



# wwPDB X-ray Structure Validation Summary Report

Oct 8, 2023 – 05:04 PM EDT

PDB ID : 4TUE  
Title : Crystal structure of ASL-SufJ bound to Codon ACC-U on the Ribosome  
Authors : Fagan, C.E.; Dunham, C.M.  
Deposited on : 2014-06-24  
Resolution : 3.50 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](mailto: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>.

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

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

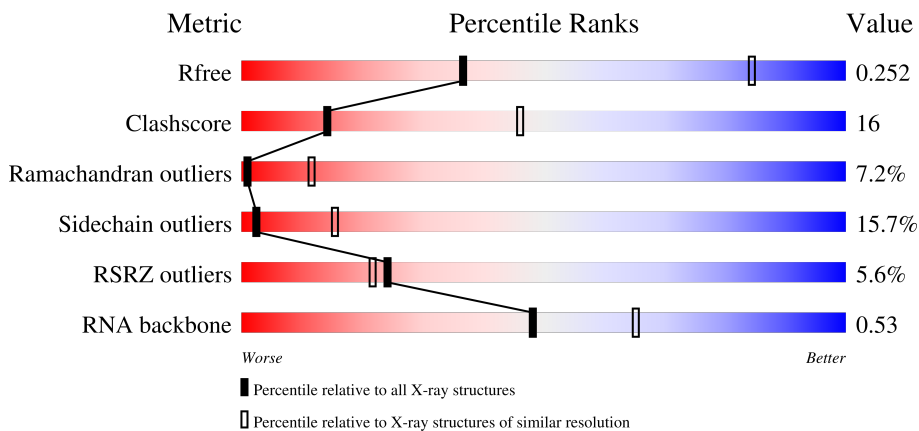
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 6% 53% 36% 8% ..
1	XA	1522	 5% 55% 34% 10% .
2	QB	256	 9% 50% 35% 7% . 7%
2	XB	256	 7% 48% 34% 9% . 7%

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Mol	Chain	Length	Quality of chain
3	QC	239	4% 53% 30% 14%
3	XC	239	3% 53% 30% 14%
4	QD	209	% 67% 27% 5%
4	XD	209	% 66% 27% 6%
5	QE	162	% 60% 28% 7%
5	XE	162	% 54% 34% 5% 7%
6	QF	101	4% 66% 30% .
6	XF	101	6% 63% 34% .
7	QG	156	5% 66% 30% . .
7	XG	156	10% 69% 28% . .
8	QH	138	62% 35% .
8	XH	138	64% 30% 5%
9	QI	128	12% 55% 38% 5% . .
9	XI	128	12% 54% 33% 12% . .
10	QJ	105	28% 44% 41% 9% . 6%
10	XJ	105	16% 40% 46% 9% 6%
11	QK	129	9% 59% 29% 5% 8%
11	XK	129	3% 61% 29% . 8%
12	QL	132	5% 29% 50% 14% . 5%
12	XL	132	3% 31% 46% 15% . 5%
13	QM	126	7% 47% 39% 10% .
13	XM	126	3% 48% 37% 10% .
14	QN	61	5% 39% 48% 11% .
14	XN	61	7% 48% 41% 8% . .
15	QO	89	% 67% 25% 7% .

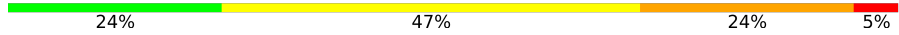
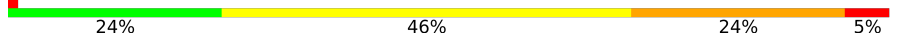

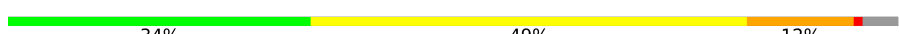


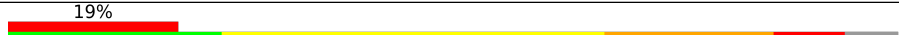
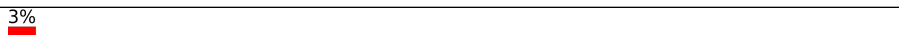
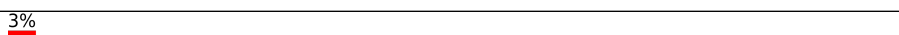
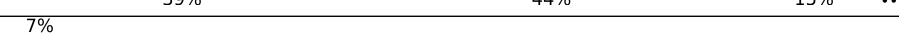
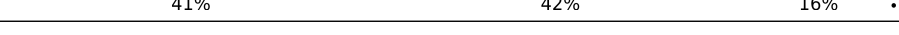
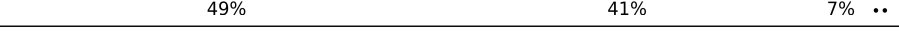





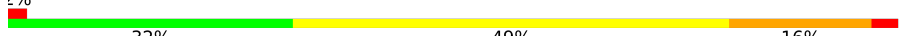
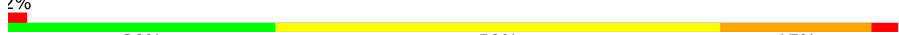






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Mol	Chain	Length	Quality of chain
15	XO	89	% 65% 26% 8% .
16	QP	88	68% 23% 5% 5%
16	XP	88	2% 53% 38% 5% 5%
17	QQ	105	2% 58% 35% .. 5%
17	XQ	105	2% 69% 23% . 5%
18	QR	88	6% 52% 22% . . 20%
18	XR	88	5% 44% 31% 5% 20%
19	QS	93	41% 31% 17% . 10%
19	XS	93	31% 44% 12% . 10%
20	QT	106	5% 46% 41% 7% 7%
20	XT	106	2% 40% 45% 8% 7%
21	QU	27	44% 44% 48% 7%
21	XU	27	33% 67% 26% 7%
22	QV	77	14% 62% 29% 9%
22	XV	77	14% 69% 19% 10% .
23	QX	25	4% 24% 12% 64%
23	XX	25	4% 16% 20% 8% 56%
24	QY	18	50% 33% 17%
24	XY	18	28% 44% 11% 17%
25	RA	2915	7% 57% 32% 9% .
25	YA	2915	6% 57% 33% 8% .
26	RB	122	% 52% 35% 10% ..
26	YB	122	9% 50% 39% 10% .
27	RD	276	54% 36% 8% .
27	YD	276	% 30% 53% 14% ..

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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	

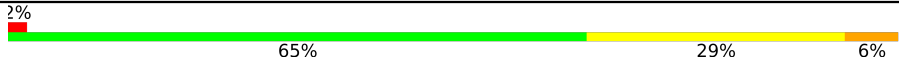
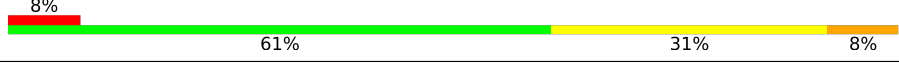
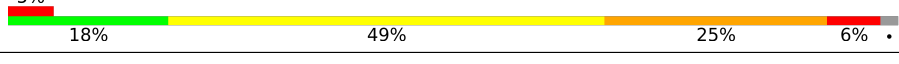
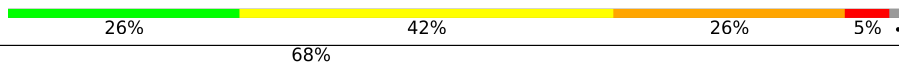



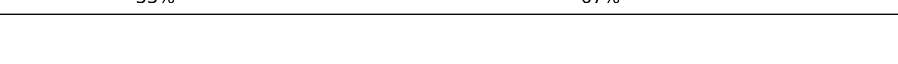
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Mol	Chain	Length	Quality of chain
40	YU	118	3% 49% 42% 8%
41	RV	101	6% 56% 33% 9%
41	YV	101	4% 42% 47% 11%
42	RW	113	63% 27% 9%
42	YW	113	66% 25% 9%
43	RX	96	54% 33% 8%
43	YX	96	52% 38% 6%
44	RY	110	19% 28% 49% 15% 7%
44	YY	110	5% 44% 33% 15% 7%
45	RZ	206	8% 53% 25% 9% 11%
45	YZ	206	5% 45% 36% 7% 11%
46	R0	85	67% 26%
46	Y0	85	58% 36%
47	R1	98	3% 61% 29% 7%
47	Y1	98	4% 56% 34% 7%
48	R2	72	56% 33% 6%
48	Y2	72	4% 25% 53% 17%
49	R3	60	3% 70% 23% 5%
49	Y3	60	57% 30% 12%
50	R4	71	6% 44% 41% 10%
50	Y4	71	4% 25% 37% 28% 10%
51	R5	60	13% 20% 48% 25% 5%
51	Y5	60	5% 40% 38% 18%
52	R6	54	48% 20% 39% 30% 9%
52	Y6	54	44% 28% 41% 19% 9%

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z5	3	
56	Z6	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1636	-	-	-	X
57	MG	QA	1656	-	-	-	X
57	MG	QA	1658	-	-	-	X
57	MG	QA	1662	-	-	-	X
57	MG	QA	1682	-	-	-	X
57	MG	QA	1686	-	-	-	X
57	MG	RA	3050	-	-	-	X
57	MG	RA	3141	-	-	-	X
57	MG	RA	3150	-	-	-	X
57	MG	RA	3178	-	-	-	X
57	MG	RA	3180	-	-	-	X
57	MG	RA	3181	-	-	-	X
57	MG	RA	3184	-	-	-	X
57	MG	RA	3222	-	-	-	X
57	MG	RA	3241	-	-	-	X
57	MG	RA	3277	-	-	-	X
57	MG	RA	3281	-	-	-	X
57	MG	RA	3286	-	-	-	X
57	MG	RA	3287	-	-	-	X
57	MG	RA	3291	-	-	-	X
57	MG	RA	3292	-	-	-	X
57	MG	RA	3294	-	-	-	X
57	MG	RA	3301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3303	-	-	-	X
57	MG	RA	3309	-	-	-	X
57	MG	RP	201	-	-	-	X
57	MG	XA	1650	-	-	-	X
57	MG	XA	1658	-	-	-	X
57	MG	XA	1672	-	-	-	X
57	MG	XA	1679	-	-	-	X
57	MG	XA	1680	-	-	-	X
57	MG	XA	1686	-	-	-	X
57	MG	XA	1692	-	-	-	X
57	MG	XA	1694	-	-	-	X
57	MG	Y0	101	-	-	-	X
57	MG	YA	3115	-	-	-	X
57	MG	YA	3119	-	-	-	X
57	MG	YA	3125	-	-	-	X
57	MG	YA	3143	-	-	-	X
57	MG	YA	3157	-	-	-	X
57	MG	YA	3165	-	-	-	X
57	MG	YA	3172	-	-	-	X
57	MG	YA	3176	-	-	-	X
57	MG	YA	3177	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3199	-	-	-	X
57	MG	YA	3204	-	-	-	X
57	MG	YA	3214	-	-	-	X
57	MG	YA	3223	-	-	-	X
57	MG	YA	3253	-	-	-	X
57	MG	YA	3261	-	-	-	X
57	MG	YA	3268	-	-	-	X
57	MG	YA	3273	-	-	-	X
57	MG	YA	3277	-	-	-	X
57	MG	YA	3280	-	-	-	X
57	MG	YA	3282	-	-	-	X
57	MG	YA	3286	-	-	-	X
57	MG	YA	3296	-	-	-	X
57	MG	YA	3313	-	-	-	X
57	MG	YA	3317	-	-	-	X
57	MG	YA	3321	-	-	-	X
57	MG	YA	3323	-	-	-	X
57	MG	YE	302	-	-	-	X



## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
10	XJ	99	801	504	157	139	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			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	QX	9	Total	C	N	O	P	0	0	0
			173	76	30	58	9			
23	XX	11	Total	C	N	O	P	0	0	0
			235	106	45	73	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			
24	XY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			

- 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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

- 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
			Total	C	N	O	P			
26	YB	120	2573	1146	476	832	119	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	RI	146	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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
42	YW	113	900	566	177	155	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	58	Total	C	N	O	S	0	0	0
			454	285	89	75	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 CC-Puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z5	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z6	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	92	Total	Mg	0	0
			92	92		
57	QF	1	Total	Mg	0	0
			1	1		
57	QK	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	2	Total	Mg	0	0
			2	2		

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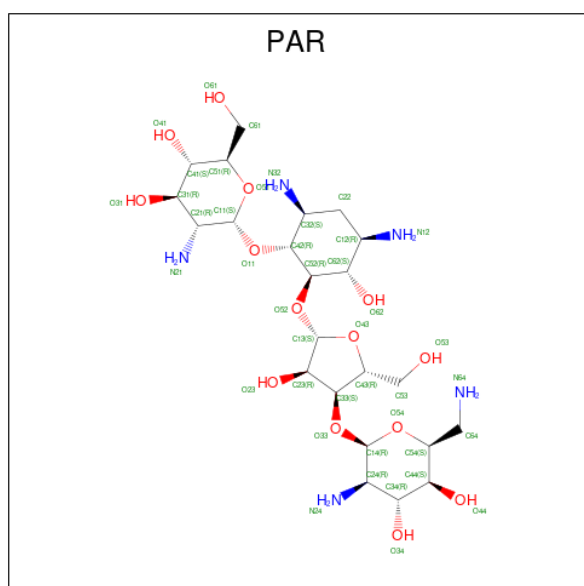
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	1	Total 1	Mg 1	0	0
57	QY	1	Total 1	Mg 1	0	0
57	RA	309	Total 309	Mg 309	0	0
57	RB	3	Total 3	Mg 3	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XA	114	Total 114	Mg 114	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	XX	1	Total 1	Mg 1	0	0
57	XY	1	Total 1	Mg 1	0	0
57	YA	326	Total 326	Mg 326	0	0
57	YB	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YD	2	Total	Mg	0	0
			2	2		
57	YE	2	Total	Mg	0	0
			2	2		
57	YP	2	Total	Mg	0	0
			2	2		
57	YQ	1	Total	Mg	0	0
			1	1		
57	YR	1	Total	Mg	0	0
			1	1		
57	YU	1	Total	Mg	0	0
			1	1		
57	YY	1	Total	Mg	0	0
			1	1		
57	Y0	2	Total	Mg	0	0
			2	2		
57	Y5	1	Total	Mg	0	0
			1	1		
57	Y7	1	Total	Mg	0	0
			1	1		

