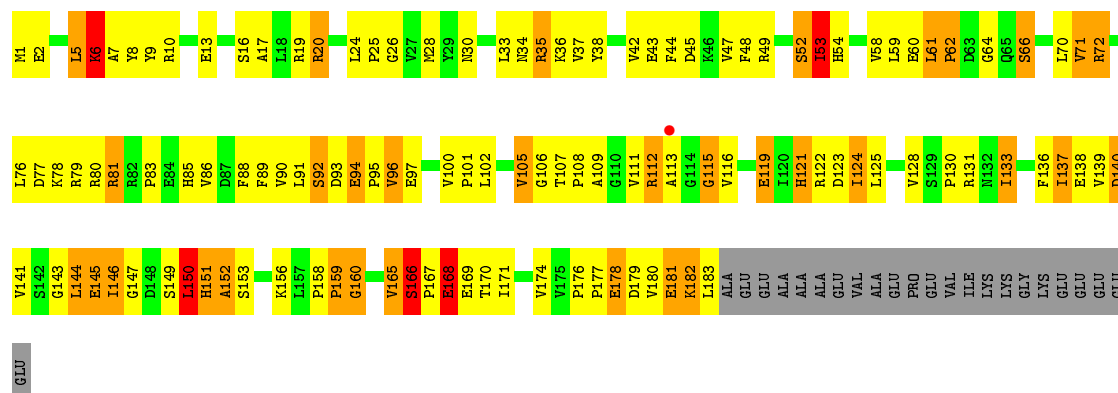
• Molecule 41: 50S ribosomal protein L24



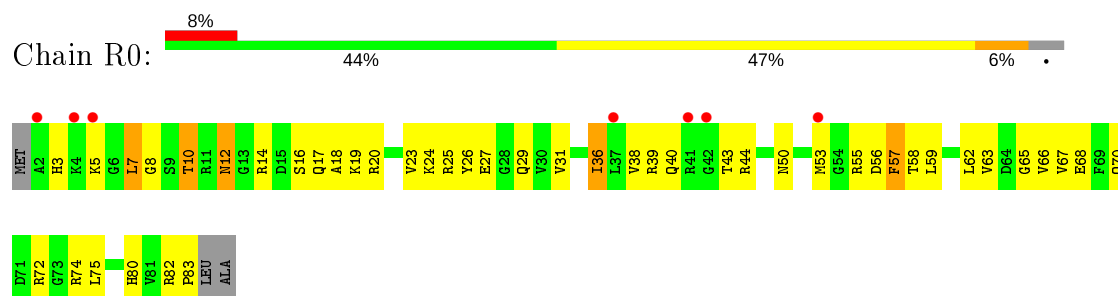
• Molecule 42: 50S ribosomal protein L25



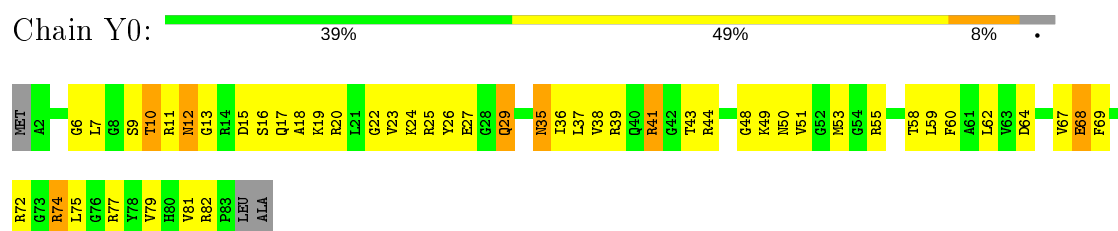
• Molecule 42: 50S ribosomal protein L25



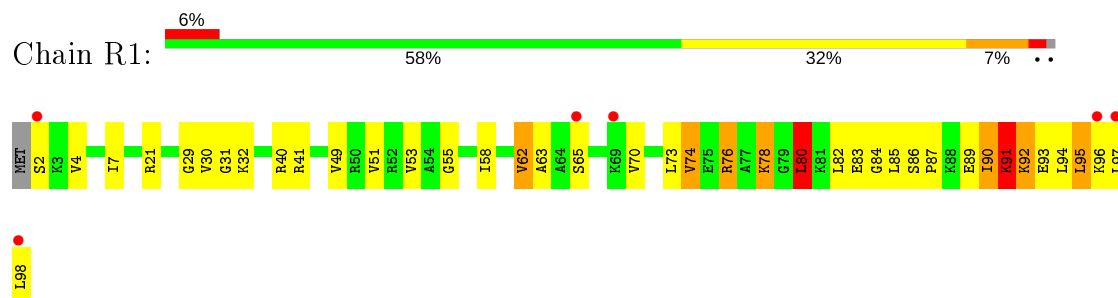
- Molecule 43: 50S ribosomal protein L27



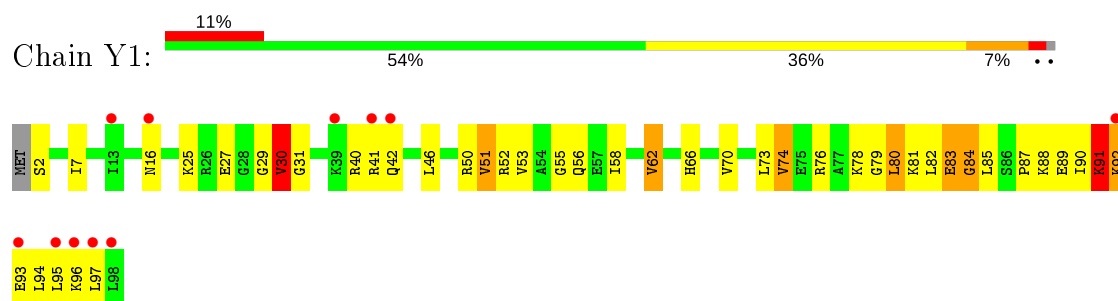
- Molecule 43: 50S ribosomal protein L27



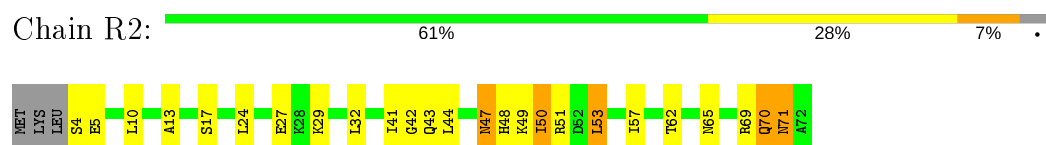
- Molecule 44: 50S ribosomal protein L28



- Molecule 44: 50S ribosomal protein L28



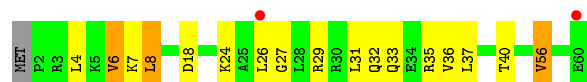
- Molecule 45: 50S ribosomal protein L29



- Molecule 45: 50S ribosomal protein L29



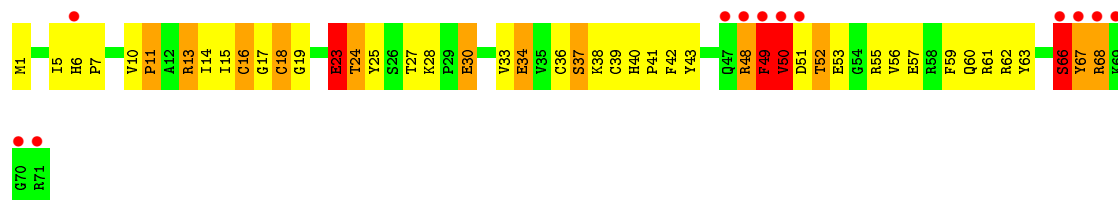
- Chain B3: 



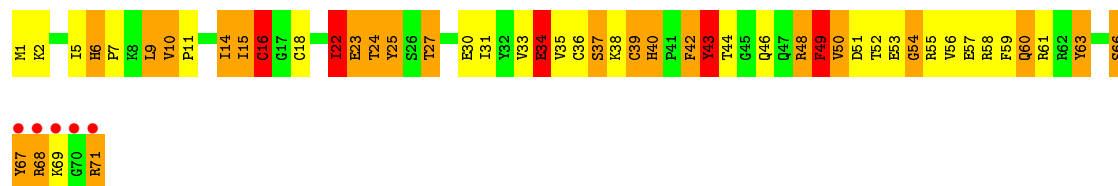
- Chain Y3: 

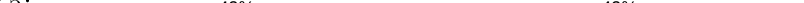


- Chain R4: 



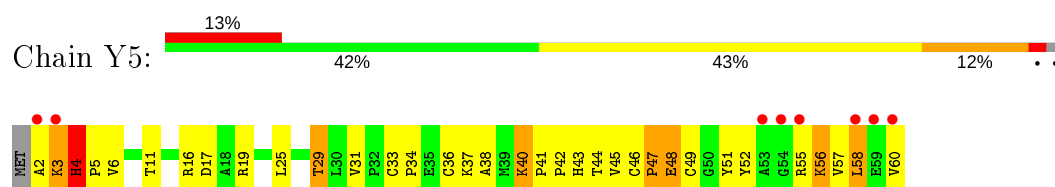
- Chain Y4: 



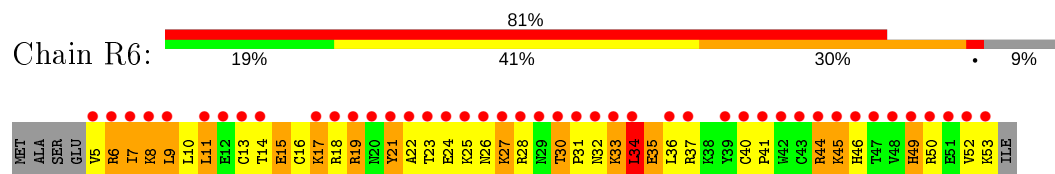
- Chain B5: 



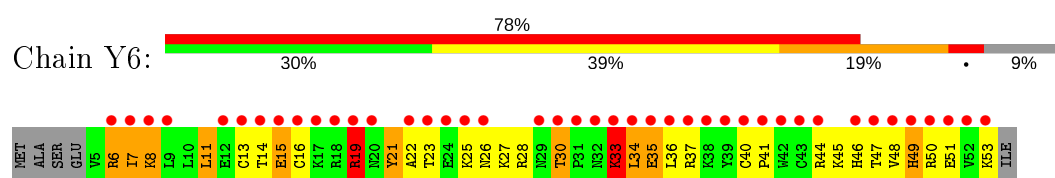
- WORLDWIDE
PDB
PROTEIN DATA BANK



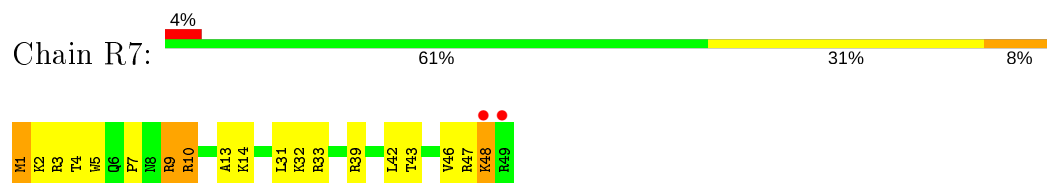
- Molecule 49: 50S ribosomal protein L33



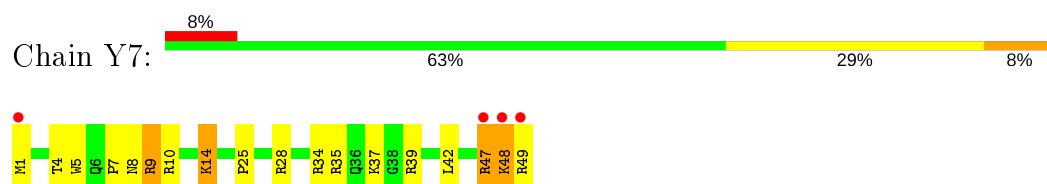
- Molecule 49: 50S ribosomal protein L33



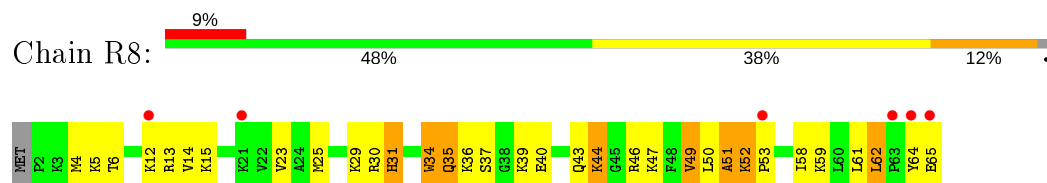
- Molecule 50: 50S ribosomal protein L34



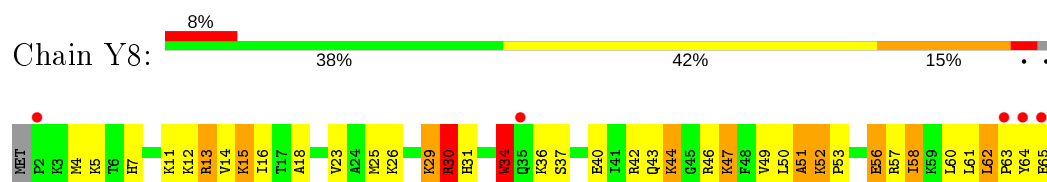
- Molecule 50: 50S ribosomal protein L34



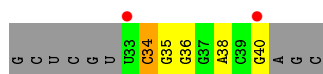
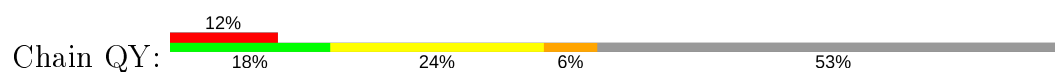
- Molecule 51: 50S ribosomal protein L35



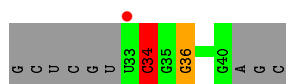
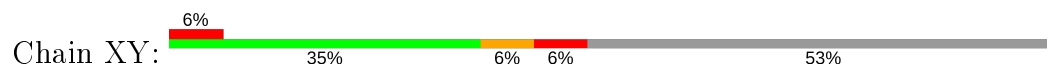
- Molecule 51: 50S ribosomal protein L35



- Molecule 55: A site ASL of tRNA-Proline CGG (unmodified)



- Molecule 55: A site ASL of tRNA-Proline CGG (unmodified)



