



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2024 – 11:53 PM EST

PDB ID : 4LNT
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-U on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-07-12
Resolution : 2.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

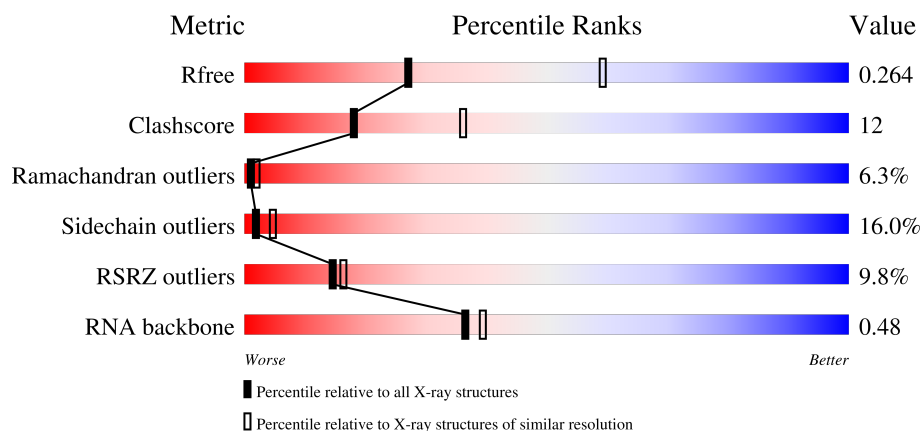
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)
RNA backbone	3690	1105 (3.18-2.70)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div>4%</div> <div>51% 36% 10% ..</div> </div>
1	XA	1522	<div> <div>2%</div> <div>50% 35% 12% ..</div> </div>
2	QB	256	<div> <div>20%</div> <div>49% 36% 7% • 7%</div> </div>
2	XB	256	<div> <div>14%</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	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QY	17	
23	XY	17	
24	QX	25	
24	XX	25	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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

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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	

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Mol	Chain	Length	Quality of chain
53	R7	49	<div><div></div><div>12%63%29%8%</div></div>
53	Y7	49	<div><div></div><div>4%61%31%8%</div></div>
54	R8	65	<div><div></div><div>14%51%35%12%.</div></div>
54	Y8	65	<div><div></div><div>18%45%35%15%..</div></div>
55	R9	37	<div><div></div><div>81%68%27%5%</div></div>
55	Y9	37	<div><div></div><div>59%70%27%. </div></div>
56	Z6	3	<div><div></div><div>33%33%33%</div></div>
56	Z8	3	<div><div></div><div>33%33%33%</div></div>

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291993 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.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			
23	XY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			

- Molecule 24 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
24	XX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	65	Total	Mg	0	0
			65	65		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		

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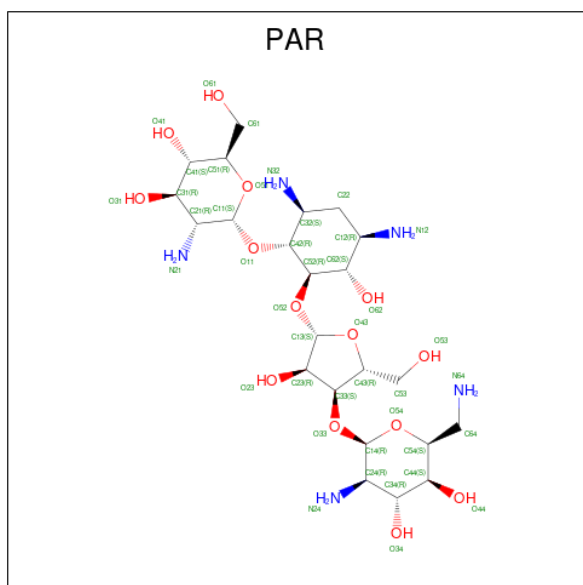
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	1	Total 1	Mg 1	0	0
57	RA	242	Total 242	Mg 242	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RU	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	268	Total 268	Mg 268	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YE	1	Total 1	Mg 1	0	0
57	YP	2	Total 2	Mg 2	0	0
57	YQ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YX	1	Total	Mg	0	0
			1	1		
57	Y5	1	Total	Mg	0	0
			1	1		

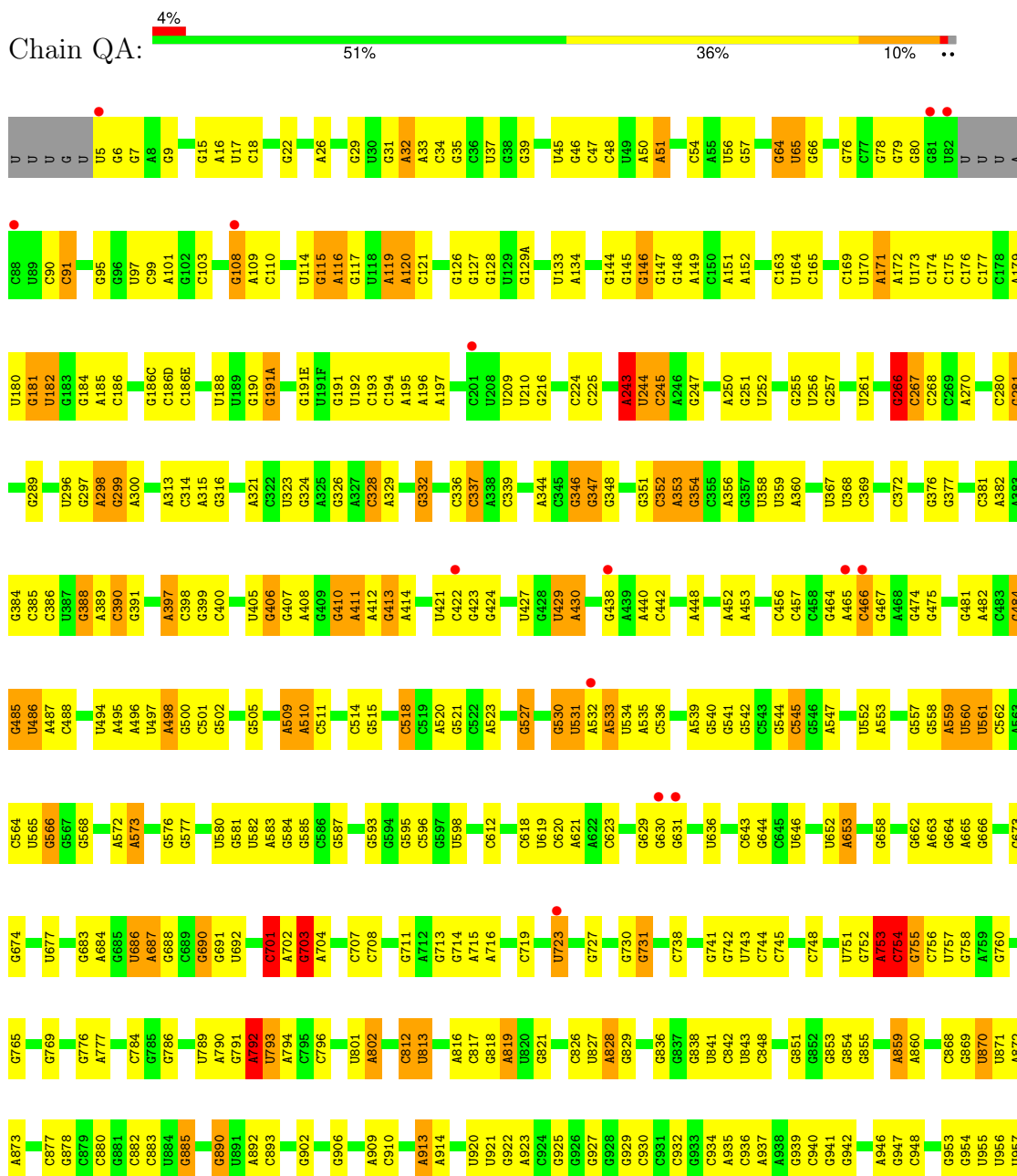
- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).

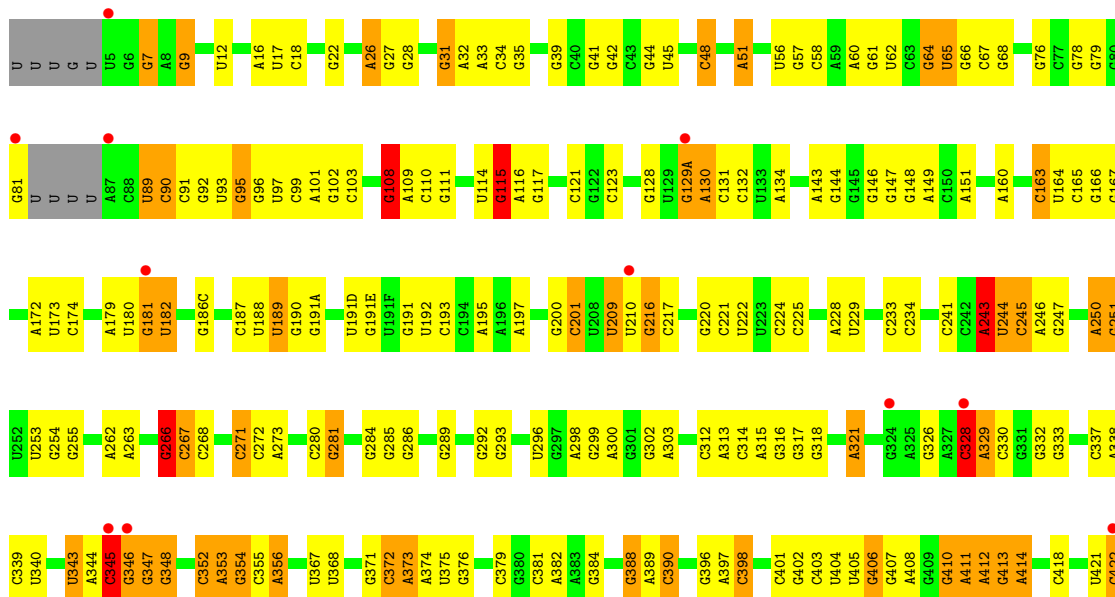


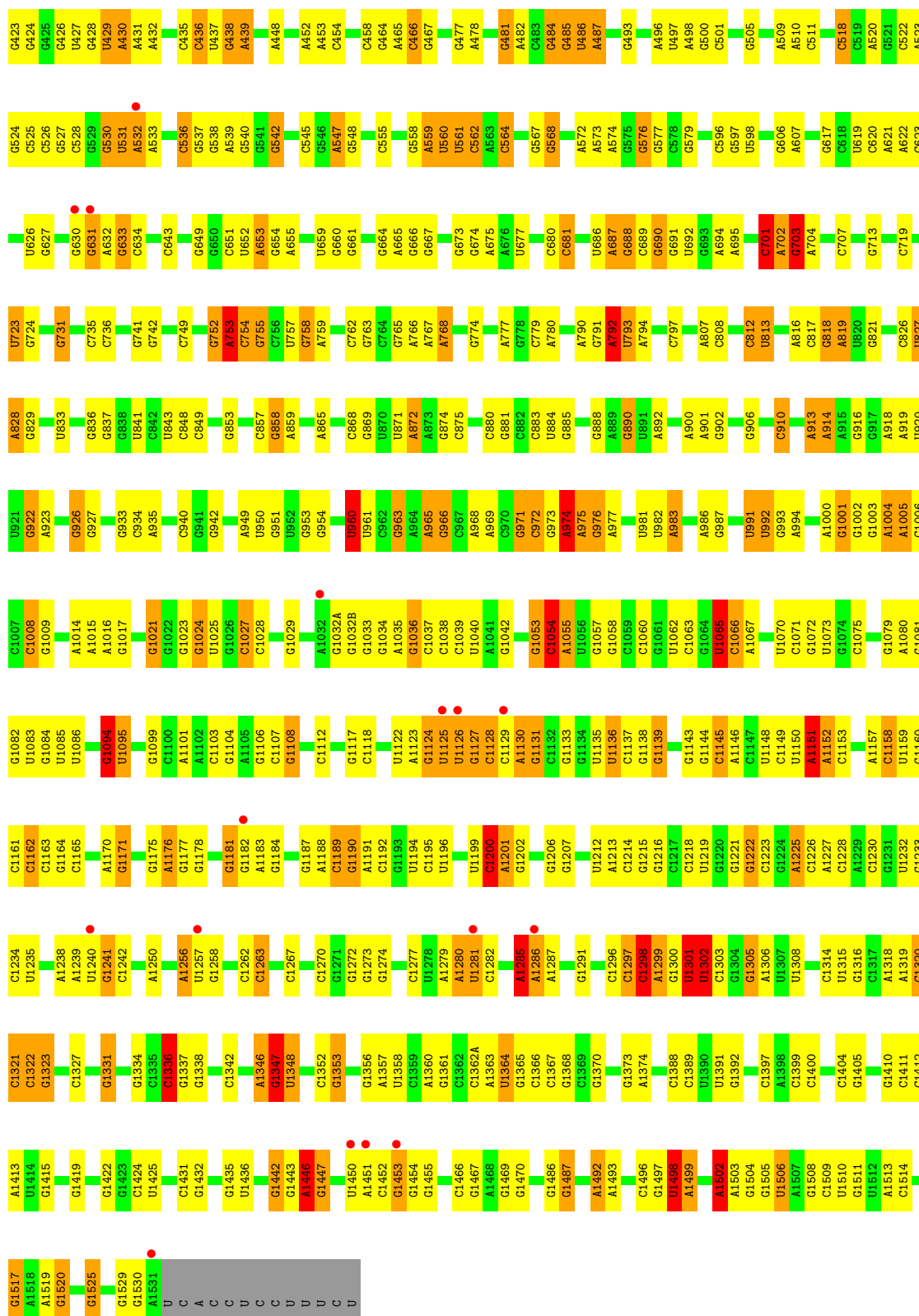
3 Residue-property plots

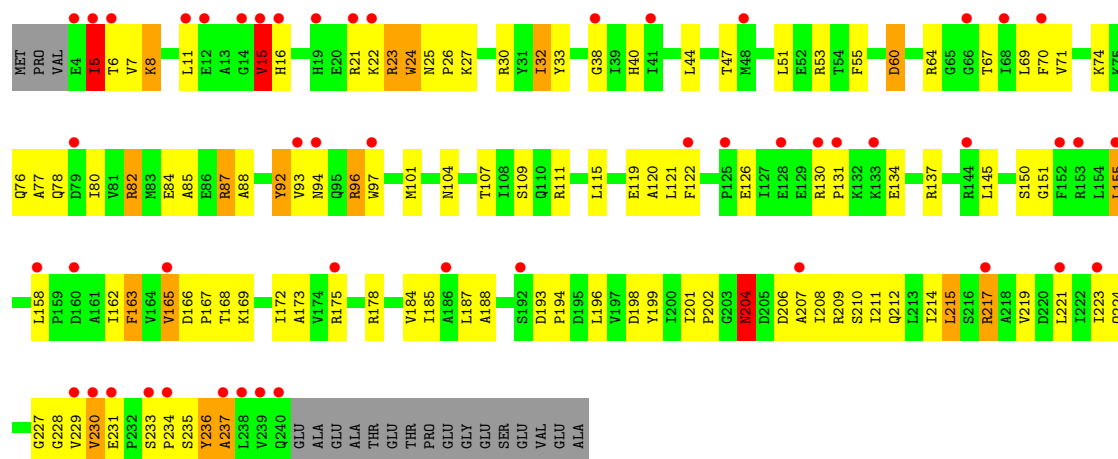
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

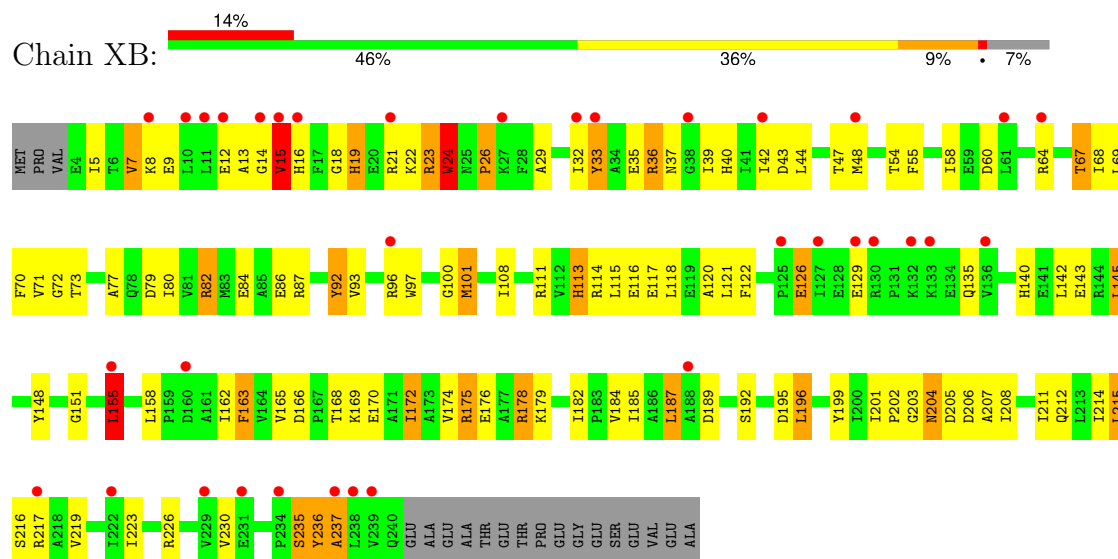




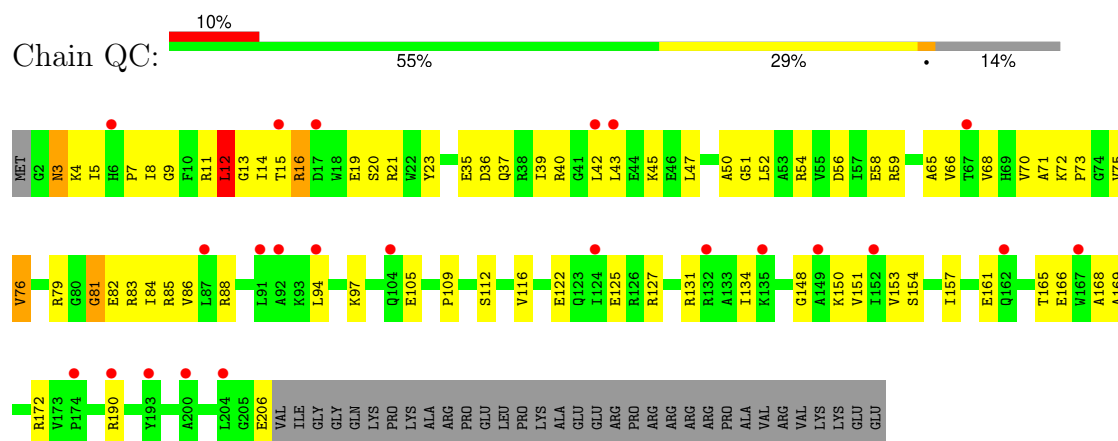




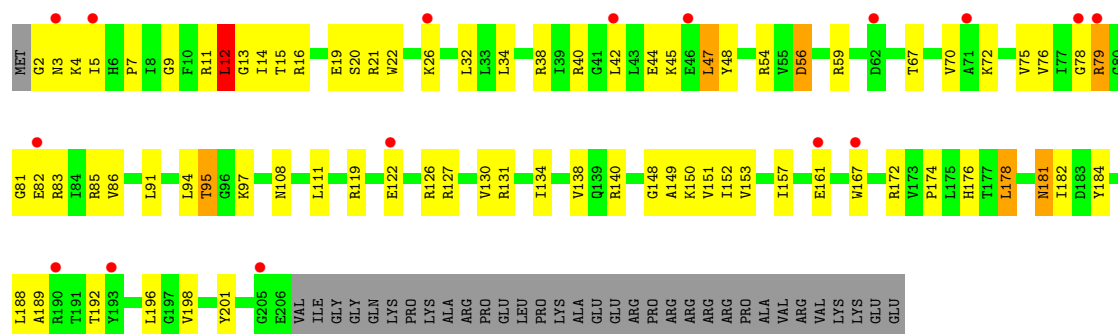
• Molecule 2: 30S ribosomal protein S2



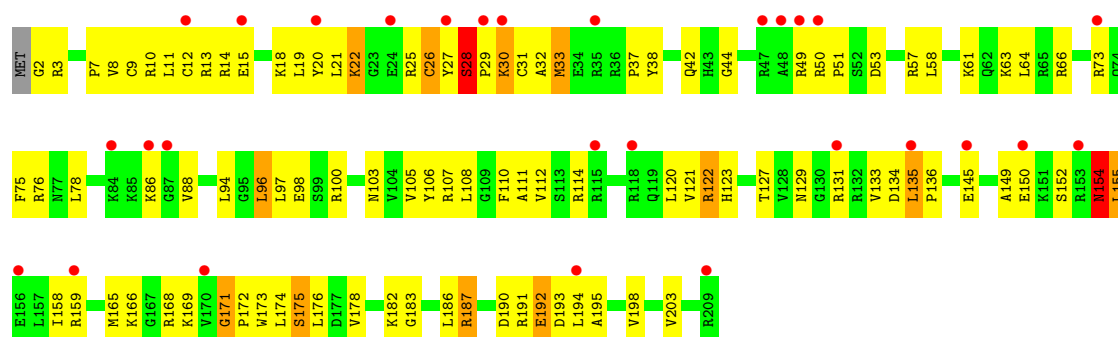
• Molecule 3: 30S ribosomal protein S3



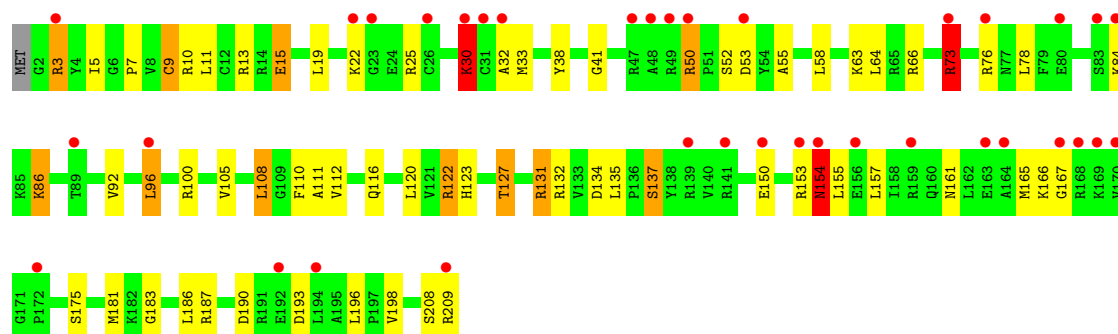
• Molecule 3: 30S ribosomal protein S3



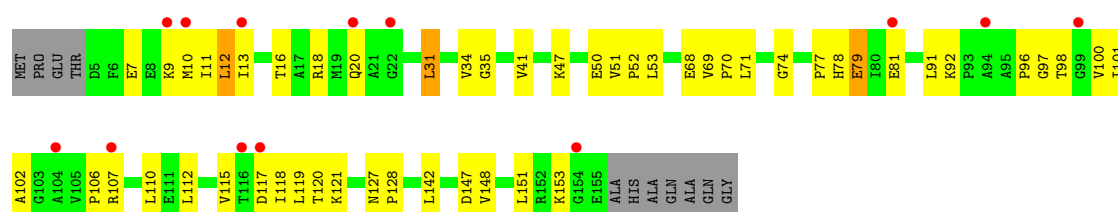
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