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



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

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

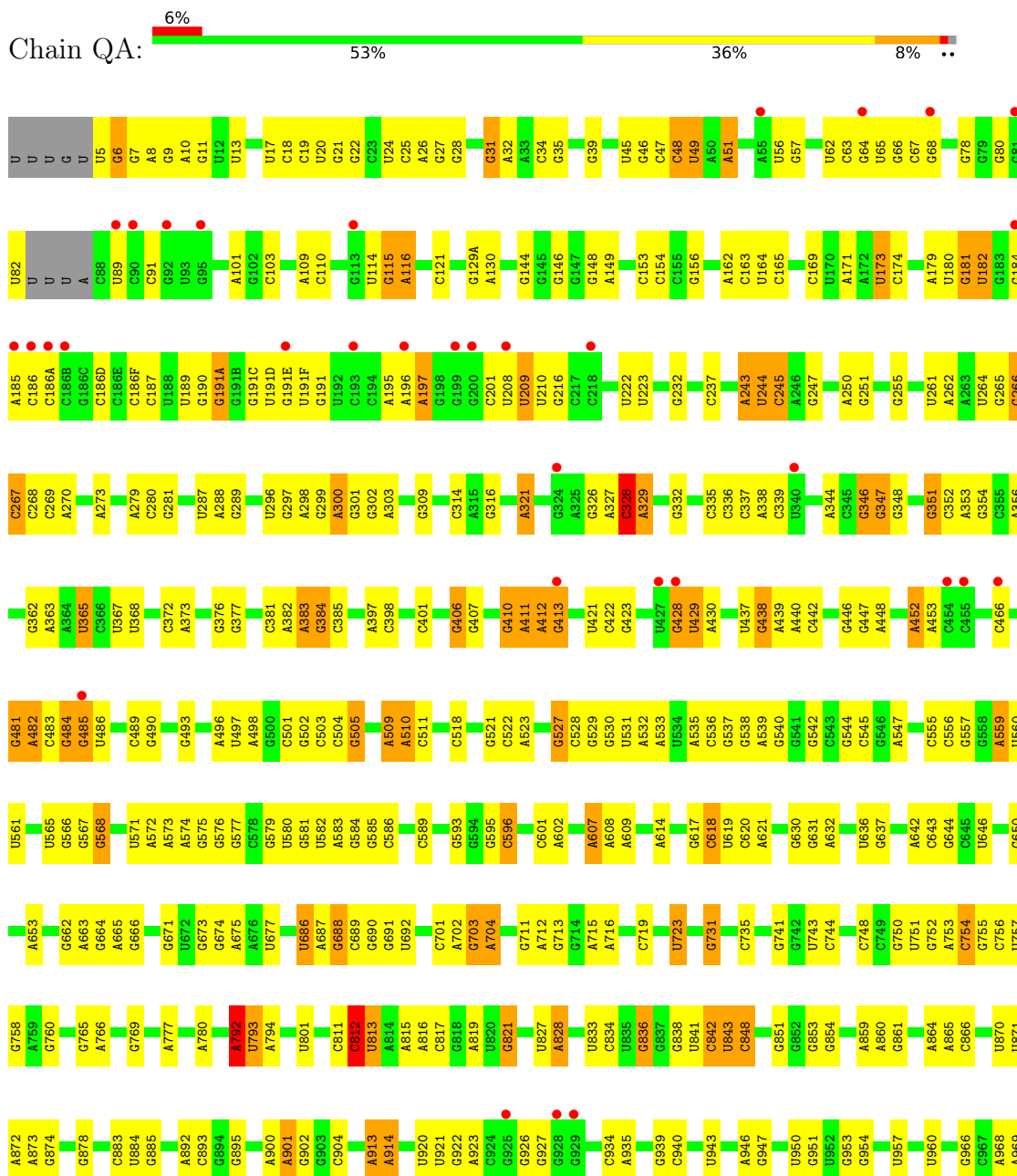
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

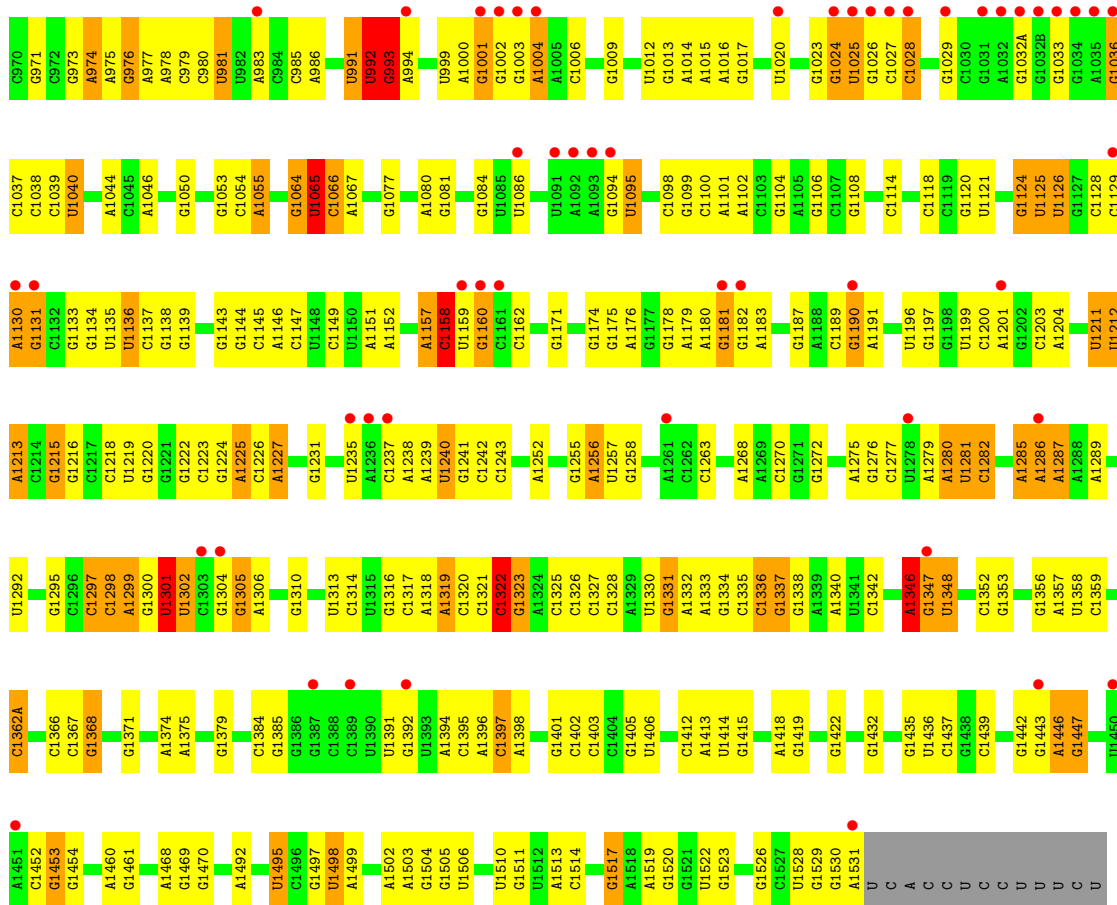
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QD	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XD	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots [i](#)

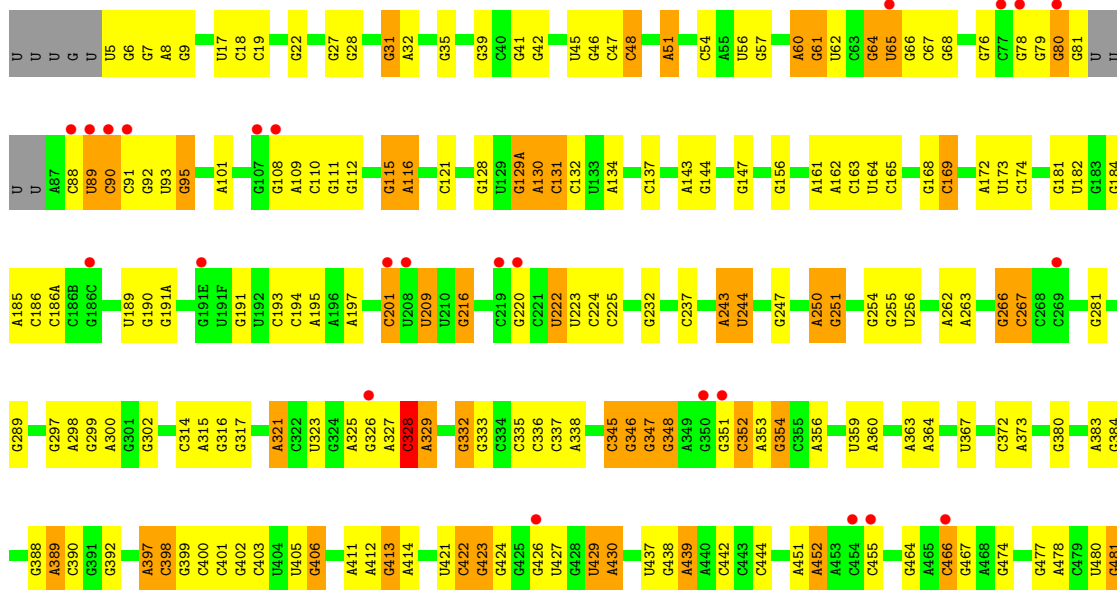
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S rRNA