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.82Å 447.39Å 619.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	187.58 – 3.68 189.96 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.1 (187.58-3.68) 99.2 (189.96-3.54)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.212 , 0.272 0.214 , 0.272	Depositor DCC
R_{free} test set	31728 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	291730	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 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	0.59	3/36098 (0.0%)	1.21	155/56341 (0.3%)
1	XA	0.65	1/36101 (0.0%)	1.27	208/56346 (0.4%)
2	QB	0.31	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.31	0/1629	0.53	0/2195
3	XC	0.37	0/1629	0.56	0/2195
4	QD	0.38	0/1733	0.58	1/2318 (0.0%)
4	XD	0.40	0/1733	0.60	0/2318
5	QE	0.35	0/1171	0.56	0/1576
5	XE	0.39	0/1171	0.59	0/1576
6	QF	0.38	0/856	0.54	0/1154
6	XF	0.38	0/856	0.58	0/1154
7	QG	0.33	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.50	0/1709
8	QH	0.33	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.35	0/814	0.60	0/1095
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.39	0/900	0.58	0/1213
12	QL	0.37	0/991	0.61	0/1327
12	XL	0.45	0/991	0.74	1/1327 (0.1%)
13	QM	0.32	0/974	0.59	0/1303
13	XM	0.37	0/974	0.63	0/1303
14	QN	0.41	0/501	0.60	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	0.31	0/765	0.59	0/1007
21	QU	0.31	0/221	0.54	0/288
21	XU	0.31	0/221	0.62	0/288
22	RA	0.72	8/69521 (0.0%)	1.34	555/108529 (0.5%)
22	YA	0.80	28/69543 (0.0%)	1.43	823/108563 (0.8%)
23	RB	0.58	0/2878	1.22	15/4490 (0.3%)
23	YB	0.63	0/2878	1.28	17/4490 (0.4%)
24	RD	0.51	0/2165	0.70	0/2919
24	YD	0.58	0/2165	0.78	1/2919 (0.0%)
25	RE	0.43	0/1601	0.73	3/2160 (0.1%)
25	YE	0.46	0/1601	0.75	2/2160 (0.1%)
26	RF	0.42	0/1620	0.62	0/2194
26	YF	0.48	0/1620	0.71	1/2194 (0.0%)
27	RG	0.31	0/1499	0.57	1/2016 (0.0%)
27	YG	0.40	0/1499	0.60	0/2016
28	RH	0.29	0/1332	0.58	0/1802
28	YH	0.45	0/1332	0.73	0/1802
29	RI	0.52	0/1151	0.79	1/1558 (0.1%)
29	YI	0.55	0/1151	0.80	0/1558
30	RN	0.41	0/1131	0.62	0/1525
30	YN	0.43	0/1131	0.64	0/1525
31	RO	0.41	0/943	0.62	1/1269 (0.1%)
31	YO	0.50	0/943	0.65	0/1269
32	RP	0.44	0/1162	0.81	1/1544 (0.1%)
32	YP	0.49	0/1162	0.90	2/1544 (0.1%)
33	RQ	0.47	0/1143	0.74	2/1527 (0.1%)
33	YQ	0.57	0/1143	0.80	1/1527 (0.1%)
34	RR	0.42	0/982	0.69	0/1312
34	YR	0.44	0/982	0.73	0/1312
35	RS	0.36	0/892	0.65	0/1187
35	YS	0.40	0/892	0.75	1/1187 (0.1%)
36	RT	0.42	0/1155	0.63	0/1542
36	YT	0.44	0/1155	0.67	0/1542
37	RU	0.40	0/982	0.65	0/1306
37	YU	0.50	0/982	0.68	0/1306
38	RV	0.38	0/790	0.61	1/1057 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YV	0.45	0/790	0.73	1/1057 (0.1%)
39	RW	0.49	0/911	0.67	0/1220
39	YW	0.45	0/911	0.68	0/1220
40	RX	0.47	0/739	0.62	0/993
40	YX	0.49	0/739	0.66	0/993
41	RY	0.44	0/798	0.68	0/1064
41	YY	0.46	0/798	0.70	0/1064
42	RZ	0.58	1/1493 (0.1%)	0.77	0/2026
42	YZ	0.56	0/1493	0.79	1/2026 (0.0%)
43	R0	0.65	0/657	0.80	0/874
43	Y0	0.74	1/657 (0.2%)	0.90	1/874 (0.1%)
44	R1	0.44	0/770	0.66	0/1022
44	Y1	0.46	0/770	0.69	0/1022
45	R2	0.39	0/583	0.65	0/771
45	Y2	0.52	0/583	0.73	0/771
46	R3	0.35	0/474	0.57	0/635
46	Y3	0.41	0/474	0.59	0/635
47	R4	0.33	0/594	0.68	0/795
47	Y4	0.37	0/594	0.68	0/795
48	R5	0.44	0/473	0.73	0/639
48	Y5	0.43	0/473	0.77	1/639 (0.2%)
49	R6	0.35	0/431	0.69	0/575
49	Y6	0.37	0/431	0.67	0/575
50	R7	0.49	0/438	0.68	0/575
50	Y7	0.57	0/438	0.71	0/575
51	R8	0.55	0/525	0.79	0/691
51	Y8	0.58	0/525	0.82	0/691
52	R9	0.26	0/310	0.45	0/407
52	Y9	0.32	0/310	0.48	0/407
53	QV	0.85	1/1836 (0.1%)	1.45	24/2859 (0.8%)
53	XV	0.89	1/1836 (0.1%)	1.54	25/2859 (0.9%)
54	QX	0.95	0/193	1.91	7/299 (2.3%)
54	XX	1.12	0/193	1.83	4/299 (1.3%)
55	QY	0.68	0/194	1.53	0/301
55	XY	0.72	0/194	1.25	1/301 (0.3%)
56	Z6	0.74	0/40	1.58	1/60 (1.7%)
56	Z8	0.92	0/40	1.50	0/60
All	All	0.64	44/316105 (0.0%)	1.20	1861/472575 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	QL	0	1
12	XL	0	1
25	RE	0	1
25	YE	0	1
26	YF	0	1
28	RH	0	2
28	YH	0	2
29	RI	0	1
35	YS	0	1
42	YZ	0	2
45	Y2	0	1
47	R4	0	1
51	R8	0	2
51	Y8	0	2
All	All	0	19

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	QV	1	C	OP3-P	-10.81	1.48	1.61
53	XV	1	C	OP3-P	-10.09	1.49	1.61
22	YA	783	A	N9-C4	-8.12	1.32	1.37
22	YA	2542	A	N9-C4	-7.43	1.33	1.37
22	YA	1966	A	N9-C4	-7.42	1.33	1.37

The worst 5 of 1861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	QV	75	C	O5'-P-OP2	-13.28	93.75	105.70
22	YA	774	A	C2-N3-C4	-12.25	104.47	110.60
22	RA	1931	U	N3-C2-O2	-12.05	113.77	122.20
22	YA	1332	G	C6-C5-N7	-11.94	123.24	130.40
22	YA	450	G	C5-C6-N1	-11.37	105.81	111.50

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
25	RE	21	VAL	Peptide
28	RH	127	GLU	Peptide
28	RH	153	LYS	Peptide

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Mol	Chain	Res	Type	Group
29	RI	134	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	775	0
1	XA	32249	0	16279	824	0
2	QB	1924	0	1975	64	0
2	XB	1924	0	1975	83	0
3	QC	1605	0	1668	50	0
3	XC	1605	0	1668	63	0
4	QD	1703	0	1763	68	0
4	XD	1703	0	1764	48	0
5	QE	1155	0	1213	36	0
5	XE	1155	0	1213	43	0
6	QF	843	0	857	20	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	41	0
7	XG	1257	0	1296	30	0
8	QH	1116	0	1177	40	0
8	XH	1116	0	1177	32	0
9	QI	1010	0	1037	43	0
9	XI	1010	0	1037	60	0
10	QJ	801	0	849	50	0
10	XJ	801	0	849	40	0
11	QK	885	0	904	29	0
11	XK	885	0	904	33	0
12	QL	975	0	1062	43	0
12	XL	975	0	1062	47	0
13	QM	964	0	1034	46	0
13	XM	964	0	1034	62	0
14	QN	492	0	529	27	0
14	XN	492	0	529	23	0
15	QO	734	0	771	23	0
15	XO	734	0	771	22	0
16	QP	705	0	725	21	0
16	XP	705	0	725	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	QQ	834	0	904	26	0
17	XQ	834	0	904	20	0
18	QR	574	0	644	13	0
18	XR	574	0	644	21	0
19	QS	674	0	699	39	0
19	XS	674	0	699	55	0
20	QT	763	0	861	25	0
20	XT	763	0	861	40	0
21	QU	217	0	234	12	0
21	XU	217	0	234	8	0
22	RA	62071	0	31292	1370	0
22	YA	62091	0	31301	1336	1
23	RB	2573	0	1306	57	0
23	YB	2573	0	1306	64	1
24	RD	2115	0	2195	107	0
24	YD	2115	0	2195	106	0
25	RE	1568	0	1634	67	0
25	YE	1568	0	1634	68	0
26	RF	1585	0	1632	76	0
26	YF	1585	0	1632	64	0
27	RG	1474	0	1535	62	0
27	YG	1474	0	1535	69	0
28	RH	1307	0	1382	67	0
28	YH	1307	0	1382	62	0
29	RI	1136	0	1223	84	0
29	YI	1136	0	1223	73	0
30	RN	1104	0	1180	38	0
30	YN	1104	0	1180	51	0
31	RO	933	0	996	23	0
31	YO	933	0	996	25	0
32	RP	1145	0	1227	79	0
32	YP	1145	0	1228	95	0
33	RQ	1122	0	1179	58	0
33	YQ	1122	0	1179	49	0
34	RR	968	0	1033	48	0
34	YR	968	0	1033	37	0
35	RS	882	0	943	45	0
35	YS	882	0	943	43	0
36	RT	1141	0	1202	51	0
36	YT	1141	0	1202	56	0
37	RU	964	0	1022	36	0
37	YU	964	0	1022	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	RV	779	0	852	24	0
38	YV	779	0	852	43	0
39	RW	900	0	964	28	0
39	YW	900	0	964	26	0
40	RX	725	0	778	31	0
40	YX	725	0	778	24	0
41	RY	785	0	878	52	0
41	YY	785	0	878	43	0
42	RZ	1461	0	1493	96	0
42	YZ	1461	0	1493	104	0
43	R0	648	0	671	37	0
43	Y0	648	0	672	41	0
44	R1	763	0	848	32	0
44	Y1	763	0	848	36	0
45	R2	581	0	629	14	0
45	Y2	581	0	629	23	0
46	R3	469	0	518	7	0
46	Y3	469	0	518	15	0
47	R4	581	0	574	30	0
47	Y4	581	0	574	76	0
48	R5	459	0	480	30	0
48	Y5	459	0	480	31	0
49	R6	424	0	450	30	0
49	Y6	424	0	450	29	0
50	R7	430	0	480	17	0
50	Y7	430	0	480	19	0
51	R8	517	0	582	36	0
51	Y8	517	0	582	43	0
52	R9	307	0	338	14	0
52	Y9	307	0	338	17	0
53	QV	1644	0	836	29	0
53	XV	1644	0	836	36	0
54	QX	173	0	88	3	0
54	XX	173	0	88	3	0
55	QY	174	0	88	4	0
55	XY	174	0	88	2	0
56	Z6	74	0	51	0	0
56	Z8	74	0	51	4	0
57	QA	42	0	45	1	0
57	XA	42	0	45	2	0
58	QA	76	0	0	0	0
58	QF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QM	1	0	0	0	0
58	QV	1	0	0	0	0
58	R0	1	0	0	0	0
58	R5	1	0	0	0	0
58	R8	2	0	0	0	0
58	RA	247	0	0	0	0
58	RB	2	0	0	0	0
58	RD	1	0	0	0	0
58	RE	2	0	0	0	0
58	RF	1	0	0	0	0
58	RP	2	0	0	0	0
58	XA	82	0	0	0	0
58	XB	1	0	0	0	0
58	XM	1	0	0	0	0
58	XV	2	0	0	0	0
58	Y0	1	0	0	0	0
58	Y5	1	0	0	0	0
58	YA	265	0	0	0	0
58	YB	3	0	0	0	0
58	YD	2	0	0	0	0
58	YP	2	0	0	0	0
58	YQ	1	0	0	0	0
58	YX	1	0	0	0	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	291730	0	198220	7613	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 7613 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)
22:RA:2701:C:H3'	22:RA:2702:U:H5''	1.27	1.07
1:XA:963:G:N3	10:XJ:55:LYS:NZ	2.02	1.07
24:YD:43:ARG:NH1	24:YD:44:ASN:OD1	1.86	1.06
22:YA:2701:C:H3'	22:YA:2702:U:H5''	1.38	1.05
22:YA:1138:G:H21	30:YN:106:MET:HE3	1.22	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:YA:1593:G:O2'	23:YB:54:G:OP1[1_655]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	174 (74%)	44 (19%)	17 (7%)	1	15
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	18
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	4	32
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	10	44
4	QD	206/209 (99%)	176 (85%)	24 (12%)	6 (3%)	4	32
4	XD	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	6	35
5	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	3	30
5	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	7	39
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	47
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	47
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	22	59
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4	32
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	26
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	4	31
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	4	31
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	21
11	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	42
12	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	1	19
12	XL	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	11
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	13
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	13
14	QN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	15
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	49
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	36
16	QP	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	13	49
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	13	49
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7	39
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	24
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10	44
19	QS	82/93 (88%)	56 (68%)	15 (18%)	11 (13%)	0	4
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	4
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	18
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	1	18
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
24	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	24
24	YD	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	4	31
25	RE	203/206 (98%)	147 (72%)	36 (18%)	20 (10%)	0	8
25	YE	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	0	8
26	RF	200/210 (95%)	167 (84%)	20 (10%)	13 (6%)	1	17
26	YF	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	3	26
27	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	13
27	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	16
28	RH	168/180 (93%)	114 (68%)	33 (20%)	21 (12%)	0	4
28	YH	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	RI	144/148 (97%)	94 (65%)	31 (22%)	19 (13%)	0	4
29	YI	144/148 (97%)	100 (69%)	23 (16%)	21 (15%)	0	3
30	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	10
30	YN	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	7
31	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	42
31	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	9	42
32	RP	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	0	9
32	YP	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	0	5
33	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	4
33	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	3
34	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	24
34	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	21
35	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	8
35	YS	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	0	5
36	RT	135/146 (92%)	106 (78%)	17 (13%)	12 (9%)	1	10
36	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	14
37	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	29
37	YU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	29
38	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	18
38	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	11
39	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3	29
39	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	8	41
40	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	37
40	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6	37
41	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	3
41	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	5
42	RZ	181/206 (88%)	118 (65%)	35 (19%)	28 (16%)	0	3
42	YZ	181/206 (88%)	113 (62%)	46 (25%)	22 (12%)	0	5
43	R0	80/85 (94%)	61 (76%)	15 (19%)	4 (5%)	2	22
43	Y0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	12	47
44	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	18
45	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1	13
45	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	10
46	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	29
46	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	41
47	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	0
47	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
48	R5	57/60 (95%)	44 (77%)	11 (19%)	2 (4%)	3	29
48	Y5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	29
49	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	0
49	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	2
50	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	38
50	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	38
51	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	11
51	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	17
52	R9	35/37 (95%)	35 (100%)	0	0	100	100
52	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	9180 (80%)	1546 (14%)	744 (6%)	1	17