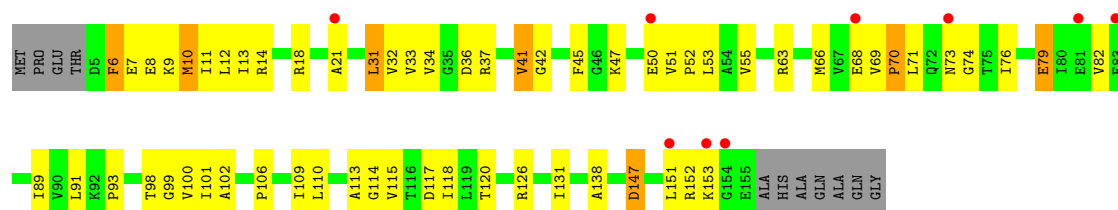


• Molecule 5: 30S ribosomal protein S5



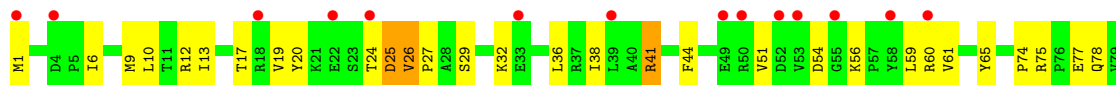
- Molecule 5: 30S ribosomal protein S5

Chain XE: 

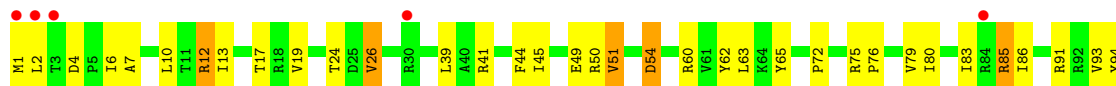




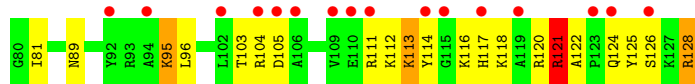
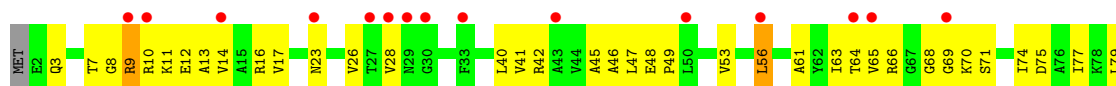
- Molecule 8: 30S ribosomal protein S8



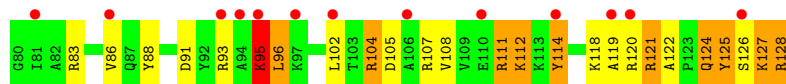
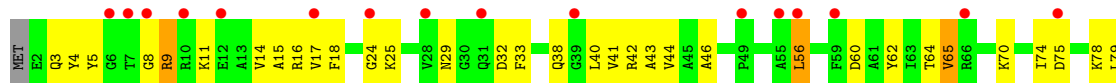
- Molecule 8: 30S ribosomal protein S8



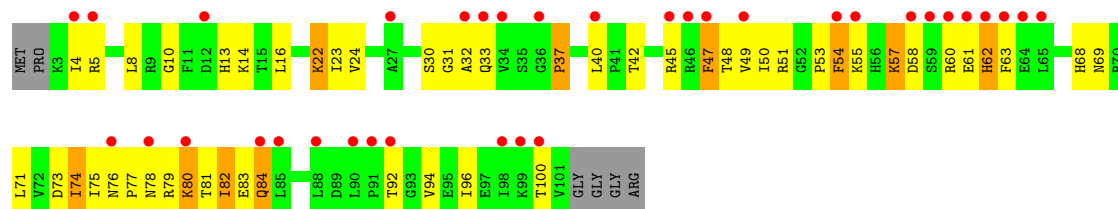
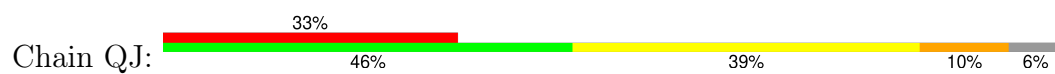
- Molecule 9: 30S ribosomal protein S9



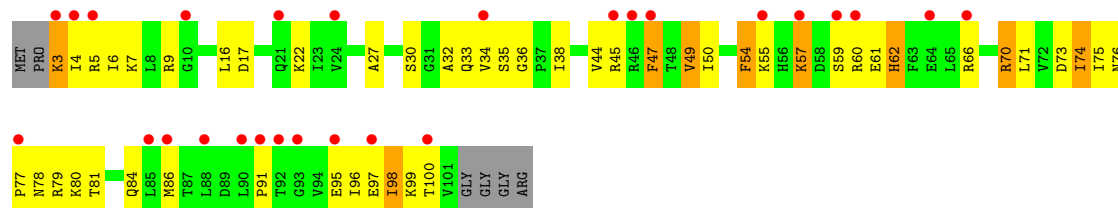
- Molecule 9: 30S ribosomal protein S9



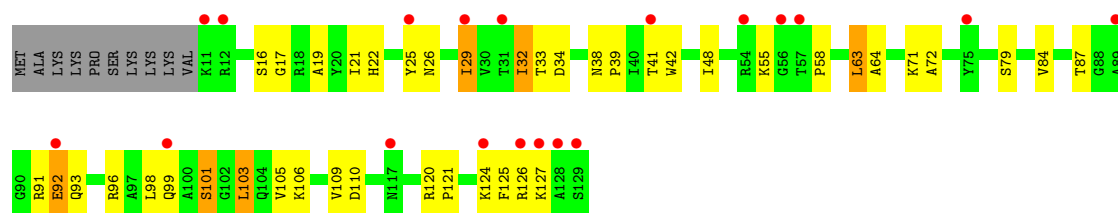
- Molecule 10: 30S ribosomal protein S10



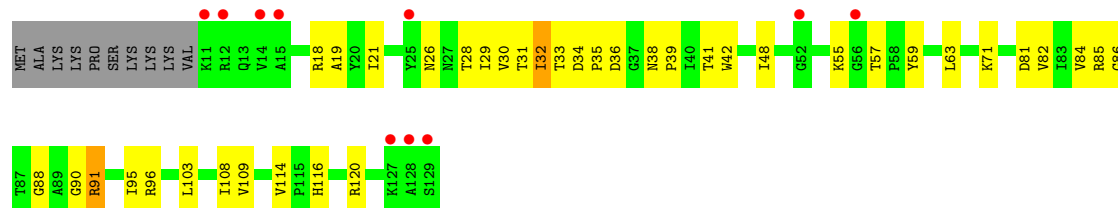
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

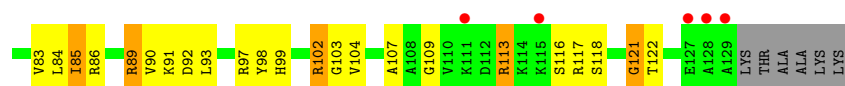


• Molecule 11: 30S ribosomal protein S11

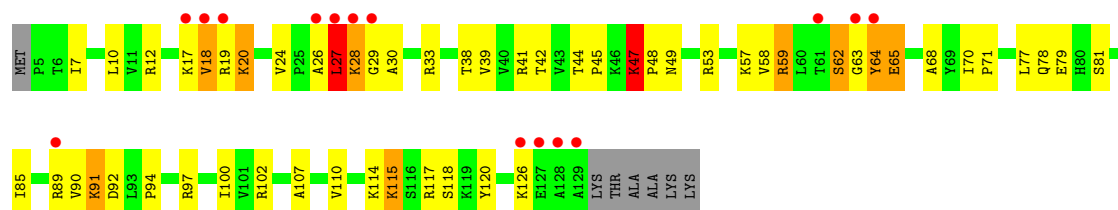


• Molecule 12: 30S ribosomal protein S12

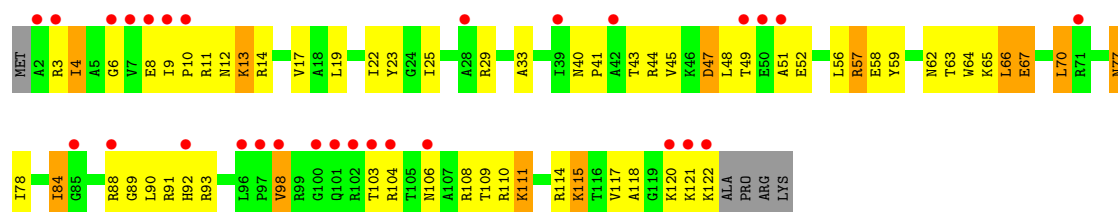




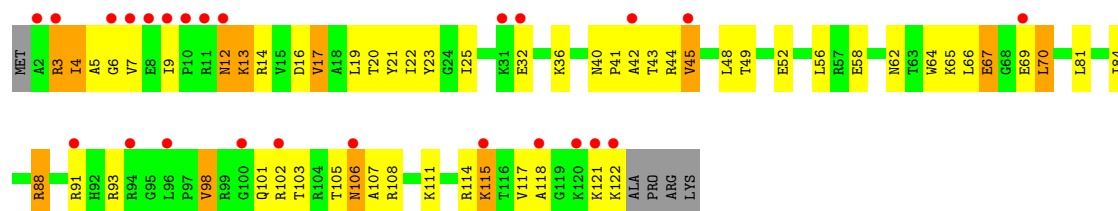
• Molecule 12: 30S ribosomal protein S12



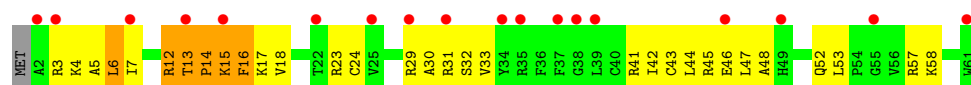
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

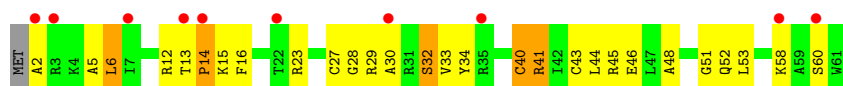


• Molecule 14: 30S ribosomal protein S14

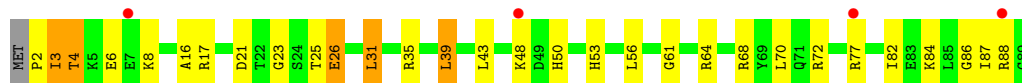


• Molecule 14: 30S ribosomal protein S14





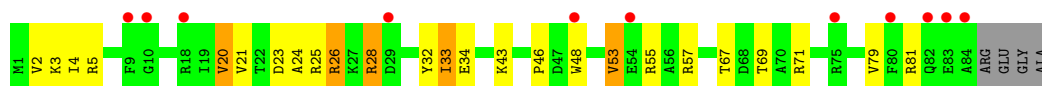
- Molecule 15: 30S ribosomal protein S15



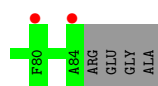
- Molecule 15: 30S ribosomal protein S15



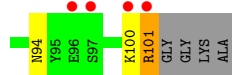
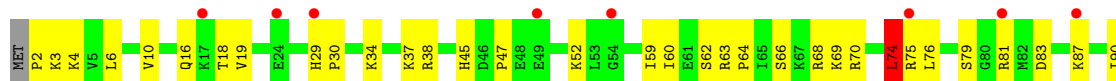
- Molecule 16: 30S ribosomal protein S16




- Molecule 16: 30S ribosomal protein S16

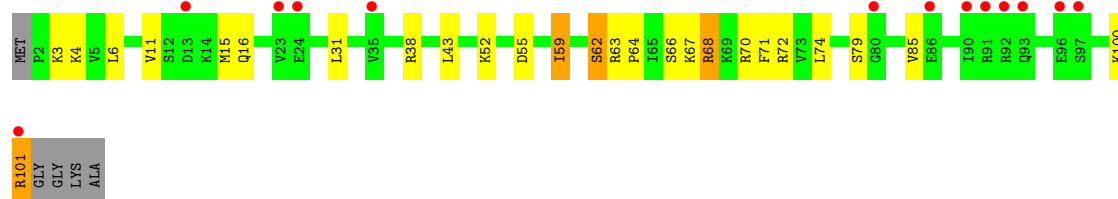


- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

Chain XQ: 



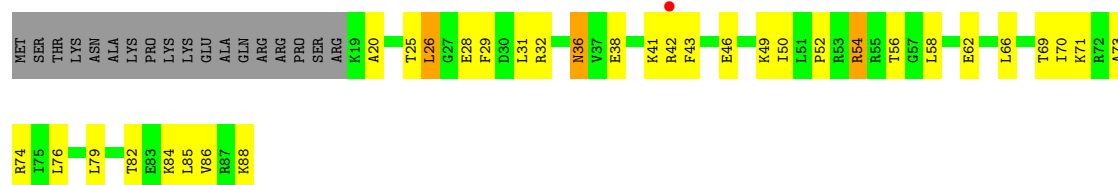
- Molecule 18: 30S ribosomal protein S18

Chain QR: 




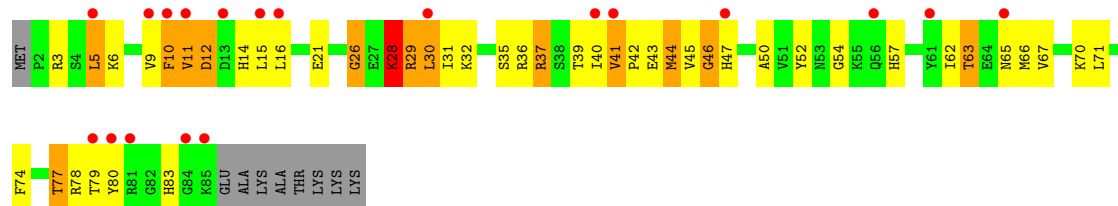
- Molecule 18: 30S ribosomal protein S18

Chain XR: 



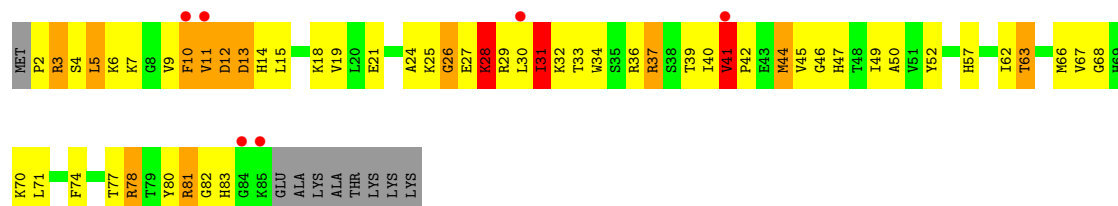
- Molecule 19: 30S ribosomal protein S19

Chain QS: 



- Molecule 19: 30S ribosomal protein S19

Chain XS: 



- Molecule 20: 30S ribosomal protein S20

Chain QT:



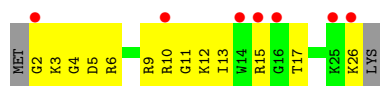
- Molecule 20: 30S ribosomal protein S20

Chain XT:



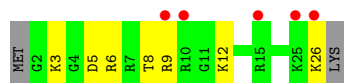
- Molecule 21: 30S ribosomal protein S21

Chain QU:



- Molecule 21: 30S ribosomal protein S21

Chain XU:



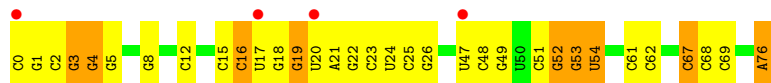
- Molecule 22: P-site tRNA fMet

Chain QV:

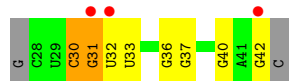
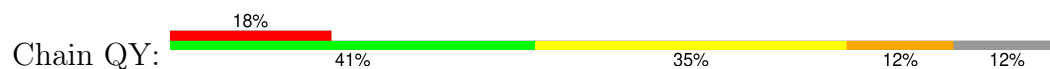


- Molecule 22: P-site tRNA fMet

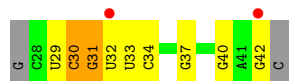
Chain XV:



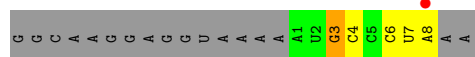
- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



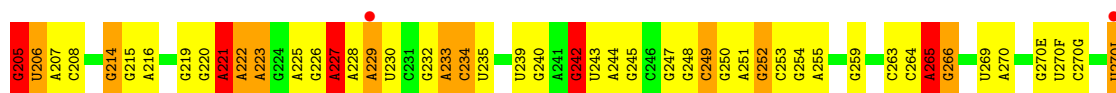
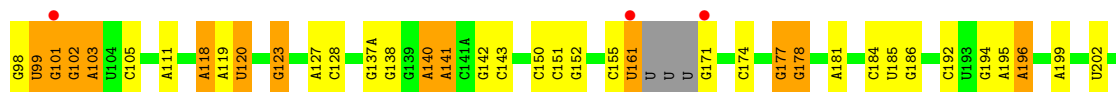
- Molecule 24: A-site ASL SufA6