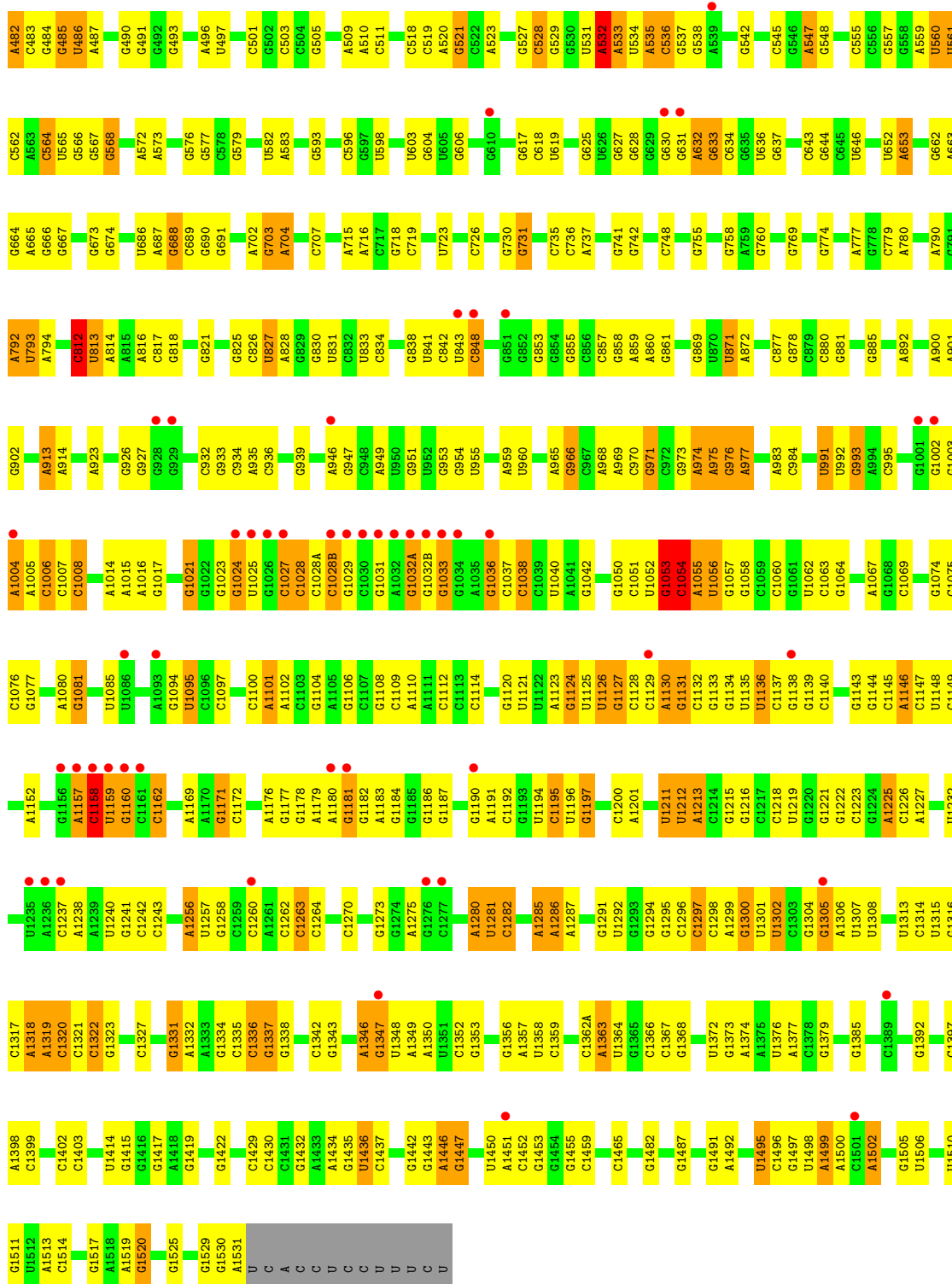




● Molecule 1: 16S rRNA

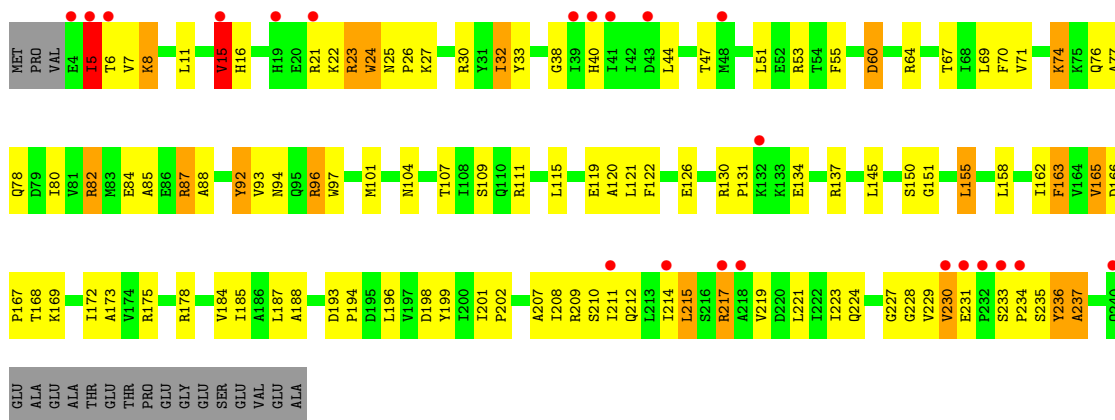




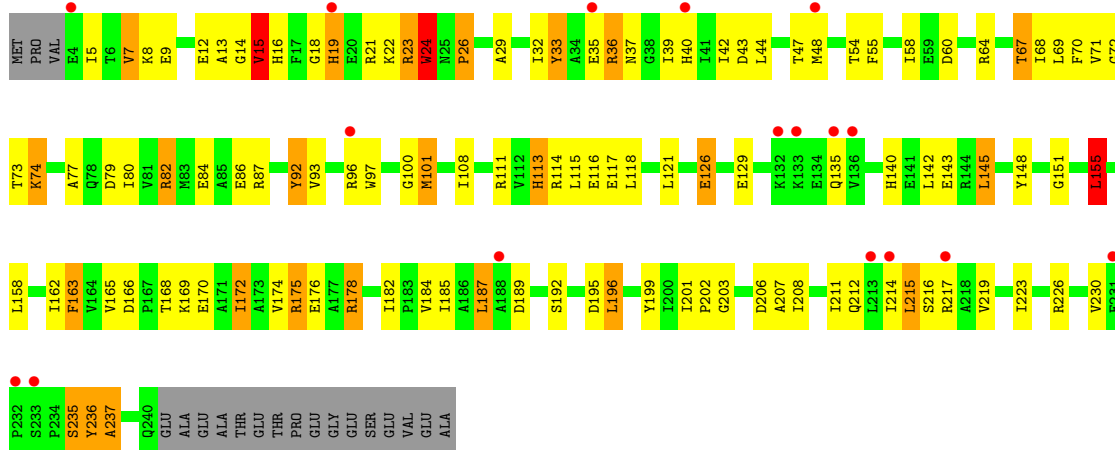


● Molecule 2: 30S ribosomal protein S2

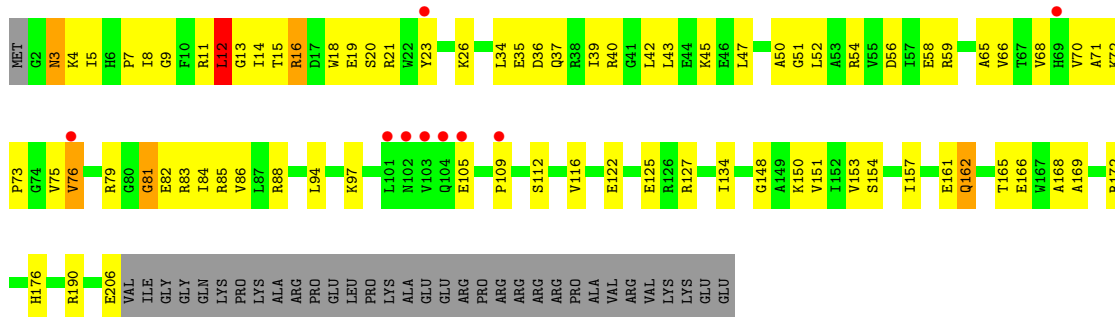




• Molecule 2: 30S ribosomal protein S2

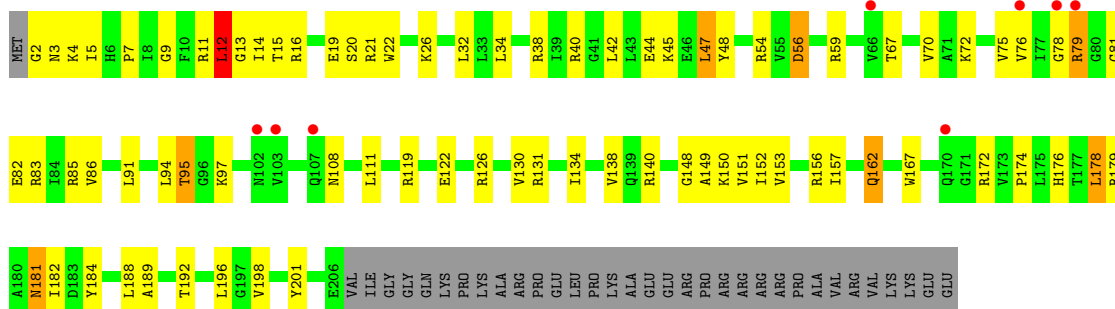


• Molecule 3: 30S ribosomal protein S3

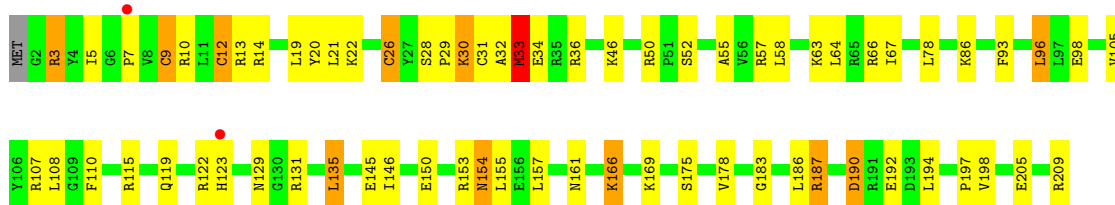


• Molecule 3: 30S ribosomal protein S3

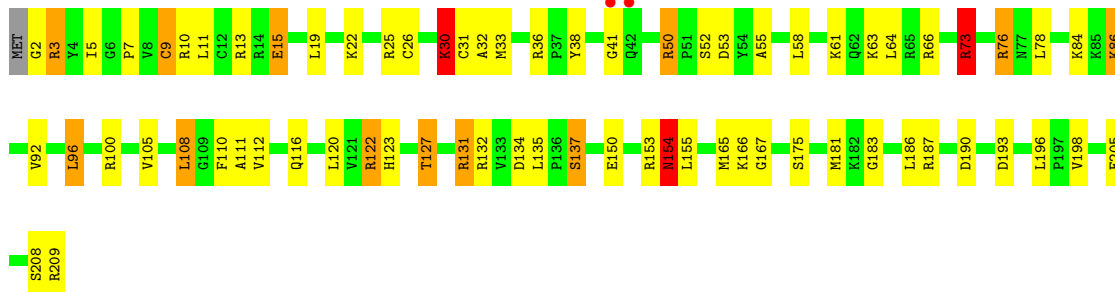




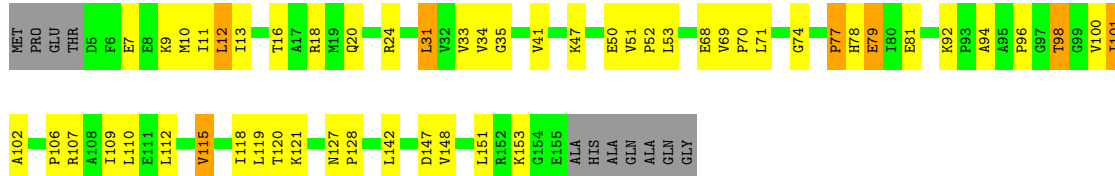
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

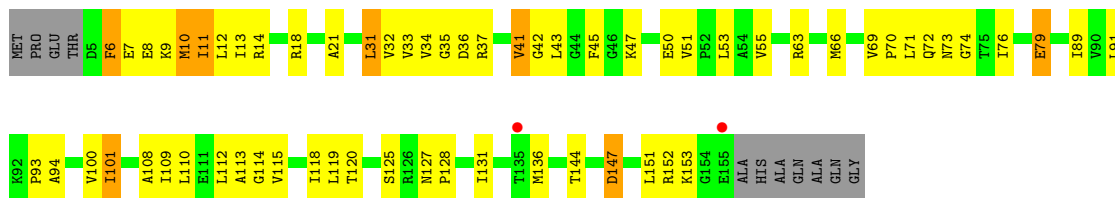


• Molecule 5: 30S ribosomal protein S5

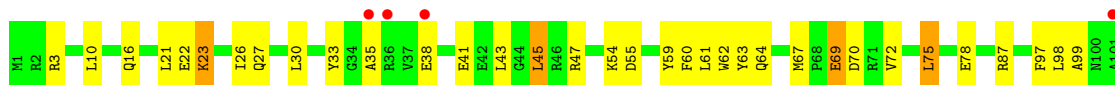


• Molecule 5: 30S ribosomal protein S5

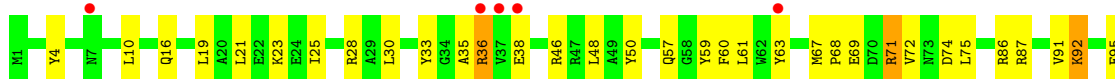




• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

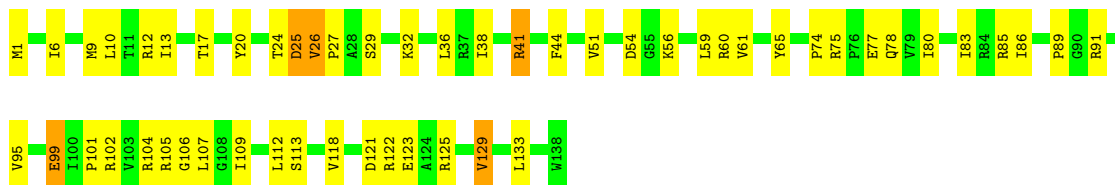


• Molecule 7: 30S ribosomal protein S7

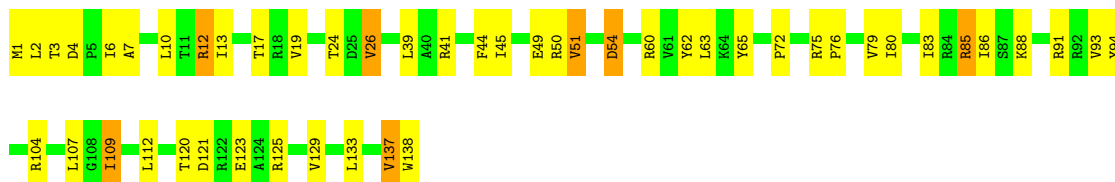


• Molecule 8: 30S ribosomal protein S8

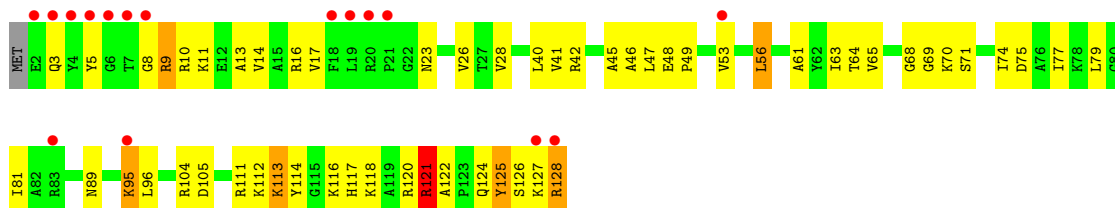




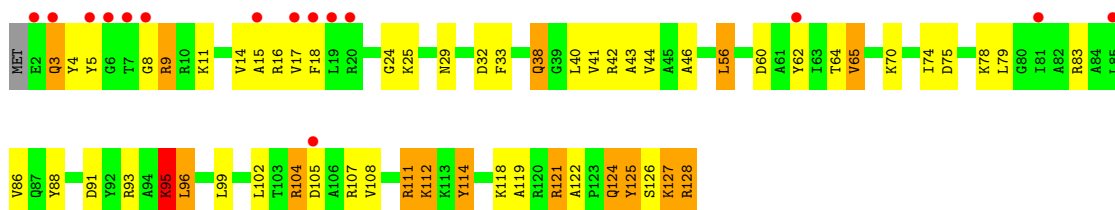
- Molecule 8: 30S ribosomal protein S8



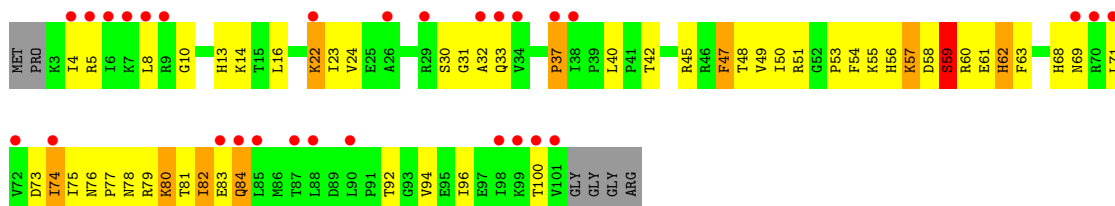
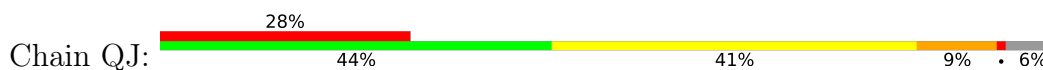
- Molecule 9: 30S ribosomal protein S9



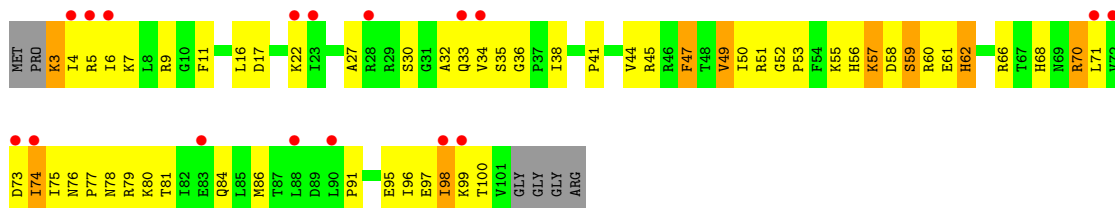
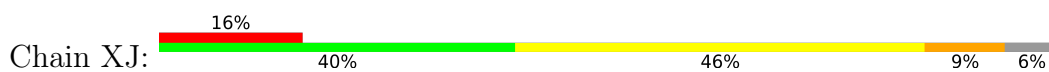
- Molecule 9: 30S ribosomal protein S9



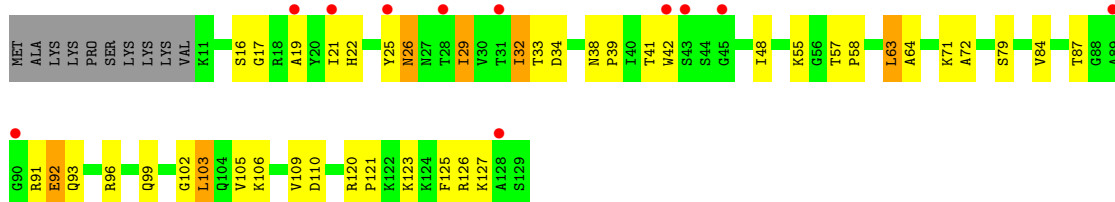
- Molecule 10: 30S ribosomal protein S10



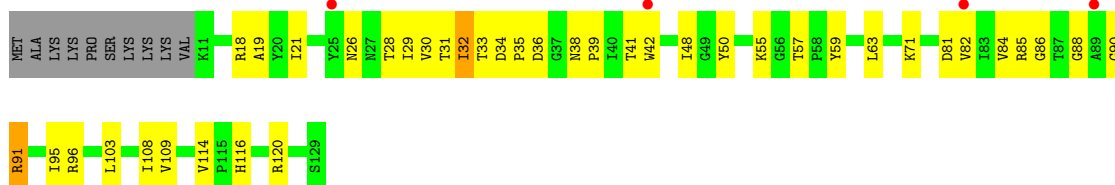
- Molecule 10: 30S ribosomal protein S10



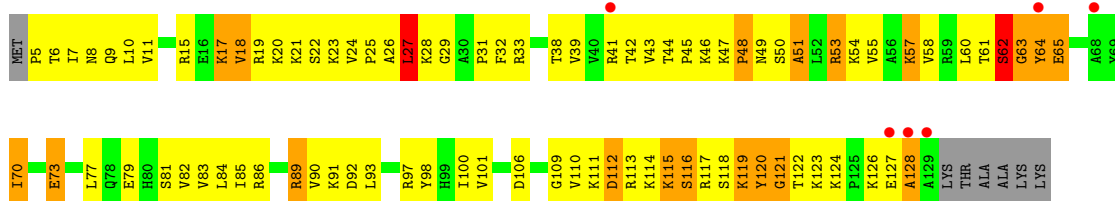
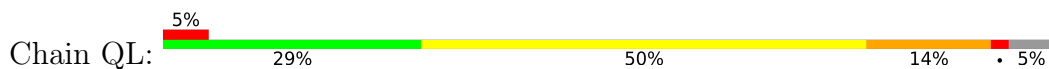
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

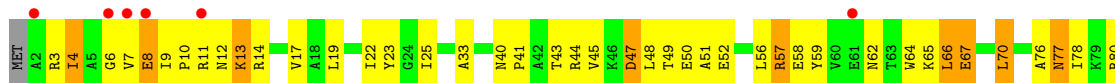


- Molecule 12: 30S ribosomal protein S12





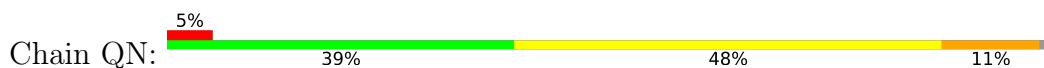
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



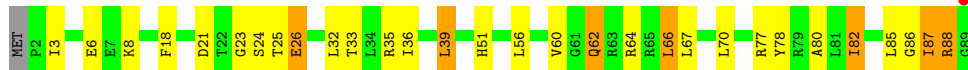
- Molecule 14: 30S ribosomal protein S14 type Z