5 of 744 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
13	QM	67	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	172 (84%)	33 (16%)	2	15
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5	24
3	QC	159/188 (85%)	145 (91%)	14 (9%)	10	38
3	XC	159/188 (85%)	146 (92%)	13 (8%)	11	41
4	QD	180/181 (99%)	157 (87%)	23 (13%)	4	22
4	XD	180/181 (99%)	154 (86%)	26 (14%)	3	19
5	QE	116/123 (94%)	104 (90%)	12 (10%)	7	31
5	XE	116/123 (94%)	104 (90%)	12 (10%)	7	31
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4	21
6	XF	90/90 (100%)	82 (91%)	8 (9%)	9	37
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8	34
7	XG	126/127 (99%)	114 (90%)	12 (10%)	8	34
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11	40
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	29
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2	12
9	XI	98/99 (99%)	80 (82%)	18 (18%)	1	10
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	21
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	13
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	32
11	XK	90/99 (91%)	82 (91%)	8 (9%)	9	37
12	QL	104/109 (95%)	87 (84%)	17 (16%)	2	15
12	XL	104/109 (95%)	93 (89%)	11 (11%)	6	30
13	QM	97/101 (96%)	73 (75%)	24 (25%)	0	5
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	9
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	19
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	37
15	XO	79/80 (99%)	69 (87%)	10 (13%)	4	23
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	23
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	23
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	11	40
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	50 (82%)	11 (18%)	1	11
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	18
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	26
20	XT	76/82 (93%)	66 (87%)	10 (13%)	4	21
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	55
24	RD	214/218 (98%)	174 (81%)	40 (19%)	1	10
24	YD	214/218 (98%)	181 (85%)	33 (15%)	2	17
25	RE	165/166 (99%)	126 (76%)	39 (24%)	1	5
25	YE	165/166 (99%)	137 (83%)	28 (17%)	2	13
26	RF	161/166 (97%)	132 (82%)	29 (18%)	1	11
26	YF	161/166 (97%)	137 (85%)	24 (15%)	3	18
27	RG	155/156 (99%)	134 (86%)	21 (14%)	4	21
27	YG	155/156 (99%)	133 (86%)	22 (14%)	3	19
28	RH	142/148 (96%)	120 (84%)	22 (16%)	2	17
28	YH	142/148 (96%)	117 (82%)	25 (18%)	2	12
29	RI	122/124 (98%)	86 (70%)	36 (30%)	0	2
29	YI	122/124 (98%)	85 (70%)	37 (30%)	0	2
30	RN	117/119 (98%)	97 (83%)	20 (17%)	2	13
30	YN	117/119 (98%)	96 (82%)	21 (18%)	2	11
31	RO	100/100 (100%)	90 (90%)	10 (10%)	7	32
31	YO	100/100 (100%)	88 (88%)	12 (12%)	5	25
32	RP	116/116 (100%)	85 (73%)	31 (27%)	0	3
32	YP	116/116 (100%)	82 (71%)	34 (29%)	0	2
33	RQ	111/111 (100%)	95 (86%)	16 (14%)	3	19
33	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	13
34	RR	101/101 (100%)	83 (82%)	18 (18%)	2	11
34	YR	101/101 (100%)	81 (80%)	20 (20%)	1	8
35	RS	87/88 (99%)	69 (79%)	18 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	YS	87/88 (99%)	68 (78%)	19 (22%)	1	7
36	RT	120/127 (94%)	102 (85%)	18 (15%)	3	17
36	YT	120/127 (94%)	98 (82%)	22 (18%)	1	10
37	RU	93/94 (99%)	78 (84%)	15 (16%)	2	15
37	YU	93/94 (99%)	77 (83%)	16 (17%)	2	13
38	RV	82/82 (100%)	66 (80%)	16 (20%)	1	9
38	YV	82/82 (100%)	67 (82%)	15 (18%)	1	10
39	RW	92/92 (100%)	73 (79%)	19 (21%)	1	7
39	YW	92/92 (100%)	76 (83%)	16 (17%)	2	12
40	RX	74/78 (95%)	64 (86%)	10 (14%)	4	21
40	YX	74/78 (95%)	60 (81%)	14 (19%)	1	9
41	RY	85/91 (93%)	63 (74%)	22 (26%)	0	4
41	YY	85/91 (93%)	64 (75%)	21 (25%)	0	5
42	RZ	162/179 (90%)	131 (81%)	31 (19%)	1	9
42	YZ	162/179 (90%)	121 (75%)	41 (25%)	0	4
43	R0	65/67 (97%)	56 (86%)	9 (14%)	3	20
43	Y0	65/67 (97%)	53 (82%)	12 (18%)	1	10
44	R1	82/83 (99%)	73 (89%)	9 (11%)	6	29
44	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	18
45	R2	64/67 (96%)	57 (89%)	7 (11%)	6	29
45	Y2	64/67 (96%)	47 (73%)	17 (27%)	0	3
46	R3	51/52 (98%)	45 (88%)	6 (12%)	5	26
46	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	16
47	R4	63/63 (100%)	45 (71%)	18 (29%)	0	2
47	Y4	63/63 (100%)	43 (68%)	20 (32%)	0	1
48	R5	51/52 (98%)	37 (72%)	14 (28%)	0	3
48	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	3
49	R6	48/52 (92%)	35 (73%)	13 (27%)	0	3
49	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
50	R7	42/42 (100%)	34 (81%)	8 (19%)	1	9
50	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	R8	54/55 (98%)	44 (82%)	10 (18%)	1	10
51	Y8	54/55 (98%)	41 (76%)	13 (24%)	0	5
52	R9	34/34 (100%)	32 (94%)	2 (6%)	19	51
52	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	51
All	All	9702/10066 (96%)	8111 (84%)	1591 (16%)	2	15

5 of 1591 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	R3	8	LEU
8	XH	41	ARG
42	YZ	153	SER
47	R4	67	TYR
2	XB	178	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
28	RH	147	ASN
29	RI	104	GLN
2	XB	204	ASN
25	RE	143	ASN
28	RH	143	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	341 (22%)	49 (3%)
1	XA	1498/1522 (98%)	352 (23%)	40 (2%)
22	RA	2879/2916 (98%)	747 (25%)	65 (2%)
22	YA	2880/2916 (98%)	734 (25%)	57 (1%)
23	RB	119/122 (97%)	29 (24%)	2 (1%)
23	YB	119/122 (97%)	32 (26%)	1 (0%)
53	QV	76/77 (98%)	22 (28%)	1 (1%)
53	XV	76/77 (98%)	24 (31%)	3 (3%)
54	QX	7/25 (28%)	4 (57%)	1 (14%)
54	XX	7/25 (28%)	3 (42%)	1 (14%)
55	QY	7/17 (41%)	3 (42%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	XY	7/17 (41%)	2 (28%)	0
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9175/9364 (97%)	2293 (24%)	220 (2%)

5 of 2293 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	7	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 220 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	RA	2351	G
1	XA	244	U
22	YA	2422	A
22	RA	2439	A
22	RA	2776	A

5.4 Non-standard residues in protein, DNA, RNA chains

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	76	56,22	32,40,41	1.02	1 (3%)	33,57,60	2.06	10 (30%)
56	PPU	Z8	76	56,22	32,40,41	1.04	3 (9%)	33,57,60	1.67	8 (24%)

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	76	56,22	-	3/21/43/44	0/4/4/4
56	PPU	Z8	76	56,22	-	1/21/43/44	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	C2'-C3'	-2.48	1.49	1.53
56	Z6	76	PPU	C5-C4	2.41	1.47	1.40
56	Z8	76	PPU	C5-C4	2.15	1.46	1.40
56	Z8	76	PPU	C4-N3	-2.11	1.32	1.35

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-5.98	114.20	123.21
56	Z6	76	PPU	N1-C6-N6	4.60	121.89	117.06
56	Z8	76	PPU	N1-C6-N6	4.54	121.83	117.06
56	Z6	76	PPU	C10-N6-C6	-3.29	109.56	119.51
56	Z6	76	PPU	CM-OC-CZ	3.24	124.55	117.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z6	76	PPU	CE1-CZ-OC-CM
56	Z6	76	PPU	CE2-CZ-OC-CM
56	Z8	76	PPU	C5-C6-N6-C9
56	Z6	76	PPU	C5-C6-N6-C9

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	4	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 706 ligands modelled in this entry, 704 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PAR	QA	1601	-	45,45,45	1.47	7 (15%)	64,67,67	1.38	9 (14%)
57	PAR	XA	1601	-	45,45,45	1.50	6 (13%)	64,67,67	1.34	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	QA	1601	-	-	8/18/94/94	0/4/4/4
57	PAR	XA	1601	-	-	6/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	QA	1601	PAR	C64-C54	5.14	1.59	1.52
57	XA	1601	PAR	C64-C54	4.91	1.58	1.52
57	QA	1601	PAR	C52-C42	3.16	1.58	1.52
57	QA	1601	PAR	O54-C14	2.86	1.49	1.41
57	XA	1601	PAR	O54-C14	2.85	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	XA	1601	PAR	O33-C14-C24	4.73	116.37	108.22
57	XA	1601	PAR	C14-O54-C54	4.30	122.13	113.69
57	QA	1601	PAR	O52-C13-C23	3.82	115.89	107.96
57	QA	1601	PAR	C14-O54-C54	3.79	121.13	113.69
57	QA	1601	PAR	O33-C14-C24	3.76	114.69	108.22

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

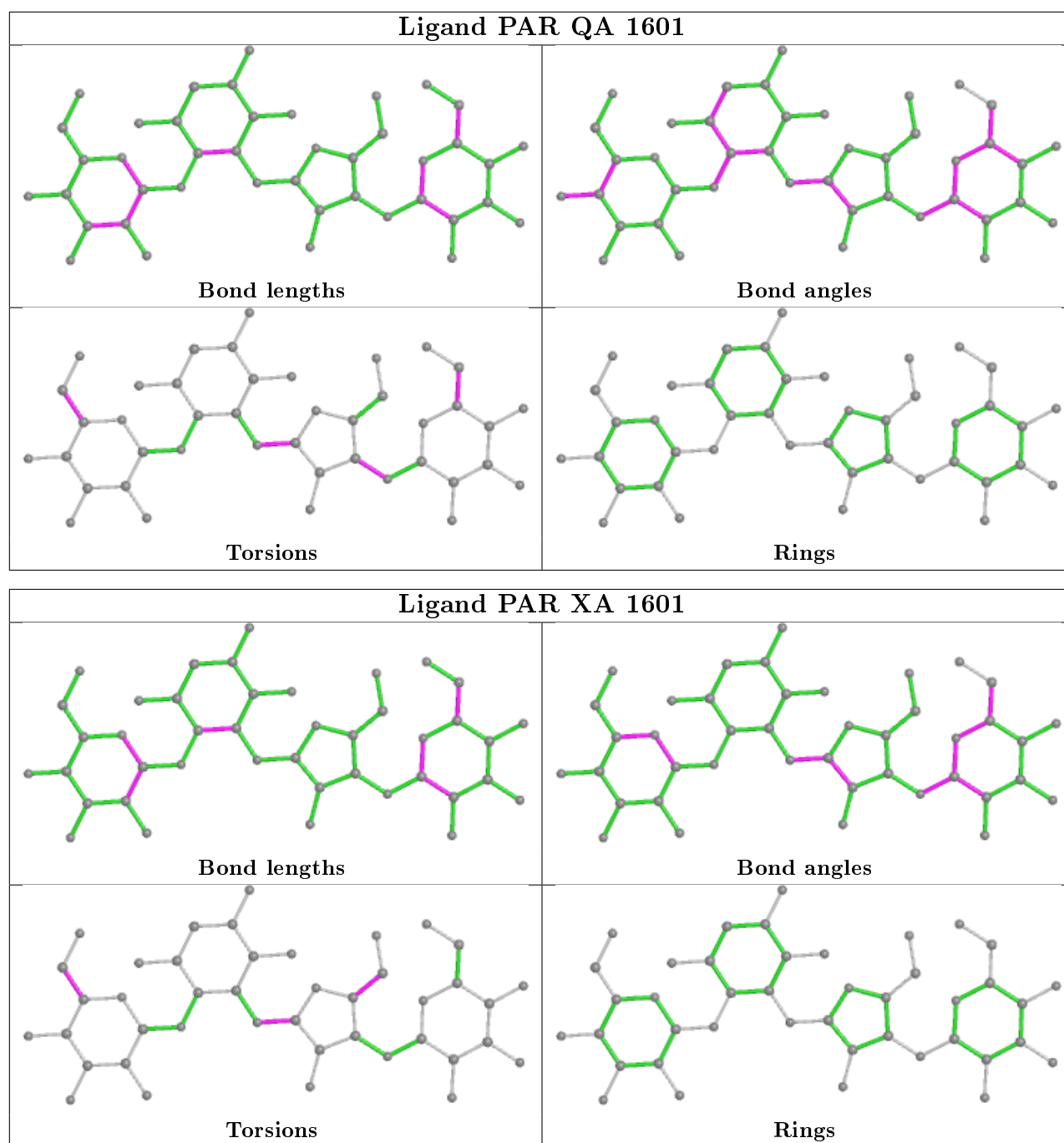
Mol	Chain	Res	Type	Atoms
57	QA	1601	PAR	C44-C54-C64-N64
57	QA	1601	PAR	O54-C54-C64-N64
57	XA	1601	PAR	O51-C51-C61-O61
57	QA	1601	PAR	O51-C51-C61-O61
57	XA	1601	PAR	C41-C51-C61-O61