- Molecule 24: A-site ASL SufA6

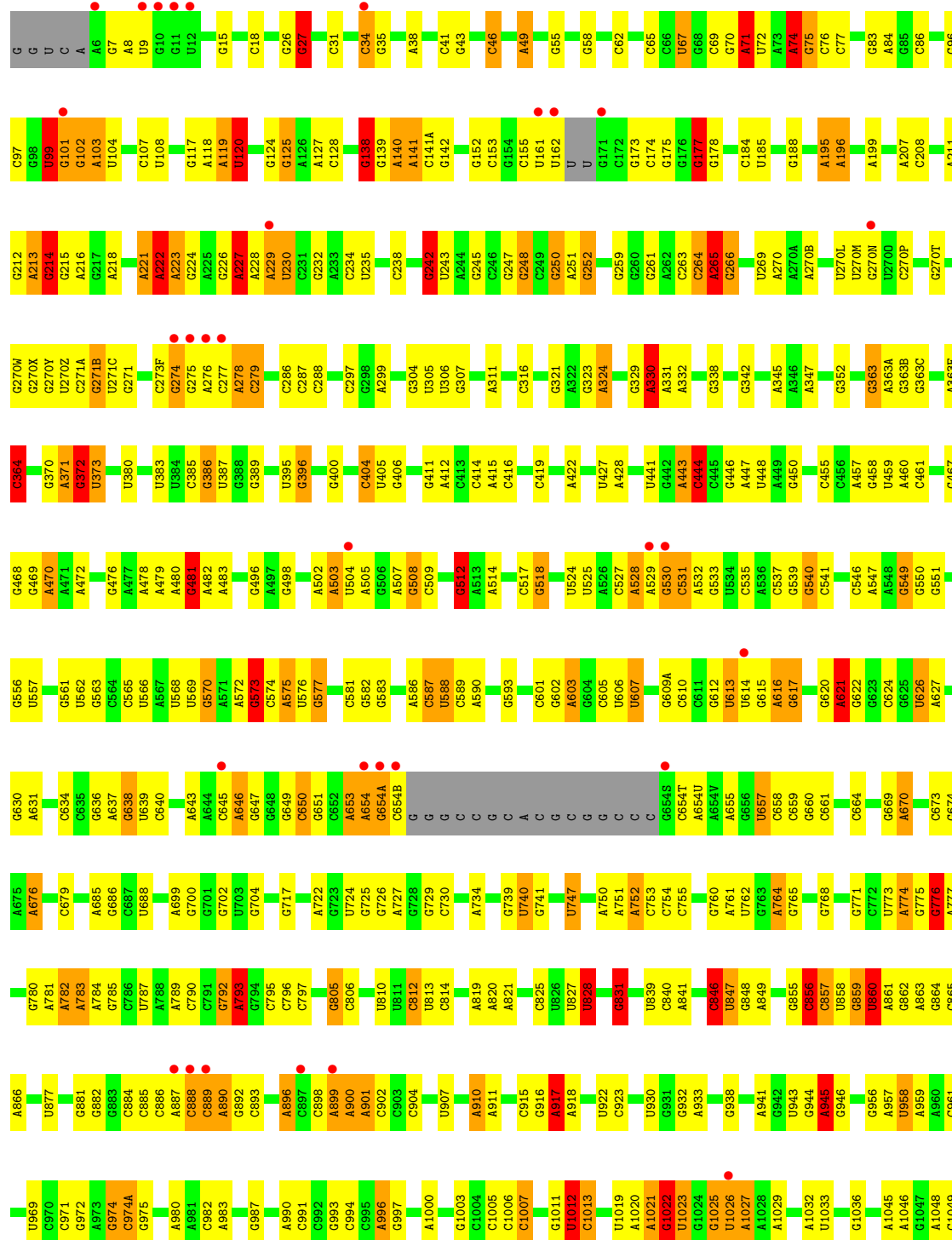


- Molecule 25: 23S rRNA

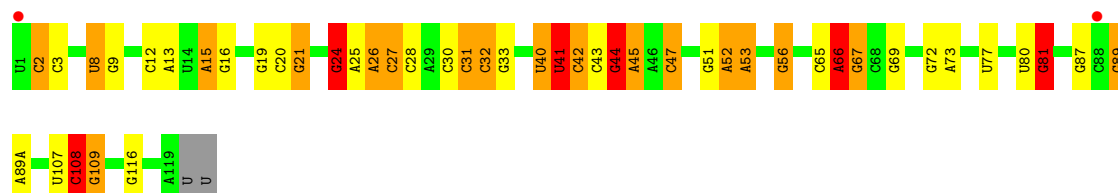




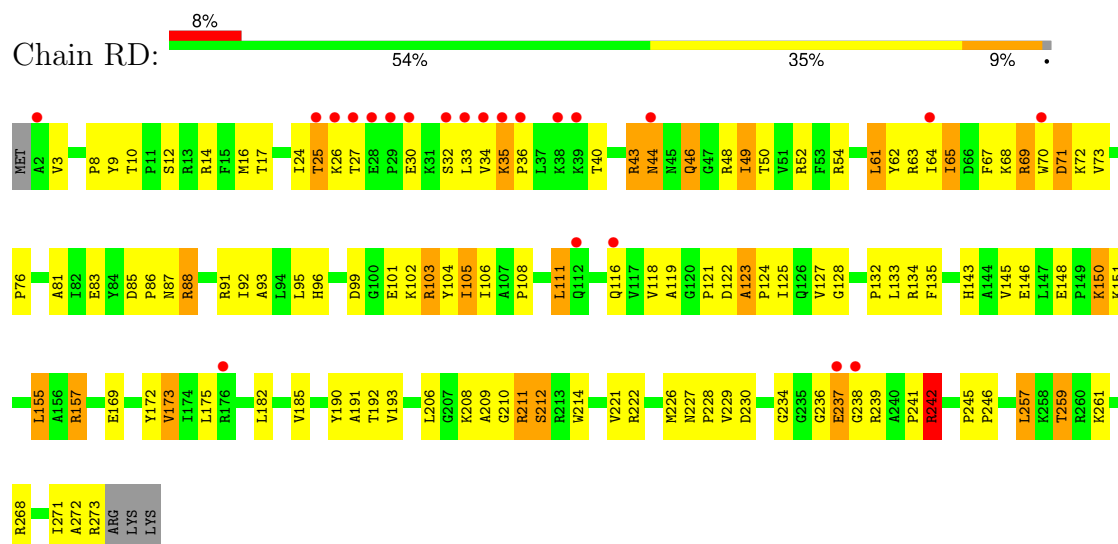
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A1803	C1804	U1805	C1806	G1807	G1816	U2011	G1817	U1818	G1819	A1819	U1732	U1820	C1827	G1828	A1829	U1833	U1834	G1835	C1836	G1837	C1838	G1839	G1763	C1843	C1844	G1845	G1846	A1847	G1848	U1951	G1849	G1850	U1851	C1852	G1857	G1858	U1859	C1860	G1861	A1865	G1866	G1867	A1868	A1869	C1870	A1871	A1872	G1878	C1882	G1883	A1884	A1885	C1886	C1887	G1888	A1981	U1796	C1797	U1798	G1799	C1800	G1801	A1802
C1902	C1905	G1906	A1913	U2011	G1914	U1915	C1925	U1926	A1927	A1928	G1929	U1930	U1931	C1934	G1935	A1936	C1937	A1938	U1939	G1945	U1946	C1947	G1950	U1951	A1952	A1953	U1955	U1956	C1957	C1958	G1962	U1963	G1964	C1967	G1968	A1969	A1970	A1971	A1972	G1973	C1974	G1980	C2070	A2071	C2065	U2068	G2069	C2070	A2071	U2074	U2075	U2079	G1899										
G1992	U1993	C2006	G2010	U2011	G2012	A2013	A2014	A2015	A2019	A2020	C2021	U2022	G2023	C2026	G2027	U2028	A2031	G2032	A2033	C2036	G2037	G2038	C2039	A2042	C2043	C2050	A2051	G2052	G2053	A2054	G2055	G2056	A2059	A2060	G2061	C2062	C2063	C2064	C2065	U2068	G2069	C2070	A2071	U2074	U2075	U2079	G1899																
U2086	G2087	G2093	U2099	G2100	G2101	U2102	C2103	C2107	C2108	U2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	U2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	C2128	G2131	U2132	G2133	A2134	A2135	C2136	C2137	C2138	C2139	C2140	G2141	C2142	C2143	U2144	C2145	C2146	G2147	G2148	G2149	U2150	G2151	G2154	G2155	G2157										
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C2342	C2343	U2344	G2345	A2346	C2347	C2350	C2359	A2360	C2364	A2369	C2374	G2375	A2376	A2377	A2378	G2383	G2384	C2385	G2389	U2390	G2391	A2392	C2394	U2401	C2402	C2403	C2404	G2405	U2406	G2410	A2411	G2415	C2416	C2417	A2418	U2419	C2420	U2423	C2424	A2425	G2429	A2430	U2431	A2432	A2433																		
A2434	A2435	U2438	A2439	C2440	C2441	C2442	G2443	G2444	C2445	U2446	C2447	A2448	A2451	G2455	C2456	A2459	U2460	C2466	A2469	G2470	C2474	C2475	A2476	C2477	G2481	G2482	C2483	G2484	G2487	G2490	U2491	U2492	U2493	G2494	G2495	C2496	A2497	C2498	C2499	U2500	C2501	G2502	A2503	A2504	G2505	U2506	C2507	G2508															
A2518	U2519	C2527	U2528	G2529	A2530	A2531	G2532	A2533	U2537	C2538	C2539	C2540	A2541	A2542	G2543	G2544	U2547	U2552	G2553	U2554	U2555	G2556	G2557	C2558	C2559	U2562	U2563	A2564	A2565	A2566	G2567	C2568	G2569	G2570	C2571	A2572	C2573	U2580	U2584	U2585	U2589	C2594	G2599	A2602	G2603	U2604	U2605	C2606															
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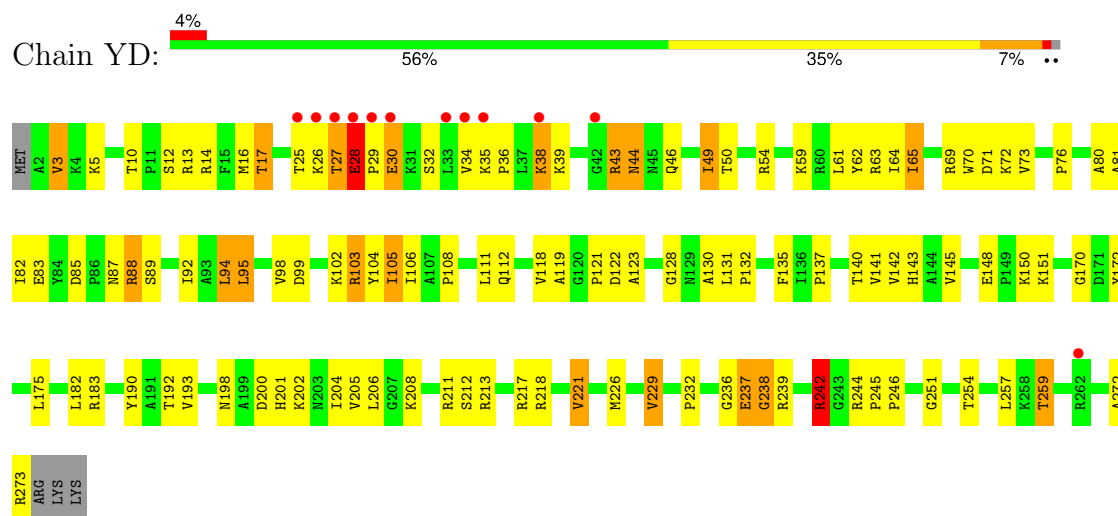




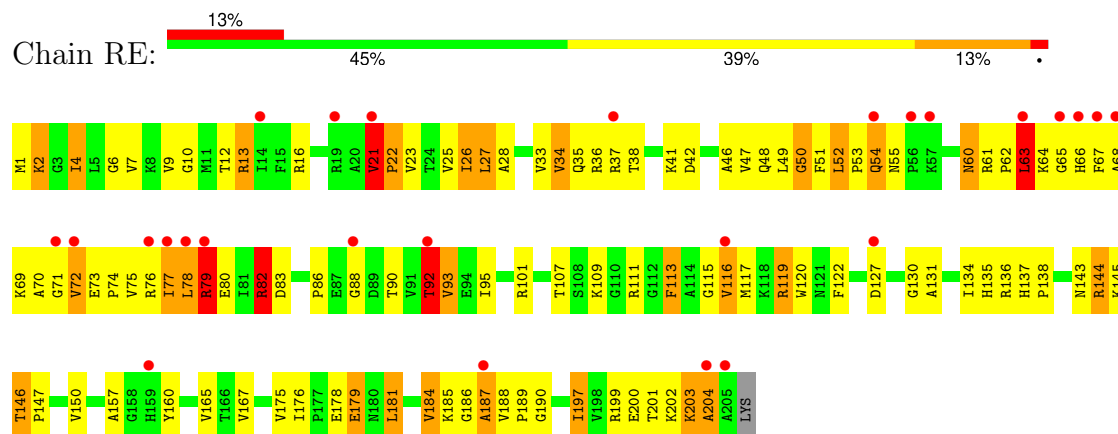
- Molecule 27: 50S ribosomal protein L2



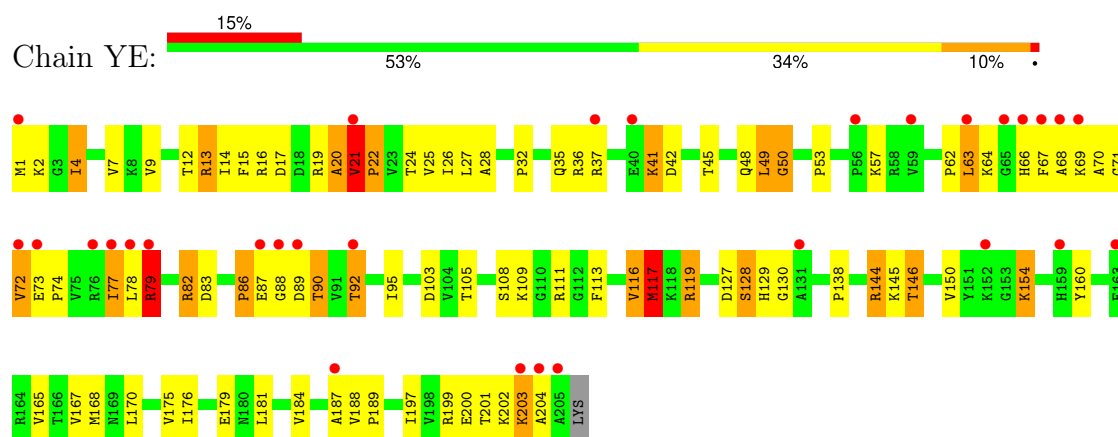
- Molecule 27: 50S ribosomal protein L2



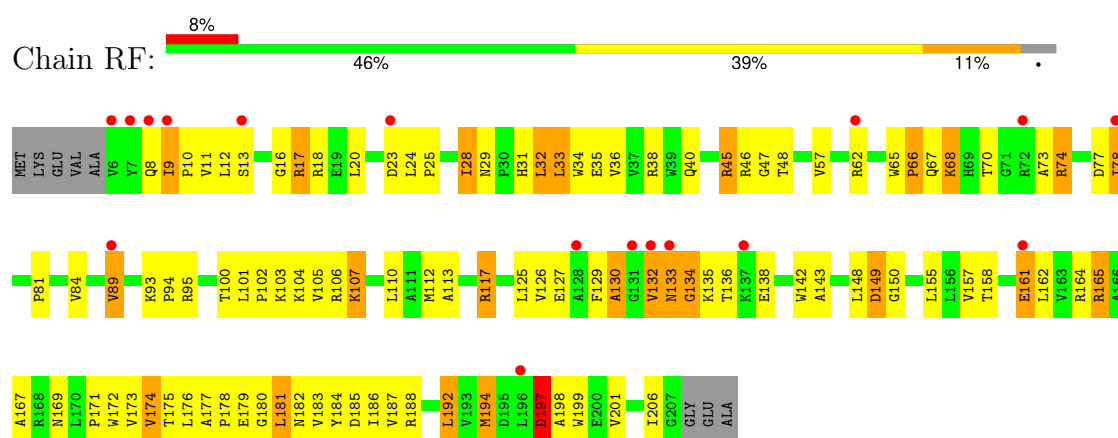
- Molecule 28: 50S ribosomal protein L3



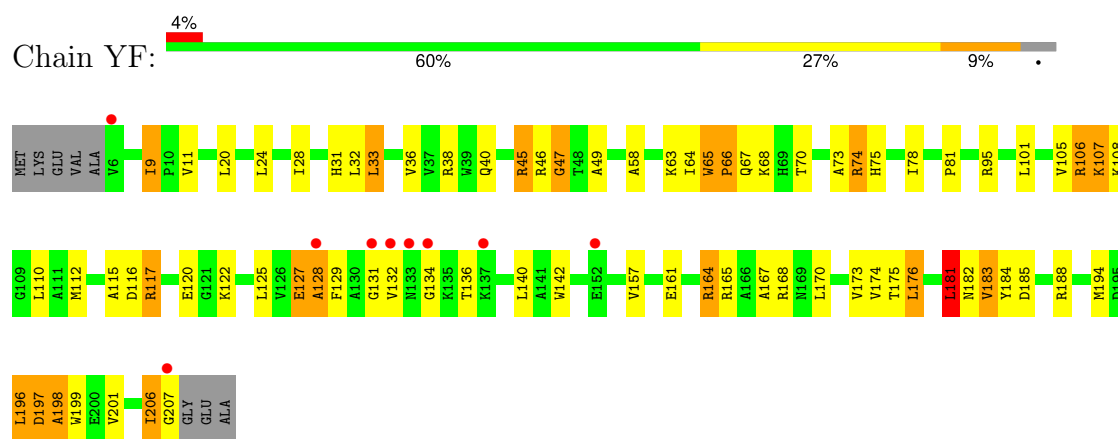
- Molecule 28: 50S ribosomal protein L3



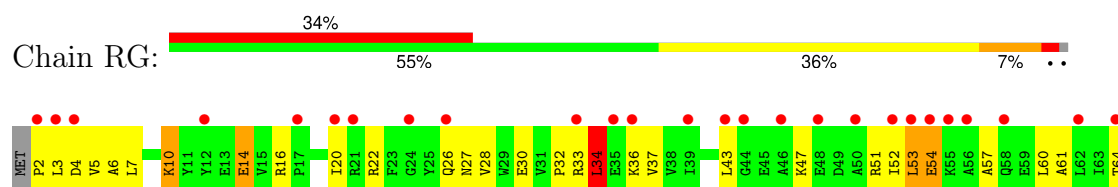
• Molecule 29: 50S ribosomal protein L4

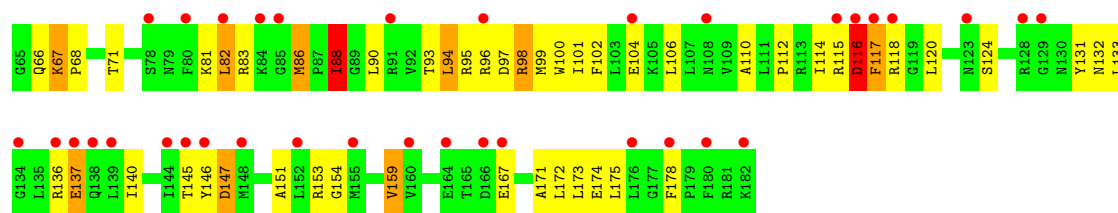


• Molecule 29: 50S ribosomal protein L4

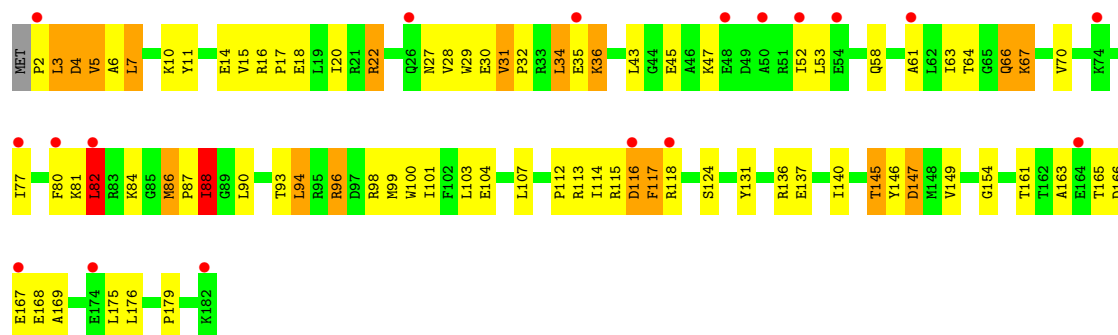


• Molecule 30: 50S ribosomal protein L5

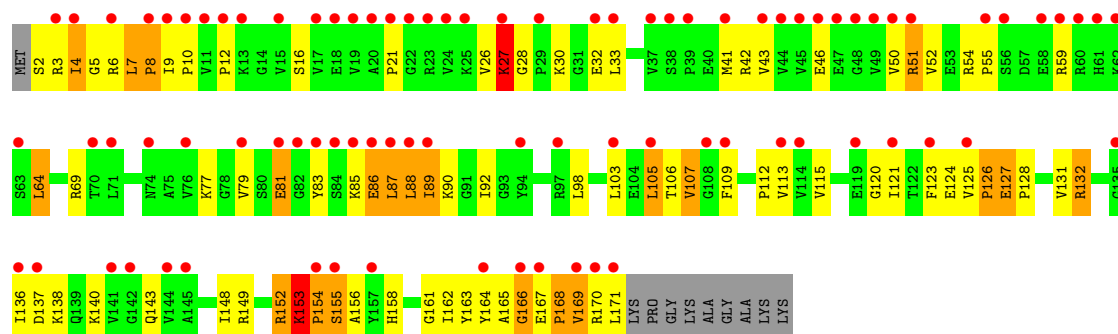




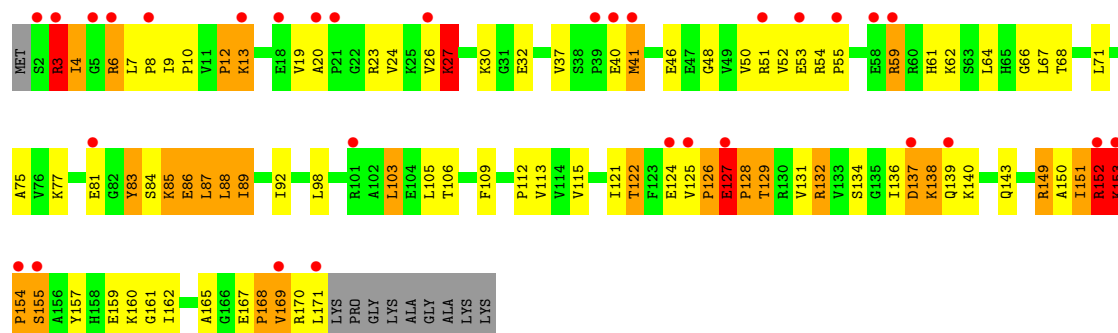
• Molecule 30: 50S ribosomal protein L5



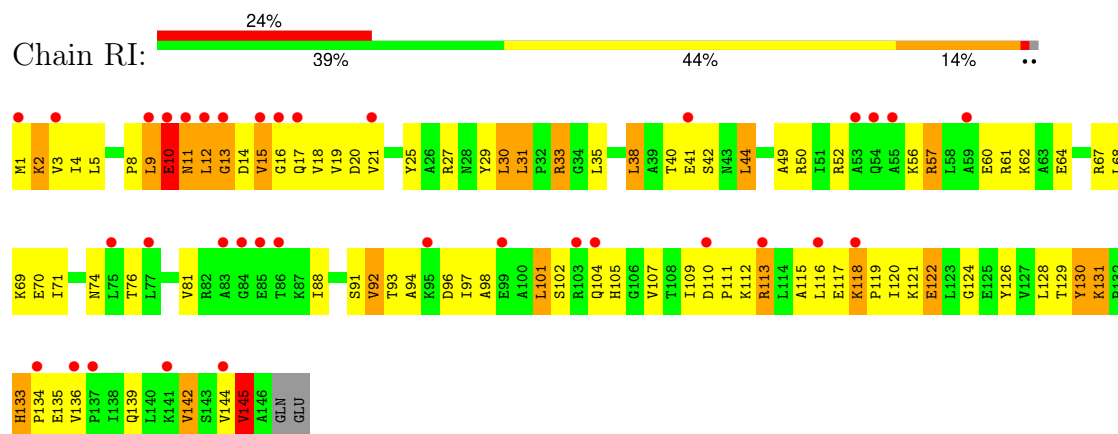
• Molecule 31: 50S ribosomal protein L6



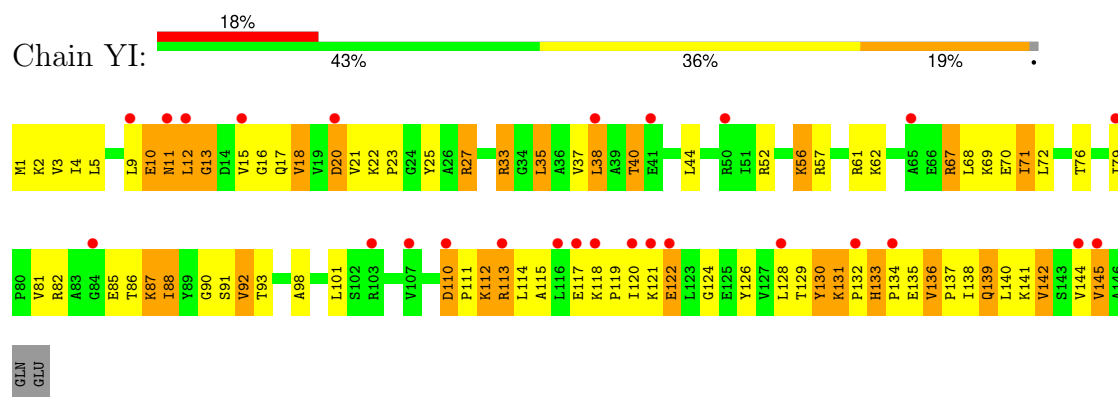
• Molecule 31: 50S ribosomal protein L6



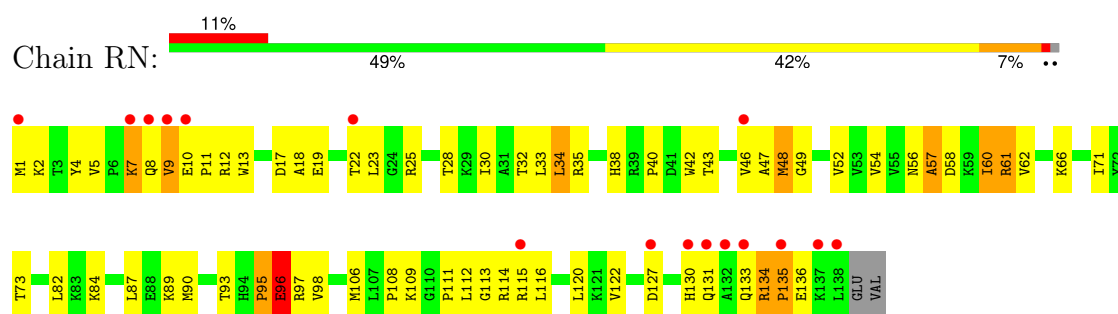
- Molecule 32: 50S ribosomal protein L9



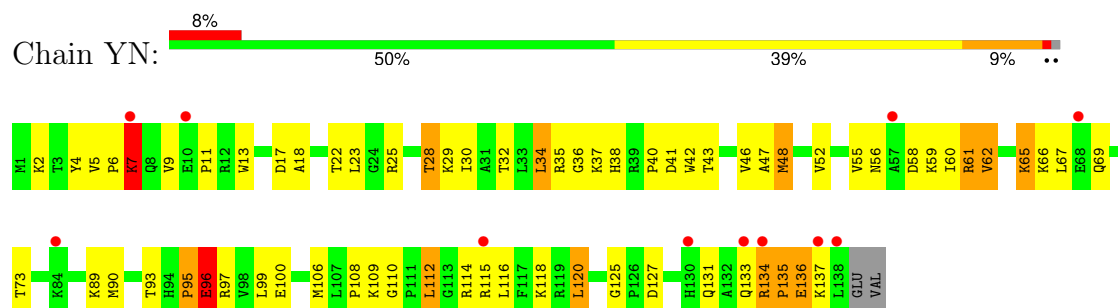
- Molecule 32: 50S ribosomal protein L9



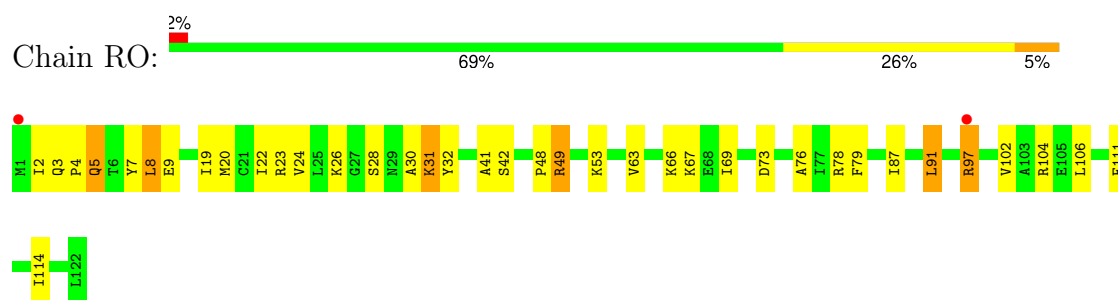
- Molecule 33: 50S ribosomal protein L13



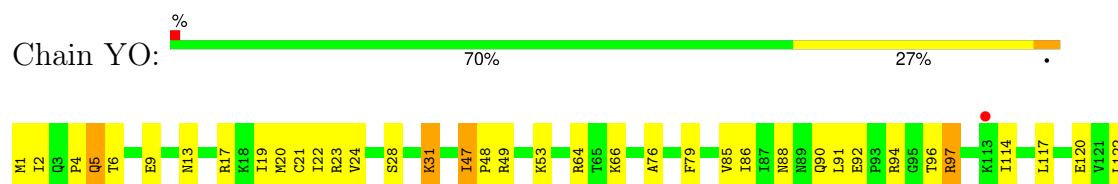
- Molecule 33: 50S ribosomal protein L13