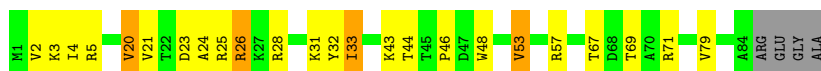
- Molecule 15: 30S ribosomal protein S15



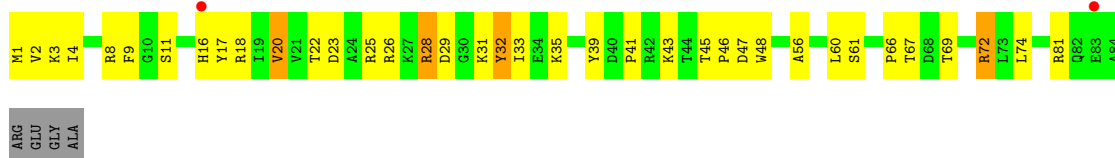
- Molecule 15: 30S ribosomal protein S15



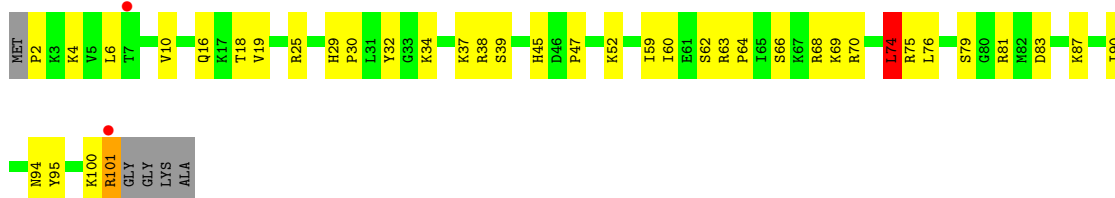
• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16



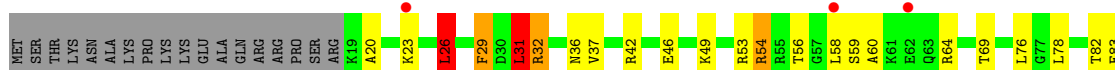
• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17



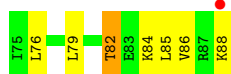
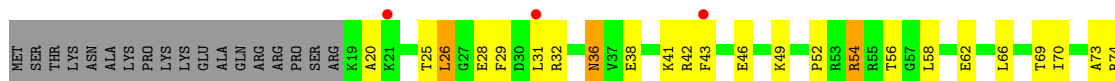
• Molecule 18: 30S ribosomal protein S18







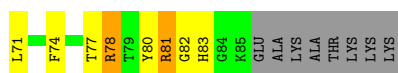
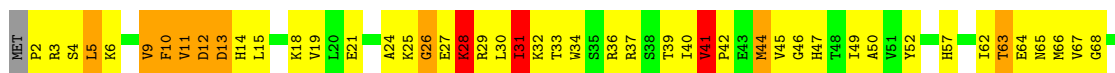
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19

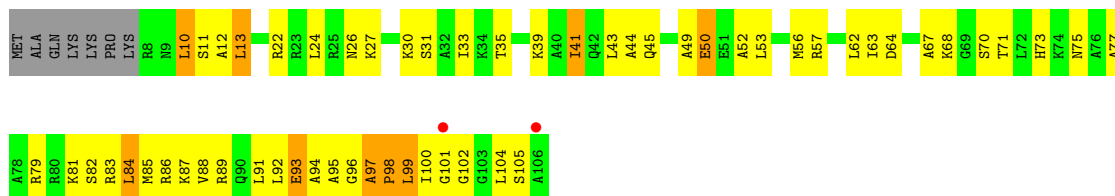


• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20

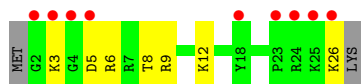




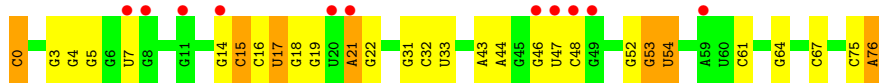
● Molecule 21: 30S ribosomal protein Thx



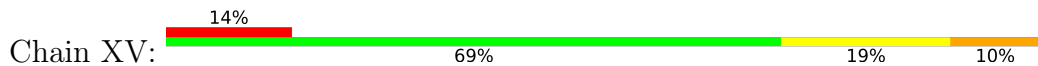
● Molecule 21: 30S ribosomal protein Thx



● Molecule 22: P-site tRNA-fMet



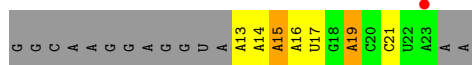
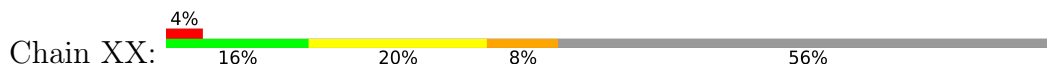
● Molecule 22: P-site tRNA-fMet