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QA	1601	PAR	1	0
57	XA	1601	PAR	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.42	75 (5%) 28 20	28, 70, 146, 264	0
1	XA	1500/1522 (98%)	0.54	83 (5%) 25 17	18, 64, 151, 247	0
2	QB	237/256 (92%)	0.13	9 (3%) 40 28	48, 115, 166, 191	0
2	XB	237/256 (92%)	-0.23	1 (0%) 92 88	35, 98, 150, 194	0
3	QC	205/239 (85%)	0.52	10 (4%) 29 21	45, 105, 149, 166	0
3	XC	205/239 (85%)	0.15	2 (0%) 82 72	35, 78, 130, 168	0
4	QD	208/209 (99%)	0.46	10 (4%) 30 21	27, 79, 119, 169	0
4	XD	208/209 (99%)	0.30	4 (1%) 66 54	34, 75, 127, 151	0
5	QE	151/162 (93%)	0.45	7 (4%) 32 22	37, 88, 135, 167	0
5	XE	151/162 (93%)	0.29	3 (1%) 65 52	29, 65, 115, 148	0
6	QF	101/101 (100%)	-0.20	1 (0%) 82 72	21, 76, 112, 185	0
6	XF	101/101 (100%)	0.21	0 100 100	32, 72, 115, 153	0
7	QG	155/156 (99%)	0.57	22 (14%) 2 2	46, 96, 152, 185	0
7	XG	155/156 (99%)	0.31	9 (5%) 23 15	40, 87, 145, 167	0
8	QH	138/138 (100%)	0.29	2 (1%) 75 63	41, 90, 125, 153	0
8	XH	138/138 (100%)	0.27	3 (2%) 62 48	33, 72, 108, 149	0
9	QI	127/128 (99%)	1.38	35 (27%) 0 0	67, 109, 148, 172	0
9	XI	127/128 (99%)	0.65	15 (11%) 4 4	28, 99, 147, 164	0
10	QJ	99/105 (94%)	0.96	16 (16%) 1 1	59, 114, 165, 205	0
10	XJ	99/105 (94%)	0.90	16 (16%) 1 1	41, 103, 147, 171	0
11	QK	119/129 (92%)	0.54	7 (5%) 22 15	35, 79, 130, 177	0
11	XK	119/129 (92%)	0.68	6 (5%) 28 20	24, 71, 125, 182	0
12	QL	125/132 (94%)	1.06	15 (12%) 4 3	30, 70, 120, 182	0
12	XL	125/132 (94%)	0.91	23 (18%) 1 1	15, 58, 120, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	1.20	30 (24%) 0 0	36, 106, 144, 196	0
13	XM	121/126 (96%)	0.53	11 (9%) 9 6	38, 88, 137, 187	0
14	QN	60/61 (98%)	2.07	30 (50%) 0 0	58, 97, 124, 142	0
14	XN	60/61 (98%)	1.09	9 (15%) 2 1	34, 75, 109, 125	0
15	QO	88/89 (98%)	0.01	0 100 100	30, 79, 123, 154	0
15	XO	88/89 (98%)	0.25	1 (1%) 80 70	28, 73, 108, 124	0
16	QP	84/88 (95%)	0.44	1 (1%) 79 68	35, 69, 107, 152	0
16	XP	84/88 (95%)	1.14	20 (23%) 0 0	34, 74, 129, 163	0
17	QQ	100/105 (95%)	1.01	14 (14%) 2 2	24, 83, 122, 140	0
17	XQ	100/105 (95%)	0.98	14 (14%) 2 2	39, 78, 113, 165	0
18	QR	70/88 (79%)	0.06	1 (1%) 75 63	26, 78, 137, 167	0
18	XR	70/88 (79%)	0.31	3 (4%) 35 25	24, 70, 120, 147	0
19	QS	84/93 (90%)	1.71	32 (38%) 0 0	68, 111, 151, 176	0
19	XS	84/93 (90%)	0.60	8 (9%) 8 5	32, 97, 148, 177	0
20	QT	99/106 (93%)	0.91	9 (9%) 9 6	34, 79, 133, 144	0
20	XT	99/106 (93%)	1.63	34 (34%) 0 0	44, 88, 140, 174	0
21	QU	25/27 (92%)	3.33	20 (80%) 0 0	36, 102, 144, 147	0
21	XU	25/27 (92%)	2.34	15 (60%) 0 0	67, 92, 119, 132	0
22	RA	2882/2916 (98%)	0.47	145 (5%) 28 20	14, 51, 198, 261	0
22	YA	2883/2916 (98%)	0.42	106 (3%) 41 29	8, 43, 187, 292	0
23	RB	120/122 (98%)	-0.05	1 (0%) 86 77	53, 81, 118, 144	0
23	YB	120/122 (98%)	-0.03	1 (0%) 86 77	36, 67, 98, 136	0
24	RD	272/276 (98%)	0.34	4 (1%) 73 62	9, 50, 100, 155	0
24	YD	272/276 (98%)	0.60	5 (1%) 68 56	2, 42, 86, 187	0
25	RE	205/206 (99%)	0.37	7 (3%) 45 33	17, 61, 126, 193	0
25	YE	205/206 (99%)	0.19	2 (0%) 82 72	3, 56, 124, 170	0
26	RF	202/210 (96%)	-0.04	0 100 100	9, 61, 124, 182	0
26	YF	202/210 (96%)	0.01	1 (0%) 91 85	10, 53, 113, 148	0
27	RG	181/182 (99%)	0.49	9 (4%) 28 20	42, 97, 145, 178	0
27	YG	181/182 (99%)	0.12	4 (2%) 62 48	40, 80, 130, 201	0
28	RH	170/180 (94%)	1.84	67 (39%) 0 0	67, 134, 177, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YH	170/180 (94%)	-0.05	1 (0%) 89 83	24, 76, 126, 177	0
29	RI	146/148 (98%)	0.05	3 (2%) 63 50	24, 87, 130, 181	0
29	YI	146/148 (98%)	-0.04	3 (2%) 63 50	19, 86, 127, 152	0
30	RN	138/140 (98%)	0.44	7 (5%) 28 19	29, 68, 121, 174	0
30	YN	138/140 (98%)	0.11	0 100 100	13, 56, 111, 173	0
31	RO	122/122 (100%)	0.53	3 (2%) 57 43	11, 55, 102, 158	0
31	YO	122/122 (100%)	0.90	11 (9%) 9 6	9, 51, 88, 123	0
32	RP	150/150 (100%)	0.63	11 (7%) 15 10	13, 69, 133, 176	0
32	YP	150/150 (100%)	0.41	5 (3%) 46 34	12, 61, 122, 182	0
33	RQ	141/141 (100%)	1.22	29 (20%) 1 0	29, 71, 124, 164	0
33	YQ	141/141 (100%)	0.43	4 (2%) 53 39	16, 56, 115, 152	0
34	RR	118/118 (100%)	0.43	4 (3%) 45 33	3, 55, 102, 136	0
34	YR	118/118 (100%)	0.77	5 (4%) 36 25	27, 57, 95, 140	0
35	RS	111/112 (99%)	0.66	10 (9%) 9 6	34, 80, 124, 162	0
35	YS	111/112 (99%)	0.17	2 (1%) 68 56	27, 73, 113, 138	0
36	RT	137/146 (93%)	0.53	7 (5%) 28 19	27, 67, 143, 169	0
36	YT	137/146 (93%)	0.53	4 (2%) 51 38	19, 65, 135, 172	0
37	RU	117/118 (99%)	0.21	2 (1%) 70 58	12, 62, 111, 167	0
37	YU	117/118 (99%)	0.36	2 (1%) 70 58	13, 45, 111, 172	0
38	RV	101/101 (100%)	0.03	2 (1%) 65 52	16, 78, 131, 186	0
38	YV	101/101 (100%)	0.34	3 (2%) 50 36	21, 68, 139, 214	0
39	RW	113/113 (100%)	0.29	1 (0%) 84 75	15, 47, 106, 158	0
39	YW	113/113 (100%)	0.27	2 (1%) 68 56	16, 46, 106, 168	0
40	RX	92/96 (95%)	0.34	0 100 100	17, 56, 103, 130	0
40	YX	92/96 (95%)	0.10	0 100 100	9, 42, 86, 138	0
41	RY	102/110 (92%)	0.41	1 (0%) 82 72	28, 86, 142, 176	0
41	YY	102/110 (92%)	0.09	1 (0%) 82 72	30, 73, 138, 185	0
42	RZ	183/206 (88%)	0.42	12 (6%) 18 11	45, 92, 141, 160	0
42	YZ	183/206 (88%)	-0.18	1 (0%) 91 85	21, 82, 136, 178	0
43	R0	82/85 (96%)	0.97	7 (8%) 10 8	9, 51, 88, 102	0
43	Y0	82/85 (96%)	0.34	0 100 100	20, 48, 73, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	R1	97/98 (98%)	0.82	6 (6%) 20 13	13, 60, 144, 182	0
44	Y1	97/98 (98%)	1.05	11 (11%) 5 4	7, 53, 136, 172	0
45	R2	69/72 (95%)	-0.06	0 100 100	36, 77, 136, 164	0
45	Y2	69/72 (95%)	-0.06	0 100 100	18, 57, 116, 159	0
46	R3	59/60 (98%)	0.80	2 (3%) 45 33	33, 76, 118, 142	0
46	Y3	59/60 (98%)	0.03	1 (1%) 70 58	19, 57, 109, 169	0
47	R4	71/71 (100%)	0.87	12 (16%) 1 1	61, 142, 196, 236	0
47	Y4	71/71 (100%)	0.14	5 (7%) 16 10	58, 131, 182, 223	0
48	R5	59/60 (98%)	0.42	2 (3%) 45 33	12, 66, 149, 160	0
48	Y5	59/60 (98%)	0.85	8 (13%) 3 2	17, 64, 166, 185	0
49	R6	49/54 (90%)	4.49	44 (89%) 0 0	101, 159, 184, 200	0
49	Y6	49/54 (90%)	3.64	42 (85%) 0 0	95, 152, 182, 209	0
50	R7	49/49 (100%)	0.39	2 (4%) 37 26	11, 41, 95, 153	0
50	Y7	49/49 (100%)	0.42	4 (8%) 11 8	6, 33, 78, 135	0
51	R8	64/65 (98%)	0.83	6 (9%) 8 5	18, 59, 121, 163	0
51	Y8	64/65 (98%)	0.74	5 (7%) 13 9	16, 52, 108, 164	0
52	R9	37/37 (100%)	8.37	37 (100%) 0 0	92, 141, 184, 204	0
52	Y9	37/37 (100%)	5.96	37 (100%) 0 0	102, 132, 168, 182	0
53	QV	77/77 (100%)	-0.12	1 (1%) 77 66	35, 82, 137, 160	0
53	XV	77/77 (100%)	-0.07	1 (1%) 77 66	11, 71, 111, 159	0
54	QX	8/25 (32%)	0.84	0 100 100	44, 56, 107, 137	0
54	XX	8/25 (32%)	1.20	2 (25%) 0 0	37, 46, 104, 148	0
55	QY	8/17 (47%)	1.51	2 (25%) 0 0	62, 74, 124, 144	0
55	XY	8/17 (47%)	0.50	1 (12%) 3 3	54, 71, 109, 122	0
56	Z6	2/3 (66%)	0.82	0 100 100	45, 45, 45, 52	0
56	Z8	2/3 (66%)	1.45	0 100 100	30, 30, 30, 32	0
All	All	20861/21492 (97%)	0.50	1352 (6%) 18 12	2, 66, 150, 292	0

The worst 5 of 1352 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R9	11	CYS	18.9
52	R9	37	GLY	15.5

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Mol	Chain	Res	Type	RSRZ
52	R9	14	CYS	14.9
52	Y9	1	MET	14.0
52	R9	36	GLN	14.0