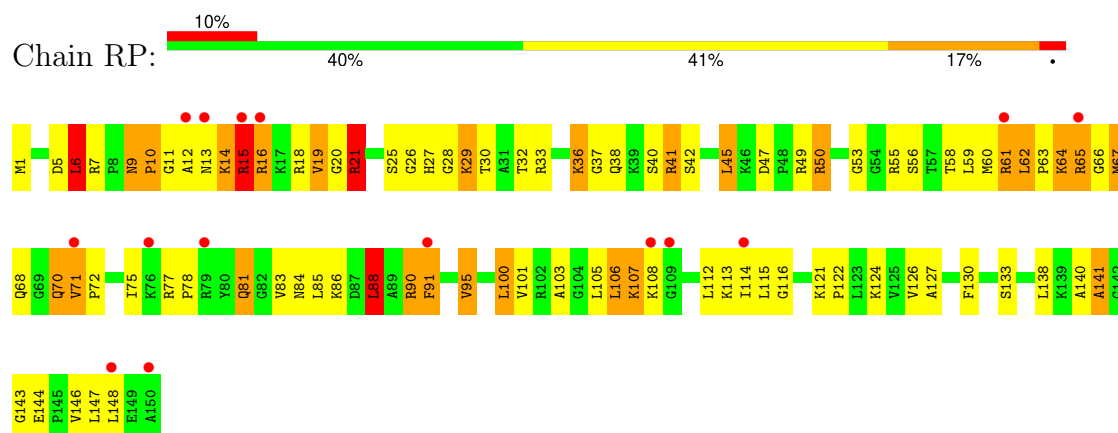
- Molecule 34: 50S ribosomal protein L14



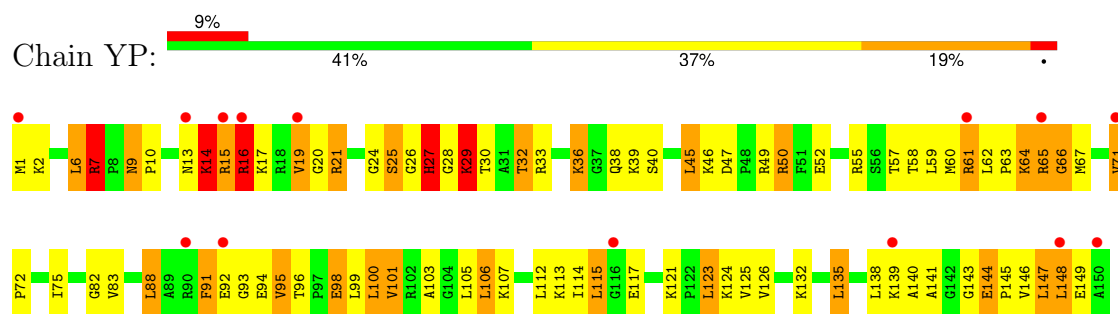
- Molecule 34: 50S ribosomal protein L14



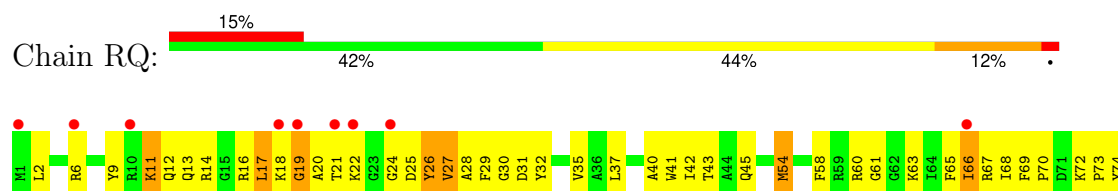
- Molecule 35: 50S ribosomal protein L15

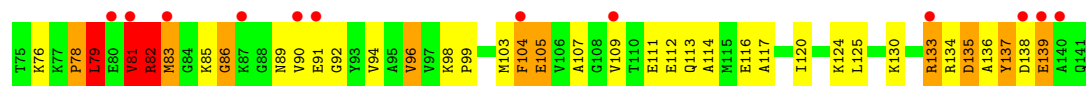


- Molecule 35: 50S ribosomal protein L15

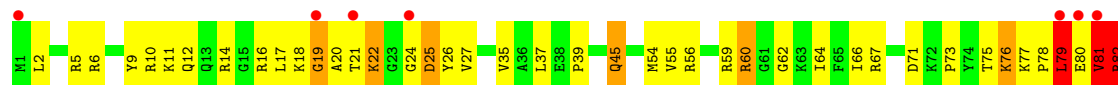


- Molecule 36: 50S ribosomal protein L16

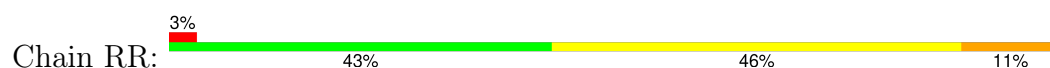




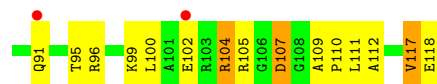
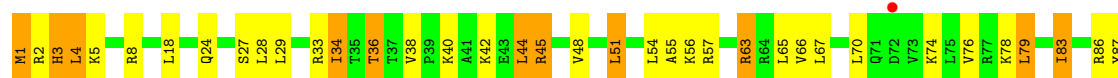
• Molecule 36: 50S ribosomal protein L16



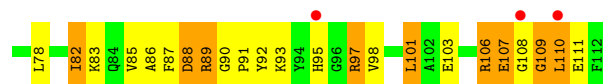
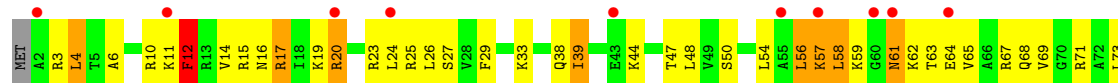
• Molecule 37: 50S ribosomal protein L17



• Molecule 37: 50S ribosomal protein L17

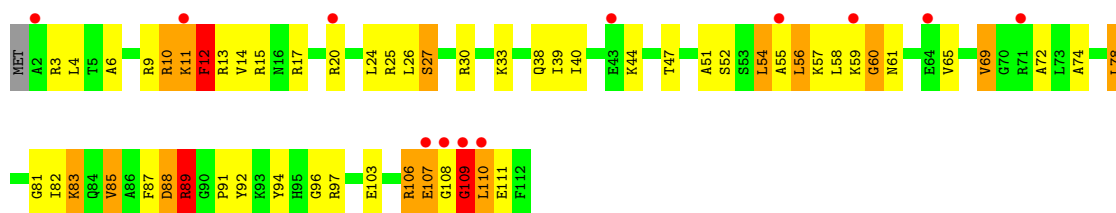


• Molecule 38: 50S ribosomal protein L18

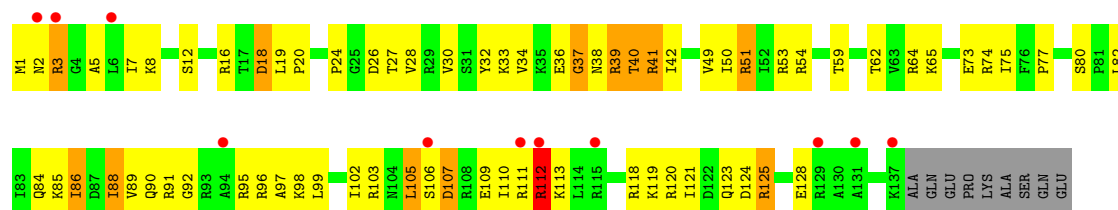


• Molecule 38: 50S ribosomal protein L18

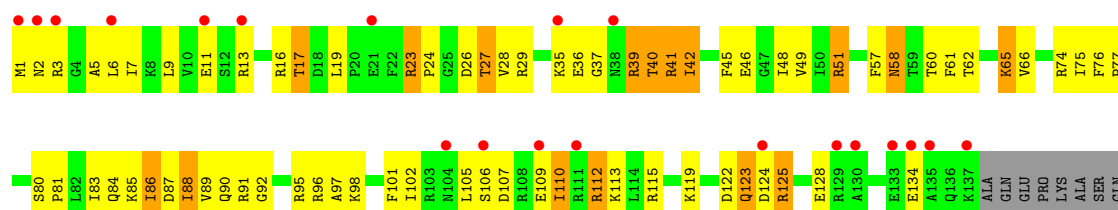
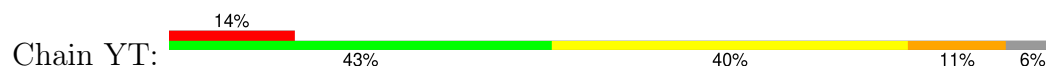




• Molecule 39: 50S ribosomal protein L19

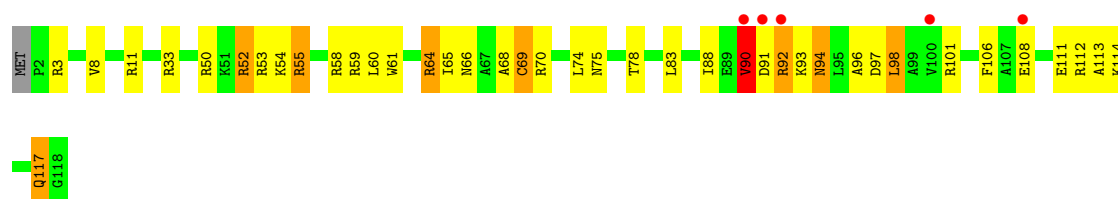


• Molecule 39: 50S ribosomal protein L19

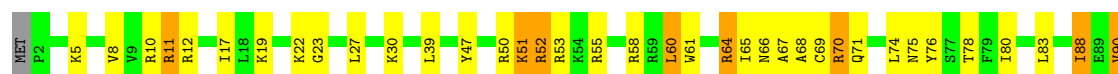


GLU

• Molecule 40: 50S ribosomal protein L20

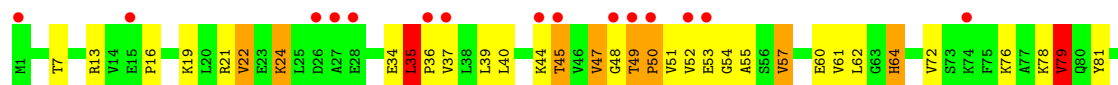


• Molecule 40: 50S ribosomal protein L20

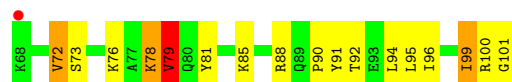
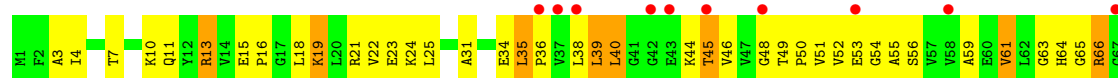
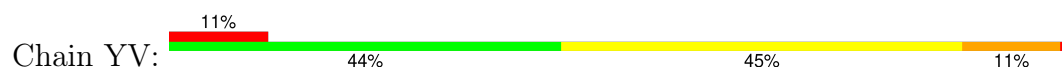




- Molecule 41: 50S ribosomal protein L21



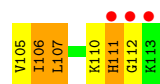
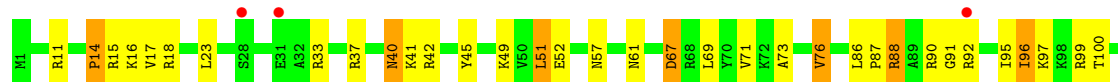
- Molecule 41: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L22

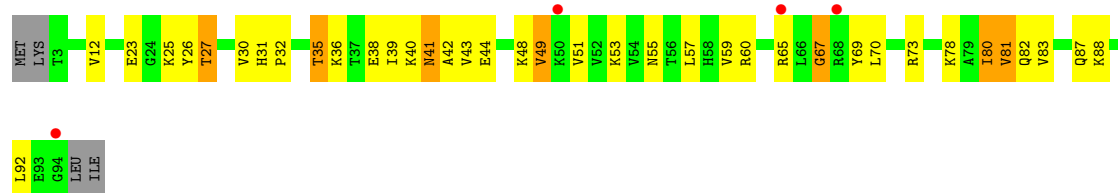


- Molecule 42: 50S ribosomal protein L22

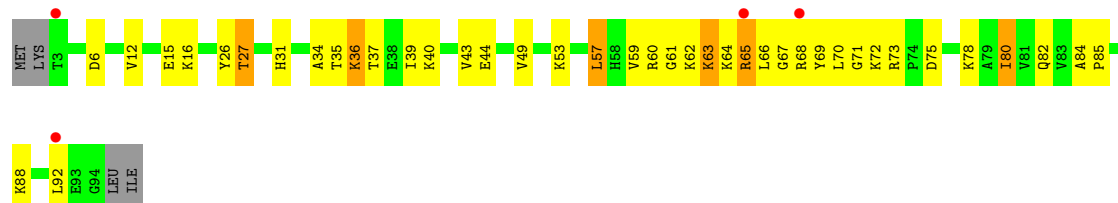


- Molecule 43: 50S ribosomal protein L23

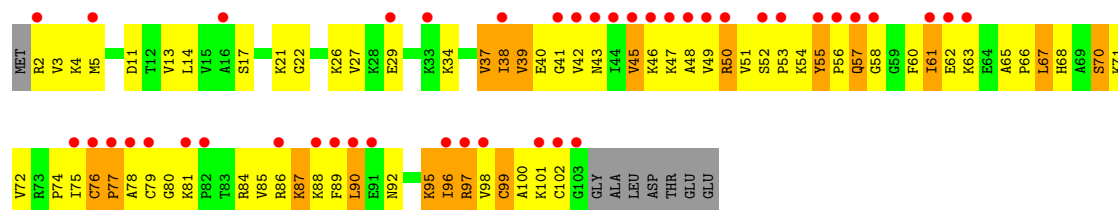




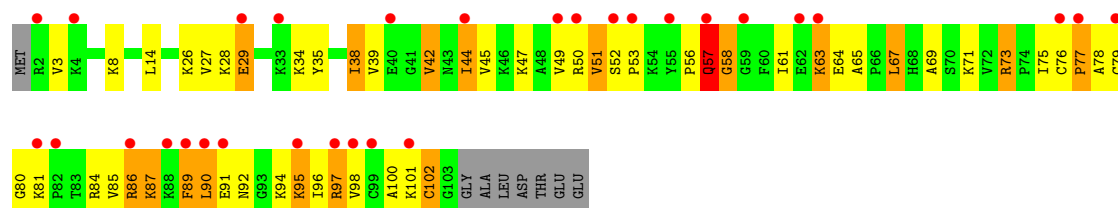
- Molecule 43: 50S ribosomal protein L23



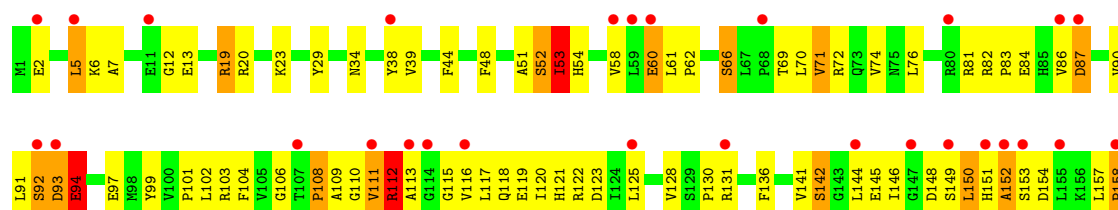
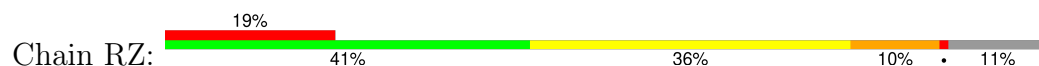
- Molecule 44: 50S ribosomal protein L24

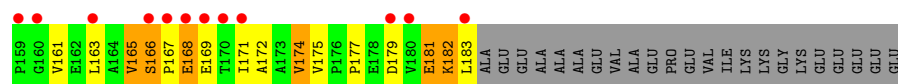


- Molecule 44: 50S ribosomal protein L24

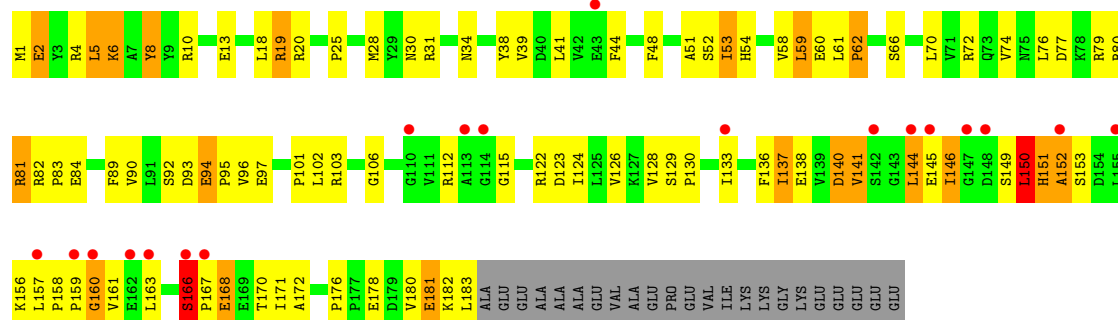
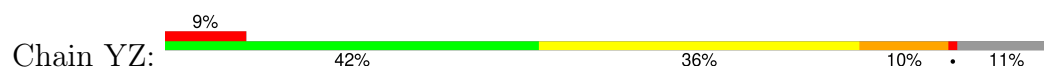


- Molecule 45: 50S ribosomal protein L25





- Molecule 45: 50S ribosomal protein L25



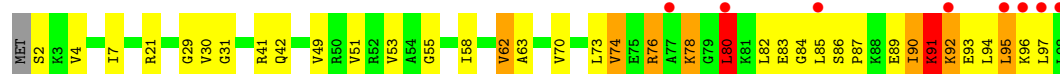
- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L28



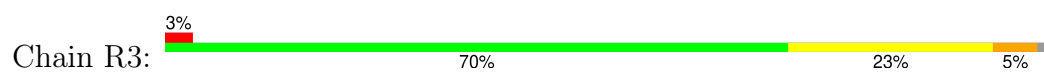
- Molecule 48: 50S ribosomal protein L29



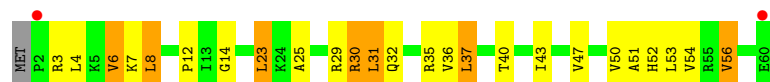
- Molecule 48: 50S ribosomal protein L29



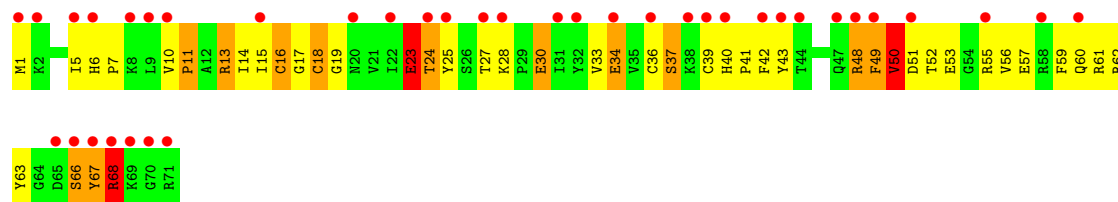
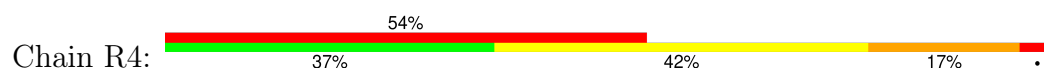
- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30



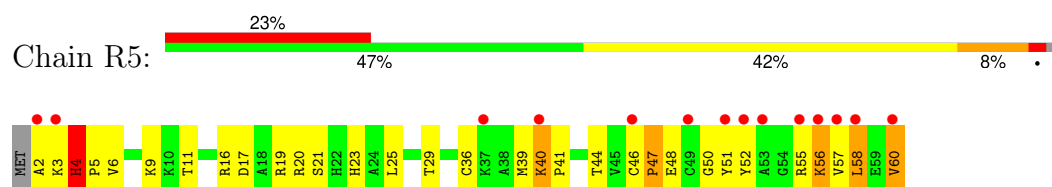
- Molecule 50: 50S ribosomal protein L31



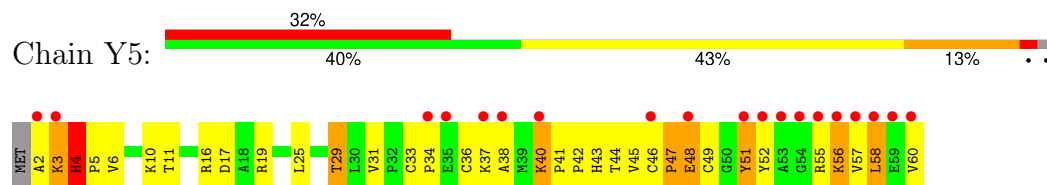
- Molecule 50: 50S ribosomal protein L31



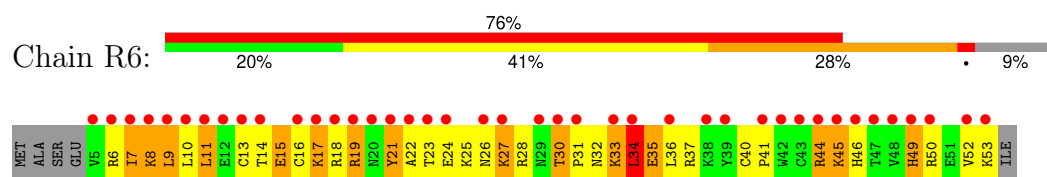
- Molecule 51: 50S ribosomal protein L32



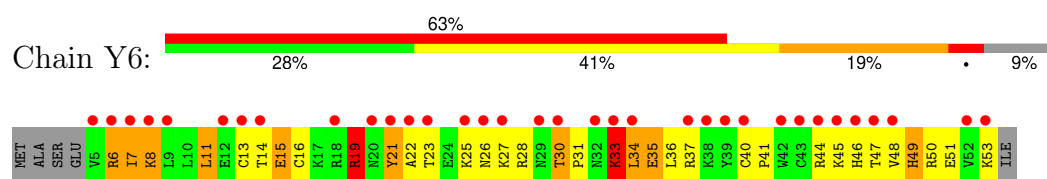
- Molecule 51: 50S ribosomal protein L32



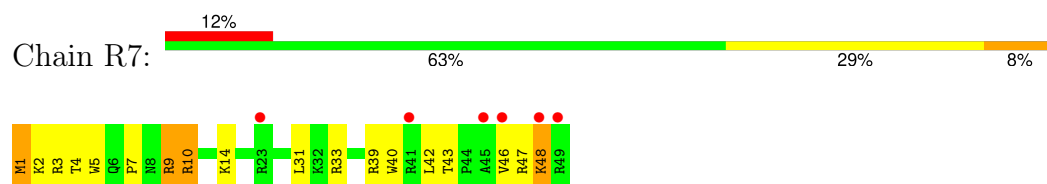
- Molecule 52: 50S ribosomal protein L33



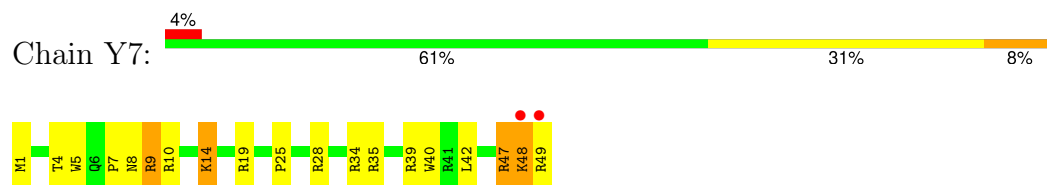
- Molecule 52: 50S ribosomal protein L33



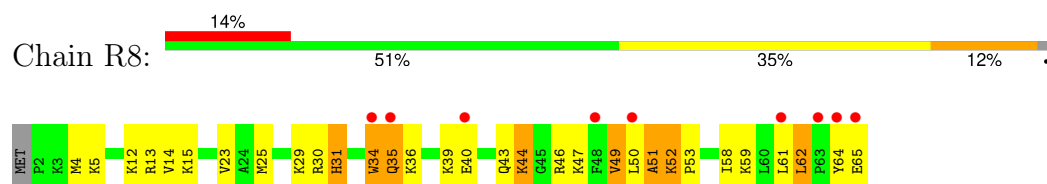
- Molecule 53: 50S ribosomal protein L34