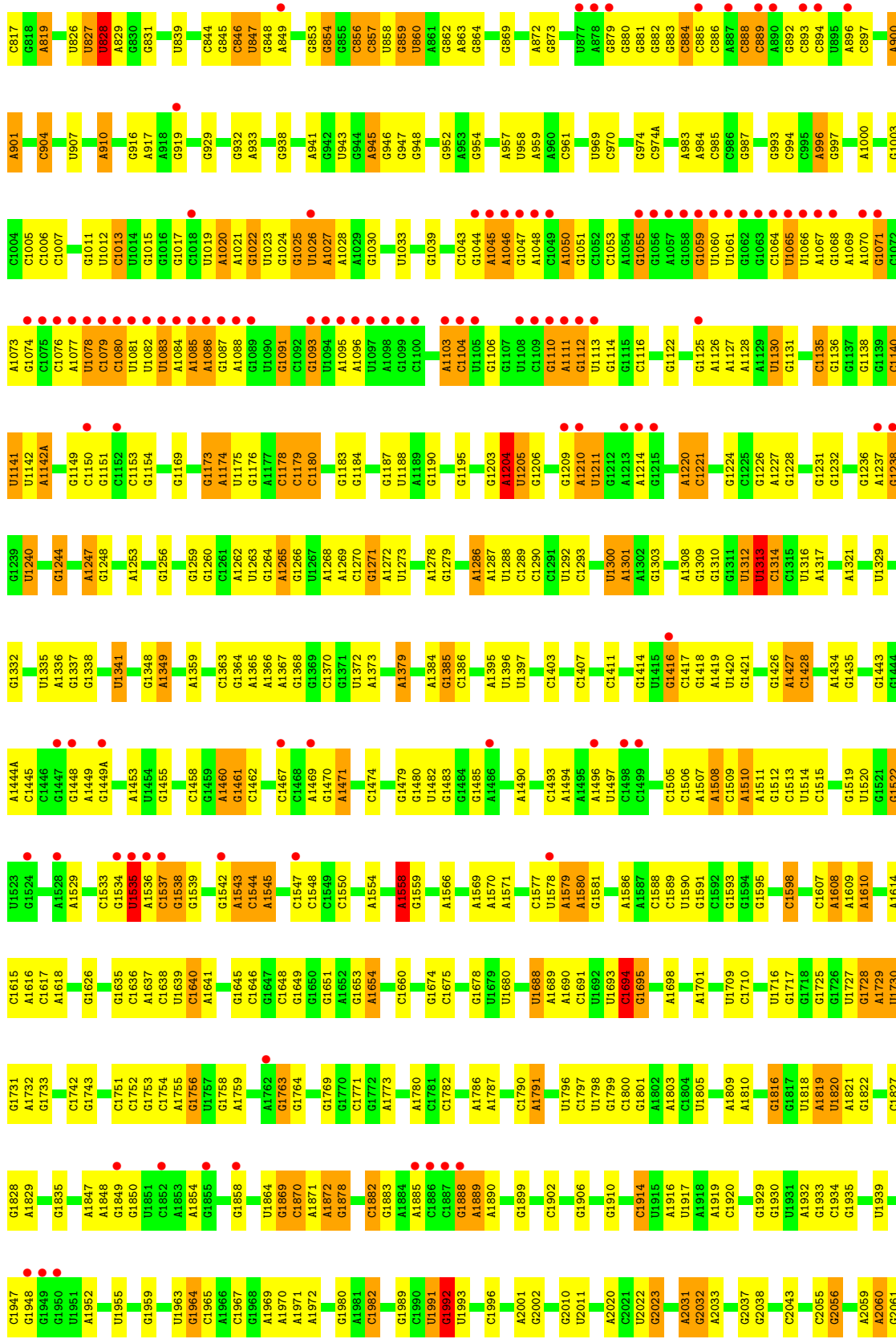
● Molecule 23: messenger RNA

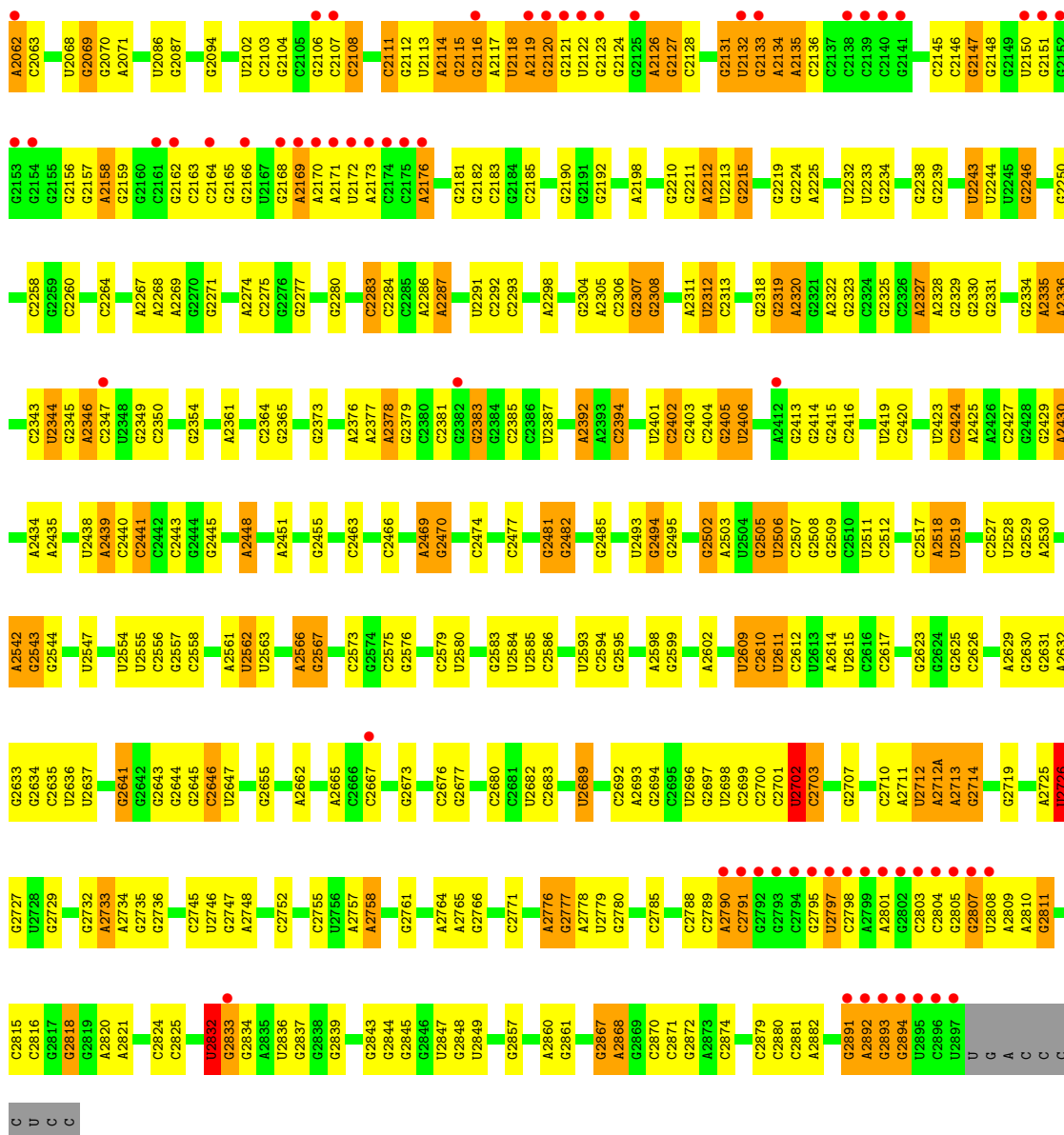


● Molecule 23: messenger RNA

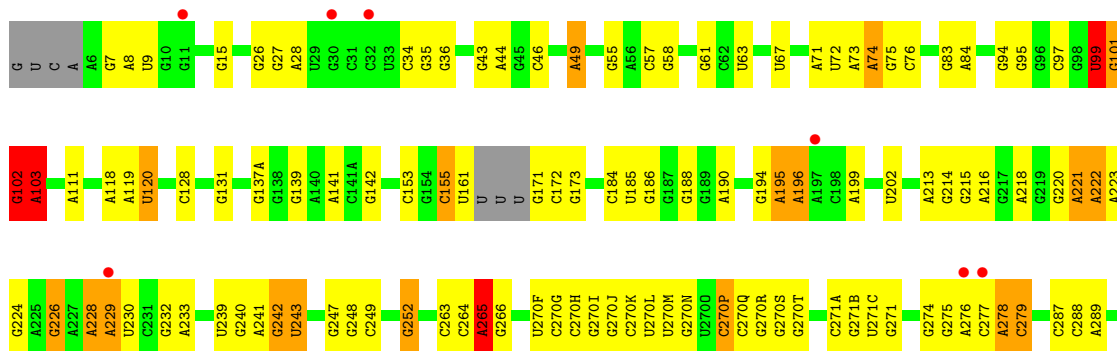


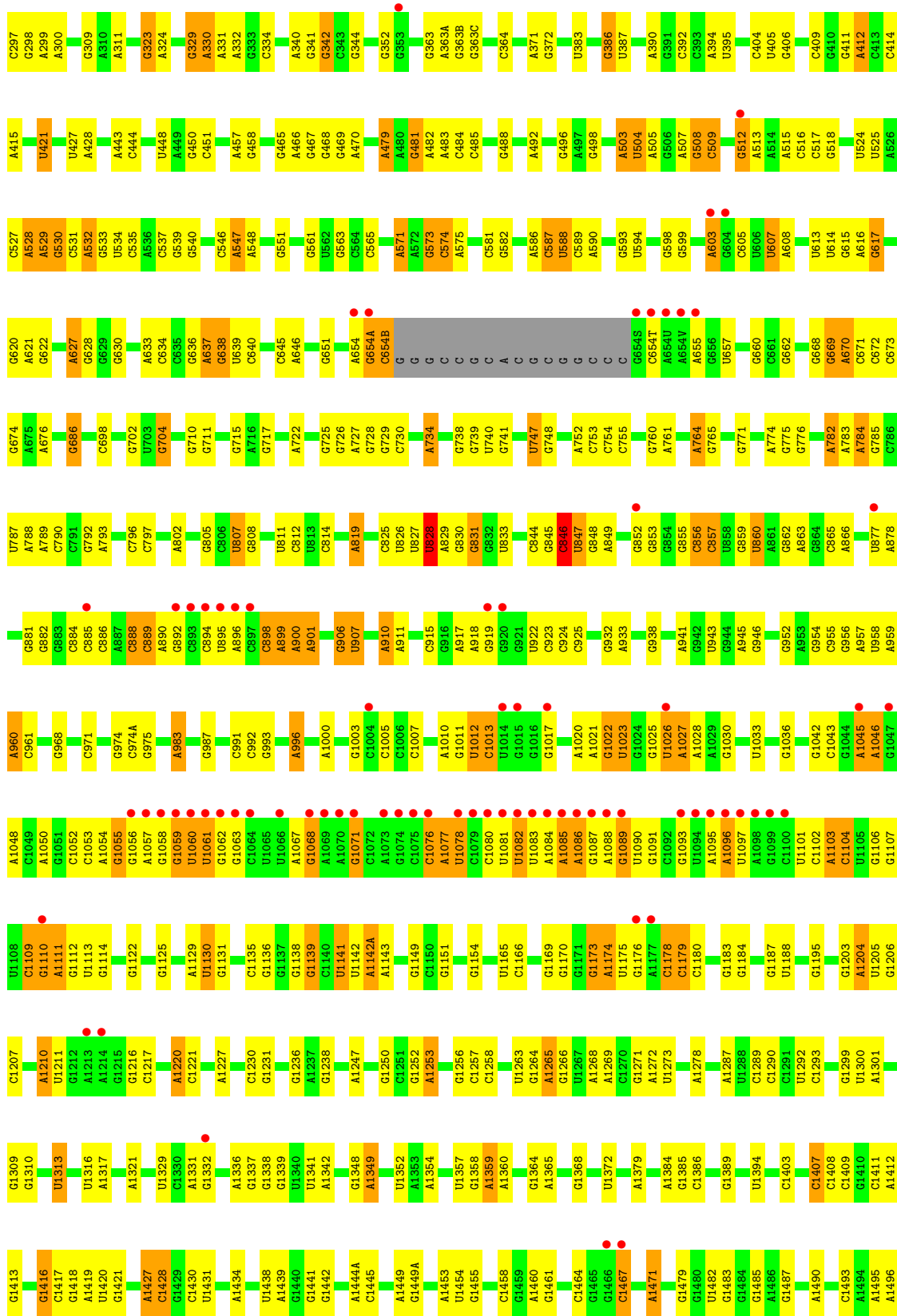


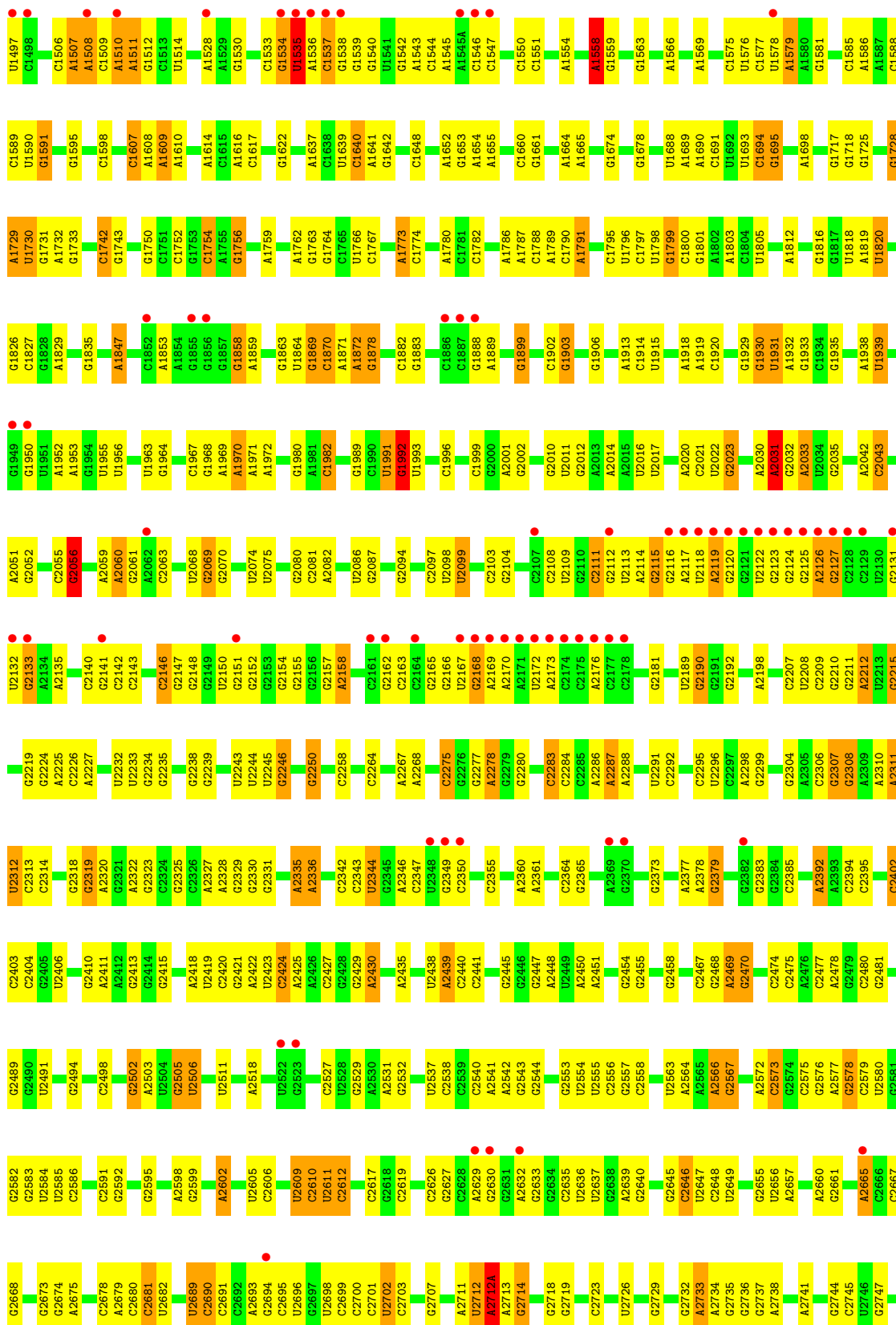


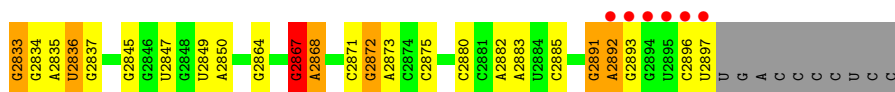
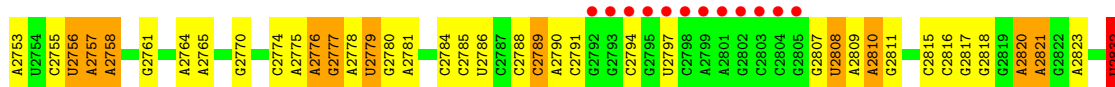


● Molecule 25: 23S rRNA

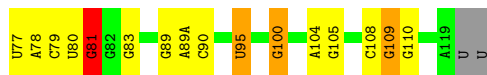








• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA



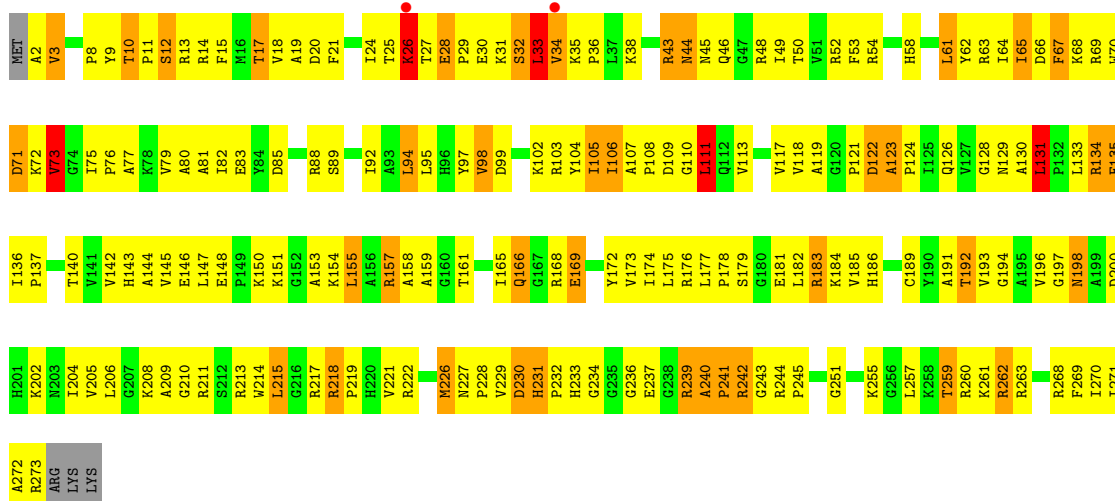
• Molecule 27: 50S ribosomal protein L2



• Molecule 27: 50S ribosomal protein L2

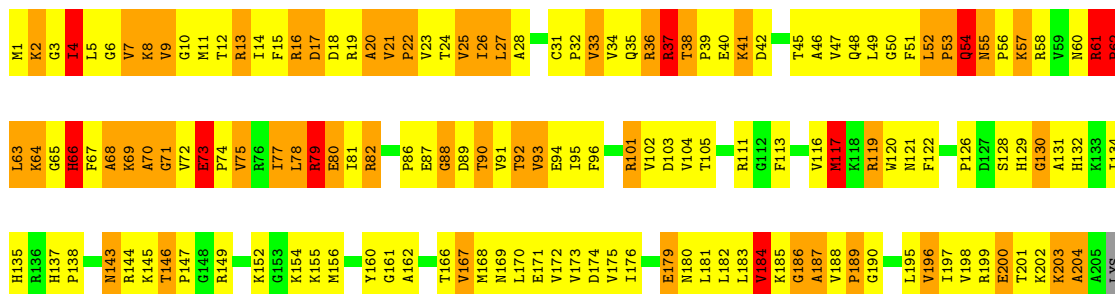






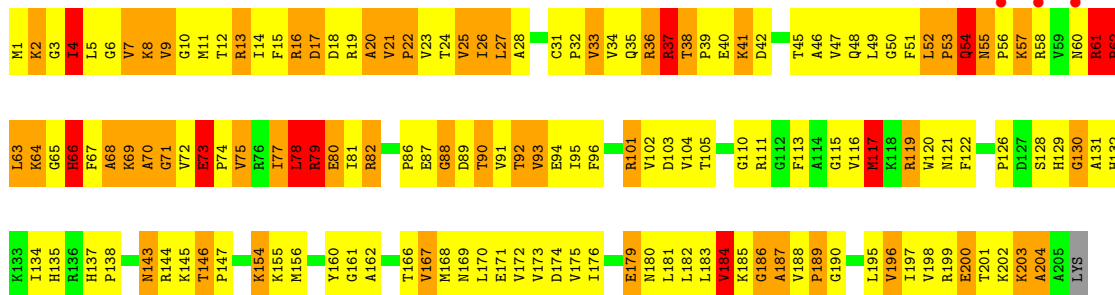
- Molecule 28: 50S ribosomal protein L3

Chain RE: 24% 47% 24% 5%



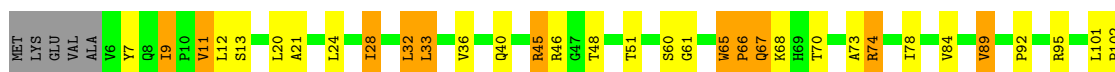
- Molecule 28: 50S ribosomal protein L3

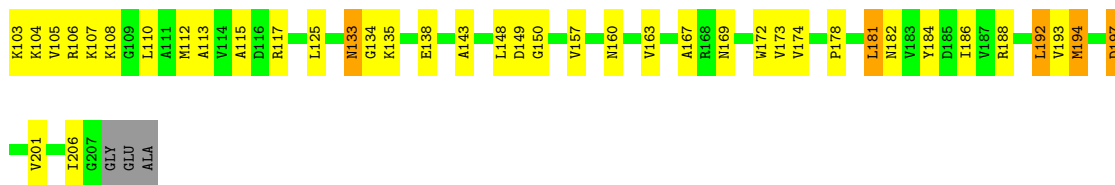
Chain YE: 24% 46% 24% 5%



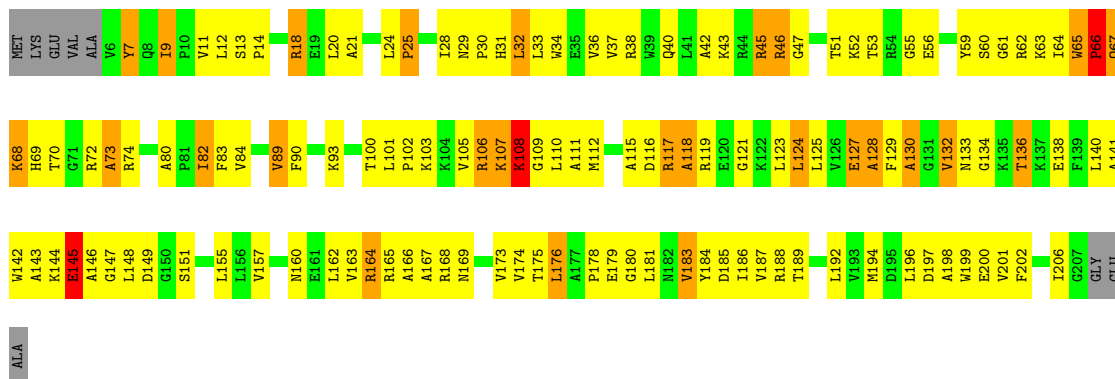
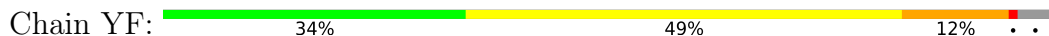
- Molecule 29: 50S ribosomal protein L4