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	Z6	76	37/38	0.96	0.40	37,37,37,37	0
56	PPU	Z8	76	37/38	0.96	0.41	30,30,30,30	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
58	MG	RA	3227	1/1	0.32	0.47	60,60,60,60	0
58	MG	RA	3212	1/1	0.57	0.75	73,73,73,73	0
58	MG	XM	201	1/1	0.58	0.35	98,98,98,98	0
58	MG	RA	3221	1/1	0.60	0.23	30,30,30,30	0
58	MG	QA	1667	1/1	0.66	0.24	35,35,35,35	0
58	MG	YA	3214	1/1	0.66	0.68	50,50,50,50	0
58	MG	YA	3170	1/1	0.67	0.33	33,33,33,33	0
58	MG	RA	3157	1/1	0.67	0.38	37,37,37,37	0
58	MG	RA	3234	1/1	0.68	0.33	69,69,69,69	0
58	MG	YA	3205	1/1	0.70	0.37	62,62,62,62	0
58	MG	RA	3204	1/1	0.71	0.24	50,50,50,50	0
58	MG	RA	3209	1/1	0.73	0.25	47,47,47,47	0
58	MG	RA	3182	1/1	0.73	0.39	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	RA	3144	1/1	0.73	0.33	32,32,32,32	0
58	MG	QA	1621	1/1	0.73	0.21	38,38,38,38	0
58	MG	RA	3225	1/1	0.74	0.39	33,33,33,33	0
58	MG	YA	3263	1/1	0.74	0.26	40,40,40,40	0
58	MG	YA	3174	1/1	0.75	0.12	10,10,10,10	0
58	MG	RA	3143	1/1	0.76	0.14	5,5,5,5	0
58	MG	RA	3002	1/1	0.76	0.46	30,30,30,30	0
58	MG	YA	3182	1/1	0.76	0.24	3,3,3,3	0
58	MG	RA	3138	1/1	0.76	0.28	38,38,38,38	0
58	MG	YA	3169	1/1	0.76	0.15	16,16,16,16	0
58	MG	QA	1604	1/1	0.76	0.25	5,5,5,5	0
58	MG	XA	1679	1/1	0.77	0.18	18,18,18,18	0
58	MG	RA	3067	1/1	0.77	0.94	74,74,74,74	0
58	MG	RA	3013	1/1	0.77	0.27	29,29,29,29	0
58	MG	RA	3171	1/1	0.77	0.29	31,31,31,31	0
58	MG	YA	3144	1/1	0.77	0.15	6,6,6,6	0
58	MG	YA	3126	1/1	0.78	0.15	0,0,0,0	0
58	MG	YA	3130	1/1	0.78	0.25	21,21,21,21	0
58	MG	RA	3164	1/1	0.78	0.30	45,45,45,45	0
58	MG	YA	3203	1/1	0.78	0.18	18,18,18,18	0
58	MG	RA	3196	1/1	0.78	0.26	63,63,63,63	0
58	MG	RA	3247	1/1	0.78	0.30	9,9,9,9	0
58	MG	YA	3254	1/1	0.79	0.29	16,16,16,16	0
58	MG	RA	3233	1/1	0.79	0.22	42,42,42,42	0
58	MG	Y0	101	1/1	0.79	0.42	74,74,74,74	0
58	MG	XA	1650	1/1	0.79	0.21	14,14,14,14	0
58	MG	XA	1680	1/1	0.79	0.31	45,45,45,45	0
58	MG	YA	3018	1/1	0.79	0.77	74,74,74,74	0
58	MG	YA	3116	1/1	0.80	0.22	14,14,14,14	0
58	MG	RA	3126	1/1	0.80	0.22	16,16,16,16	0
58	MG	YA	3222	1/1	0.81	0.19	13,13,13,13	0
58	MG	YA	3179	1/1	0.81	0.23	26,26,26,26	0
58	MG	RA	3232	1/1	0.81	0.11	15,15,15,15	0
58	MG	RA	3229	1/1	0.81	0.24	23,23,23,23	0
58	MG	RA	3006	1/1	0.81	0.41	10,10,10,10	0
58	MG	RA	3056	1/1	0.81	0.54	74,74,74,74	0
58	MG	QA	1603	1/1	0.81	0.23	11,11,11,11	0
58	MG	YA	3164	1/1	0.81	0.39	44,44,44,44	0
58	MG	YA	3228	1/1	0.81	0.14	9,9,9,9	0
58	MG	XA	1635	1/1	0.82	0.17	26,26,26,26	0
58	MG	QA	1677	1/1	0.83	0.19	47,47,47,47	0
58	MG	YA	3132	1/1	0.83	0.17	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	RA	3201	1/1	0.83	0.25	34,34,34,34	0
58	MG	YA	3080	1/1	0.83	0.56	74,74,74,74	0
58	MG	XA	1632	1/1	0.83	0.14	9,9,9,9	0
58	MG	XA	1667	1/1	0.83	0.21	34,34,34,34	0
58	MG	YA	3165	1/1	0.83	0.22	1,1,1,1	0
58	MG	RA	3004	1/1	0.83	0.43	40,40,40,40	0
58	MG	YA	3236	1/1	0.83	0.22	18,18,18,18	0
58	MG	RA	3105	1/1	0.83	0.15	14,14,14,14	0
58	MG	YA	3151	1/1	0.83	0.21	3,3,3,3	0
58	MG	YA	3250	1/1	0.84	0.33	15,15,15,15	0
58	MG	RA	3203	1/1	0.84	0.18	15,15,15,15	0
58	MG	XA	1630	1/1	0.84	0.16	15,15,15,15	0
58	MG	YA	3259	1/1	0.84	0.28	5,5,5,5	0
58	MG	YA	3233	1/1	0.84	0.22	34,34,34,34	0
58	MG	YA	3218	1/1	0.84	0.82	59,59,59,59	0
58	MG	RA	3183	1/1	0.84	0.29	11,11,11,11	0
58	MG	YA	3133	1/1	0.84	0.25	32,32,32,32	0
58	MG	YA	3155	1/1	0.84	0.25	45,45,45,45	0
58	MG	XA	1681	1/1	0.84	0.20	31,31,31,31	0
58	MG	RA	3161	1/1	0.85	0.23	10,10,10,10	0
58	MG	RA	3220	1/1	0.85	0.15	13,13,13,13	0
58	MG	YD	301	1/1	0.85	0.46	74,74,74,74	0
58	MG	YA	3246	1/1	0.85	0.22	0,0,0,0	0
58	MG	XA	1602	1/1	0.85	0.23	15,15,15,15	0
58	MG	YA	3249	1/1	0.85	0.33	20,20,20,20	0
58	MG	YA	3099	1/1	0.85	0.58	74,74,74,74	0
58	MG	YA	3207	1/1	0.85	0.34	55,55,55,55	0
58	MG	RA	3228	1/1	0.85	0.16	13,13,13,13	0
58	MG	YA	3234	1/1	0.85	0.21	17,17,17,17	0
58	MG	RA	3005	1/1	0.86	0.22	24,24,24,24	0
58	MG	XA	1651	1/1	0.86	0.28	33,33,33,33	0
58	MG	YA	3183	1/1	0.86	0.12	19,19,19,19	0
58	MG	RA	3177	1/1	0.86	0.35	15,15,15,15	0
58	MG	XA	1658	1/1	0.86	0.14	3,3,3,3	0
58	MG	RA	3130	1/1	0.86	0.20	15,15,15,15	0
58	MG	XA	1656	1/1	0.86	0.20	17,17,17,17	0
58	MG	XA	1628	1/1	0.86	0.14	18,18,18,18	0
58	MG	YA	3105	1/1	0.86	0.19	19,19,19,19	0
58	MG	QA	1672	1/1	0.86	0.32	19,19,19,19	0
58	MG	YA	3248	1/1	0.86	0.20	8,8,8,8	0
58	MG	RA	3074	1/1	0.86	0.20	6,6,6,6	0
58	MG	RA	3205	1/1	0.86	0.46	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	YA	3162	1/1	0.86	0.35	11,11,11,11	0
58	MG	YA	3118	1/1	0.86	0.35	8,8,8,8	0
58	MG	YA	3014	1/1	0.87	0.46	74,74,74,74	0
58	MG	XA	1646	1/1	0.87	0.14	21,21,21,21	0
58	MG	YA	3191	1/1	0.87	0.28	9,9,9,9	0
58	MG	YA	3217	1/1	0.87	0.13	18,18,18,18	0
58	MG	RA	3243	1/1	0.87	0.26	1,1,1,1	0
58	MG	QA	1675	1/1	0.87	0.26	32,32,32,32	0
58	MG	QA	1671	1/1	0.87	0.16	6,6,6,6	0
58	MG	RA	3159	1/1	0.87	0.12	23,23,23,23	0
58	MG	RA	3188	1/1	0.87	0.48	48,48,48,48	0
58	MG	QA	1645	1/1	0.87	0.29	4,4,4,4	0
58	MG	YA	3245	1/1	0.87	0.18	33,33,33,33	0
58	MG	YA	3120	1/1	0.87	0.29	46,46,46,46	0
58	MG	QA	1664	1/1	0.87	0.16	56,56,56,56	0
58	MG	RA	3199	1/1	0.87	0.78	63,63,63,63	0
58	MG	YA	3208	1/1	0.87	0.41	35,35,35,35	0
58	MG	XA	1672	1/1	0.87	0.19	16,16,16,16	0
58	MG	QA	1653	1/1	0.87	0.17	0,0,0,0	0
58	MG	YA	3181	1/1	0.87	0.26	0,0,0,0	0
58	MG	YA	3184	1/1	0.87	0.20	23,23,23,23	0
58	MG	YA	3216	1/1	0.87	0.34	55,55,55,55	0
58	MG	YA	3145	1/1	0.87	0.20	20,20,20,20	0
58	MG	RA	3158	1/1	0.87	0.22	15,15,15,15	0
58	MG	YA	3244	1/1	0.88	0.25	0,0,0,0	0
58	MG	YQ	201	1/1	0.88	0.11	90,90,90,90	0
58	MG	RA	3216	1/1	0.88	0.28	2,2,2,2	0
58	MG	YA	3187	1/1	0.88	0.29	41,41,41,41	0
58	MG	XA	1663	1/1	0.88	0.21	32,32,32,32	0
58	MG	YA	3102	1/1	0.88	0.10	8,8,8,8	0
58	MG	YA	3156	1/1	0.88	0.57	29,29,29,29	0
58	MG	YB	202	1/1	0.88	0.34	19,19,19,19	0
58	MG	RA	3235	1/1	0.88	0.47	74,74,74,74	0
58	MG	XA	1636	1/1	0.88	0.18	8,8,8,8	0
58	MG	YA	3223	1/1	0.88	0.21	34,34,34,34	0
58	MG	QA	1674	1/1	0.88	0.18	8,8,8,8	0
58	MG	RA	3193	1/1	0.88	0.23	47,47,47,47	0
58	MG	YA	3200	1/1	0.88	0.15	6,6,6,6	0
58	MG	YA	3013	1/1	0.88	0.32	3,3,3,3	0
58	MG	RA	3172	1/1	0.88	0.24	42,42,42,42	0
58	MG	YA	3247	1/1	0.88	0.49	34,34,34,34	0
58	MG	XB	301	1/1	0.88	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	XA	1682	1/1	0.88	0.20	35,35,35,35	0
58	MG	YA	3041	1/1	0.88	0.56	74,74,74,74	0
58	MG	XA	1621	1/1	0.89	0.10	19,19,19,19	0
58	MG	RA	3214	1/1	0.89	0.26	24,24,24,24	0
58	MG	RA	3154	1/1	0.89	0.20	59,59,59,59	0
58	MG	YA	3127	1/1	0.89	0.30	23,23,23,23	0
58	MG	QA	1660	1/1	0.89	0.10	36,36,36,36	0
58	MG	YA	3075	1/1	0.89	0.15	12,12,12,12	0
58	MG	RA	3124	1/1	0.89	0.16	2,2,2,2	0
58	MG	RA	3073	1/1	0.89	0.21	10,10,10,10	0
58	MG	RA	3014	1/1	0.89	0.19	28,28,28,28	0
58	MG	YA	3262	1/1	0.89	0.23	26,26,26,26	0
58	MG	RA	3120	1/1	0.89	0.18	4,4,4,4	0
58	MG	RA	3223	1/1	0.89	0.32	54,54,54,54	0
58	MG	YA	3199	1/1	0.89	0.25	12,12,12,12	0
58	MG	YA	3163	1/1	0.89	0.29	21,21,21,21	0
58	MG	YB	201	1/1	0.89	0.25	33,33,33,33	0
58	MG	XA	1639	1/1	0.89	0.21	45,45,45,45	0
58	MG	RA	3202	1/1	0.89	0.30	0,0,0,0	0
58	MG	RA	3207	1/1	0.89	0.20	7,7,7,7	0
58	MG	YA	3150	1/1	0.89	0.30	16,16,16,16	0
58	MG	YA	3226	1/1	0.89	0.14	11,11,11,11	0
58	MG	RF	301	1/1	0.89	0.22	13,13,13,13	0
58	MG	QA	1640	1/1	0.89	0.27	13,13,13,13	0
58	MG	YA	3256	1/1	0.89	0.60	74,74,74,74	0
58	MG	RA	3148	1/1	0.89	0.39	47,47,47,47	0
58	MG	YA	3173	1/1	0.89	0.25	15,15,15,15	0
58	MG	QA	1632	1/1	0.89	0.17	42,42,42,42	0
58	MG	QA	1643	1/1	0.89	0.23	21,21,21,21	0
58	MG	YD	302	1/1	0.89	0.21	5,5,5,5	0
58	MG	XA	1676	1/1	0.89	0.34	19,19,19,19	0
58	MG	YA	3081	1/1	0.90	0.29	10,10,10,10	0
58	MG	YA	3012	1/1	0.90	0.29	10,10,10,10	0
58	MG	XA	1617	1/1	0.90	0.36	74,74,74,74	0
58	MG	RA	3094	1/1	0.90	0.28	16,16,16,16	0
58	MG	QA	1658	1/1	0.90	0.16	39,39,39,39	0
58	MG	YA	3197	1/1	0.90	1.19	42,42,42,42	0
58	MG	XA	1607	1/1	0.90	0.28	7,7,7,7	0
58	MG	YA	3072	1/1	0.90	0.21	22,22,22,22	0
58	MG	QA	1668	1/1	0.90	0.17	0,0,0,0	0
58	MG	XA	1610	1/1	0.90	0.21	6,6,6,6	0
58	MG	RA	3191	1/1	0.90	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	YA	3158	1/1	0.90	0.36	21,21,21,21	0
58	MG	RA	3242	1/1	0.90	0.32	13,13,13,13	0
58	MG	RA	3017	1/1	0.90	0.35	18,18,18,18	0
58	MG	RA	3136	1/1	0.90	0.20	5,5,5,5	0
58	MG	YA	3135	1/1	0.90	0.22	6,6,6,6	0
58	MG	YA	3235	1/1	0.90	0.21	26,26,26,26	0
58	MG	XA	1665	1/1	0.90	0.15	33,33,33,33	0
58	MG	YA	3194	1/1	0.90	0.26	36,36,36,36	0
58	MG	YA	3176	1/1	0.90	0.13	45,45,45,45	0
58	MG	XA	1642	1/1	0.90	0.16	47,47,47,47	0
58	MG	YA	3210	1/1	0.90	0.20	17,17,17,17	0
58	MG	RA	3226	1/1	0.90	0.32	1,1,1,1	0
58	MG	RA	3238	1/1	0.90	0.24	32,32,32,32	0
58	MG	XV	102	1/1	0.90	0.18	2,2,2,2	0
58	MG	RA	3068	1/1	0.90	0.25	13,13,13,13	0
58	MG	RA	3088	1/1	0.90	0.16	7,7,7,7	0
58	MG	RA	3198	1/1	0.90	0.19	26,26,26,26	0
58	MG	YA	3161	1/1	0.90	0.26	23,23,23,23	0
58	MG	RA	3215	1/1	0.90	0.09	13,13,13,13	0
58	MG	XA	1604	1/1	0.90	0.29	9,9,9,9	0
58	MG	YA	3239	1/1	0.90	0.17	41,41,41,41	0
58	MG	RA	3010	1/1	0.91	0.47	14,14,14,14	0
58	MG	XA	1609	1/1	0.91	0.09	51,51,51,51	0
58	MG	YA	3219	1/1	0.91	0.42	22,22,22,22	0
58	MG	RA	3156	1/1	0.91	0.17	9,9,9,9	0
58	MG	YA	3142	1/1	0.91	0.61	31,31,31,31	0
58	MG	RA	3208	1/1	0.91	0.16	30,30,30,30	0
58	MG	QF	201	1/1	0.91	0.25	36,36,36,36	0
58	MG	YA	3056	1/1	0.91	0.22	5,5,5,5	0
58	MG	XA	1620	1/1	0.91	0.33	15,15,15,15	0
58	MG	YA	3036	1/1	0.91	0.28	11,11,11,11	0
58	MG	RA	3241	1/1	0.91	0.13	8,8,8,8	0
58	MG	YA	3090	1/1	0.91	0.27	26,26,26,26	0
58	MG	YA	3112	1/1	0.91	0.17	13,13,13,13	0
58	MG	YA	3251	1/1	0.91	0.57	10,10,10,10	0
58	MG	YA	3257	1/1	0.91	0.26	14,14,14,14	0
58	MG	RA	3155	1/1	0.91	0.16	54,54,54,54	0
58	MG	YA	3011	1/1	0.91	0.20	9,9,9,9	0
58	MG	YA	3230	1/1	0.91	0.15	42,42,42,42	0
58	MG	YA	3054	1/1	0.91	0.26	14,14,14,14	0
58	MG	QA	1673	1/1	0.91	0.24	9,9,9,9	0
58	MG	QA	1602	1/1	0.91	0.21	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	XA	1655	1/1	0.91	0.29	68,68,68,68	0
58	MG	YA	3071	1/1	0.91	0.21	1,1,1,1	0
58	MG	RA	3012	1/1	0.91	0.40	31,31,31,31	0
58	MG	RA	3101	1/1	0.91	0.18	18,18,18,18	0
58	MG	RA	3072	1/1	0.91	0.29	18,18,18,18	0
58	MG	XA	1670	1/1	0.91	0.19	27,27,27,27	0
58	MG	QA	1627	1/1	0.91	0.18	30,30,30,30	0
58	MG	RA	3051	1/1	0.91	0.31	1,1,1,1	0
58	MG	YA	3264	1/1	0.91	0.35	5,5,5,5	0
58	MG	YA	3028	1/1	0.91	0.19	15,15,15,15	0
58	MG	YA	3137	1/1	0.91	0.11	10,10,10,10	0
58	MG	YA	3035	1/1	0.91	0.33	12,12,12,12	0
58	MG	RA	3237	1/1	0.91	0.38	6,6,6,6	0
58	MG	RA	3146	1/1	0.91	0.16	25,25,25,25	0
58	MG	RA	3135	1/1	0.91	0.13	12,12,12,12	0
58	MG	YA	3051	1/1	0.92	0.25	13,13,13,13	0
58	MG	QA	1618	1/1	0.92	0.09	17,17,17,17	0
58	MG	RA	3218	1/1	0.92	0.12	17,17,17,17	0
58	MG	YA	3206	1/1	0.92	0.27	52,52,52,52	0
58	MG	RE	301	1/1	0.92	0.20	9,9,9,9	0
58	MG	XA	1624	1/1	0.92	0.10	22,22,22,22	0
58	MG	RA	3063	1/1	0.92	0.24	19,19,19,19	0
58	MG	RA	3184	1/1	0.92	0.35	23,23,23,23	0
58	MG	RA	3162	1/1	0.92	0.52	18,18,18,18	0
58	MG	RA	3003	1/1	0.92	0.18	4,4,4,4	0
58	MG	YA	3115	1/1	0.92	0.22	17,17,17,17	0
58	MG	XA	1675	1/1	0.92	0.32	14,14,14,14	0
58	MG	YA	3188	1/1	0.92	0.13	13,13,13,13	0
58	MG	RA	3140	1/1	0.92	0.32	34,34,34,34	0
58	MG	RA	3224	1/1	0.92	0.83	142,142,142,142	0
58	MG	YA	3190	1/1	0.92	0.15	8,8,8,8	0
58	MG	YA	3139	1/1	0.92	0.15	8,8,8,8	0
58	MG	QA	1647	1/1	0.92	0.32	38,38,38,38	0
58	MG	RA	3181	1/1	0.92	0.33	21,21,21,21	0
58	MG	QA	1617	1/1	0.92	0.18	46,46,46,46	0
58	MG	YA	3160	1/1	0.92	0.14	16,16,16,16	0
58	MG	QA	1626	1/1	0.92	0.11	17,17,17,17	0
58	MG	YA	3093	1/1	0.92	0.27	10,10,10,10	0
58	MG	XA	1677	1/1	0.92	0.16	2,2,2,2	0
58	MG	RA	3092	1/1	0.92	0.32	0,0,0,0	0
58	MG	YA	3171	1/1	0.92	0.22	22,22,22,22	0
58	MG	YA	3255	1/1	0.92	0.38	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	PAR	QA	1601	42/42	0.92	0.35	42,42,42,42	0
58	MG	XA	1647	1/1	0.92	0.12	22,22,22,22	0
58	MG	QA	1612	1/1	0.92	0.29	15,15,15,15	0
58	MG	YA	3096	1/1	0.92	0.20	6,6,6,6	0
58	MG	YA	3152	1/1	0.92	0.24	27,27,27,27	0
58	MG	RA	3104	1/1	0.92	0.18	11,11,11,11	0
58	MG	QA	1616	1/1	0.92	0.15	52,52,52,52	0
58	MG	RA	3031	1/1	0.92	0.36	9,9,9,9	0
58	MG	YA	3140	1/1	0.92	0.34	8,8,8,8	0
58	MG	RA	3160	1/1	0.92	0.19	19,19,19,19	0
58	MG	RA	3033	1/1	0.92	0.37	6,6,6,6	0
58	MG	RA	3141	1/1	0.92	0.59	40,40,40,40	0
58	MG	XA	1637	1/1	0.92	0.16	14,14,14,14	0
58	MG	RA	3121	1/1	0.92	0.17	36,36,36,36	0
58	MG	RA	3001	1/1	0.92	0.27	16,16,16,16	0
58	MG	RA	3180	1/1	0.92	0.24	17,17,17,17	0
58	MG	YP	202	1/1	0.92	0.10	1,1,1,1	0
58	MG	RA	3129	1/1	0.92	0.23	21,21,21,21	0
58	MG	QA	1655	1/1	0.92	0.21	14,14,14,14	0
58	MG	XA	1611	1/1	0.92	0.15	11,11,11,11	0
58	MG	RA	3106	1/1	0.93	0.14	6,6,6,6	0
58	MG	YA	3040	1/1	0.93	0.17	19,19,19,19	0
58	MG	QA	1676	1/1	0.93	0.14	13,13,13,13	0
58	MG	RA	3173	1/1	0.93	0.28	35,35,35,35	0
58	MG	XA	1641	1/1	0.93	0.24	11,11,11,11	0
58	MG	YA	3231	1/1	0.93	0.20	34,34,34,34	0
58	MG	RA	3086	1/1	0.93	0.22	22,22,22,22	0
58	MG	YA	3049	1/1	0.93	0.39	74,74,74,74	0
58	MG	XA	1634	1/1	0.93	0.17	7,7,7,7	0
58	MG	R5	101	1/1	0.93	0.32	11,11,11,11	0
58	MG	YA	3153	1/1	0.93	0.11	14,14,14,14	0
58	MG	RA	3231	1/1	0.93	0.17	16,16,16,16	0
58	MG	YA	3243	1/1	0.93	0.21	13,13,13,13	0
58	MG	XA	1678	1/1	0.93	0.23	2,2,2,2	0
58	MG	XA	1664	1/1	0.93	0.19	22,22,22,22	0
58	MG	XA	1613	1/1	0.93	0.12	8,8,8,8	0
58	MG	QA	1622	1/1	0.93	0.09	12,12,12,12	0
58	MG	RA	3036	1/1	0.93	0.48	18,18,18,18	0
58	MG	YA	3146	1/1	0.93	0.23	40,40,40,40	0
58	MG	XA	1619	1/1	0.93	0.24	5,5,5,5	0
58	MG	YA	3172	1/1	0.93	0.37	40,40,40,40	0
58	MG	RA	3095	1/1	0.93	0.25	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	RA	3062	1/1	0.93	0.36	21,21,21,21	0
58	MG	YA	3195	1/1	0.93	0.19	5,5,5,5	0
58	MG	YA	3154	1/1	0.93	0.44	11,11,11,11	0
58	MG	YA	3237	1/1	0.93	0.32	36,36,36,36	0
58	MG	YA	3060	1/1	0.93	0.24	8,8,8,8	0
58	MG	RA	3075	1/1	0.93	0.14	9,9,9,9	0
58	MG	XA	1640	1/1	0.93	0.26	27,27,27,27	0
58	MG	YA	3055	1/1	0.93	0.28	6,6,6,6	0
57	PAR	XA	1601	42/42	0.93	0.30	38,38,38,38	0
58	MG	RA	3185	1/1	0.93	0.22	16,16,16,16	0
58	MG	RA	3125	1/1	0.93	0.30	19,19,19,19	0
58	MG	RA	3076	1/1	0.93	0.15	7,7,7,7	0
58	MG	YA	3078	1/1	0.93	0.17	9,9,9,9	0
58	MG	QA	1670	1/1	0.93	0.34	5,5,5,5	0
58	MG	R0	101	1/1	0.93	0.09	2,2,2,2	0
58	MG	YA	3159	1/1	0.93	0.15	12,12,12,12	0
58	MG	YA	3141	1/1	0.93	0.13	19,19,19,19	0
58	MG	YA	3058	1/1	0.93	0.17	20,20,20,20	0
58	MG	RA	3142	1/1	0.93	0.38	20,20,20,20	0
58	MG	YA	3227	1/1	0.93	0.40	39,39,39,39	0
58	MG	YA	3002	1/1	0.94	0.22	0,0,0,0	0
58	MG	QA	1642	1/1	0.94	0.18	38,38,38,38	0
58	MG	RA	3186	1/1	0.94	0.28	17,17,17,17	0
58	MG	RA	3022	1/1	0.94	0.20	24,24,24,24	0
58	MG	XA	1626	1/1	0.94	0.13	15,15,15,15	0
58	MG	YA	3198	1/1	0.94	0.27	18,18,18,18	0
58	MG	YA	3074	1/1	0.94	0.12	1,1,1,1	0
58	MG	RA	3222	1/1	0.94	0.12	2,2,2,2	0
58	MG	YA	3220	1/1	0.94	0.16	1,1,1,1	0
58	MG	YA	3192	1/1	0.94	0.30	21,21,21,21	0