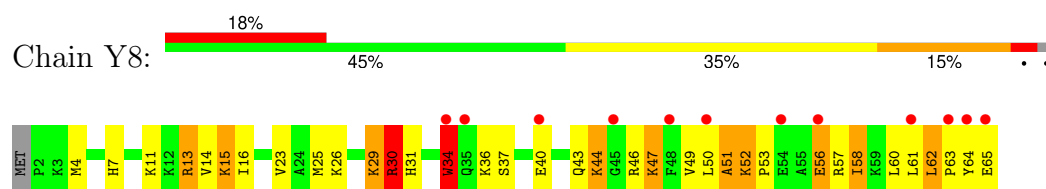
- Molecule 53: 50S ribosomal protein L34



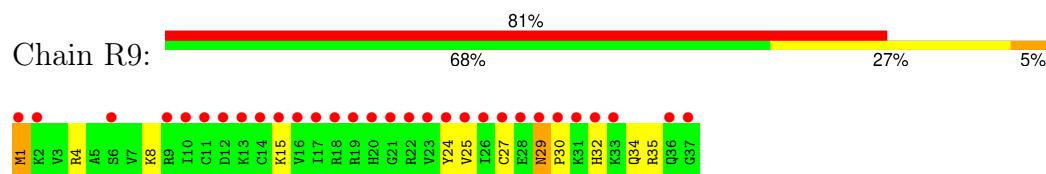
- Molecule 54: 50S ribosomal protein L35



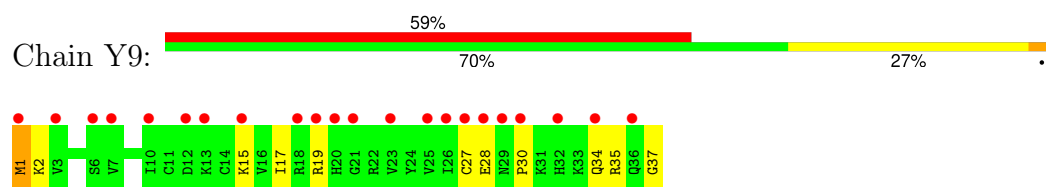
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- 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	209.81Å 449.41Å 620.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.22 – 2.94 155.22 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.6 (155.22-2.94) 98.6 (155.22-2.94)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.265 0.220 , 0.264	Depositor DCC
R_{free} test set	57063 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	291993	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: 1MG, PPU, ZN, PAR, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	QA	0.46	0/36098	1.01	71/56341 (0.1%)
1	XA	0.54	0/36101	1.09	114/56346 (0.2%)
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	0.36	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	0.33	0/1029	0.57	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.35	0/814	0.59	0/1095
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.38	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	0.36	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	0.53	0/992
15	XO	0.39	0/745	0.54	0/992
16	QP	0.36	0/721	0.56	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.35	0/847	0.53	0/1131
17	XQ	0.35	0/847	0.54	0/1131
18	QR	0.35	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.33	0/689	0.60	0/926
19	XS	0.37	0/689	0.69	1/926 (0.1%)
20	QT	0.35	0/765	0.63	0/1007
20	XT	0.31	0/765	0.59	0/1007
21	QU	0.30	0/221	0.54	0/288
21	XU	0.31	0/221	0.61	0/288
22	QV	0.52	1/1836 (0.1%)	0.98	4/2859 (0.1%)
22	XV	0.59	1/1836 (0.1%)	1.06	4/2859 (0.1%)
23	QY	0.34	0/333	0.91	0/517
23	XY	0.40	0/333	0.94	0/517
24	QX	0.44	0/185	1.15	2/285 (0.7%)
24	XX	0.67	0/185	1.08	0/285
25	RA	0.63	8/69521 (0.0%)	1.16	318/108529 (0.3%)
25	YA	0.72	19/69543 (0.0%)	1.26	504/108563 (0.5%)
26	RB	0.49	0/2878	1.05	6/4490 (0.1%)
26	YB	0.56	0/2878	1.15	18/4490 (0.4%)
27	RD	0.50	0/2165	0.70	0/2919
27	YD	0.58	0/2165	0.78	1/2919 (0.0%)
28	RE	0.43	0/1601	0.73	3/2160 (0.1%)
28	YE	0.46	0/1601	0.75	2/2160 (0.1%)
29	RF	0.42	0/1620	0.62	0/2194
29	YF	0.48	0/1620	0.71	1/2194 (0.0%)
30	RG	0.31	0/1499	0.57	1/2016 (0.0%)
30	YG	0.39	0/1499	0.60	0/2016
31	RH	0.28	0/1332	0.58	0/1802
31	YH	0.45	0/1332	0.73	0/1802
32	RI	0.35	0/1151	0.67	0/1558
32	YI	0.35	0/1151	0.66	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.43	0/1131	0.64	0/1525
34	RO	0.41	0/943	0.62	1/1269 (0.1%)
34	YO	0.49	0/943	0.65	0/1269
35	RP	0.43	0/1162	0.81	1/1544 (0.1%)
35	YP	0.49	0/1162	0.90	2/1544 (0.1%)
36	RQ	0.47	0/1143	0.73	2/1527 (0.1%)
36	YQ	0.57	0/1143	0.80	1/1527 (0.1%)
37	RR	0.42	0/982	0.69	0/1312
37	YR	0.44	0/982	0.73	0/1312
38	RS	0.36	0/892	0.64	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.40	0/892	0.75	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.44	0/1155	0.67	0/1542
40	RU	0.39	0/982	0.65	0/1306
40	YU	0.50	0/982	0.68	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.45	0/790	0.73	1/1057 (0.1%)
42	RW	0.49	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.50	0/739	0.66	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.46	0/798	0.69	0/1064
45	RZ	0.34	0/1493	0.59	0/2026
45	YZ	0.37	0/1493	0.64	2/2026 (0.1%)
46	R0	0.45	0/657	0.65	0/874
46	Y0	0.48	0/657	0.69	0/874
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.39	0/583	0.65	0/771
48	Y2	0.52	0/583	0.73	0/771
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.41	0/474	0.59	0/635
50	R4	0.33	0/594	0.68	0/795
50	Y4	0.37	0/594	0.68	0/795
51	R5	0.43	0/473	0.73	0/639
51	Y5	0.43	0/473	0.77	1/639 (0.2%)
52	R6	0.35	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.68	0/575
53	Y7	0.57	0/438	0.71	0/575
54	R8	0.55	0/525	0.79	0/691
54	Y8	0.58	0/525	0.82	0/691
55	R9	0.26	0/310	0.45	0/407
55	Y9	0.32	0/310	0.48	0/407
56	Z6	0.80	0/40	1.80	1/60 (1.7%)
56	Z8	0.78	0/40	1.81	1/60 (1.7%)
All	All	0.56	29/316367 (0.0%)	1.04	1068/472979 (0.2%)

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
28	RE	0	1
28	YE	0	1
29	YF	0	1
31	RH	0	2
31	YH	0	2
38	YS	0	1
45	YZ	0	1
48	Y2	0	1
54	R8	0	2
54	Y8	0	2
All	All	0	16

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.50	1.48	1.61
22	XV	0	C	OP3-P	-10.49	1.48	1.61
25	YA	528	A	N9-C4	-9.10	1.32	1.37
25	YA	783	A	N9-C4	-7.66	1.33	1.37
25	YA	783	A	N3-C4	-7.55	1.30	1.34

The worst 5 of 1068 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	1786	A	N7-C8-N9	13.21	120.41	113.80
25	YA	528	A	C2-N3-C4	-13.10	104.05	110.60
25	YA	783	A	C2-N3-C4	-12.39	104.41	110.60
25	YA	1786	A	C5-N7-C8	-12.26	97.77	103.90
25	YA	1786	A	C2-N3-C4	-11.73	104.73	110.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
54	R8	30	ARG	Peptide
28	RE	21	VAL	Peptide
31	RH	127	GLU	Peptide
31	RH	153	LYS	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	16278	492	0
1	XA	32249	0	16279	529	1
2	QB	1924	0	1975	64	0
2	XB	1924	0	1975	80	0
3	QC	1605	0	1668	41	0
3	XC	1605	0	1668	63	0
4	QD	1703	0	1763	63	0
4	XD	1703	0	1764	47	0
5	QE	1155	0	1213	28	0
5	XE	1155	0	1213	42	0
6	QF	843	0	857	20	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	37	0
7	XG	1257	0	1296	24	0
8	QH	1116	0	1175	37	0
8	XH	1116	0	1177	25	0
9	QI	1010	0	1037	34	0
9	XI	1010	0	1037	50	0
10	QJ	801	0	849	48	0
10	XJ	801	0	849	42	0
11	QK	885	0	904	25	0
11	XK	885	0	904	28	0
12	QL	975	0	1062	35	0
12	XL	975	0	1062	46	0
13	QM	964	0	1034	40	0
13	XM	964	0	1034	39	0
14	QN	492	0	529	24	0
14	XN	492	0	529	17	0
15	QO	734	0	771	21	0
15	XO	734	0	771	19	0
16	QP	705	0	725	18	0
16	XP	705	0	725	26	0
17	QQ	834	0	904	19	0
17	XQ	834	0	904	19	0
18	QR	574	0	644	11	0
18	XR	574	0	644	21	0
19	QS	674	0	699	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	44	0
20	QT	763	0	860	26	0
20	XT	763	0	861	36	0
21	QU	217	0	234	11	0
21	XU	217	0	234	4	0
22	QV	1644	0	836	26	0
22	XV	1644	0	836	18	0
23	QY	323	0	165	3	0
23	XY	323	0	165	4	0
24	QX	167	0	87	0	0
24	XX	167	0	87	0	0
25	RA	62071	0	31288	921	1
25	YA	62091	0	31295	872	0
26	RB	2573	0	1306	40	1
26	YB	2573	0	1306	32	0
27	RD	2115	0	2195	96	0
27	YD	2115	0	2195	97	0
28	RE	1568	0	1634	72	0
28	YE	1568	0	1634	64	0
29	RF	1585	0	1632	80	0
29	YF	1585	0	1632	64	0
30	RG	1474	0	1535	54	0
30	YG	1474	0	1535	57	0
31	RH	1307	0	1382	61	0
31	YH	1307	0	1382	66	0
32	RI	1136	0	1223	59	1
32	YI	1136	0	1223	49	0
33	RN	1104	0	1180	40	0
33	YN	1104	0	1180	50	0
34	RO	933	0	996	26	0
34	YO	933	0	996	25	0
35	RP	1145	0	1227	87	0
35	YP	1145	0	1227	94	0
36	RQ	1122	0	1179	61	0
36	YQ	1122	0	1178	48	0
37	RR	968	0	1033	48	0
37	YR	968	0	1033	36	0
38	RS	882	0	943	48	0
38	YS	882	0	943	40	0
39	RT	1141	0	1202	53	0
39	YT	1141	0	1202	50	0
40	RU	964	0	1022	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YU	964	0	1022	58	0
41	RV	779	0	852	20	0
41	YV	779	0	852	42	0
42	RW	900	0	964	27	0
42	YW	900	0	964	28	0
43	RX	725	0	778	28	0
43	YX	725	0	778	25	0
44	RY	785	0	878	52	0
44	YY	785	0	878	39	0
45	RZ	1461	0	1493	59	0
45	YZ	1461	0	1493	56	0
46	R0	648	0	672	20	0
46	Y0	648	0	672	27	0
47	R1	763	0	848	26	0
47	Y1	763	0	848	28	0
48	R2	581	0	629	19	0
48	Y2	581	0	629	26	0
49	R3	469	0	518	7	0
49	Y3	469	0	518	17	0
50	R4	581	0	574	25	0
50	Y4	581	0	574	45	0
51	R5	459	0	480	25	0
51	Y5	459	0	480	33	0
52	R6	424	0	450	27	0
52	Y6	424	0	450	30	0
53	R7	430	0	480	14	0
53	Y7	430	0	480	17	0
54	R8	517	0	582	30	0
54	Y8	517	0	582	40	0
55	R9	307	0	338	9	0
55	Y9	307	0	338	7	0
56	Z6	74	0	51	6	0
56	Z8	74	0	51	5	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	RA	242	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RR	1	0	0	0	0
57	RU	1	0	0	0	0
57	XA	72	0	0	0	0
57	XM	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y5	1	0	0	0	0
57	YA	268	0	0	0	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	1	0	0	0	0
57	YX	1	0	0	0	0
58	QA	42	0	45	2	0
58	XA	42	0	45	1	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291993	0	198359	5830	2

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

The worst 5 of 5830 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)
4:QD:22:LYS:HG3	4:QD:26:CYS:SG	1.85	1.16
25:RA:2701:C:H3'	25:RA:2702:U:H5''	1.30	1.13
25:YA:2701:C:H3'	25:YA:2702:U:H5''	1.32	1.07
25:RA:1359:A:N6	25:RA:1372:U:O4	1.87	1.07
27:YD:43:ARG:NH1	27:YD:44:ASN:OD1	1.86	1.06

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:1593:G:O2'	26:RB:54:G:OP1[1_655]	2.12	0.08
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	175 (74%)	43 (18%)	17 (7%)	1	1
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	2
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	3	9
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	8	24
4	QD	206/209 (99%)	175 (85%)	25 (12%)	6 (3%)	3	10
4	XD	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	5	14
5	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	3	7
5	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	6	17
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%)	10	26
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	10	26
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	19	41
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	3	10
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	2	5
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	3	8
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	3	9
10	XJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	1	3
11	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	4	12
11	XK	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	7	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	1	2
12	XL	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	1
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	1
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	1
14	QN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	1
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	1
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	11	28
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	15
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	11	28
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	11	28
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	6	17
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	4
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	24
19	QS	82/93 (88%)	56 (68%)	15 (18%)	11 (13%)	0	0
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	0
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	2
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	1	2
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	4
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	4
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	4
27	YD	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	3	8
28	RE	203/206 (98%)	147 (72%)	36 (18%)	20 (10%)	0	1
28	YE	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	0	1
29	RF	200/210 (95%)	167 (84%)	20 (10%)	13 (6%)	1	2
29	YF	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	2	5
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	1
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	1
31	RH	168/180 (93%)	114 (68%)	33 (20%)	21 (12%)	0	0
31	YH	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	0
32	RI	144/148 (97%)	101 (70%)	30 (21%)	13 (9%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	YI	144/148 (97%)	104 (72%)	23 (16%)	17 (12%)	0	0
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	0	1
33	YN	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	1
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	21
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	7	21
35	RP	148/150 (99%)	106 (72%)	28 (19%)	14 (10%)	0	1
35	YP	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	0	0
36	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	0
36	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	0
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	4
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	1	3
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	1
38	YS	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	0	0
39	RT	135/146 (92%)	106 (78%)	17 (13%)	12 (9%)	0	1
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	1
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	7
40	YU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	7
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	2
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	1
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3	7
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	7	20
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	16
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	5	16
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	0
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	0
45	RZ	181/206 (88%)	124 (68%)	32 (18%)	25 (14%)	0	0
45	YZ	181/206 (88%)	124 (68%)	40 (22%)	17 (9%)	0	1
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	10	26
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	1
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1	1
48	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	0	1
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	7
49	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	7	20
50	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
51	R5	57/60 (95%)	44 (77%)	11 (19%)	2 (4%)	3	7
51	Y5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	7
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	0
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	0
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	16
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	5	16
54	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	1
54	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	2
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	9215 (80%)	1533 (13%)	722 (6%)	1	2

5 of 722 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	4
2	XB	205/220 (93%)	180 (88%)	25 (12%)	4	11
3	QC	159/188 (85%)	145 (91%)	14 (9%)	8	21
3	XC	159/188 (85%)	146 (92%)	13 (8%)	9	23
4	QD	180/181 (99%)	157 (87%)	23 (13%)	3	10
4	XD	180/181 (99%)	154 (86%)	26 (14%)	2	7
5	QE	116/123 (94%)	104 (90%)	12 (10%)	6	16
5	XE	116/123 (94%)	104 (90%)	12 (10%)	6	16
6	QF	90/90 (100%)	78 (87%)	12 (13%)	3	9
6	XF	90/90 (100%)	82 (91%)	8 (9%)	8	20
7	QG	126/127 (99%)	114 (90%)	12 (10%)	7	18
7	XG	126/127 (99%)	114 (90%)	12 (10%)	7	18
8	QH	119/119 (100%)	109 (92%)	10 (8%)	9	22
8	XH	119/119 (100%)	106 (89%)	13 (11%)	5	14
9	QI	98/99 (99%)	81 (83%)	17 (17%)	1	3
9	XI	98/99 (99%)	80 (82%)	18 (18%)	1	3
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	3	8
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	1	4
11	QK	90/99 (91%)	81 (90%)	9 (10%)	6	17
11	XK	90/99 (91%)	81 (90%)	9 (10%)	6	17
12	QL	104/109 (95%)	87 (84%)	17 (16%)	2	4
12	XL	104/109 (95%)	93 (89%)	11 (11%)	5	15
13	QM	97/101 (96%)	73 (75%)	24 (25%)	0	0
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	2
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	3
14	XN	49/50 (98%)	42 (86%)	7 (14%)	2	7
15	QO	79/80 (99%)	72 (91%)	7 (9%)	8	20
15	XO	79/80 (99%)	69 (87%)	10 (13%)	3	10
16	QP	72/74 (97%)	63 (88%)	9 (12%)	3	10
16	XP	72/74 (97%)	64 (89%)	8 (11%)	5	13
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	9	22
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	15	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	50 (82%)	11 (18%)	1	3
18	XR	61/77 (79%)	52 (85%)	9 (15%)	2	6
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	2
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	1
20	QT	76/82 (93%)	67 (88%)	9 (12%)	4	12
20	XT	76/82 (93%)	66 (87%)	10 (13%)	3	9
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	20	42
27	RD	214/218 (98%)	175 (82%)	39 (18%)	1	3
27	YD	214/218 (98%)	181 (85%)	33 (15%)	2	5
28	RE	165/166 (99%)	126 (76%)	39 (24%)	0	0
28	YE	165/166 (99%)	137 (83%)	28 (17%)	1	4
29	RF	161/166 (97%)	132 (82%)	29 (18%)	1	3
29	YF	161/166 (97%)	137 (85%)	24 (15%)	2	6
30	RG	155/156 (99%)	134 (86%)	21 (14%)	3	8
30	YG	155/156 (99%)	133 (86%)	22 (14%)	2	7
31	RH	142/148 (96%)	121 (85%)	21 (15%)	2	6
31	YH	142/148 (96%)	115 (81%)	27 (19%)	1	2
32	RI	122/124 (98%)	99 (81%)	23 (19%)	1	2
32	YI	122/124 (98%)	92 (75%)	30 (25%)	0	0
33	RN	117/119 (98%)	97 (83%)	20 (17%)	1	3
33	YN	117/119 (98%)	96 (82%)	21 (18%)	1	3
34	RO	100/100 (100%)	90 (90%)	10 (10%)	6	17
34	YO	100/100 (100%)	89 (89%)	11 (11%)	5	13
35	RP	116/116 (100%)	85 (73%)	31 (27%)	0	0
35	YP	116/116 (100%)	82 (71%)	34 (29%)	0	0
36	RQ	111/111 (100%)	95 (86%)	16 (14%)	2	7
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	1	3
37	RR	101/101 (100%)	83 (82%)	18 (18%)	1	3
37	YR	101/101 (100%)	80 (79%)	21 (21%)	1	1
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	YS	87/88 (99%)	68 (78%)	19 (22%)	1	1
39	RT	120/127 (94%)	102 (85%)	18 (15%)	2	6
39	YT	120/127 (94%)	98 (82%)	22 (18%)	1	3
40	RU	93/94 (99%)	78 (84%)	15 (16%)	2	4
40	YU	93/94 (99%)	77 (83%)	16 (17%)	1	3
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	2
41	YV	82/82 (100%)	67 (82%)	15 (18%)	1	3
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	1
42	YW	92/92 (100%)	76 (83%)	16 (17%)	1	3
43	RX	74/78 (95%)	64 (86%)	10 (14%)	3	8
43	YX	74/78 (95%)	60 (81%)	14 (19%)	1	2
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	0
44	YY	85/91 (93%)	64 (75%)	21 (25%)	0	0
45	RZ	162/179 (90%)	133 (82%)	29 (18%)	1	3
45	YZ	162/179 (90%)	130 (80%)	32 (20%)	1	2
46	R0	65/67 (97%)	60 (92%)	5 (8%)	10	25
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	7	19
47	R1	82/83 (99%)	73 (89%)	9 (11%)	5	13
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	2	7
48	R2	64/67 (96%)	57 (89%)	7 (11%)	5	14
48	Y2	64/67 (96%)	47 (73%)	17 (27%)	0	0
49	R3	51/52 (98%)	45 (88%)	6 (12%)	4	12
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	5
50	R4	63/63 (100%)	45 (71%)	18 (29%)	0	0
50	Y4	63/63 (100%)	43 (68%)	20 (32%)	0	0
51	R5	51/52 (98%)	37 (72%)	14 (28%)	0	0
51	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	0
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	0
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	1
53	R7	42/42 (100%)	34 (81%)	8 (19%)	1	2
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	R8	54/55 (98%)	44 (82%)	10 (18%)	1	3
54	Y8	54/55 (98%)	41 (76%)	13 (24%)	0	0
55	R9	34/34 (100%)	32 (94%)	2 (6%)	16	36
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	16	36
All	All	9702/10066 (96%)	8152 (84%)	1550 (16%)	2	5

5 of 1550 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	XL	81	SER
31	YH	152	ARG
14	XN	40	CYS
12	XL	62	SER
27	YD	217	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
55	R9	29	ASN
2	XB	204	ASN
2	XB	19	HIS
2	XB	212	GLN
13	QM	92	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	304 (20%)	48 (3%)
1	XA	1498/1522 (98%)	311 (20%)	50 (3%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QY	14/17 (82%)	5 (35%)	1 (7%)
23	XY	14/17 (82%)	6 (42%)	1 (7%)
24	QX	7/25 (28%)	3 (42%)	2 (28%)
24	XX	7/25 (28%)	1 (14%)	0
25	RA	2879/2916 (98%)	659 (22%)	74 (2%)
25	YA	2880/2916 (98%)	623 (21%)	75 (2%)
26	RB	119/122 (97%)	29 (24%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	YB	119/122 (97%)	29 (24%)	3 (2%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9364 (98%)	2008 (21%)	258 (2%)

5 of 2008 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	29	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 258 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	1819	A
25	YA	2126	A
25	RA	1608	A
25	RA	1312	U
25	YA	2439	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	PPU	Z6	76	56,25	33,40,41	2.68	8 (24%)	33,57,60	2.65	8 (24%)
56	PPU	Z8	76	56,25	33,40,41	2.67	8 (24%)	33,57,60	2.63	8 (24%)
23	1MG	QY	37	23	19,26,27	2.49	3 (15%)	18,39,42	2.20	5 (27%)
23	1MG	XY	37	23	19,26,27	2.49	3 (15%)	18,39,42	2.12	5 (27%)

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	56,25	-	2/21/43/44	0/4/4/4
56	PPU	Z8	76	56,25	-	2/21/43/44	0/4/4/4
23	1MG	QY	37	23	-	0/3/25/26	0/3/3/3
23	1MG	XY	37	23	-	0/3/25/26	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.65	1.41	1.23
56	Z8	76	PPU	O-C	9.58	1.41	1.23
23	XY	37	1MG	C2-N2	7.98	1.48	1.34
23	QY	37	1MG	C2-N2	7.76	1.47	1.34
56	Z6	76	PPU	C9-N6	-6.23	1.31	1.45