Chain RF: 61% 27% 8%

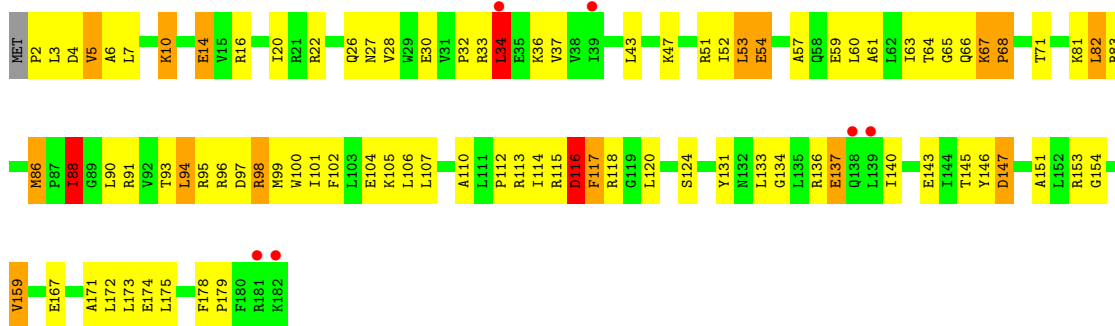




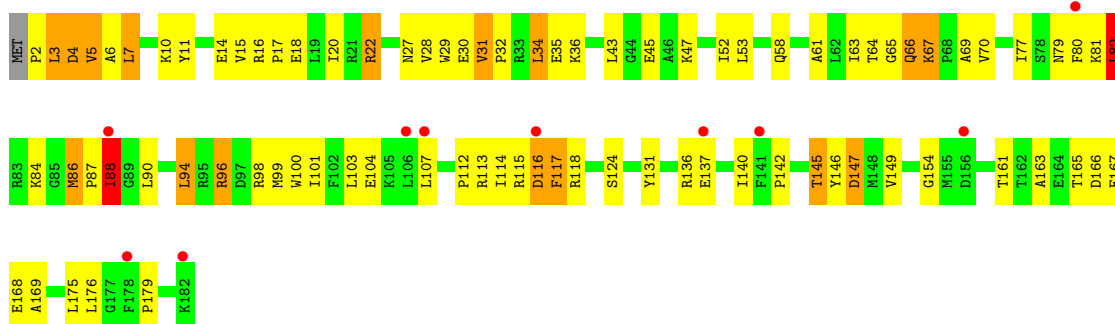
• Molecule 29: 50S ribosomal protein L4



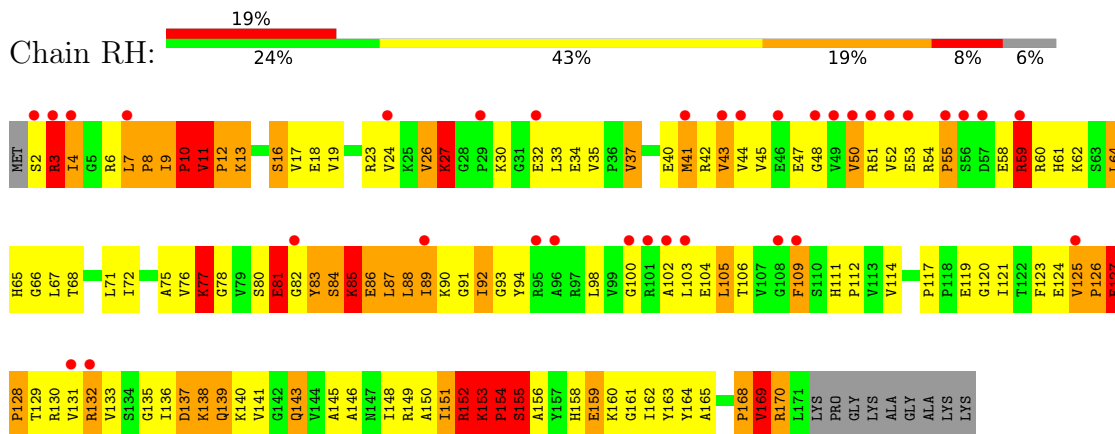
• Molecule 30: 50S ribosomal protein L5



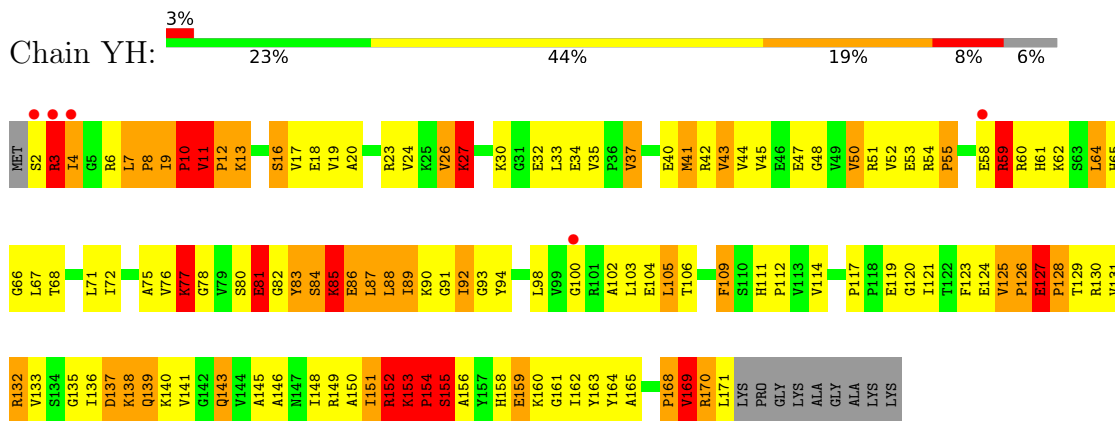
• Molecule 30: 50S ribosomal protein L5



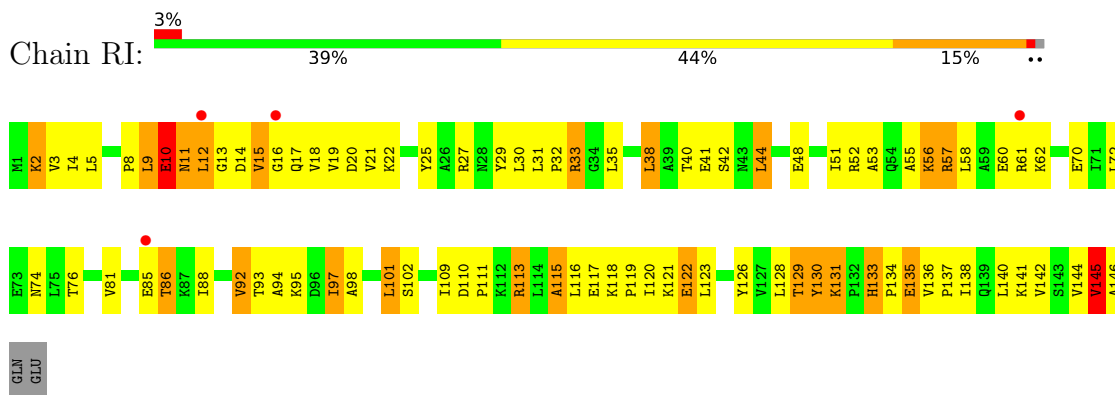
- Molecule 31: 50S ribosomal protein L6



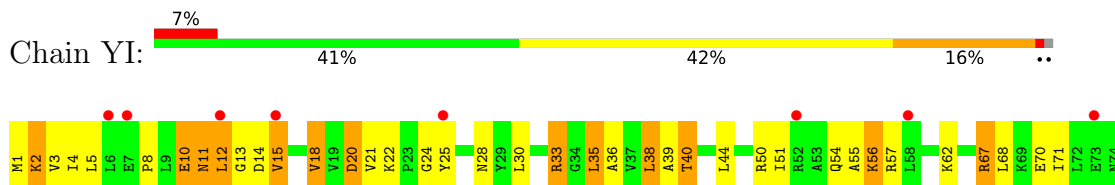
- Molecule 31: 50S ribosomal protein L6

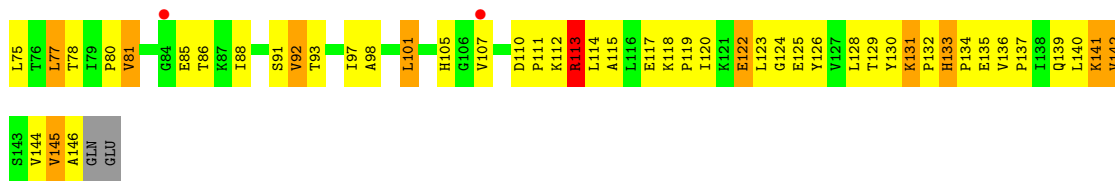


- Molecule 32: 50S ribosomal protein L9

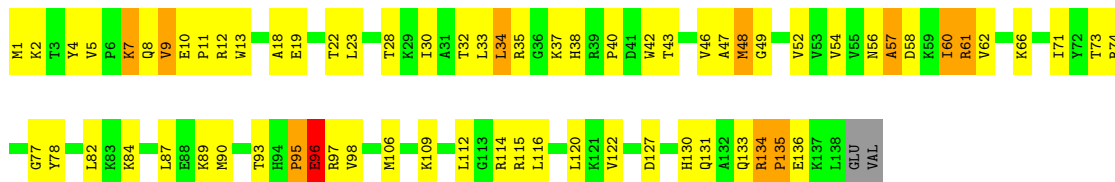


- Molecule 32: 50S ribosomal protein L9

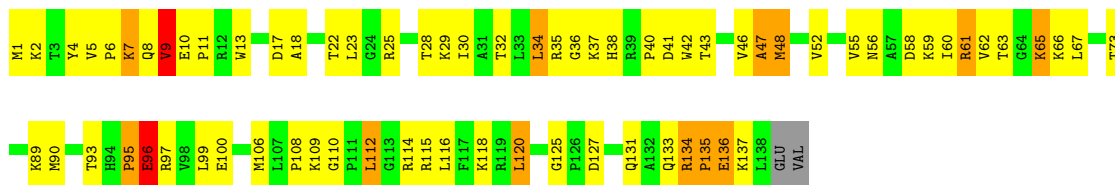




• Molecule 33: 50S ribosomal protein L13



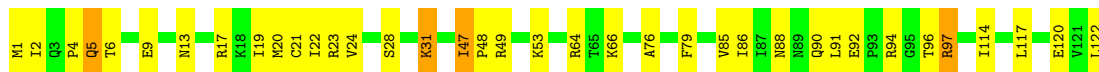
• Molecule 33: 50S ribosomal protein L13



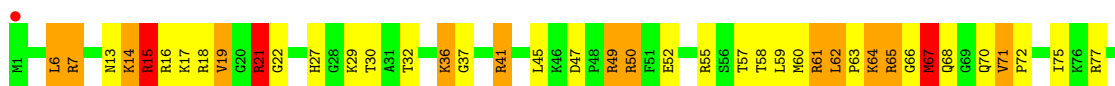
• Molecule 34: 50S ribosomal protein L14



• Molecule 34: 50S ribosomal protein L14

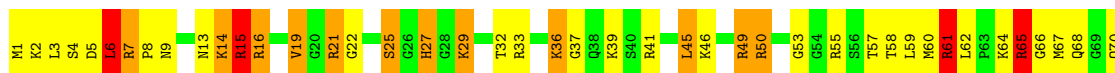


• Molecule 35: 50S ribosomal protein L15





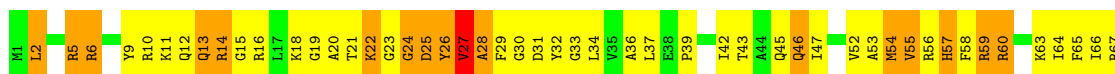
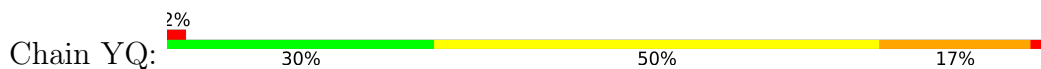
• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L16

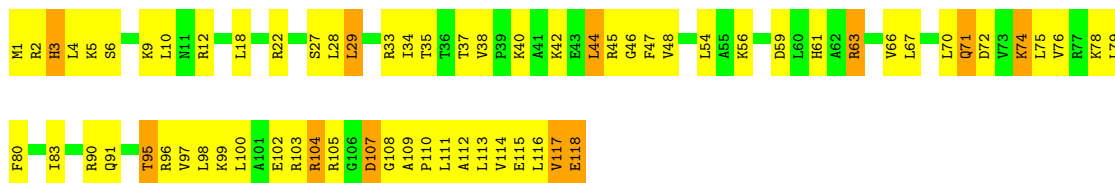


• Molecule 36: 50S ribosomal protein L16

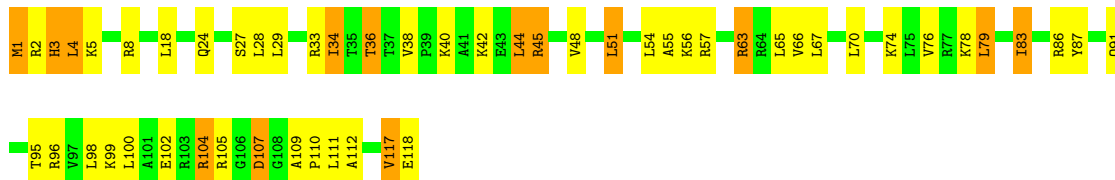


• Molecule 37: 50S ribosomal protein L17

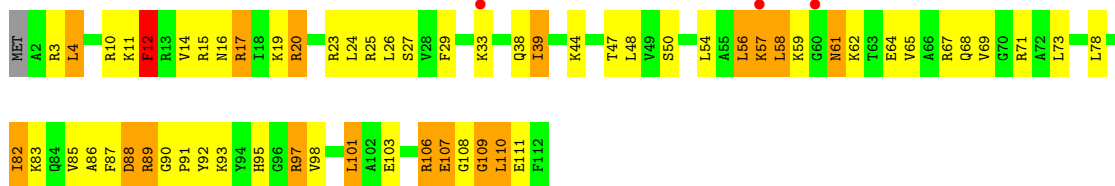




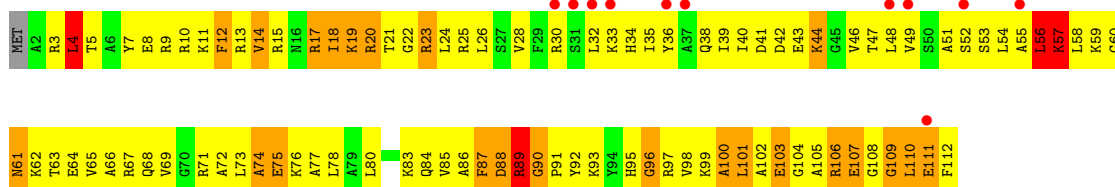
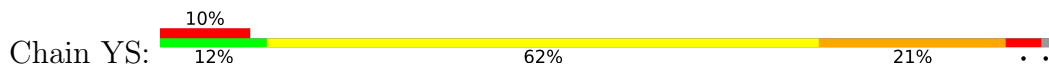
• Molecule 37: 50S ribosomal protein L17



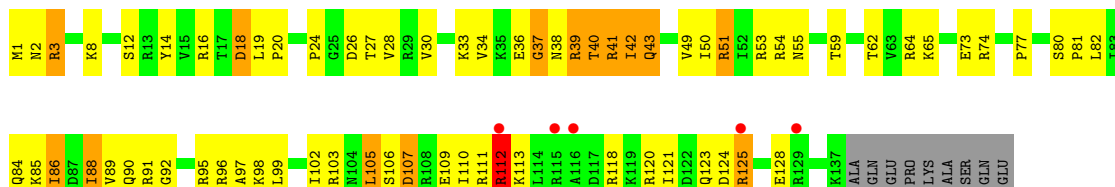
• Molecule 38: 50S ribosomal protein L18



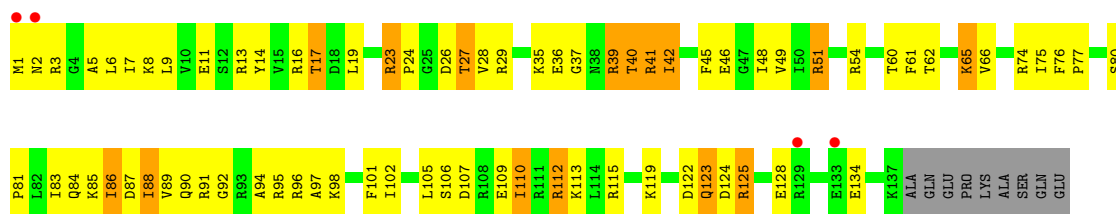
• Molecule 38: 50S ribosomal protein L18



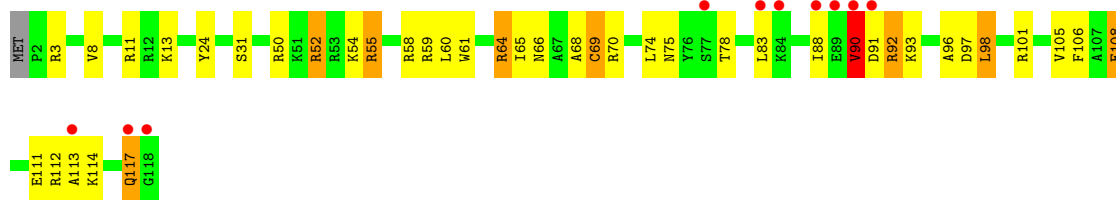
• Molecule 39: 50S ribosomal protein L19