58	MG	QM	201	1/1	0.94	0.06	51,51,51,51	0
58	MG	YA	3024	1/1	0.94	0.24	10,10,10,10	0
58	MG	YA	3032	1/1	0.94	0.22	1,1,1,1	0
58	MG	RA	3127	1/1	0.94	0.16	22,22,22,22	0
58	MG	RA	3187	1/1	0.94	0.21	42,42,42,42	0
58	MG	YA	3215	1/1	0.94	0.13	42,42,42,42	0
58	MG	YA	3070	1/1	0.94	0.20	1,1,1,1	0
58	MG	QA	1636	1/1	0.94	0.18	1,1,1,1	0
58	MG	XA	1671	1/1	0.94	0.38	33,33,33,33	0
58	MG	RA	3230	1/1	0.94	0.20	41,41,41,41	0
58	MG	XA	1631	1/1	0.94	0.21	4,4,4,4	0
58	MG	RA	3115	1/1	0.94	0.26	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	YA	3242	1/1	0.94	0.14	9,9,9,9	0
58	MG	RA	3149	1/1	0.94	0.25	4,4,4,4	0
58	MG	YA	3001	1/1	0.94	0.20	23,23,23,23	0
58	MG	YA	3046	1/1	0.94	0.50	74,74,74,74	0
58	MG	QA	1666	1/1	0.94	0.12	68,68,68,68	0
58	MG	RA	3163	1/1	0.94	0.26	34,34,34,34	0
58	MG	YA	3119	1/1	0.94	0.24	9,9,9,9	0
58	MG	RA	3178	1/1	0.94	0.13	25,25,25,25	0
58	MG	YA	3193	1/1	0.94	0.08	14,14,14,14	0
58	MG	YA	3108	1/1	0.94	0.30	7,7,7,7	0
58	MG	XA	1627	1/1	0.94	0.17	12,12,12,12	0
58	MG	YA	3020	1/1	0.94	0.41	8,8,8,8	0
58	MG	RA	3147	1/1	0.94	0.37	32,32,32,32	0
58	MG	YA	3260	1/1	0.94	0.71	74,74,74,74	0
58	MG	RD	301	1/1	0.94	0.33	12,12,12,12	0
58	MG	YA	3211	1/1	0.94	0.50	55,55,55,55	0
58	MG	RA	3122	1/1	0.94	0.15	5,5,5,5	0
58	MG	YA	3134	1/1	0.94	0.13	19,19,19,19	0
58	MG	QA	1641	1/1	0.94	0.14	43,43,43,43	0
58	MG	YA	3031	1/1	0.94	0.18	5,5,5,5	0
58	MG	XA	1661	1/1	0.94	0.09	2,2,2,2	0
58	MG	RA	3245	1/1	0.94	0.36	7,7,7,7	0
58	MG	RA	3190	1/1	0.94	0.07	40,40,40,40	0
58	MG	YA	3178	1/1	0.94	0.26	17,17,17,17	0
58	MG	QA	1665	1/1	0.94	0.09	37,37,37,37	0
58	MG	YA	3106	1/1	0.94	0.15	16,16,16,16	0
58	MG	YA	3053	1/1	0.94	0.22	8,8,8,8	0
58	MG	YA	3136	1/1	0.94	0.17	0,0,0,0	0
58	MG	YA	3003	1/1	0.94	0.42	74,74,74,74	0
58	MG	XA	1648	1/1	0.94	0.16	19,19,19,19	0
58	MG	QA	1639	1/1	0.94	0.22	33,33,33,33	0
58	MG	YA	3103	1/1	0.94	0.25	8,8,8,8	0
58	MG	XA	1643	1/1	0.94	0.34	74,74,74,74	0
58	MG	XA	1683	1/1	0.94	0.10	10,10,10,10	0
58	MG	QA	1629	1/1	0.94	0.20	11,11,11,11	0
58	MG	QA	1635	1/1	0.94	0.39	76,76,76,76	0
58	MG	YA	3124	1/1	0.94	0.23	6,6,6,6	0
58	MG	RA	3008	1/1	0.94	0.46	6,6,6,6	0
58	MG	XA	1654	1/1	0.94	0.27	54,54,54,54	0
58	MG	YA	3252	1/1	0.94	0.36	1,1,1,1	0
58	MG	XA	1633	1/1	0.94	0.10	7,7,7,7	0
58	MG	QA	1663	1/1	0.94	0.21	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	YA	3059	1/1	0.94	0.14	11,11,11,11	0
58	MG	RA	3107	1/1	0.94	0.17	2,2,2,2	0
58	MG	YA	3016	1/1	0.94	0.10	7,7,7,7	0
58	MG	QA	1628	1/1	0.94	0.26	10,10,10,10	0
58	MG	RA	3009	1/1	0.95	0.94	74,74,74,74	0
58	MG	YA	3121	1/1	0.95	0.11	6,6,6,6	0
58	MG	QA	1619	1/1	0.95	0.25	12,12,12,12	0
58	MG	RA	3240	1/1	0.95	0.29	5,5,5,5	0
58	MG	YA	3147	1/1	0.95	0.27	9,9,9,9	0
58	MG	RA	3090	1/1	0.95	0.20	6,6,6,6	0
58	MG	RA	3044	1/1	0.95	0.21	8,8,8,8	0
58	MG	YA	3265	1/1	0.95	0.17	24,24,24,24	0
58	MG	XA	1662	1/1	0.95	0.14	12,12,12,12	0
58	MG	YA	3047	1/1	0.95	0.31	3,3,3,3	0
58	MG	QA	1634	1/1	0.95	0.42	23,23,23,23	0
58	MG	XA	1629	1/1	0.95	0.23	4,4,4,4	0
58	MG	QA	1649	1/1	0.95	0.14	32,32,32,32	0
58	MG	RA	3195	1/1	0.95	0.14	7,7,7,7	0
58	MG	QA	1615	1/1	0.95	0.21	9,9,9,9	0
58	MG	XA	1615	1/1	0.95	0.08	19,19,19,19	0
58	MG	XA	1618	1/1	0.95	0.12	0,0,0,0	0
58	MG	RA	3108	1/1	0.95	0.10	6,6,6,6	0
58	MG	RA	3042	1/1	0.95	0.23	1,1,1,1	0
58	MG	XA	1660	1/1	0.95	0.18	22,22,22,22	0
58	MG	QA	1630	1/1	0.95	0.17	7,7,7,7	0
58	MG	XA	1603	1/1	0.95	0.11	1,1,1,1	0
58	MG	XA	1606	1/1	0.95	0.23	3,3,3,3	0
58	MG	RA	3179	1/1	0.95	0.14	4,4,4,4	0
58	MG	RA	3071	1/1	0.95	0.24	11,11,11,11	0
58	MG	QA	1662	1/1	0.95	0.12	0,0,0,0	0
58	MG	RA	3175	1/1	0.95	0.27	14,14,14,14	0
58	MG	RA	3054	1/1	0.95	0.25	18,18,18,18	0
58	MG	RA	3114	1/1	0.95	0.16	10,10,10,10	0
58	MG	RA	3043	1/1	0.95	0.27	10,10,10,10	0
58	MG	QA	1613	1/1	0.95	0.36	8,8,8,8	0
58	MG	YA	3008	1/1	0.95	0.24	8,8,8,8	0
58	MG	XA	1673	1/1	0.95	0.12	6,6,6,6	0
58	MG	RA	3027	1/1	0.95	0.21	15,15,15,15	0
58	MG	YA	3007	1/1	0.95	0.16	8,8,8,8	0
58	MG	YA	3029	1/1	0.95	0.22	12,12,12,12	0
58	MG	YA	3019	1/1	0.95	0.34	13,13,13,13	0
58	MG	RA	3165	1/1	0.95	0.23	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	QA	1625	1/1	0.95	0.29	29,29,29,29	0
58	MG	YA	3241	1/1	0.95	0.17	18,18,18,18	0
58	MG	RB	201	1/1	0.95	0.08	16,16,16,16	0
58	MG	YA	3258	1/1	0.95	0.34	4,4,4,4	0
58	MG	YA	3057	1/1	0.95	0.34	11,11,11,11	0
58	MG	YA	3065	1/1	0.95	0.22	31,31,31,31	0
58	MG	RA	3018	1/1	0.95	0.26	5,5,5,5	0
58	MG	QA	1669	1/1	0.95	0.20	18,18,18,18	0
58	MG	QA	1646	1/1	0.95	0.16	28,28,28,28	0
58	MG	RA	3102	1/1	0.95	0.33	21,21,21,21	0
58	MG	QA	1606	1/1	0.95	0.43	10,10,10,10	0
58	MG	RA	3219	1/1	0.95	0.24	8,8,8,8	0
58	MG	QA	1624	1/1	0.95	0.12	26,26,26,26	0
58	MG	YA	3030	1/1	0.95	0.61	18,18,18,18	0
58	MG	YA	3149	1/1	0.95	0.21	16,16,16,16	0
58	MG	RA	3055	1/1	0.95	0.12	10,10,10,10	0
58	MG	RA	3019	1/1	0.95	0.11	8,8,8,8	0
58	MG	XA	1669	1/1	0.95	0.06	55,55,55,55	0
58	MG	QA	1633	1/1	0.95	0.23	15,15,15,15	0
58	MG	YA	3186	1/1	0.95	0.24	25,25,25,25	0
58	MG	YA	3084	1/1	0.95	0.15	12,12,12,12	0
58	MG	XA	1622	1/1	0.95	0.23	6,6,6,6	0
58	MG	YA	3086	1/1	0.96	0.20	3,3,3,3	0
58	MG	XA	1605	1/1	0.96	0.35	15,15,15,15	0
58	MG	YA	3048	1/1	0.96	0.15	4,4,4,4	0
58	MG	YA	3004	1/1	0.96	0.15	11,11,11,11	0
58	MG	RA	3032	1/1	0.96	0.25	14,14,14,14	0
58	MG	YA	3015	1/1	0.96	0.52	74,74,74,74	0
58	MG	QA	1610	1/1	0.96	0.22	21,21,21,21	0
58	MG	RA	3064	1/1	0.96	0.24	4,4,4,4	0
58	MG	XA	1608	1/1	0.96	0.17	1,1,1,1	0
58	MG	XA	1623	1/1	0.96	0.05	28,28,28,28	0
58	MG	YA	3026	1/1	0.96	0.26	5,5,5,5	0
58	MG	RA	3119	1/1	0.96	0.16	20,20,20,20	0
58	MG	QA	1652	1/1	0.96	0.10	13,13,13,13	0
58	MG	YA	3076	1/1	0.96	0.34	10,10,10,10	0
58	MG	YA	3113	1/1	0.96	0.22	17,17,17,17	0
58	MG	RA	3038	1/1	0.96	0.22	4,4,4,4	0
58	MG	RA	3189	1/1	0.96	0.12	14,14,14,14	0
58	MG	YA	3143	1/1	0.96	0.09	0,0,0,0	0
58	MG	RA	3109	1/1	0.96	0.20	0,0,0,0	0
58	MG	RA	3034	1/1	0.96	0.27	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	YA	3117	1/1	0.96	0.11	28,28,28,28	0
58	MG	YA	3043	1/1	0.96	0.28	5,5,5,5	0
58	MG	YA	3022	1/1	0.96	0.26	7,7,7,7	0
58	MG	RA	3166	1/1	0.96	0.23	5,5,5,5	0
58	MG	YA	3094	1/1	0.96	0.17	12,12,12,12	0
58	MG	XA	1674	1/1	0.96	0.17	4,4,4,4	0
58	MG	RA	3041	1/1	0.96	0.26	9,9,9,9	0
58	MG	YA	3177	1/1	0.96	0.13	4,4,4,4	0
58	MG	RA	3169	1/1	0.96	0.20	13,13,13,13	0
58	MG	RA	3167	1/1	0.96	0.18	1,1,1,1	0
58	MG	RA	3206	1/1	0.96	0.14	5,5,5,5	0
58	MG	RA	3197	1/1	0.96	0.18	81,81,81,81	0
58	MG	RA	3100	1/1	0.96	0.13	0,0,0,0	0
58	MG	YA	3079	1/1	0.96	0.19	22,22,22,22	0
58	MG	RA	3097	1/1	0.96	0.21	5,5,5,5	0
58	MG	YA	3240	1/1	0.96	0.15	12,12,12,12	0
58	MG	YA	3052	1/1	0.96	0.16	12,12,12,12	0
58	MG	YA	3189	1/1	0.96	0.07	30,30,30,30	0
58	MG	RA	3217	1/1	0.96	0.09	8,8,8,8	0
58	MG	YA	3034	1/1	0.96	0.22	7,7,7,7	0
58	MG	R8	101	1/1	0.96	0.15	6,6,6,6	0
58	MG	RA	3123	1/1	0.96	0.08	10,10,10,10	0
58	MG	RA	3060	1/1	0.96	0.20	15,15,15,15	0
58	MG	XA	1659	1/1	0.96	0.12	36,36,36,36	0
58	MG	YA	3067	1/1	0.96	0.27	17,17,17,17	0
58	MG	XA	1653	1/1	0.96	0.37	42,42,42,42	0
58	MG	RA	3070	1/1	0.96	0.17	4,4,4,4	0
58	MG	RA	3213	1/1	0.96	0.13	9,9,9,9	0
58	MG	YA	3077	1/1	0.96	0.25	6,6,6,6	0
58	MG	RA	3015	1/1	0.96	0.27	0,0,0,0	0
58	MG	RA	3079	1/1	0.96	0.07	25,25,25,25	0
58	MG	RA	3168	1/1	0.96	0.19	3,3,3,3	0
58	MG	RA	3046	1/1	0.96	0.36	24,24,24,24	0
58	MG	RA	3011	1/1	0.96	0.23	0,0,0,0	0
58	MG	YA	3261	1/1	0.96	0.49	16,16,16,16	0
58	MG	RA	3045	1/1	0.96	0.15	2,2,2,2	0
58	MG	YA	3224	1/1	0.96	0.26	18,18,18,18	0
58	MG	RA	3134	1/1	0.96	0.26	17,17,17,17	0
58	MG	RA	3150	1/1	0.96	0.23	27,27,27,27	0
58	MG	RA	3153	1/1	0.96	0.12	0,0,0,0	0
58	MG	QA	1637	1/1	0.96	0.09	17,17,17,17	0
58	MG	QA	1657	1/1	0.96	0.12	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	XA	1649	1/1	0.96	0.13	17,17,17,17	0
58	MG	QA	1644	1/1	0.96	0.11	26,26,26,26	0
58	MG	YA	3005	1/1	0.96	0.22	26,26,26,26	0
58	MG	RA	3039	1/1	0.96	0.29	7,7,7,7	0
58	MG	YA	3196	1/1	0.96	0.11	41,41,41,41	0
58	MG	RA	3137	1/1	0.96	0.25	14,14,14,14	0
58	MG	RA	3007	1/1	0.96	0.42	8,8,8,8	0
58	MG	YX	101	1/1	0.96	0.19	47,47,47,47	0
58	MG	RA	3058	1/1	0.96	0.11	5,5,5,5	0
58	MG	RA	3133	1/1	0.96	0.16	7,7,7,7	0
58	MG	XA	1666	1/1	0.96	0.52	85,85,85,85	0
58	MG	RA	3026	1/1	0.96	0.24	7,7,7,7	0
58	MG	YA	3045	1/1	0.96	0.25	5,5,5,5	0
58	MG	YA	3212	1/1	0.96	0.09	10,10,10,10	0
58	MG	RA	3089	1/1	0.96	0.16	6,6,6,6	0
58	MG	RA	3084	1/1	0.96	0.20	14,14,14,14	0
58	MG	QA	1648	1/1	0.96	0.12	43,43,43,43	0
58	MG	RA	3025	1/1	0.96	0.23	3,3,3,3	0
58	MG	RA	3081	1/1	0.96	0.39	18,18,18,18	0
58	MG	RA	3111	1/1	0.96	0.20	12,12,12,12	0
58	MG	RA	3152	1/1	0.97	0.24	14,14,14,14	0
58	MG	YA	3039	1/1	0.97	0.17	20,20,20,20	0
58	MG	XA	1638	1/1	0.97	0.15	4,4,4,4	0
58	MG	YA	3044	1/1	0.97	0.24	2,2,2,2	0
58	MG	RA	3112	1/1	0.97	0.18	7,7,7,7	0
58	MG	YA	3209	1/1	0.97	0.14	7,7,7,7	0
58	MG	RA	3085	1/1	0.97	0.23	7,7,7,7	0
58	MG	YA	3068	1/1	0.97	0.19	20,20,20,20	0
58	MG	RA	3210	1/1	0.97	0.22	8,8,8,8	0
58	MG	RA	3116	1/1	0.97	0.11	8,8,8,8	0
58	MG	YA	3038	1/1	0.97	0.33	16,16,16,16	0
58	MG	YA	3225	1/1	0.97	0.14	12,12,12,12	0
58	MG	QA	1605	1/1	0.97	0.28	6,6,6,6	0
58	MG	YA	3037	1/1	0.97	0.14	16,16,16,16	0
58	MG	YA	3085	1/1	0.97	0.25	17,17,17,17	0
58	MG	YA	3025	1/1	0.97	0.13	16,16,16,16	0
58	MG	YA	3033	1/1	0.97	0.17	12,12,12,12	0
58	MG	RA	3077	1/1	0.97	0.18	6,6,6,6	0
58	MG	RA	3145	1/1	0.97	0.17	3,3,3,3	0
58	MG	RA	3049	1/1	0.97	0.23	12,12,12,12	0
58	MG	YA	3088	1/1	0.97	0.20	6,6,6,6	0
58	MG	RA	3028	1/1	0.97	0.30	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	RA	3023	1/1	0.97	0.23	9,9,9,9	0
58	MG	RA	3170	1/1	0.97	0.09	9,9,9,9	0
58	MG	YA	3110	1/1	0.97	0.14	4,4,4,4	0
58	MG	RA	3211	1/1	0.97	0.20	16,16,16,16	0
58	MG	RA	3192	1/1	0.97	0.24	17,17,17,17	0
58	MG	YA	3095	1/1	0.97	0.20	19,19,19,19	0
58	MG	YA	3123	1/1	0.97	0.21	1,1,1,1	0
58	MG	YA	3114	1/1	0.97	0.22	6,6,6,6	0
58	MG	YA	3109	1/1	0.97	0.08	10,10,10,10	0
58	MG	YA	3221	1/1	0.97	0.08	19,19,19,19	0
58	MG	RA	3029	1/1	0.97	0.23	2,2,2,2	0
58	MG	RA	3113	1/1	0.97	0.13	1,1,1,1	0
58	MG	RA	3053	1/1	0.97	0.10	2,2,2,2	0
58	MG	YA	3167	1/1	0.97	0.12	15,15,15,15	0
58	MG	YA	3069	1/1	0.97	0.26	12,12,12,12	0
58	MG	XA	1652	1/1	0.97	0.07	32,32,32,32	0
58	MG	RA	3083	1/1	0.97	0.22	32,32,32,32	0
58	MG	QA	1651	1/1	0.97	0.11	5,5,5,5	0
58	MG	QA	1654	1/1	0.97	0.14	12,12,12,12	0
58	MG	YA	3129	1/1	0.97	0.16	20,20,20,20	0
58	MG	R8	102	1/1	0.97	0.20	2,2,2,2	0
58	MG	YA	3202	1/1	0.97	0.21	38,38,38,38	0
58	MG	YB	203	1/1	0.97	0.14	4,4,4,4	0
58	MG	XA	1657	1/1	0.97	0.18	19,19,19,19	0
58	MG	RA	3244	1/1	0.97	0.17	0,0,0,0	0
58	MG	QA	1620	1/1	0.97	0.10	3,3,3,3	0
58	MG	RA	3246	1/1	0.97	0.17	33,33,33,33	0
58	MG	YA	3122	1/1	0.97	0.15	9,9,9,9	0
58	MG	YA	3175	1/1	0.97	0.25	14,14,14,14	0
58	MG	RA	3061	1/1	0.97	0.16	0,0,0,0	0
58	MG	YA	3125	1/1	0.97	0.14	11,11,11,11	0
58	MG	YA	3042	1/1	0.97	0.23	15,15,15,15	0
58	MG	RA	3057	1/1	0.97	0.14	4,4,4,4	0
58	MG	XA	1625	1/1	0.97	0.11	5,5,5,5	0
58	MG	RA	3103	1/1	0.97	0.28	5,5,5,5	0
58	MG	RA	3066	1/1	0.97	0.16	7,7,7,7	0
58	MG	RA	3050	1/1	0.97	0.18	9,9,9,9	0
58	MG	RA	3069	1/1	0.97	0.17	19,19,19,19	0
58	MG	XA	1616	1/1	0.97	0.18	5,5,5,5	0
58	MG	RA	3093	1/1	0.97	0.24	12,12,12,12	0
58	MG	YA	3166	1/1	0.97	0.12	11,11,11,11	0
58	MG	YA	3062	1/1	0.97	0.20	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	RA	3059	1/1	0.97	0.23	8,8,8,8	0
58	MG	YA	3204	1/1	0.97	0.59	42,42,42,42	0
58	MG	YA	3050	1/1	0.97	0.23	5,5,5,5	0
58	MG	RA	3131	1/1	0.97	0.30	7,7,7,7	0
58	MG	XA	1645	1/1	0.97	0.18	5,5,5,5	0
58	MG	RA	3030	1/1	0.97	0.19	8,8,8,8	0
58	MG	YA	3097	1/1	0.97	0.14	11,11,11,11	0
58	MG	RA	3099	1/1	0.97	0.31	11,11,11,11	0
58	MG	RA	3132	1/1	0.97	0.20	9,9,9,9	0
58	MG	RA	3052	1/1	0.97	0.17	1,1,1,1	0
58	MG	RA	3024	1/1	0.97	0.29	11,11,11,11	0
58	MG	RA	3236	1/1	0.97	0.37	13,13,13,13	0
58	MG	RA	3176	1/1	0.97	0.06	21,21,21,21	0
58	MG	YA	3104	1/1	0.97	0.09	0,0,0,0	0
58	MG	YA	3006	1/1	0.97	0.16	26,26,26,26	0
58	MG	RA	3037	1/1	0.98	0.88	74,74,74,74	0
58	MG	RA	3128	1/1	0.98	0.11	9,9,9,9	0
58	MG	RA	3139	1/1	0.98	0.19	12,12,12,12	0
58	MG	YA	3128	1/1	0.98	0.46	6,6,6,6	0
58	MG	RA	3117	1/1	0.98	0.12	11,11,11,11	0
58	MG	QV	101	1/1	0.98	0.20	22,22,22,22	0
58	MG	YA	3017	1/1	0.98	0.14	11,11,11,11	0
58	MG	YA	3229	1/1	0.98	0.15	14,14,14,14	0
58	MG	YA	3010	1/1	0.98	0.28	15,15,15,15	0
58	MG	YA	3082	1/1	0.98	0.13	17,17,17,17	0
58	MG	YA	3100	1/1	0.98	0.23	8,8,8,8	0
58	MG	RA	3020	1/1	0.98	0.20	4,4,4,4	0
58	MG	QA	1611	1/1	0.98	0.11	1,1,1,1	0
58	MG	XA	1668	1/1	0.98	0.13	0,0,0,0	0
58	MG	YA	3092	1/1	0.98	0.14	28,28,28,28	0
58	MG	YA	3101	1/1	0.98	0.32	5,5,5,5	0
58	MG	QA	1608	1/1	0.98	0.06	4,4,4,4	0
58	MG	YA	3157	1/1	0.98	0.17	0,0,0,0	0
58	MG	RA	3239	1/1	0.98	0.23	0,0,0,0	0
58	MG	YA	3253	1/1	0.98	0.14	22,22,22,22	0
58	MG	QA	1607	1/1	0.98	0.15	22,22,22,22	0
58	MG	QA	1609	1/1	0.98	0.10	32,32,32,32	0
58	MG	YA	3083	1/1	0.98	0.25	5,5,5,5	0
58	MG	YA	3087	1/1	0.98	0.19	5,5,5,5	0
58	MG	YP	201	1/1	0.98	1.20	54,54,54,54	0
58	MG	QA	1638	1/1	0.98	0.10	14,14,14,14	0
58	MG	RA	3200	1/1	0.98	0.12	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	QA	1650	1/1	0.98	0.17	53,53,53,53	0
58	MG	RP	202	1/1	0.98	0.43	76,76,76,76	0
58	MG	XA	1614	1/1	0.98	0.10	21,21,21,21	0
58	MG	YA	3232	1/1	0.98	0.24	35,35,35,35	0
58	MG	XA	1612	1/1	0.98	0.24	10,10,10,10	0
58	MG	RA	3091	1/1	0.98	0.28	9,9,9,9	0
58	MG	YA	3201	1/1	0.98	0.13	57,57,57,57	0
58	MG	QA	1656	1/1	0.98	0.27	44,44,44,44	0
58	MG	YA	3089	1/1	0.98	0.26	13,13,13,13	0
58	MG	QA	1661	1/1	0.98	0.16	50,50,50,50	0
58	MG	YA	3009	1/1	0.98	0.17	15,15,15,15	0
58	MG	YA	3073	1/1	0.98	0.10	4,4,4,4	0
58	MG	YA	3091	1/1	0.98	0.22	29,29,29,29	0
58	MG	RA	3082	1/1	0.98	0.18	10,10,10,10	0
58	MG	YA	3131	1/1	0.98	0.14	16,16,16,16	0
58	MG	QA	1623	1/1	0.98	0.13	46,46,46,46	0
58	MG	RB	202	1/1	0.98	0.13	29,29,29,29	0
58	MG	YA	3023	1/1	0.98	0.29	18,18,18,18	0
58	MG	RA	3118	1/1	0.98	0.24	16,16,16,16	0
58	MG	RA	3040	1/1	0.98	0.20	13,13,13,13	0
58	MG	YA	3185	1/1	0.98	0.28	22,22,22,22	0
58	MG	YA	3061	1/1	0.98	0.14	15,15,15,15	0
58	MG	RE	302	1/1	0.98	0.23	15,15,15,15	0
58	MG	YA	3066	1/1	0.98	0.31	6,6,6,6	0
58	MG	XV	101	1/1	0.98	0.12	3,3,3,3	0
58	MG	RA	3047	1/1	0.98	0.15	19,19,19,19	0
58	MG	RA	3110	1/1	0.98	0.13	19,19,19,19	0
58	MG	RA	3065	1/1	0.98	0.19	0,0,0,0	0
58	MG	RP	201	1/1	0.98	0.92	118,118,118,118	0
59	ZN	XN	101	1/1	0.98	0.12	70,70,70,70	0
58	MG	YA	3138	1/1	0.98	0.18	6,6,6,6	0
58	MG	RA	3098	1/1	0.98	0.12	10,10,10,10	0
58	MG	RA	3078	1/1	0.98	0.21	16,16,16,16	0
58	MG	YA	3107	1/1	0.98	0.17	9,9,9,9	0
58	MG	QA	1631	1/1	0.98	0.14	50,50,50,50	0
58	MG	RA	3194	1/1	0.98	0.25	0,0,0,0	0
58	MG	RA	3021	1/1	0.98	0.22	18,18,18,18	0
58	MG	YA	3064	1/1	0.98	0.14	4,4,4,4	0
58	MG	YA	3098	1/1	0.98	0.33	8,8,8,8	0
58	MG	Y5	101	1/1	0.98	0.26	13,13,13,13	0
58	MG	RA	3096	1/1	0.98	0.30	17,17,17,17	0
58	MG	QA	1614	1/1	0.98	0.13	2,2,2,2	0