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.55	110.19	123.20
56	Z8	76	PPU	C3'-N3'-C	-8.53	110.22	123.20
23	QY	37	1MG	N2-C2-N1	6.47	123.99	118.79
23	XY	37	1MG	N2-C2-N1	5.83	123.47	118.79
56	Z8	76	PPU	N3-C2-N1	-5.38	121.37	128.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z6	76	PPU	O-C-CA-N
56	Z8	76	PPU	O-C-CA-N
56	Z6	76	PPU	N3'-C-CA-N
56	Z8	76	PPU	N3'-C-CA-N

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	76	PPU	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 683 ligands modelled in this entry, 681 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	PAR	XA	1673	-	44,45,45	1.33	6 (13%)	63,67,67	1.30	4 (6%)
58	PAR	QA	1666	-	44,45,45	1.28	6 (13%)	63,67,67	1.33	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	XA	1673	-	-	6/18/94/94	0/4/4/4
58	PAR	QA	1666	-	-	8/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C52-C42	3.13	1.58	1.52
58	XA	1673	PAR	C52-C42	3.00	1.58	1.52
58	XA	1673	PAR	O54-C14	2.86	1.49	1.41
58	XA	1673	PAR	C11-C21	2.86	1.57	1.52
58	QA	1666	PAR	O54-C14	2.85	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1673	PAR	O33-C14-C24	5.04	116.32	108.08
58	XA	1673	PAR	C14-O54-C54	4.32	122.16	113.72
58	QA	1666	PAR	O33-C14-C24	4.04	114.69	108.08
58	QA	1666	PAR	C14-O54-C54	3.84	121.21	113.72
58	QA	1666	PAR	O11-C42-C52	3.16	115.44	107.42

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

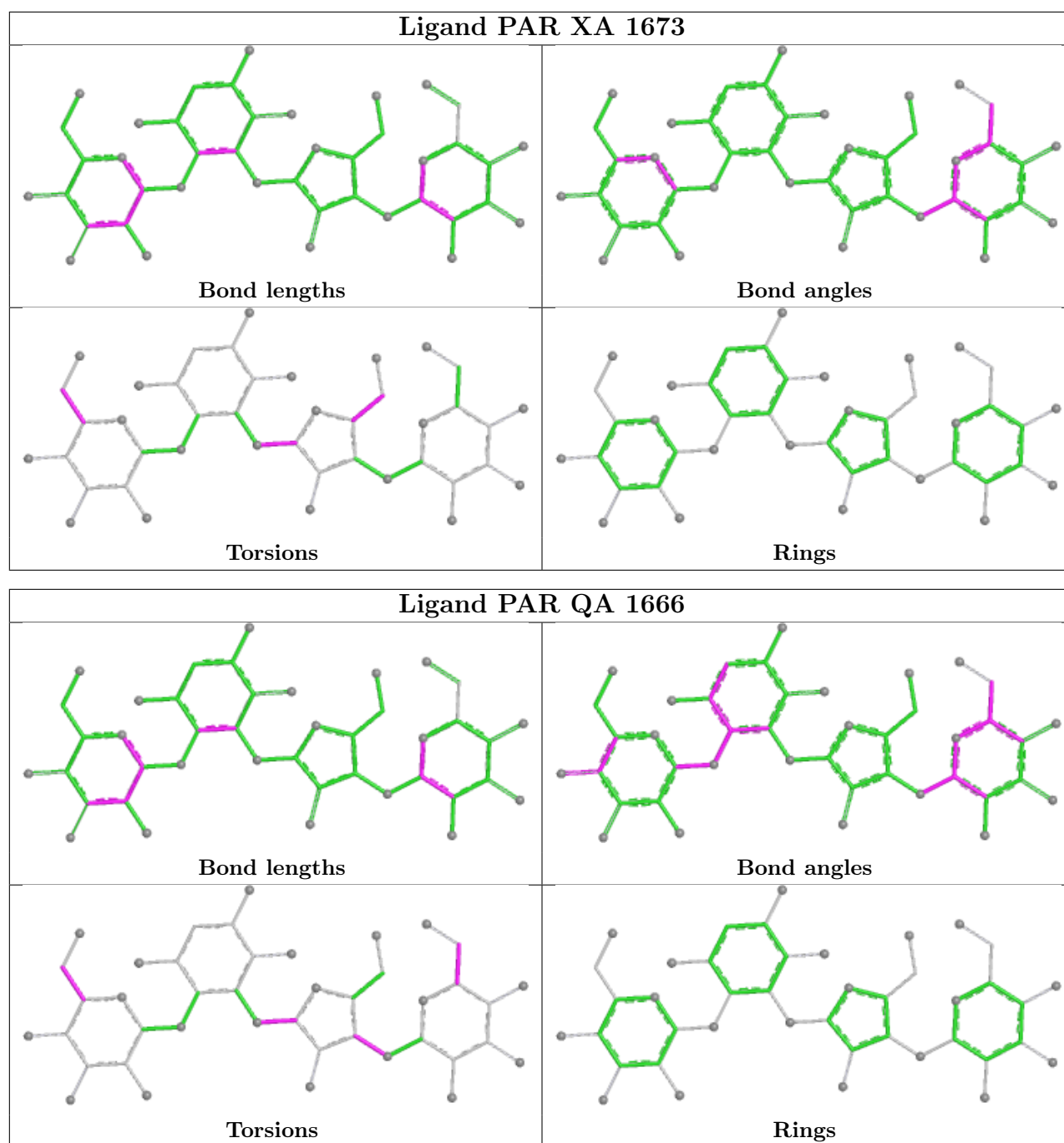
Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	XA	1673	PAR	O51-C51-C61-O61
58	QA	1666	PAR	O51-C51-C61-O61
58	XA	1673	PAR	C41-C51-C61-O61

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1673	PAR	1	0
58	QA	1666	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%)	0.24	55 (3%) 45 43	14, 55, 134, 294	0
1	XA	1500/1522 (98%)	-0.01	27 (1%) 67 65	7, 42, 133, 270	0
2	QB	237/256 (92%)	1.34	50 (21%) 3 5	42, 98, 171, 216	0
2	XB	237/256 (92%)	0.99	35 (14%) 7 9	27, 78, 141, 206	0
3	QC	205/239 (85%)	1.02	23 (11%) 11 14	37, 91, 139, 192	0
3	XC	205/239 (85%)	0.57	16 (7%) 20 21	11, 53, 103, 148	0
4	QD	208/209 (99%)	0.80	28 (13%) 8 11	23, 54, 106, 136	0
4	XD	208/209 (99%)	0.86	36 (17%) 5 7	17, 51, 103, 175	0
5	QE	151/162 (93%)	0.59	13 (8%) 18 19	29, 65, 114, 172	0
5	XE	151/162 (93%)	0.28	9 (5%) 29 27	15, 43, 86, 138	0
6	QF	101/101 (100%)	0.17	4 (3%) 43 39	13, 48, 78, 119	0
6	XF	101/101 (100%)	0.11	2 (1%) 64 62	12, 46, 76, 153	0
7	QG	155/156 (99%)	0.69	15 (9%) 15 16	23, 73, 121, 172	0
7	XG	155/156 (99%)	0.47	13 (8%) 18 20	18, 62, 109, 143	0
8	QH	138/138 (100%)	0.99	21 (15%) 6 9	30, 67, 99, 116	0
8	XH	138/138 (100%)	0.53	9 (6%) 26 25	13, 48, 84, 127	0
9	QI	127/128 (99%)	1.31	31 (24%) 2 3	33, 89, 129, 180	0
9	XI	127/128 (99%)	1.36	29 (22%) 2 4	19, 69, 124, 167	0
10	QJ	99/105 (94%)	1.64	35 (35%) 1 1	27, 98, 176, 200	0
10	XJ	99/105 (94%)	1.28	27 (27%) 2 2	5, 72, 131, 162	0
11	QK	119/129 (92%)	1.01	19 (15%) 6 8	22, 55, 110, 180	0
11	XK	119/129 (92%)	0.23	10 (8%) 18 20	16, 43, 106, 177	0
12	QL	125/132 (94%)	0.93	22 (17%) 4 7	14, 47, 100, 195	0
12	XL	125/132 (94%)	0.40	15 (12%) 10 13	7, 30, 103, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	1.50	29 (23%) 2 3	27, 84, 121, 226	0
13	XM	121/126 (96%)	1.12	25 (20%) 3 5	24, 57, 113, 211	0
14	QN	60/61 (98%)	1.39	18 (30%) 1 2	38, 80, 105, 122	0
14	XN	60/61 (98%)	0.82	10 (16%) 5 7	22, 43, 76, 100	0
15	QO	88/89 (98%)	0.35	4 (4%) 39 36	15, 52, 101, 137	0
15	XO	88/89 (98%)	0.17	3 (3%) 48 45	10, 42, 80, 97	0
16	QP	84/88 (95%)	0.78	11 (13%) 8 12	26, 50, 96, 135	0
16	XP	84/88 (95%)	0.84	12 (14%) 7 10	25, 57, 102, 179	0
17	QQ	100/105 (95%)	0.77	12 (12%) 10 13	27, 56, 100, 119	0
17	XQ	100/105 (95%)	0.63	13 (13%) 9 12	23, 55, 94, 109	0
18	QR	70/88 (79%)	0.33	5 (7%) 23 23	18, 55, 97, 111	0
18	XR	70/88 (79%)	0.13	1 (1%) 73 70	16, 50, 102, 113	0
19	QS	84/93 (90%)	1.25	19 (22%) 3 4	50, 96, 144, 180	0
19	XS	84/93 (90%)	0.44	6 (7%) 23 23	20, 65, 113, 176	0
20	QT	99/106 (93%)	0.86	17 (17%) 5 7	20, 59, 117, 189	0
20	XT	99/106 (93%)	1.04	18 (18%) 4 6	30, 68, 122, 151	0
21	QU	25/27 (92%)	1.12	7 (28%) 2 2	30, 73, 126, 140	0
21	XU	25/27 (92%)	0.74	5 (20%) 3 5	31, 45, 98, 136	0
22	QV	77/77 (100%)	0.49	5 (6%) 26 25	13, 59, 116, 149	0
22	XV	77/77 (100%)	-0.00	4 (5%) 34 31	3, 42, 86, 154	0
23	QY	14/17 (82%)	1.51	3 (21%) 3 4	60, 101, 150, 155	0
23	XY	14/17 (82%)	0.56	2 (14%) 7 10	24, 79, 120, 138	0
24	QX	8/25 (32%)	0.74	1 (12%) 9 13	30, 49, 70, 98	0
24	XX	8/25 (32%)	-0.44	0 100 100	15, 25, 40, 55	0
25	RA	2882/2916 (98%)	-0.25	117 (4%) 42 39	1, 31, 175, 318	0
25	YA	2883/2916 (98%)	-0.40	116 (4%) 43 39	0, 21, 170, 311	0
26	RB	120/122 (98%)	0.24	2 (1%) 69 66	29, 55, 88, 110	0
26	YB	120/122 (98%)	-0.28	2 (1%) 69 66	14, 37, 58, 106	0
27	RD	272/276 (98%)	0.13	22 (8%) 19 21	0, 24, 63, 135	0
27	YD	272/276 (98%)	-0.23	12 (4%) 39 37	0, 14, 46, 168	0
28	RE	205/206 (99%)	0.38	26 (12%) 9 13	1, 36, 109, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.60	30 (14%) 7 9	0, 32, 113, 183	0
29	RF	202/210 (96%)	0.36	17 (8%) 18 20	2, 41, 94, 154	0
29	YF	202/210 (96%)	-0.02	9 (4%) 39 36	0, 27, 83, 144	0
30	RG	181/182 (99%)	1.61	61 (33%) 1 2	26, 79, 130, 185	0
30	YG	181/182 (99%)	0.49	18 (9%) 14 16	14, 43, 93, 158	0
31	RH	170/180 (94%)	2.07	86 (50%) 0 1	42, 117, 172, 219	0
31	YH	170/180 (94%)	0.98	31 (18%) 4 6	12, 50, 96, 160	0
32	RI	146/148 (98%)	1.32	35 (23%) 2 3	22, 74, 128, 179	0
32	YI	146/148 (98%)	1.04	26 (17%) 4 7	16, 74, 128, 161	0
33	RN	138/140 (98%)	0.52	16 (11%) 11 14	16, 43, 86, 150	0
33	YN	138/140 (98%)	0.42	11 (7%) 20 21	10, 35, 87, 139	0
34	RO	122/122 (100%)	-0.20	2 (1%) 70 68	10, 34, 75, 103	0
34	YO	122/122 (100%)	-0.29	1 (0%) 82 81	1, 25, 48, 76	0
35	RP	150/150 (100%)	0.61	15 (10%) 14 16	3, 48, 112, 222	0
35	YP	150/150 (100%)	0.29	14 (9%) 16 17	2, 32, 95, 190	0
36	RQ	141/141 (100%)	0.69	21 (14%) 7 9	4, 47, 104, 139	0
36	YQ	141/141 (100%)	0.06	13 (9%) 16 17	1, 27, 82, 153	0
37	RR	118/118 (100%)	-0.15	3 (2%) 58 55	3, 30, 55, 88	0
37	YR	118/118 (100%)	-0.05	3 (2%) 58 55	6, 31, 58, 113	0
38	RS	111/112 (99%)	0.69	13 (11%) 10 14	23, 58, 109, 127	0
38	YS	111/112 (99%)	0.44	12 (10%) 12 15	13, 40, 93, 150	0
39	RT	137/146 (93%)	0.40	11 (8%) 20 21	16, 42, 124, 206	0
39	YT	137/146 (93%)	0.65	20 (14%) 7 9	9, 35, 131, 196	0
40	RU	117/118 (99%)	0.33	5 (4%) 40 37	6, 34, 96, 165	0
40	YU	117/118 (99%)	-0.05	8 (6%) 25 24	2, 21, 85, 144	0
41	RV	101/101 (100%)	0.71	16 (15%) 6 8	7, 53, 108, 198	0
41	YV	101/101 (100%)	0.44	11 (10%) 12 15	0, 46, 93, 208	0
42	RW	113/113 (100%)	-0.04	7 (6%) 28 26	3, 25, 69, 172	0
42	YW	113/113 (100%)	-0.06	6 (5%) 33 30	1, 25, 79, 174	0
43	RX	92/96 (95%)	0.08	4 (4%) 40 37	0, 33, 64, 106	0
43	YX	92/96 (95%)	-0.16	4 (4%) 40 37	0, 22, 59, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.95	43 (42%) 1 1	10, 65, 132, 205	0
44	YY	102/110 (92%)	1.47	30 (29%) 1 2	8, 46, 109, 201	0
45	RZ	183/206 (88%)	1.19	40 (21%) 3 4	28, 81, 152, 203	0
45	YZ	183/206 (88%)	0.58	19 (10%) 13 15	16, 59, 135, 195	0
46	R0	82/85 (96%)	0.12	4 (4%) 36 33	13, 36, 60, 83	0
46	Y0	82/85 (96%)	-0.39	2 (2%) 59 57	2, 22, 41, 74	0
47	R1	97/98 (98%)	0.47	8 (8%) 19 20	5, 33, 134, 196	0
47	Y1	97/98 (98%)	0.51	12 (12%) 9 13	1, 29, 123, 178	0
48	R2	69/72 (95%)	0.36	7 (10%) 14 16	15, 51, 121, 133	0
48	Y2	69/72 (95%)	0.45	7 (10%) 14 16	8, 32, 85, 167	0
49	R3	59/60 (98%)	0.19	2 (3%) 48 45	15, 41, 78, 134	0
49	Y3	59/60 (98%)	-0.02	2 (3%) 48 45	10, 30, 81, 142	0
50	R4	71/71 (100%)	2.51	38 (53%) 0 1	59, 140, 202, 292	0
50	Y4	71/71 (100%)	2.30	34 (47%) 0 1	39, 97, 174, 227	0
51	R5	59/60 (98%)	0.87	14 (23%) 2 3	2, 33, 145, 188	0
51	Y5	59/60 (98%)	0.95	19 (32%) 1 2	1, 39, 172, 198	0
52	R6	49/54 (90%)	3.59	41 (83%) 0 0	68, 125, 194, 221	0
52	Y6	49/54 (90%)	2.99	34 (69%) 0 0	70, 113, 183, 206	0
53	R7	49/49 (100%)	-0.11	6 (12%) 10 13	2, 12, 67, 170	0
53	Y7	49/49 (100%)	-0.20	2 (4%) 42 39	0, 7, 50, 140	0
54	R8	64/65 (98%)	0.45	9 (14%) 7 10	8, 31, 93, 151	0
54	Y8	64/65 (98%)	0.57	12 (18%) 4 6	0, 25, 81, 172	0
55	R9	37/37 (100%)	3.26	30 (81%) 0 0	55, 105, 158, 176	0
55	Y9	37/37 (100%)	2.82	22 (59%) 0 0	47, 87, 153, 202	0
56	Z6	2/3 (66%)	0.33	0 100 100	21, 21, 21, 24	0
56	Z8	2/3 (66%)	0.02	0 100 100	5, 5, 5, 14	0
All	All	20873/21492 (97%)	0.31	2037 (9%) 14 16	0, 43, 135, 318	0

The worst 5 of 2037 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	11.7
11	QK	128	ALA	10.7

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Mol	Chain	Res	Type	RSRZ
11	QK	127	LYS	10.6
11	XK	129	SER	9.8
14	XN	2	ALA	9.7