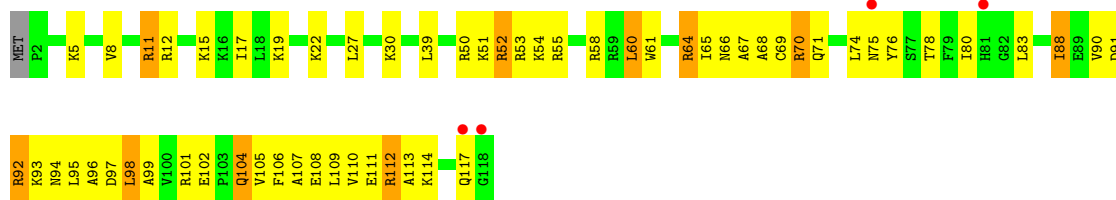
• Molecule 39: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L20



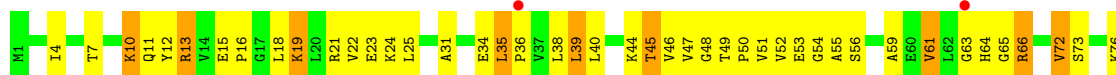
• Molecule 40: 50S ribosomal protein L20



• Molecule 41: 50S ribosomal protein L21

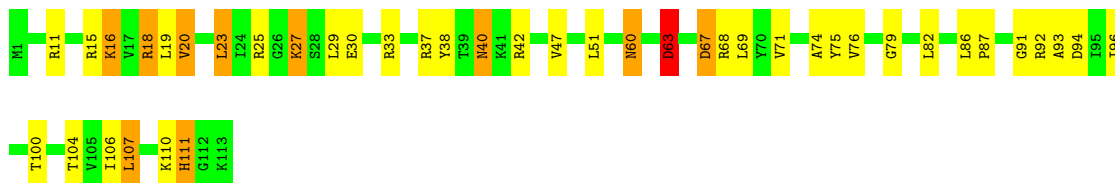


• Molecule 41: 50S ribosomal protein L21





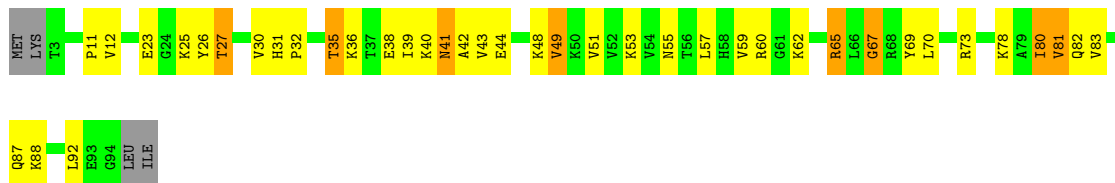
- Molecule 42: 50S ribosomal protein L22



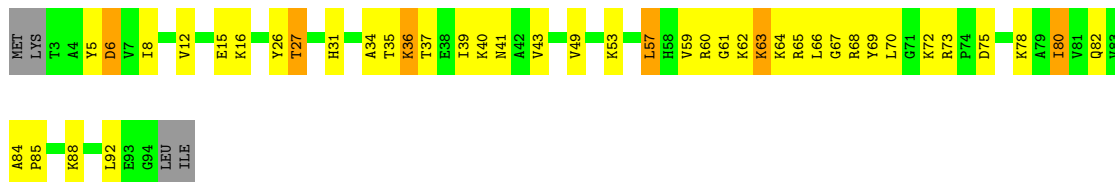
- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23



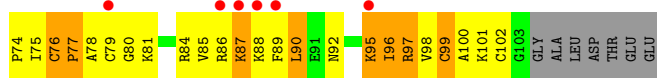
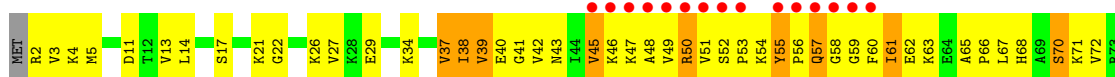
- Molecule 43: 50S ribosomal protein L23



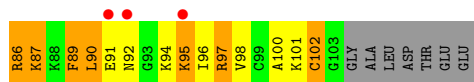
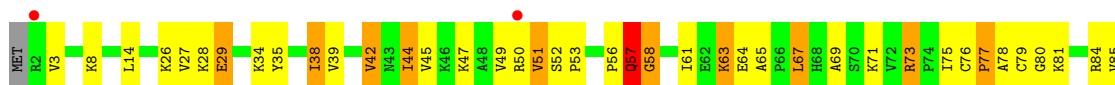
- Molecule 44: 50S ribosomal protein L24



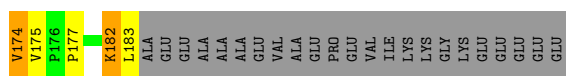
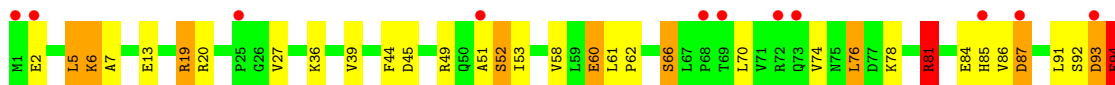




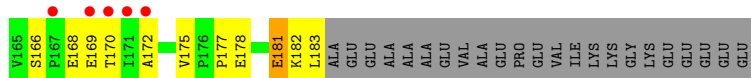
• Molecule 44: 50S ribosomal protein L24



• Molecule 45: 50S ribosomal protein L25



• Molecule 45: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L27





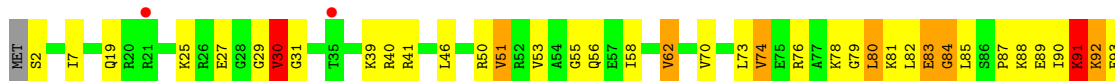
- Molecule 46: 50S ribosomal protein L27



- 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

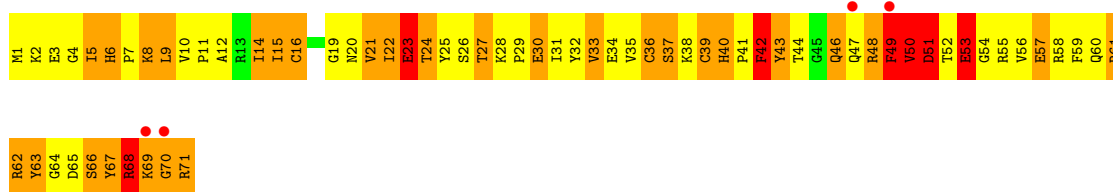




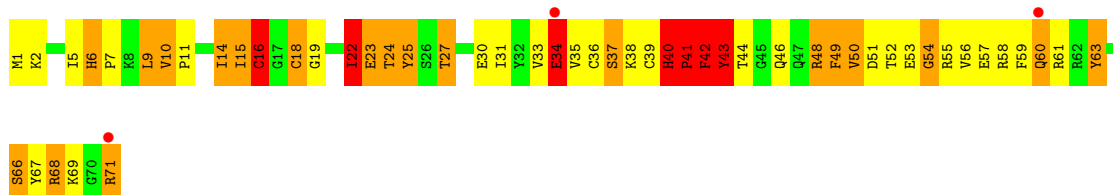
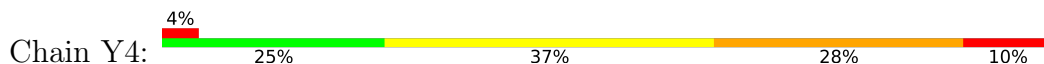
- Molecule 49: 50S ribosomal protein L30



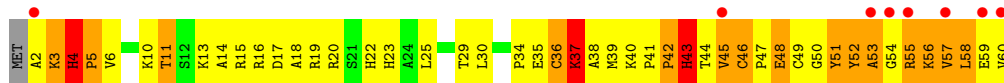
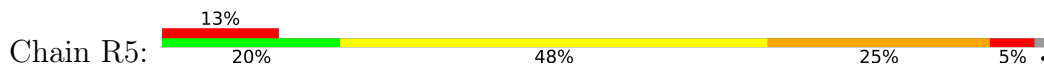
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31



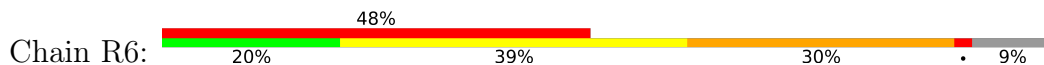
- Molecule 51: 50S ribosomal protein L32

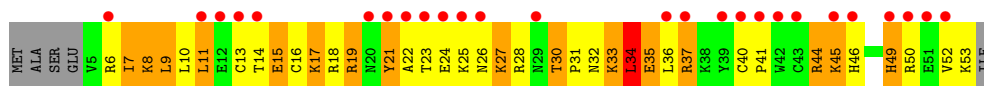


- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33





• Molecule 52: 50S ribosomal protein L33



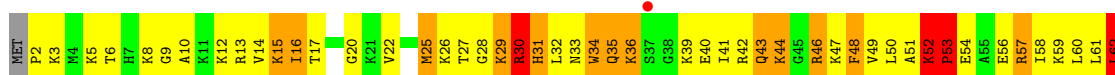
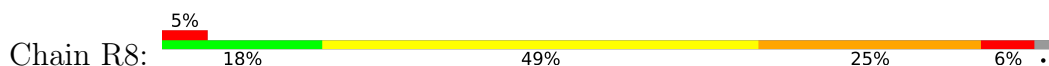
• Molecule 53: 50S ribosomal protein L34



• Molecule 53: 50S ribosomal protein L34



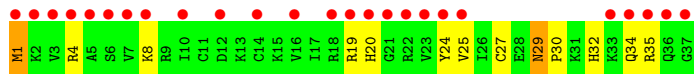
• Molecule 54: 50S ribosomal protein L35



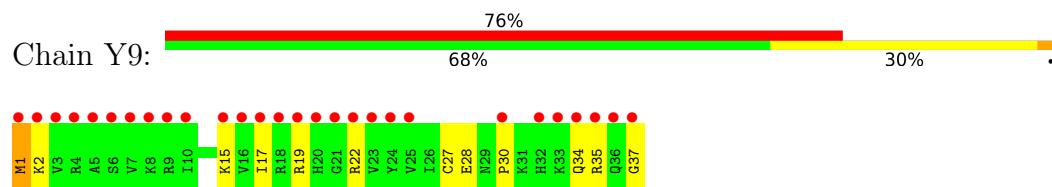
• Molecule 54: 50S ribosomal protein L35



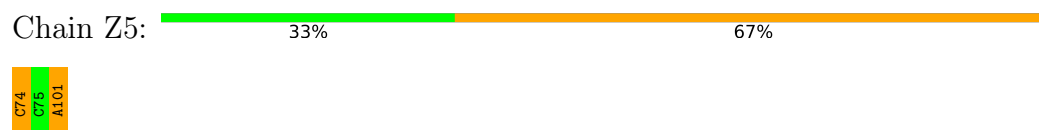
• Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-Puro



- Molecule 56: CC-Puro



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.28Å 448.36Å 616.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.50 49.80 – 3.47	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.80-3.50) 98.1 (49.80-3.47)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.214 , 0.250 0.220 , 0.252	Depositor DCC
$R_{free}$ test set	33377 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.6	Xtrriage
Anisotropy	0.106	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 96.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	292242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

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	0.27	0/36098	0.83	42/56341 (0.1%)
1	XA	0.30	1/36101 (0.0%)	0.85	45/56346 (0.1%)
2	QB	0.32	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.54	0/2195
3	XC	0.37	0/1629	0.57	0/2195
4	QD	0.27	0/1733	0.45	0/2318
4	XD	0.40	0/1733	0.60	0/2318
5	QE	0.35	0/1171	0.57	0/1576
5	XE	0.43	0/1171	0.63	1/1576 (0.1%)
6	QF	0.39	0/856	0.55	0/1154
6	XF	0.39	0/856	0.58	0/1154
7	QG	0.34	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.51	0/1709
8	QH	0.34	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.37	0/814	0.63	2/1095 (0.2%)
10	XJ	0.39	1/814 (0.1%)	0.63	1/1095 (0.1%)
11	QK	0.39	0/900	0.59	1/1213 (0.1%)
11	XK	0.39	0/900	0.59	0/1213
12	QL	0.49	1/991 (0.1%)	0.80	1/1327 (0.1%)
12	XL	0.49	0/991	0.83	3/1327 (0.2%)
13	QM	0.32	0/974	0.58	0/1303
13	XM	0.37	0/974	0.62	0/1303
14	QN	0.37	0/501	0.62	0/664
14	XN	0.43	0/501	0.66	0/664
15	QO	0.36	0/745	0.54	0/992
15	XO	0.40	0/745	0.55	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.36	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.36	0/847	0.54	0/1131
18	QR	0.36	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.60	0/768
19	QS	0.34	0/689	0.61	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.37	0/765	0.66	0/1007
20	XT	0.31	0/765	0.60	0/1007
21	QU	0.31	0/221	0.55	0/288
21	XU	0.31	0/221	0.62	0/288
22	QV	0.41	1/1836 (0.1%)	0.85	0/2859
22	XV	0.41	1/1836 (0.1%)	0.85	1/2859 (0.0%)
23	QX	0.24	0/192	0.72	0/297
23	XX	1.13	1/263 (0.4%)	1.41	2/407 (0.5%)
24	QY	0.29	0/355	0.82	0/551
24	XY	0.71	0/355	1.50	8/551 (1.5%)
25	RA	0.30	0/69521	0.84	41/108529 (0.0%)
25	YA	0.32	0/69521	0.86	45/108529 (0.0%)
26	RB	0.37	0/2878	0.95	5/4490 (0.1%)
26	YB	0.35	0/2878	0.97	9/4490 (0.2%)
27	RD	0.51	0/2165	0.70	0/2919
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.30	0/1620	0.48	0/2194
29	YF	0.49	0/1620	0.75	0/2194
30	RG	0.32	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	3/1802 (0.2%)
32	RI	0.28	0/1151	0.56	0/1558
32	YI	0.32	0/1151	0.54	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.43	0/1131	0.63	0/1525
34	RO	0.42	0/943	0.62	1/1269 (0.1%)
34	YO	0.50	0/943	0.65	0/1269
35	RP	0.29	0/1162	0.60	1/1544 (0.1%)
35	YP	0.33	0/1162	0.64	0/1544
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.43	0/982	0.70	0/1312
37	YR	0.45	0/982	0.73	0/1312
38	RS	0.36	0/892	0.65	0/1187