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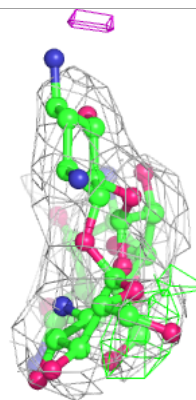
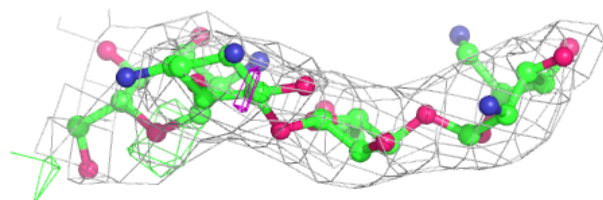
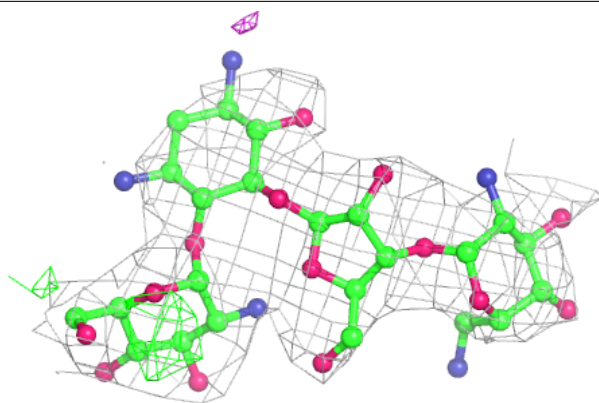
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	YA	3168	1/1	0.99	0.26	3,3,3,3	0
58	MG	RA	3080	1/1	0.99	0.25	10,10,10,10	0
58	MG	YA	3180	1/1	0.99	0.24	19,19,19,19	0
58	MG	YA	3148	1/1	0.99	0.12	15,15,15,15	0
58	MG	YA	3213	1/1	0.99	0.12	31,31,31,31	0
58	MG	YA	3238	1/1	0.99	0.27	76,76,76,76	0
58	MG	RA	3151	1/1	0.99	0.38	3,3,3,3	0
58	MG	YA	3111	1/1	0.99	0.08	26,26,26,26	0
58	MG	RA	3087	1/1	0.99	0.18	10,10,10,10	0
58	MG	RA	3174	1/1	0.99	0.06	17,17,17,17	0
58	MG	QA	1659	1/1	0.99	0.09	42,42,42,42	0
59	ZN	QN	101	1/1	0.99	0.07	86,86,86,86	0
58	MG	YA	3027	1/1	0.99	0.22	21,21,21,21	0
58	MG	RA	3035	1/1	0.99	0.11	2,2,2,2	0
58	MG	RA	3048	1/1	0.99	0.17	2,2,2,2	0
58	MG	RA	3016	1/1	0.99	0.18	8,8,8,8	0
58	MG	YA	3021	1/1	0.99	0.26	8,8,8,8	0
58	MG	XA	1644	1/1	0.99	0.13	4,4,4,4	0
58	MG	YA	3063	1/1	0.99	0.36	12,12,12,12	0
59	ZN	QD	301	1/1	1.00	0.23	27,27,27,27	0
59	ZN	XD	301	1/1	1.00	0.29	10,10,10,10	0