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	0.92	0.15	27,27,27,27	0
56	PPU	Z8	76	37/38	0.93	0.13	14,14,14,14	0
23	1MG	QY	37	24/25	0.95	0.09	53,53,53,53	0
23	1MG	XY	37	24/25	0.96	0.08	30,30,30,30	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	YA	3139	1/1	-0.04	0.36	55,55,55,55	0
57	MG	QH	201	1/1	0.11	0.23	74,74,74,74	0
57	MG	QA	1625	1/1	0.27	0.20	70,70,70,70	0
57	MG	RA	3192	1/1	0.33	0.22	68,68,68,68	0
57	MG	RA	3091	1/1	0.34	0.21	23,23,23,23	0
57	MG	RA	3120	1/1	0.39	0.36	80,80,80,80	0
57	MG	RA	3193	1/1	0.40	0.23	63,63,63,63	0
57	MG	RA	3139	1/1	0.49	0.33	59,59,59,59	0
57	MG	RA	3227	1/1	0.52	0.15	32,32,32,32	0
57	MG	YA	3104	1/1	0.53	0.16	3,3,3,3	0
57	MG	RA	3223	1/1	0.54	0.28	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	QA	1661	1/1	0.60	0.17	138,138,138,138	0
57	MG	XA	1629	1/1	0.60	0.25	32,32,32,32	0
57	MG	YA	3120	1/1	0.61	0.22	21,21,21,21	0
57	MG	XA	1665	1/1	0.63	0.23	56,56,56,56	0
57	MG	RA	3130	1/1	0.63	0.16	43,43,43,43	0
57	MG	QA	1628	1/1	0.64	0.18	37,37,37,37	0
57	MG	QA	1656	1/1	0.65	0.20	89,89,89,89	0
57	MG	RA	3135	1/1	0.65	0.22	31,31,31,31	0
57	MG	YA	3016	1/1	0.66	0.13	0,0,0,0	0
57	MG	XA	1670	1/1	0.67	0.12	35,35,35,35	0
57	MG	YA	3140	1/1	0.67	0.14	2,2,2,2	0
57	MG	YA	3165	1/1	0.67	0.29	40,40,40,40	0
57	MG	YA	3130	1/1	0.72	0.19	20,20,20,20	0
57	MG	XA	1653	1/1	0.73	0.27	70,70,70,70	0
57	MG	RA	3194	1/1	0.74	0.17	13,13,13,13	0
57	MG	YA	3084	1/1	0.74	0.17	2,2,2,2	0
57	MG	RB	202	1/1	0.75	0.20	46,46,46,46	0
57	MG	RP	202	1/1	0.75	0.26	85,85,85,85	0
57	MG	YA	3266	1/1	0.75	0.34	51,51,51,51	0
57	MG	YA	3160	1/1	0.76	0.10	18,18,18,18	0
57	MG	QA	1636	1/1	0.77	0.27	39,39,39,39	0
57	MG	XA	1669	1/1	0.78	0.15	49,49,49,49	0
57	MG	XA	1652	1/1	0.78	0.14	47,47,47,47	0
57	MG	RA	3206	1/1	0.78	0.24	44,44,44,44	0
57	MG	YA	3240	1/1	0.78	0.12	32,32,32,32	0
57	MG	QA	1637	1/1	0.78	0.18	16,16,16,16	0
57	MG	RA	3026	1/1	0.79	0.15	3,3,3,3	0
57	MG	RA	3187	1/1	0.80	0.29	66,66,66,66	0
57	MG	YA	3164	1/1	0.80	0.24	45,45,45,45	0
57	MG	RA	3138	1/1	0.80	0.16	6,6,6,6	0
57	MG	XA	1631	1/1	0.80	0.20	33,33,33,33	0
57	MG	XA	1639	1/1	0.80	0.23	58,58,58,58	0
57	MG	QA	1608	1/1	0.81	0.10	22,22,22,22	0
57	MG	QA	1629	1/1	0.81	0.17	30,30,30,30	0
57	MG	YA	3197	1/1	0.81	0.17	42,42,42,42	0
57	MG	RD	301	1/1	0.81	0.17	35,35,35,35	0
57	MG	RA	3155	1/1	0.81	0.12	10,10,10,10	0
57	MG	YA	3204	1/1	0.82	0.12	17,17,17,17	0
57	MG	YB	201	1/1	0.82	0.12	39,39,39,39	0
57	MG	YP	201	1/1	0.82	0.15	96,96,96,96	0
57	MG	QA	1655	1/1	0.83	0.21	38,38,38,38	0
57	MG	QA	1630	1/1	0.83	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3115	1/1	0.83	0.12	5,5,5,5	0
57	MG	XA	1672	1/1	0.83	0.20	27,27,27,27	0
57	MG	XM	201	1/1	0.84	0.09	58,58,58,58	0
57	MG	QF	201	1/1	0.84	0.30	54,54,54,54	0
57	MG	QA	1632	1/1	0.84	0.12	88,88,88,88	0
57	MG	YA	3102	1/1	0.84	0.22	44,44,44,44	0
57	MG	YA	3198	1/1	0.84	0.31	69,69,69,69	0
57	MG	XA	1663	1/1	0.84	0.15	38,38,38,38	0
57	MG	QA	1631	1/1	0.84	0.11	39,39,39,39	0
57	MG	RA	3209	1/1	0.84	0.26	47,47,47,47	0
57	MG	RA	3045	1/1	0.84	0.17	6,6,6,6	0
57	MG	RA	3058	1/1	0.84	0.19	34,34,34,34	0
57	MG	YA	3071	1/1	0.85	0.09	0,0,0,0	0
57	MG	RA	3101	1/1	0.85	0.10	2,2,2,2	0
57	MG	QA	1660	1/1	0.85	0.19	38,38,38,38	0
57	MG	YA	3207	1/1	0.85	0.34	46,46,46,46	0
57	MG	YA	3150	1/1	0.85	0.28	62,62,62,62	0
57	MG	RA	3228	1/1	0.85	0.18	43,43,43,43	0
57	MG	YA	3054	1/1	0.85	0.22	48,48,48,48	0
57	MG	YA	3127	1/1	0.85	0.18	26,26,26,26	0
58	PAR	QA	1666	42/42	0.85	0.19	43,43,43,43	0
57	MG	RB	201	1/1	0.86	0.12	41,41,41,41	0
57	MG	XX	101	1/1	0.86	0.15	45,45,45,45	0
57	MG	YA	3220	1/1	0.86	0.18	32,32,32,32	0
57	MG	RA	3220	1/1	0.86	0.10	31,31,31,31	0
57	MG	RA	3175	1/1	0.86	0.13	19,19,19,19	0
57	MG	RA	3238	1/1	0.86	0.18	14,14,14,14	0
57	MG	YA	3131	1/1	0.86	0.28	34,34,34,34	0
57	MG	YP	202	1/1	0.86	0.11	5,5,5,5	0
57	MG	YQ	201	1/1	0.86	0.24	142,142,142,142	0
57	MG	R0	101	1/1	0.86	0.20	15,15,15,15	0
57	MG	QA	1657	1/1	0.87	0.12	37,37,37,37	0
57	MG	YA	3173	1/1	0.87	0.11	49,49,49,49	0
57	MG	RA	3171	1/1	0.87	0.25	33,33,33,33	0
57	MG	QA	1647	1/1	0.87	0.08	32,32,32,32	0
57	MG	QA	1622	1/1	0.87	0.18	40,40,40,40	0
57	MG	RA	3121	1/1	0.87	0.20	36,36,36,36	0
57	MG	YA	3129	1/1	0.87	0.19	28,28,28,28	0
57	MG	YA	3221	1/1	0.87	0.17	29,29,29,29	0
57	MG	QA	1663	1/1	0.87	0.14	67,67,67,67	0
57	MG	YA	3242	1/1	0.87	0.20	33,33,33,33	0
57	MG	RA	3068	1/1	0.87	0.14	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3196	1/1	0.87	0.19	42,42,42,42	0
57	MG	RA	3203	1/1	0.87	0.11	47,47,47,47	0
57	MG	RA	3084	1/1	0.87	0.10	7,7,7,7	0
57	MG	QA	1633	1/1	0.87	0.36	35,35,35,35	0
57	MG	YX	101	1/1	0.87	0.15	46,46,46,46	0
57	MG	RA	3142	1/1	0.87	0.15	32,32,32,32	0
57	MG	YA	3235	1/1	0.88	0.23	30,30,30,30	0
57	MG	RA	3124	1/1	0.88	0.23	24,24,24,24	0
57	MG	YA	3178	1/1	0.88	0.18	29,29,29,29	0
57	MG	YA	3182	1/1	0.88	0.15	18,18,18,18	0
57	MG	XA	1622	1/1	0.88	0.18	33,33,33,33	0
57	MG	RA	3078	1/1	0.88	0.23	23,23,23,23	0
57	MG	RA	3118	1/1	0.88	0.12	22,22,22,22	0
57	MG	RA	3145	1/1	0.88	0.26	27,27,27,27	0
57	MG	YA	3061	1/1	0.88	0.13	17,17,17,17	0
57	MG	XA	1651	1/1	0.88	0.09	95,95,95,95	0
57	MG	YA	3039	1/1	0.89	0.17	10,10,10,10	0
57	MG	YA	3045	1/1	0.89	0.19	1,1,1,1	0
57	MG	QX	101	1/1	0.89	0.22	26,26,26,26	0
57	MG	XA	1607	1/1	0.89	0.16	22,22,22,22	0
57	MG	YA	3070	1/1	0.89	0.20	18,18,18,18	0
57	MG	RA	3242	1/1	0.89	0.33	31,31,31,31	0
57	MG	XA	1624	1/1	0.89	0.21	16,16,16,16	0
57	MG	RA	3156	1/1	0.89	0.12	31,31,31,31	0
57	MG	RU	201	1/1	0.89	0.27	117,117,117,117	0
57	MG	YA	3106	1/1	0.89	0.20	12,12,12,12	0
58	PAR	XA	1673	42/42	0.89	0.14	31,31,31,31	0
57	MG	QA	1603	1/1	0.90	0.23	22,22,22,22	0
57	MG	RA	3170	1/1	0.90	0.16	33,33,33,33	0
57	MG	YA	3180	1/1	0.90	0.27	41,41,41,41	0
57	MG	QA	1652	1/1	0.90	0.16	32,32,32,32	0
57	MG	YA	3184	1/1	0.90	0.17	26,26,26,26	0
57	MG	YA	3193	1/1	0.90	0.22	18,18,18,18	0
57	MG	RA	3174	1/1	0.90	0.13	25,25,25,25	0
57	MG	YA	3117	1/1	0.90	0.36	24,24,24,24	0
57	MG	RA	3010	1/1	0.90	0.27	38,38,38,38	0
57	MG	R5	101	1/1	0.90	0.10	21,21,21,21	0
57	MG	RA	3221	1/1	0.90	0.14	39,39,39,39	0
57	MG	XA	1614	1/1	0.90	0.09	7,7,7,7	0
57	MG	RA	3222	1/1	0.90	0.14	36,36,36,36	0
57	MG	RA	3176	1/1	0.90	0.14	10,10,10,10	0
57	MG	QA	1665	1/1	0.90	0.21	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3249	1/1	0.90	0.32	42,42,42,42	0
57	MG	RA	3189	1/1	0.90	0.18	46,46,46,46	0
57	MG	YA	3154	1/1	0.90	0.07	3,3,3,3	0
57	MG	YA	3155	1/1	0.90	0.41	50,50,50,50	0
57	MG	YA	3158	1/1	0.90	0.16	14,14,14,14	0
57	MG	RA	3044	1/1	0.90	0.17	18,18,18,18	0
57	MG	YA	3161	1/1	0.90	0.37	34,34,34,34	0
57	MG	RA	3146	1/1	0.90	0.20	27,27,27,27	0
57	MG	QA	1627	1/1	0.90	0.16	22,22,22,22	0
57	MG	XA	1664	1/1	0.91	0.17	44,44,44,44	0
57	MG	QA	1662	1/1	0.91	0.12	58,58,58,58	0
57	MG	QA	1649	1/1	0.91	0.14	31,31,31,31	0
57	MG	RA	3191	1/1	0.91	0.08	16,16,16,16	0
57	MG	RA	3119	1/1	0.91	0.13	30,30,30,30	0
57	MG	YA	3232	1/1	0.91	0.28	47,47,47,47	0
57	MG	RA	3092	1/1	0.91	0.18	17,17,17,17	0
57	MG	YA	3172	1/1	0.91	0.13	25,25,25,25	0
57	MG	YA	3241	1/1	0.91	0.20	37,37,37,37	0
57	MG	XA	1657	1/1	0.91	0.15	21,21,21,21	0
57	MG	YA	3245	1/1	0.91	0.29	28,28,28,28	0
57	MG	YA	3174	1/1	0.91	0.07	7,7,7,7	0
57	MG	YA	3251	1/1	0.91	0.27	38,38,38,38	0
57	MG	XA	1658	1/1	0.91	0.23	12,12,12,12	0
57	MG	YA	3143	1/1	0.91	0.23	33,33,33,33	0
57	MG	YA	3148	1/1	0.91	0.13	21,21,21,21	0
57	MG	YA	3105	1/1	0.91	0.15	24,24,24,24	0
57	MG	YA	3186	1/1	0.91	0.11	15,15,15,15	0
57	MG	YA	3153	1/1	0.91	0.12	13,13,13,13	0
57	MG	YA	3196	1/1	0.91	0.18	54,54,54,54	0
57	MG	RA	3050	1/1	0.91	0.30	30,30,30,30	0
57	MG	YA	3166	1/1	0.92	0.32	156,156,156,156	0
57	MG	RA	3212	1/1	0.92	0.05	13,13,13,13	0
57	MG	YA	3046	1/1	0.92	0.25	20,20,20,20	0
57	MG	XA	1621	1/1	0.92	0.28	23,23,23,23	0
57	MG	RA	3213	1/1	0.92	0.14	17,17,17,17	0
57	MG	RA	3216	1/1	0.92	0.19	33,33,33,33	0
57	MG	XA	1627	1/1	0.92	0.24	28,28,28,28	0
57	MG	RA	3172	1/1	0.92	0.08	15,15,15,15	0
57	MG	QA	1640	1/1	0.92	0.21	24,24,24,24	0
57	MG	RA	3029	1/1	0.92	0.19	3,3,3,3	0
57	MG	XA	1646	1/1	0.92	0.22	30,30,30,30	0
57	MG	RA	3041	1/1	0.92	0.28	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3224	1/1	0.92	0.09	18,18,18,18	0
57	MG	RA	3181	1/1	0.92	0.17	29,29,29,29	0
57	MG	YA	3122	1/1	0.92	0.16	3,3,3,3	0
57	MG	XA	1655	1/1	0.92	0.26	39,39,39,39	0
57	MG	RA	3141	1/1	0.92	0.17	15,15,15,15	0
57	MG	YA	3223	1/1	0.92	0.17	20,20,20,20	0
57	MG	YA	3226	1/1	0.92	0.22	4,4,4,4	0
57	MG	QM	201	1/1	0.92	0.14	58,58,58,58	0
57	MG	XA	1661	1/1	0.92	0.12	23,23,23,23	0
57	MG	YA	3239	1/1	0.92	0.15	38,38,38,38	0
57	MG	XA	1662	1/1	0.92	0.38	40,40,40,40	0
57	MG	RA	3241	1/1	0.92	0.22	13,13,13,13	0
57	MG	QA	1621	1/1	0.92	0.10	30,30,30,30	0
57	MG	QA	1653	1/1	0.92	0.11	88,88,88,88	0
57	MG	RA	3153	1/1	0.92	0.19	29,29,29,29	0
57	MG	YA	3152	1/1	0.92	0.19	31,31,31,31	0
57	MG	YA	3265	1/1	0.92	0.16	17,17,17,17	0
57	MG	RA	3126	1/1	0.92	0.34	33,33,33,33	0
57	MG	YA	3267	1/1	0.92	0.30	24,24,24,24	0
57	MG	RA	3053	1/1	0.92	0.20	12,12,12,12	0
57	MG	YE	301	1/1	0.92	0.14	0,0,0,0	0
57	MG	RA	3161	1/1	0.92	0.07	17,17,17,17	0
57	MG	RA	3204	1/1	0.92	0.26	33,33,33,33	0
57	MG	RA	3132	1/1	0.92	0.25	24,24,24,24	0
57	MG	YA	3024	1/1	0.92	0.21	1,1,1,1	0
57	MG	YA	3033	1/1	0.92	0.28	9,9,9,9	0
57	MG	RA	3134	1/1	0.92	0.18	23,23,23,23	0
57	MG	XA	1618	1/1	0.93	0.21	11,11,11,11	0
57	MG	YA	3015	1/1	0.93	0.27	15,15,15,15	0
57	MG	XA	1620	1/1	0.93	0.16	10,10,10,10	0
57	MG	YA	3018	1/1	0.93	0.25	16,16,16,16	0
57	MG	RA	3112	1/1	0.93	0.23	21,21,21,21	0
57	MG	YA	3171	1/1	0.93	0.26	29,29,29,29	0
57	MG	YA	3027	1/1	0.93	0.18	9,9,9,9	0
57	MG	QA	1615	1/1	0.93	0.12	28,28,28,28	0
57	MG	XA	1623	1/1	0.93	0.17	13,13,13,13	0
57	MG	RA	3070	1/1	0.93	0.27	13,13,13,13	0
57	MG	RA	3180	1/1	0.93	0.16	18,18,18,18	0
57	MG	RA	3018	1/1	0.93	0.13	17,17,17,17	0
57	MG	YA	3059	1/1	0.93	0.19	19,19,19,19	0
57	MG	YA	3185	1/1	0.93	0.08	8,8,8,8	0
57	MG	XA	1630	1/1	0.93	0.14	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3189	1/1	0.93	0.08	1,1,1,1	0
57	MG	RA	3182	1/1	0.93	0.09	6,6,6,6	0
57	MG	YA	3195	1/1	0.93	0.18	26,26,26,26	0
57	MG	XA	1633	1/1	0.93	0.17	16,16,16,16	0
57	MG	YA	3075	1/1	0.93	0.28	24,24,24,24	0
57	MG	XA	1634	1/1	0.93	0.09	6,6,6,6	0
57	MG	YA	3201	1/1	0.93	0.05	2,2,2,2	0
57	MG	XA	1636	1/1	0.93	0.20	24,24,24,24	0
57	MG	YA	3205	1/1	0.93	0.18	27,27,27,27	0
57	MG	YA	3103	1/1	0.93	0.17	8,8,8,8	0
57	MG	YA	3208	1/1	0.93	0.10	29,29,29,29	0
57	MG	YA	3216	1/1	0.93	0.24	30,30,30,30	0
57	MG	RA	3143	1/1	0.93	0.11	35,35,35,35	0
57	MG	RA	3188	1/1	0.93	0.17	29,29,29,29	0
57	MG	XA	1650	1/1	0.93	0.12	27,27,27,27	0
57	MG	RA	3082	1/1	0.93	0.21	35,35,35,35	0
57	MG	YA	3229	1/1	0.93	0.12	19,19,19,19	0
57	MG	QA	1617	1/1	0.93	0.28	31,31,31,31	0
57	MG	YA	3234	1/1	0.93	0.19	25,25,25,25	0
57	MG	RA	3149	1/1	0.93	0.16	22,22,22,22	0
57	MG	YA	3238	1/1	0.93	0.12	26,26,26,26	0
57	MG	YA	3124	1/1	0.93	0.21	9,9,9,9	0
57	MG	XA	1654	1/1	0.93	0.12	37,37,37,37	0
57	MG	RA	3085	1/1	0.93	0.13	6,6,6,6	0
57	MG	RA	3086	1/1	0.93	0.27	13,13,13,13	0
57	MG	YA	3243	1/1	0.93	0.17	21,21,21,21	0
57	MG	RA	3127	1/1	0.93	0.16	12,12,12,12	0
57	MG	YA	3133	1/1	0.93	0.16	26,26,26,26	0
57	MG	XA	1659	1/1	0.93	0.14	43,43,43,43	0
57	MG	YA	3262	1/1	0.93	0.15	4,4,4,4	0
57	MG	RA	3201	1/1	0.93	0.05	17,17,17,17	0
57	MG	RA	3088	1/1	0.93	0.27	25,25,25,25	0
57	MG	YA	3146	1/1	0.93	0.29	37,37,37,37	0
57	MG	RR	201	1/1	0.93	0.15	20,20,20,20	0
57	MG	YB	202	1/1	0.93	0.19	16,16,16,16	0
57	MG	RA	3168	1/1	0.93	0.12	19,19,19,19	0
57	MG	RA	3052	1/1	0.93	0.19	7,7,7,7	0
57	MG	QA	1613	1/1	0.93	0.30	37,37,37,37	0
57	MG	RA	3211	1/1	0.93	0.18	30,30,30,30	0
57	MG	XA	1608	1/1	0.93	0.07	34,34,34,34	0
57	MG	YA	3157	1/1	0.93	0.18	23,23,23,23	0
57	MG	QA	1642	1/1	0.93	0.19	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3068	1/1	0.94	0.25	12,12,12,12	0
57	MG	YA	3179	1/1	0.94	0.27	35,35,35,35	0
57	MG	QA	1624	1/1	0.94	0.19	30,30,30,30	0
57	MG	XA	1645	1/1	0.94	0.13	15,15,15,15	0
57	MG	YA	3073	1/1	0.94	0.17	8,8,8,8	0
57	MG	YA	3074	1/1	0.94	0.11	2,2,2,2	0
57	MG	RA	3177	1/1	0.94	0.18	24,24,24,24	0
57	MG	QA	1646	1/1	0.94	0.19	38,38,38,38	0
57	MG	YA	3089	1/1	0.94	0.23	16,16,16,16	0
57	MG	RA	3236	1/1	0.94	0.23	28,28,28,28	0
57	MG	RA	3137	1/1	0.94	0.23	7,7,7,7	0
57	MG	QA	1658	1/1	0.94	0.18	39,39,39,39	0
57	MG	RA	3184	1/1	0.94	0.06	26,26,26,26	0
57	MG	RA	3099	1/1	0.94	0.25	12,12,12,12	0
57	MG	YA	3112	1/1	0.94	0.16	11,11,11,11	0
57	MG	QA	1612	1/1	0.94	0.24	9,9,9,9	0
57	MG	RA	3102	1/1	0.94	0.18	28,28,28,28	0
57	MG	RP	201	1/1	0.94	0.35	144,144,144,144	0
57	MG	RA	3190	1/1	0.94	0.22	27,27,27,27	0
57	MG	RA	3109	1/1	0.94	0.08	3,3,3,3	0
57	MG	YA	3128	1/1	0.94	0.20	3,3,3,3	0
57	MG	RA	3111	1/1	0.94	0.25	14,14,14,14	0
57	MG	RA	3057	1/1	0.94	0.14	6,6,6,6	0
57	MG	RA	3147	1/1	0.94	0.10	14,14,14,14	0
57	MG	RA	3113	1/1	0.94	0.20	29,29,29,29	0
57	MG	YA	3134	1/1	0.94	0.17	19,19,19,19	0
57	MG	RA	3197	1/1	0.94	0.10	9,9,9,9	0
57	MG	XA	1610	1/1	0.94	0.12	7,7,7,7	0
57	MG	QA	1648	1/1	0.94	0.17	34,34,34,34	0
57	MG	YA	3145	1/1	0.94	0.14	18,18,18,18	0
57	MG	RA	3154	1/1	0.94	0.25	26,26,26,26	0
57	MG	YA	3003	1/1	0.94	0.13	1,1,1,1	0
57	MG	YA	3006	1/1	0.94	0.24	0,0,0,0	0
57	MG	YA	3011	1/1	0.94	0.25	14,14,14,14	0
57	MG	RA	3059	1/1	0.94	0.15	4,4,4,4	0
57	MG	RA	3023	1/1	0.94	0.18	5,5,5,5	0
57	MG	RA	3157	1/1	0.94	0.21	25,25,25,25	0
57	MG	YA	3263	1/1	0.94	0.23	16,16,16,16	0
57	MG	RA	3210	1/1	0.94	0.15	18,18,18,18	0
57	MG	QA	1618	1/1	0.94	0.14	13,13,13,13	0
57	MG	YA	3032	1/1	0.94	0.21	4,4,4,4	0
57	MG	RA	3162	1/1	0.94	0.07	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3163	1/1	0.94	0.20	25,25,25,25	0
57	MG	YB	203	1/1	0.94	0.15	18,18,18,18	0
57	MG	RA	3074	1/1	0.94	0.15	0,0,0,0	0
57	MG	YA	3044	1/1	0.94	0.19	4,4,4,4	0
57	MG	RA	3028	1/1	0.94	0.19	2,2,2,2	0
57	MG	QA	1620	1/1	0.94	0.13	16,16,16,16	0
57	MG	QA	1602	1/1	0.94	0.27	22,22,22,22	0
57	MG	RA	3043	1/1	0.94	0.18	7,7,7,7	0
57	MG	QA	1610	1/1	0.94	0.24	14,14,14,14	0
57	MG	YA	3049	1/1	0.95	0.23	8,8,8,8	0
57	MG	YA	3053	1/1	0.95	0.19	0,0,0,0	0
57	MG	RA	3002	1/1	0.95	0.16	26,26,26,26	0
57	MG	YA	3055	1/1	0.95	0.17	11,11,11,11	0
57	MG	YA	3170	1/1	0.95	0.05	15,15,15,15	0
57	MG	XA	1641	1/1	0.95	0.18	33,33,33,33	0
57	MG	XA	1644	1/1	0.95	0.23	23,23,23,23	0
57	MG	RA	3007	1/1	0.95	0.24	5,5,5,5	0
57	MG	RA	3239	1/1	0.95	0.30	28,28,28,28	0
57	MG	RA	3008	1/1	0.95	0.23	30,30,30,30	0
57	MG	QA	1664	1/1	0.95	0.15	17,17,17,17	0
57	MG	RA	3158	1/1	0.95	0.25	40,40,40,40	0
57	MG	RA	3011	1/1	0.95	0.37	36,36,36,36	0
57	MG	YA	3077	1/1	0.95	0.21	6,6,6,6	0
57	MG	YA	3078	1/1	0.95	0.21	14,14,14,14	0
57	MG	YA	3082	1/1	0.95	0.09	0,0,0,0	0
57	MG	YA	3187	1/1	0.95	0.13	25,25,25,25	0
57	MG	YA	3188	1/1	0.95	0.29	33,33,33,33	0
57	MG	QA	1616	1/1	0.95	0.19	28,28,28,28	0
57	MG	RE	302	1/1	0.95	0.17	5,5,5,5	0
57	MG	YA	3096	1/1	0.95	0.14	5,5,5,5	0
57	MG	RA	3198	1/1	0.95	0.06	27,27,27,27	0
57	MG	RA	3163	1/1	0.95	0.14	19,19,19,19	0
57	MG	RA	3166	1/1	0.95	0.18	28,28,28,28	0
57	MG	YA	3200	1/1	0.95	0.18	12,12,12,12	0
57	MG	RA	3022	1/1	0.95	0.17	3,3,3,3	0
57	MG	RA	3096	1/1	0.95	0.15	18,18,18,18	0
57	MG	YA	3108	1/1	0.95	0.22	12,12,12,12	0
57	MG	YA	3206	1/1	0.95	0.18	14,14,14,14	0
57	MG	YA	3110	1/1	0.95	0.17	14,14,14,14	0
57	MG	RA	3136	1/1	0.95	0.04	14,14,14,14	0
57	MG	YA	3214	1/1	0.95	0.12	25,25,25,25	0
57	MG	YA	3113	1/1	0.95	0.12	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3217	1/1	0.95	0.06	9,9,9,9	0
57	MG	YA	3115	1/1	0.95	0.22	18,18,18,18	0
57	MG	XA	1602	1/1	0.95	0.19	18,18,18,18	0
57	MG	XA	1603	1/1	0.95	0.27	13,13,13,13	0
57	MG	YA	3224	1/1	0.95	0.10	14,14,14,14	0
57	MG	YA	3225	1/1	0.95	0.13	3,3,3,3	0
57	MG	YA	3121	1/1	0.95	0.20	27,27,27,27	0
57	MG	YA	3228	1/1	0.95	0.05	11,11,11,11	0
57	MG	XA	1666	1/1	0.95	0.05	13,13,13,13	0
57	MG	YA	3231	1/1	0.95	0.20	20,20,20,20	0
57	MG	QA	1654	1/1	0.95	0.10	36,36,36,36	0
57	MG	YA	3125	1/1	0.95	0.13	9,9,9,9	0
57	MG	RA	3025	1/1	0.95	0.18	12,12,12,12	0
57	MG	XA	1671	1/1	0.95	0.07	18,18,18,18	0
57	MG	QA	1619	1/1	0.95	0.09	1,1,1,1	0
57	MG	RA	3062	1/1	0.95	0.11	29,29,29,29	0
57	MG	RA	3215	1/1	0.95	0.07	24,24,24,24	0
57	MG	QA	1644	1/1	0.95	0.09	21,21,21,21	0
57	MG	RA	3219	1/1	0.95	0.24	159,159,159,159	0
57	MG	YA	3135	1/1	0.95	0.09	3,3,3,3	0
57	MG	YA	3009	1/1	0.95	0.26	2,2,2,2	0
57	MG	QA	1638	1/1	0.95	0.18	27,27,27,27	0
57	MG	YA	3260	1/1	0.95	0.20	13,13,13,13	0
57	MG	YA	3141	1/1	0.95	0.09	17,17,17,17	0
57	MG	YA	3142	1/1	0.95	0.04	8,8,8,8	0
57	MG	RA	3071	1/1	0.95	0.22	22,22,22,22	0
57	MG	RA	3073	1/1	0.95	0.10	10,10,10,10	0
57	MG	YA	3017	1/1	0.95	0.14	18,18,18,18	0
57	MG	RA	3032	1/1	0.95	0.26	27,27,27,27	0
57	MG	YA	3023	1/1	0.95	0.22	6,6,6,6	0
57	MG	XA	1628	1/1	0.95	0.05	1,1,1,1	0
57	MG	RA	3034	1/1	0.95	0.23	17,17,17,17	0
57	MG	RA	3226	1/1	0.95	0.14	15,15,15,15	0
57	MG	RA	3150	1/1	0.95	0.12	25,25,25,25	0
57	MG	XA	1632	1/1	0.95	0.18	21,21,21,21	0
57	MG	RA	3081	1/1	0.95	0.09	10,10,10,10	0
57	MG	Y5	101	1/1	0.95	0.12	12,12,12,12	0
57	MG	RA	3232	1/1	0.95	0.18	10,10,10,10	0
57	MG	RA	3235	1/1	0.95	0.24	28,28,28,28	0
57	MG	YA	3047	1/1	0.96	0.20	4,4,4,4	0
57	MG	YA	3162	1/1	0.96	0.06	16,16,16,16	0
57	MG	RA	3097	1/1	0.96	0.18	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3098	1/1	0.96	0.22	7,7,7,7	0
57	MG	XA	1635	1/1	0.96	0.28	12,12,12,12	0
57	MG	RA	3178	1/1	0.96	0.11	26,26,26,26	0
57	MG	YA	3167	1/1	0.96	0.09	1,1,1,1	0
57	MG	YA	3169	1/1	0.96	0.21	12,12,12,12	0
57	MG	XA	1637	1/1	0.96	0.13	20,20,20,20	0
57	MG	YA	3060	1/1	0.96	0.21	1,1,1,1	0
57	MG	RA	3179	1/1	0.96	0.04	2,2,2,2	0
57	MG	YA	3062	1/1	0.96	0.15	7,7,7,7	0
57	MG	YA	3064	1/1	0.96	0.13	6,6,6,6	0
57	MG	YA	3176	1/1	0.96	0.09	2,2,2,2	0
57	MG	YA	3177	1/1	0.96	0.08	12,12,12,12	0
57	MG	RA	3140	1/1	0.96	0.18	17,17,17,17	0
57	MG	RA	3017	1/1	0.96	0.12	0,0,0,0	0
57	MG	RA	3064	1/1	0.96	0.24	13,13,13,13	0
57	MG	RA	3065	1/1	0.96	0.14	9,9,9,9	0
57	MG	YA	3183	1/1	0.96	0.17	13,13,13,13	0
57	MG	RA	3185	1/1	0.96	0.04	16,16,16,16	0
57	MG	RA	3103	1/1	0.96	0.06	2,2,2,2	0
57	MG	RA	3240	1/1	0.96	0.21	14,14,14,14	0
57	MG	RA	3037	1/1	0.96	0.12	11,11,11,11	0
57	MG	RA	3069	1/1	0.96	0.04	1,1,1,1	0
57	MG	RA	3148	1/1	0.96	0.20	15,15,15,15	0
57	MG	YA	3192	1/1	0.96	0.12	19,19,19,19	0
57	MG	YA	3085	1/1	0.96	0.15	9,9,9,9	0
57	MG	YA	3194	1/1	0.96	0.07	17,17,17,17	0
57	MG	XA	1656	1/1	0.96	0.25	31,31,31,31	0
57	MG	YA	3090	1/1	0.96	0.32	39,39,39,39	0
57	MG	YA	3091	1/1	0.96	0.16	29,29,29,29	0
57	MG	RA	3039	1/1	0.96	0.15	10,10,10,10	0
57	MG	YA	3101	1/1	0.96	0.16	3,3,3,3	0
57	MG	QA	1645	1/1	0.96	0.09	20,20,20,20	0
57	MG	YA	3203	1/1	0.96	0.05	25,25,25,25	0
57	MG	RA	3114	1/1	0.96	0.16	19,19,19,19	0
57	MG	QA	1614	1/1	0.96	0.08	20,20,20,20	0
57	MG	RA	3003	1/1	0.96	0.25	4,4,4,4	0
57	MG	RA	3004	1/1	0.96	0.22	14,14,14,14	0
57	MG	RA	3046	1/1	0.96	0.14	8,8,8,8	0
57	MG	YA	3210	1/1	0.96	0.12	26,26,26,26	0
57	MG	YA	3212	1/1	0.96	0.06	20,20,20,20	0
57	MG	YA	3109	1/1	0.96	0.08	5,5,5,5	0
57	MG	RA	3199	1/1	0.96	0.05	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3048	1/1	0.96	0.18	1,1,1,1	0
57	MG	YA	3219	1/1	0.96	0.10	31,31,31,31	0
57	MG	RA	3202	1/1	0.96	0.15	15,15,15,15	0
57	MG	YA	3114	1/1	0.96	0.18	13,13,13,13	0
57	MG	RA	3159	1/1	0.96	0.16	24,24,24,24	0
57	MG	YA	3116	1/1	0.96	0.23	39,39,39,39	0
57	MG	XA	1604	1/1	0.96	0.34	19,19,19,19	0
57	MG	YA	3118	1/1	0.96	0.27	22,22,22,22	0
57	MG	YA	3227	1/1	0.96	0.12	8,8,8,8	0
57	MG	XA	1605	1/1	0.96	0.24	17,17,17,17	0
57	MG	XA	1606	1/1	0.96	0.26	12,12,12,12	0
57	MG	YA	3230	1/1	0.96	0.17	18,18,18,18	0
57	MG	RA	3122	1/1	0.96	0.24	32,32,32,32	0
57	MG	YA	3002	1/1	0.96	0.19	1,1,1,1	0
57	MG	YA	3233	1/1	0.96	0.04	6,6,6,6	0
57	MG	RA	3083	1/1	0.96	0.18	17,17,17,17	0
57	MG	YA	3126	1/1	0.96	0.10	1,1,1,1	0
57	MG	YA	3237	1/1	0.96	0.25	25,25,25,25	0
57	MG	YA	3005	1/1	0.96	0.13	6,6,6,6	0
57	MG	XA	1609	1/1	0.96	0.23	14,14,14,14	0
57	MG	YA	3008	1/1	0.96	0.16	2,2,2,2	0
57	MG	RA	3207	1/1	0.96	0.07	60,60,60,60	0
57	MG	RA	3208	1/1	0.96	0.11	7,7,7,7	0
57	MG	XA	1615	1/1	0.96	0.18	2,2,2,2	0
57	MG	YA	3244	1/1	0.96	0.25	30,30,30,30	0
57	MG	QA	1659	1/1	0.96	0.14	21,21,21,21	0
57	MG	YA	3246	1/1	0.96	0.14	26,26,26,26	0
57	MG	RA	3164	1/1	0.96	0.18	20,20,20,20	0
57	MG	YA	3136	1/1	0.96	0.17	14,14,14,14	0
57	MG	YA	3255	1/1	0.96	0.28	20,20,20,20	0
57	MG	RA	3165	1/1	0.96	0.07	14,14,14,14	0
57	MG	YA	3261	1/1	0.96	0.22	19,19,19,19	0
57	MG	YA	3019	1/1	0.96	0.21	8,8,8,8	0
57	MG	YA	3022	1/1	0.96	0.14	1,1,1,1	0
57	MG	YA	3264	1/1	0.96	0.09	7,7,7,7	0
57	MG	RA	3027	1/1	0.96	0.20	1,1,1,1	0
57	MG	QA	1604	1/1	0.96	0.15	4,4,4,4	0
57	MG	YA	3026	1/1	0.96	0.22	2,2,2,2	0
57	MG	YA	3268	1/1	0.96	0.17	17,17,17,17	0
57	MG	RA	3214	1/1	0.96	0.17	13,13,13,13	0
57	MG	YA	3028	1/1	0.96	0.14	2,2,2,2	0
57	MG	RA	3169	1/1	0.96	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
57	MG	YA	3151	1/1	0.96	0.28	30,30,30,30	0
57	MG	RA	3087	1/1	0.96	0.17	25,25,25,25	0
57	MG	YA	3036	1/1	0.96	0.12	4,4,4,4	0
57	MG	RA	3054	1/1	0.96	0.13	2,2,2,2	0
57	MG	YA	3040	1/1	0.96	0.19	0,0,0,0	0
57	MG	QA	1601	1/1	0.96	0.27	34,34,34,34	0
57	MG	RA	3030	1/1	0.96	0.18	0,0,0,0	0
57	MG	QA	1609	1/1	0.96	0.11	13,13,13,13	0
57	MG	YA	3037	1/1	0.97	0.15	0,0,0,0	0
57	MG	YA	3156	1/1	0.97	0.18	13,13,13,13	0
57	MG	YA	3038	1/1	0.97	0.09	4,4,4,4	0
57	MG	RA	3217	1/1	0.97	0.08	14,14,14,14	0
57	MG	RA	3218	1/1	0.97	0.17	17,17,17,17	0
57	MG	YA	3041	1/1	0.97	0.20	2,2,2,2	0
57	MG	YA	3042	1/1	0.97	0.14	4,4,4,4	0
57	MG	YA	3043	1/1	0.97	0.18	1,1,1,1	0
57	MG	RA	3116	1/1	0.97	0.14	0,0,0,0	0
57	MG	RA	3035	1/1	0.97	0.17	0,0,0,0	0
57	MG	RA	3072	1/1	0.97	0.15	3,3,3,3	0
57	MG	QA	1623	1/1	0.97	0.20	19,19,19,19	0
57	MG	RA	3173	1/1	0.97	0.04	1,1,1,1	0
57	MG	YA	3051	1/1	0.97	0.27	15,15,15,15	0
57	MG	RA	3012	1/1	0.97	0.12	7,7,7,7	0
57	MG	XA	1638	1/1	0.97	0.05	20,20,20,20	0
57	MG	RA	3225	1/1	0.97	0.10	40,40,40,40	0
57	MG	YA	3057	1/1	0.97	0.20	1,1,1,1	0
57	MG	YA	3175	1/1	0.97	0.23	23,23,23,23	0
57	MG	YA	3058	1/1	0.97	0.14	0,0,0,0	0
57	MG	XA	1640	1/1	0.97	0.20	15,15,15,15	0
57	MG	RA	3075	1/1	0.97	0.07	6,6,6,6	0
57	MG	RA	3123	1/1	0.97	0.18	28,28,28,28	0
57	MG	RA	3077	1/1	0.97	0.16	13,13,13,13	0
57	MG	YA	3181	1/1	0.97	0.24	36,36,36,36	0
57	MG	RA	3230	1/1	0.97	0.21	7,7,7,7	0
57	MG	YA	3065	1/1	0.97	0.15	0,0,0,0	0
57	MG	XA	1647	1/1	0.97	0.12	23,23,23,23	0
57	MG	YA	3069	1/1	0.97	0.11	6,6,6,6	0
57	MG	XA	1648	1/1	0.97	0.04	14,14,14,14	0
57	MG	RA	3013	1/1	0.97	0.20	11,11,11,11	0
57	MG	YA	3072	1/1	0.97	0.18	9,9,9,9	0
57	MG	RA	3233	1/1	0.97	0.09	13,13,13,13	0
57	MG	YA	3191	1/1	0.97	0.17	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3234	1/1	0.97	0.15	10,10,10,10	0
57	MG	RA	3080	1/1	0.97	0.21	17,17,17,17	0
57	MG	YA	3076	1/1	0.97	0.26	15,15,15,15	0
57	MG	RA	3042	1/1	0.97	0.18	10,10,10,10	0
57	MG	RA	3014	1/1	0.97	0.17	3,3,3,3	0
57	MG	YA	3080	1/1	0.97	0.18	1,1,1,1	0
57	MG	YA	3081	1/1	0.97	0.18	10,10,10,10	0
57	MG	RA	3015	1/1	0.97	0.11	5,5,5,5	0
57	MG	RA	3016	1/1	0.97	0.18	1,1,1,1	0
57	MG	QA	1634	1/1	0.97	0.10	35,35,35,35	0
57	MG	YA	3087	1/1	0.97	0.19	1,1,1,1	0
57	MG	YA	3088	1/1	0.97	0.19	5,5,5,5	0
57	MG	RA	3186	1/1	0.97	0.05	14,14,14,14	0
57	MG	XA	1660	1/1	0.97	0.06	6,6,6,6	0
57	MG	RA	3047	1/1	0.97	0.24	12,12,12,12	0
57	MG	YA	3209	1/1	0.97	0.05	11,11,11,11	0
57	MG	YA	3093	1/1	0.97	0.16	9,9,9,9	0
57	MG	YA	3094	1/1	0.97	0.11	4,4,4,4	0
57	MG	YA	3213	1/1	0.97	0.06	6,6,6,6	0
57	MG	QA	1635	1/1	0.97	0.11	18,18,18,18	0
57	MG	YA	3215	1/1	0.97	0.05	18,18,18,18	0
57	MG	YA	3097	1/1	0.97	0.15	14,14,14,14	0
57	MG	YA	3099	1/1	0.97	0.20	9,9,9,9	0
57	MG	YA	3100	1/1	0.97	0.19	1,1,1,1	0
57	MG	RA	3021	1/1	0.97	0.20	2,2,2,2	0
57	MG	RA	3089	1/1	0.97	0.13	2,2,2,2	0
57	MG	YA	3222	1/1	0.97	0.12	27,27,27,27	0
57	MG	RA	3090	1/1	0.97	0.11	8,8,8,8	0
57	MG	QA	1611	1/1	0.97	0.21	12,12,12,12	0
57	MG	XA	1667	1/1	0.97	0.26	29,29,29,29	0
57	MG	XA	1668	1/1	0.97	0.19	15,15,15,15	0
57	MG	QA	1607	1/1	0.97	0.07	10,10,10,10	0
57	MG	RA	3093	1/1	0.97	0.20	8,8,8,8	0
57	MG	RA	3195	1/1	0.97	0.07	1,1,1,1	0
57	MG	RA	3094	1/1	0.97	0.15	8,8,8,8	0
57	MG	RA	3095	1/1	0.97	0.21	6,6,6,6	0
57	MG	XV	101	1/1	0.97	0.13	0,0,0,0	0
57	MG	RA	3024	1/1	0.97	0.14	7,7,7,7	0
57	MG	YA	3001	1/1	0.97	0.18	1,1,1,1	0
57	MG	RA	3056	1/1	0.97	0.19	1,1,1,1	0
57	MG	YA	3236	1/1	0.97	0.04	24,24,24,24	0
57	MG	RA	3200	1/1	0.97	0.31	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3119	1/1	0.97	0.25	23,23,23,23	0
57	MG	YA	3004	1/1	0.97	0.17	0,0,0,0	0
57	MG	QA	1626	1/1	0.97	0.11	21,21,21,21	0
57	MG	QA	1639	1/1	0.97	0.09	25,25,25,25	0
57	MG	YA	3123	1/1	0.97	0.18	4,4,4,4	0
57	MG	YA	3007	1/1	0.97	0.14	9,9,9,9	0
57	MG	RA	3100	1/1	0.97	0.09	6,6,6,6	0
57	MG	QA	1650	1/1	0.97	0.17	20,20,20,20	0
57	MG	RA	3205	1/1	0.97	0.18	5,5,5,5	0
57	MG	YA	3012	1/1	0.97	0.25	2,2,2,2	0
57	MG	YA	3250	1/1	0.97	0.25	22,22,22,22	0
57	MG	YA	3014	1/1	0.97	0.21	4,4,4,4	0
57	MG	YA	3253	1/1	0.97	0.24	2,2,2,2	0
57	MG	YA	3254	1/1	0.97	0.15	18,18,18,18	0
57	MG	RA	3060	1/1	0.97	0.20	0,0,0,0	0
57	MG	YA	3257	1/1	0.97	0.23	3,3,3,3	0
57	MG	RA	3005	1/1	0.97	0.23	9,9,9,9	0
57	MG	XA	1617	1/1	0.97	0.12	8,8,8,8	0
57	MG	RA	3104	1/1	0.97	0.08	9,9,9,9	0
57	MG	XA	1619	1/1	0.97	0.10	7,7,7,7	0
57	MG	YA	3021	1/1	0.97	0.13	1,1,1,1	0
57	MG	YA	3137	1/1	0.97	0.11	1,1,1,1	0
57	MG	YA	3138	1/1	0.97	0.13	0,0,0,0	0
57	MG	RA	3108	1/1	0.97	0.12	8,8,8,8	0
57	MG	RA	3006	1/1	0.97	0.23	17,17,17,17	0
57	MG	RA	3110	1/1	0.97	0.16	2,2,2,2	0
57	MG	YA	3025	1/1	0.97	0.12	6,6,6,6	0
57	MG	QA	1651	1/1	0.97	0.12	18,18,18,18	0
57	MG	RA	3067	1/1	0.97	0.13	3,3,3,3	0
57	MG	XA	1625	1/1	0.97	0.08	6,6,6,6	0
57	MG	YA	3029	1/1	0.97	0.17	1,1,1,1	0
57	MG	YA	3030	1/1	0.97	0.26	6,6,6,6	0
57	MG	QA	1606	1/1	0.97	0.12	11,11,11,11	0
57	MG	RA	3033	1/1	0.97	0.25	3,3,3,3	0
57	MG	YA	3034	1/1	0.97	0.22	13,13,13,13	0
57	MG	QA	1641	1/1	0.97	0.14	22,22,22,22	0
57	MG	RA	3107	1/1	0.98	0.12	6,6,6,6	0
57	MG	YA	3159	1/1	0.98	0.21	16,16,16,16	0
57	MG	YA	3218	1/1	0.98	0.05	1,1,1,1	0
57	MG	YA	3107	1/1	0.98	0.17	2,2,2,2	0
57	MG	RA	3019	1/1	0.98	0.15	13,13,13,13	0
57	MG	RA	3066	1/1	0.98	0.28	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RE	301	1/1	0.98	0.09	1,1,1,1	0
57	MG	YA	3111	1/1	0.98	0.07	8,8,8,8	0
57	MG	RA	3076	1/1	0.98	0.13	0,0,0,0	0
57	MG	RF	301	1/1	0.98	0.16	24,24,24,24	0
57	MG	YA	3063	1/1	0.98	0.13	3,3,3,3	0
57	MG	RA	3020	1/1	0.98	0.14	8,8,8,8	0
57	MG	RA	3160	1/1	0.98	0.06	12,12,12,12	0
57	MG	YA	3066	1/1	0.98	0.26	12,12,12,12	0
57	MG	QA	1605	1/1	0.98	0.31	23,23,23,23	0
57	MG	RA	3125	1/1	0.98	0.08	13,13,13,13	0
57	MG	QV	101	1/1	0.98	0.17	9,9,9,9	0
57	MG	RA	3144	1/1	0.98	0.21	8,8,8,8	0
57	MG	R8	101	1/1	0.98	0.15	25,25,25,25	0
57	MG	XA	1601	1/1	0.98	0.19	7,7,7,7	0
57	MG	RA	3229	1/1	0.98	0.09	26,26,26,26	0
57	MG	YA	3031	1/1	0.98	0.23	1,1,1,1	0
57	MG	QA	1643	1/1	0.98	0.04	21,21,21,21	0
57	MG	RA	3231	1/1	0.98	0.16	1,1,1,1	0
57	MG	RA	3128	1/1	0.98	0.12	4,4,4,4	0
57	MG	YA	3035	1/1	0.98	0.12	1,1,1,1	0
57	MG	RA	3167	1/1	0.98	0.09	22,22,22,22	0
57	MG	RA	3129	1/1	0.98	0.06	10,10,10,10	0
57	MG	YA	3132	1/1	0.98	0.07	5,5,5,5	0
57	MG	YA	3083	1/1	0.98	0.13	0,0,0,0	0
57	MG	RA	3061	1/1	0.98	0.16	2,2,2,2	0
57	MG	YA	3247	1/1	0.98	0.24	16,16,16,16	0
57	MG	YA	3248	1/1	0.98	0.28	30,30,30,30	0
57	MG	XA	1643	1/1	0.98	0.11	12,12,12,12	0
57	MG	YA	3190	1/1	0.98	0.08	0,0,0,0	0
57	MG	YA	3086	1/1	0.98	0.17	10,10,10,10	0
57	MG	RA	3001	1/1	0.98	0.12	4,4,4,4	0
57	MG	RA	3237	1/1	0.98	0.33	28,28,28,28	0
57	MG	XA	1611	1/1	0.98	0.23	7,7,7,7	0
57	MG	YA	3256	1/1	0.98	0.22	3,3,3,3	0
57	MG	XA	1612	1/1	0.98	0.10	3,3,3,3	0
57	MG	YA	3259	1/1	0.98	0.23	13,13,13,13	0
57	MG	XA	1613	1/1	0.98	0.04	6,6,6,6	0
57	MG	XA	1649	1/1	0.98	0.13	8,8,8,8	0
57	MG	RA	3133	1/1	0.98	0.07	6,6,6,6	0
57	MG	YA	3199	1/1	0.98	0.20	11,11,11,11	0
57	MG	YA	3144	1/1	0.98	0.10	11,11,11,11	0
57	MG	YA	3095	1/1	0.98	0.13	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3202	1/1	0.98	0.09	13,13,13,13	0
57	MG	RA	3151	1/1	0.98	0.06	0,0,0,0	0
57	MG	YA	3147	1/1	0.98	0.10	2,2,2,2	0
57	MG	YA	3048	1/1	0.98	0.21	11,11,11,11	0
57	MG	YA	3149	1/1	0.98	0.10	9,9,9,9	0
57	MG	YA	3098	1/1	0.98	0.18	2,2,2,2	0
57	MG	YA	3010	1/1	0.98	0.15	1,1,1,1	0
57	MG	YA	3050	1/1	0.98	0.17	2,2,2,2	0
57	MG	RA	3152	1/1	0.98	0.15	11,11,11,11	0
57	MG	YA	3211	1/1	0.98	0.02	0,0,0,0	0
57	MG	YA	3052	1/1	0.98	0.11	1,1,1,1	0
57	MG	RA	3117	1/1	0.98	0.12	2,2,2,2	0
57	MG	YA	3013	1/1	0.98	0.20	7,7,7,7	0
57	MG	RA	3055	1/1	0.98	0.10	8,8,8,8	0
59	ZN	QD	301	1/1	0.98	0.11	58,58,58,58	0
59	ZN	QN	101	1/1	0.98	0.06	95,95,95,95	0
59	ZN	XD	301	1/1	0.98	0.16	39,39,39,39	0
57	MG	RA	3131	1/1	0.99	0.11	13,13,13,13	0
57	MG	YA	3020	1/1	0.99	0.23	10,10,10,10	0
57	MG	XA	1616	1/1	0.99	0.14	6,6,6,6	0
57	MG	YA	3056	1/1	0.99	0.14	1,1,1,1	0
57	MG	RA	3063	1/1	0.99	0.24	1,1,1,1	0
57	MG	RA	3049	1/1	0.99	0.05	1,1,1,1	0
57	MG	RA	3031	1/1	0.99	0.13	3,3,3,3	0
57	MG	RA	3183	1/1	0.99	0.13	1,1,1,1	0
57	MG	RA	3051	1/1	0.99	0.08	4,4,4,4	0
57	MG	RA	3040	1/1	0.99	0.20	15,15,15,15	0
57	MG	RA	3036	1/1	0.99	0.14	2,2,2,2	0
57	MG	RA	3009	1/1	0.99	0.04	0,0,0,0	0
57	MG	RA	3105	1/1	0.99	0.10	6,6,6,6	0
57	MG	XA	1626	1/1	0.99	0.12	9,9,9,9	0
57	MG	YA	3067	1/1	0.99	0.10	2,2,2,2	0
57	MG	YA	3252	1/1	0.99	0.36	17,17,17,17	0
57	MG	YA	3168	1/1	0.99	0.09	0,0,0,0	0
57	MG	XA	1642	1/1	0.99	0.11	7,7,7,7	0
57	MG	RA	3106	1/1	0.99	0.10	4,4,4,4	0
57	MG	RA	3038	1/1	0.99	0.11	1,1,1,1	0
57	MG	RA	3079	1/1	0.99	0.15	11,11,11,11	0
57	MG	YA	3258	1/1	0.99	0.14	2,2,2,2	0
57	MG	YA	3092	1/1	0.99	0.13	3,3,3,3	0
59	ZN	XN	101	1/1	0.99	0.02	42,42,42,42	0
57	MG	YA	3079	1/1	1.00	0.05	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.