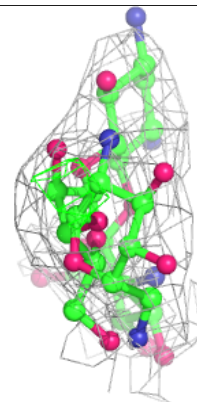
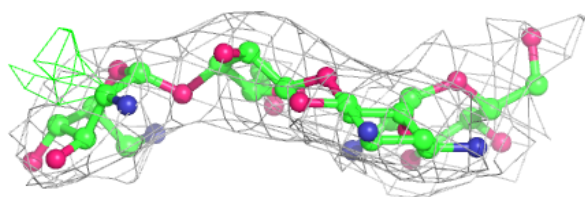
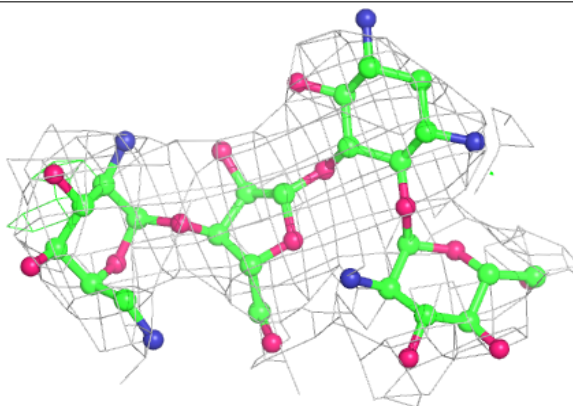
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR QA 1601:

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

**Electron density around PAR XA 1601:**

$2mF_o-DF_c$ (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.