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YS	0.46	0/892	0.83	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.44	0/1155	0.66	0/1542
40	RU	0.40	0/982	0.65	0/1306
40	YU	0.51	0/982	0.70	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.46	0/790	0.73	1/1057 (0.1%)
42	RW	0.50	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.48	0/739	0.65	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.46	0/798	0.69	0/1064
45	RZ	0.27	0/1493	0.52	0/2026
45	YZ	0.28	0/1493	0.55	0/2026
46	R0	0.46	0/657	0.68	0/874
46	Y0	0.49	0/657	0.70	0/874
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.38	0/583	0.64	0/771
48	Y2	0.50	0/583	0.83	1/771 (0.1%)
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.42	0/474	0.59	0/635
50	R4	0.39	0/594	0.78	1/795 (0.1%)
50	Y4	0.44	0/594	0.72	2/795 (0.3%)
51	R5	0.56	1/473 (0.2%)	0.78	1/639 (0.2%)
51	Y5	0.49	0/468	0.72	0/632
52	R6	0.35	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.67	0/575
53	Y7	0.56	0/438	0.70	0/575
54	R8	0.61	0/525	0.91	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.26	0/310	0.46	0/407
55	Y9	0.32	0/310	0.48	0/407
56	Z5	0.78	0/40	1.80	1/60 (1.7%)
56	Z6	0.79	0/40	1.81	1/60 (1.7%)
All	All	0.34	7/316469 (0.0%)	0.81	244/473140 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.58	1.48	1.61
22	XV	0	C	OP3-P	-10.41	1.48	1.61
1	XA	1056	U	N1-C2	-5.87	1.33	1.38
23	XX	16	A	N7-C5	-5.79	1.35	1.39
12	QL	48	PRO	N-CD	5.49	1.55	1.47

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1195	C	C6-N1-C2	-11.67	115.63	120.30
1	XA	529	G	N1-C6-O6	11.48	126.79	119.90
28	RE	21	VAL	C-N-CD	-10.10	98.38	120.60
28	YE	21	VAL	C-N-CD	-10.10	98.38	120.60
1	QA	1158	C	N1-C2-O2	8.76	124.15	118.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	459	0
1	XA	32249	0	16279	459	0
2	QB	1924	0	1975	63	0
2	XB	1924	0	1975	81	0
3	QC	1605	0	1668	51	0
3	XC	1605	0	1668	62	0
4	QD	1703	0	1764	60	0
4	XD	1703	0	1762	51	0
5	QE	1155	0	1213	49	0
5	XE	1155	0	1213	46	0
6	QF	843	0	857	21	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	31	0
8	QH	1116	0	1177	39	0
8	XH	1116	0	1177	28	0
9	QI	1010	0	1037	39	0
9	XI	1010	0	1037	56	0
10	QJ	801	0	849	68	0
10	XJ	801	0	849	63	0
11	QK	885	0	904	26	0
11	XK	885	0	904	29	0
12	QL	975	0	1062	101	0
12	XL	975	0	1062	95	0
13	QM	964	0	1034	67	0
13	XM	964	0	1034	47	0
14	QN	492	0	529	28	0
14	XN	492	0	529	26	0
15	QO	734	0	771	20	0
15	XO	734	0	771	19	0
16	QP	705	0	725	15	0
16	XP	705	0	725	26	0
17	QQ	834	0	904	27	0
17	XQ	834	0	904	20	0
18	QR	574	0	644	13	0
18	XR	574	0	644	21	0
19	QS	674	0	699	77	0
19	XS	674	0	699	54	0
20	QT	763	0	860	44	0
20	XT	763	0	861	80	0
21	QU	217	0	234	11	0
21	XU	217	0	234	5	0
22	QV	1644	0	835	14	0
22	XV	1644	0	836	14	0
23	QX	173	0	86	2	0
23	XX	235	0	120	7	0
24	QY	319	0	162	1	0
24	XY	319	0	162	9	0
25	RA	62071	0	31285	816	0
25	YA	62071	0	31288	817	0
26	RB	2573	0	1306	42	0
26	YB	2573	0	1306	47	0
27	RD	2115	0	2195	98	0
27	YD	2115	0	2195	324	0
28	RE	1568	0	1634	272	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	276	0
29	RF	1585	0	1632	52	0
29	YF	1585	0	1632	169	0
30	RG	1474	0	1535	95	0
30	YG	1474	0	1535	68	0
31	RH	1307	0	1382	228	0
31	YH	1307	0	1382	228	0
32	RI	1136	0	1223	62	0
32	YI	1136	0	1223	56	0
33	RN	1104	0	1180	41	0
33	YN	1104	0	1180	57	0
34	RO	933	0	996	21	0
34	YO	933	0	996	24	0
35	RP	1145	0	1227	66	0
35	YP	1145	0	1227	77	0
36	RQ	1122	0	1179	162	0
36	YQ	1122	0	1179	166	0
37	RR	968	0	1033	50	0
37	YR	968	0	1033	34	0
38	RS	882	0	943	44	0
38	YS	882	0	943	161	0
39	RT	1141	0	1202	66	0
39	YT	1141	0	1202	59	0
40	RU	964	0	1021	36	0
40	YU	964	0	1021	58	0
41	RV	779	0	852	24	0
41	YV	779	0	852	48	0
42	RW	900	0	964	25	0
42	YW	900	0	964	25	0
43	RX	725	0	778	31	0
43	YX	725	0	778	23	0
44	RY	785	0	878	50	0
44	YY	785	0	878	40	0
45	RZ	1461	0	1493	43	0
45	YZ	1461	0	1493	55	0
46	R0	648	0	672	28	0
46	Y0	648	0	672	38	0
47	R1	763	0	848	25	0
47	Y1	763	0	848	32	0
48	R2	581	0	629	19	0
48	Y2	581	0	629	76	0
49	R3	469	0	518	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	18	0
50	R4	581	0	575	219	0
50	Y4	581	0	577	84	0
51	R5	459	0	480	78	0
51	Y5	454	0	475	40	0
52	R6	424	0	450	35	0
52	Y6	424	0	450	29	0
53	R7	430	0	480	17	0
53	Y7	430	0	480	24	0
54	R8	517	0	582	107	0
54	Y8	517	0	582	87	0
55	R9	307	0	338	12	0
55	Y9	307	0	338	11	0
56	Z5	74	0	51	17	0
56	Z6	74	0	51	13	0
57	QA	92	0	0	0	0
57	QF	1	0	0	0	0
57	QK	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	2	0	0	0	0
57	QX	1	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	309	0	0	0	0
57	RB	3	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	1	0	0	0	0
57	RQ	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	114	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XV	3	0	0	0	0
57	XX	1	0	0	0	0
57	XY	1	0	0	0	0
57	Y0	2	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YA	326	0	0	0	0
57	YB	2	0	0	0	0
57	YD	2	0	0	0	0
57	YE	2	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	1	0	0	0	0
57	YR	1	0	0	0	0
57	YU	1	0	0	0	0
57	YY	1	0	0	0	0
58	QA	42	0	45	1	0
58	XA	42	0	45	0	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	292242	0	198373	7614	0

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

The worst 5 of 7614 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
30:RG:112:PRO:CB	50:R4:37:SER:HB2	1.50	1.39
30:RG:112:PRO:HB3	50:R4:37:SER:CB	1.53	1.37
30:RG:67:LYS:HE2	50:R4:6:HIS:CE1	1.60	1.36

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	174 (74%)	45 (19%)	16 (7%)	1	13
2	XB	235/256 (92%)	177 (75%)	43 (18%)	15 (6%)	1	14
3	QC	203/239 (85%)	164 (81%)	33 (16%)	6 (3%)	4	30
3	XC	203/239 (85%)	173 (85%)	27 (13%)	3 (2%)	10	45
4	QD	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	10	45
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	6	35
5	QE	149/162 (92%)	137 (92%)	8 (5%)	4 (3%)	5	33
5	XE	149/162 (92%)	135 (91%)	11 (7%)	3 (2%)	7	39
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	12	48
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	48
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	22	61
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4	31
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	24
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	4	29
10	QJ	97/105 (92%)	77 (79%)	16 (16%)	4 (4%)	3	23
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	18
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	42
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	42
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	10
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	10
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	12
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	7
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	50
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	36
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	13	50
16	XP	82/88 (93%)	72 (88%)	9 (11%)	1 (1%)	13	50
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7	39
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	21
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10	45
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	4
19	XS	82/93 (88%)	54 (66%)	18 (22%)	10 (12%)	0	5
20	QT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	1	15
20	XT	97/106 (92%)	75 (77%)	18 (19%)	4 (4%)	3	23
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	22
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	22
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	21
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	12
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	181 (90%)	13 (6%)	6 (3%)	4	30
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	7
30	RG	179/182 (98%)	139 (78%)	25 (14%)	15 (8%)	1	9
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	13
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	109 (76%)	24 (17%)	11 (8%)	1	10
32	YI	144/148 (97%)	108 (75%)	23 (16%)	13 (9%)	1	8
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	8
33	YN	136/140 (97%)	107 (79%)	16 (12%)	13 (10%)	0	8
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	42
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	9	42
35	RP	148/150 (99%)	109 (74%)	26 (18%)	13 (9%)	1	8
35	YP	148/150 (99%)	101 (68%)	35 (24%)	12 (8%)	1	9
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	7
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	7
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	22
37	YR	116/118 (98%)	98 (84%)	12 (10%)	6 (5%)	2	18
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	2
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1	8
39	YT	135/146 (92%)	107 (79%)	18 (13%)	10 (7%)	1	11
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	27
40	YU	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	9	42
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	15
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	9
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3	26
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	8	41
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	37
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6	37
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	2
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	5
45	RZ	181/206 (88%)	127 (70%)	34 (19%)	20 (11%)	0	6
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	0	7
46	R0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	12	48
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	8
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	14
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	1	15
48	Y2	67/72 (93%)	47 (70%)	12 (18%)	8 (12%)	0	5
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	27
49	Y3	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	41
50	R4	69/71 (97%)	22 (32%)	21 (30%)	26 (38%)	0	0
50	Y4	69/71 (97%)	34 (49%)	14 (20%)	21 (30%)	0	0
51	R5	57/60 (95%)	33 (58%)	10 (18%)	14 (25%)	0	0
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	3	26
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	1
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	2
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	38
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	38 (61%)	14 (23%)	10 (16%)	0	2
54	Y8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	3
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11469/12128 (95%)	9035 (79%)	1606 (14%)	828 (7%)	1	11

5 of 828 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	172 (84%)	33 (16%)	2	14
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5	23
3	QC	159/188 (85%)	145 (91%)	14 (9%)	10	38
3	XC	159/188 (85%)	145 (91%)	14 (9%)	10	38
4	QD	180/181 (99%)	161 (89%)	19 (11%)	6	30
4	XD	180/181 (99%)	154 (86%)	26 (14%)	3	18
5	QE	116/123 (94%)	104 (90%)	12 (10%)	7	32
5	XE	116/123 (94%)	104 (90%)	12 (10%)	7	32
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4	21
6	XF	90/90 (100%)	82 (91%)	8 (9%)	9	37
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8	34
7	XG	126/127 (99%)	114 (90%)	12 (10%)	8	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11	40
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	29
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2	11
9	XI	98/99 (99%)	78 (80%)	20 (20%)	1	6
10	QJ	89/92 (97%)	79 (89%)	10 (11%)	6	27
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	2	15
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	32
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	32
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	21
12	XL	104/109 (95%)	89 (86%)	15 (14%)	3	18
13	QM	97/101 (96%)	73 (75%)	24 (25%)	0	4
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	7
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	8
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	19
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	37
15	XO	79/80 (99%)	69 (87%)	10 (13%)	4	22
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	23
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6	28
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	11	40
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	51
18	QR	61/77 (79%)	50 (82%)	11 (18%)	1	9
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	17
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	7
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	5
20	QT	76/82 (93%)	67 (88%)	9 (12%)	5	25
20	XT	76/82 (93%)	67 (88%)	9 (12%)	5	25
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	58
27	RD	214/218 (98%)	175 (82%)	39 (18%)	1	9
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	11
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	4
29	RF	161/166 (97%)	142 (88%)	19 (12%)	5	25
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	21
30	RG	155/156 (99%)	134 (86%)	21 (14%)	4	21
30	YG	155/156 (99%)	133 (86%)	22 (14%)	3	19
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	7
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	7
32	RI	122/124 (98%)	99 (81%)	23 (19%)	1	8
32	YI	122/124 (98%)	97 (80%)	25 (20%)	1	6
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	12
33	YN	117/119 (98%)	95 (81%)	22 (19%)	1	8
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	32
34	YO	100/100 (100%)	88 (88%)	12 (12%)	5	24
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0	3
35	YP	116/116 (100%)	79 (68%)	37 (32%)	0	2
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	14
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	12
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	10
37	YR	101/101 (100%)	80 (79%)	21 (21%)	1	6
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	6
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	17
39	RT	120/127 (94%)	101 (84%)	19 (16%)	2	15
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	10
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	17
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2	11
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	7
41	YV	82/82 (100%)	67 (82%)	15 (18%)	1	8
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	6
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	11
43	RX	74/78 (95%)	64 (86%)	10 (14%)	4	21
43	YX	74/78 (95%)	60 (81%)	14 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	3
44	YY	85/91 (93%)	64 (75%)	21 (25%)	0	4
45	RZ	162/179 (90%)	137 (85%)	25 (15%)	2	16
45	YZ	162/179 (90%)	144 (89%)	18 (11%)	6	28
46	R0	65/67 (97%)	60 (92%)	5 (8%)	13	42
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	9	36
47	R1	82/83 (99%)	73 (89%)	9 (11%)	6	29
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	18
48	R2	64/67 (96%)	55 (86%)	9 (14%)	3	19
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	29
49	R3	51/52 (98%)	45 (88%)	6 (12%)	5	25
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	15
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0	3
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	4
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	4
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	3
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	6
53	R7	42/42 (100%)	34 (81%)	8 (19%)	1	8
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	12
54	R8	54/55 (98%)	38 (70%)	16 (30%)	0	2
54	Y8	54/55 (98%)	38 (70%)	16 (30%)	0	2
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	53
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	53
All	All	9702/10066 (96%)	8178 (84%)	1524 (16%)	2	15

5 of 1524 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	XM	17	VAL
31	YH	132	ARG
15	XO	26	GLU
13	XM	13	LYS
27	YD	237	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
55	R9	29	ASN
48	Y2	9	GLN
5	XE	72	GLN
27	YD	198	ASN
2	XB	212	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	272 (18%)	41 (2%)
1	XA	1499/1522 (98%)	285 (19%)	36 (2%)
22	QV	76/77 (98%)	18 (23%)	1 (1%)
22	XV	76/77 (98%)	15 (19%)	1 (1%)
23	QX	7/25 (28%)	1 (14%)	0
23	XX	10/25 (40%)	4 (40%)	0
24	QY	14/18 (77%)	4 (28%)	0
24	XY	14/18 (77%)	3 (21%)	0
25	RA	2879/2915 (98%)	559 (19%)	48 (1%)
25	YA	2879/2915 (98%)	557 (19%)	47 (1%)
26	RB	119/122 (97%)	19 (15%)	1 (0%)
26	YB	119/122 (97%)	21 (17%)	1 (0%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9193/9364 (98%)	1758 (19%)	176 (1%)

5 of 1758 RNA backbone outliers are listed below:

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

5 of 176 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	913	A
25	YA	856	C
1	XA	1200	C

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Mol	Chain	Res	Type
25	YA	195	A
25	YA	1109	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	PPU	Z5	101	25,56	32,40,41	2.56	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z6	101	25,56	32,40,41	2.56	6 (18%)	33,57,60	2.14	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z5	101	25,56	-	2/21/43/44	0/4/4/4
56	PPU	Z6	101	25,56	-	2/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	101	PPU	O-C	9.30	1.41	1.23
56	Z5	101	PPU	O-C	9.30	1.41	1.23
56	Z6	101	PPU	C9-N6	-5.96	1.31	1.45
56	Z5	101	PPU	C9-N6	-5.93	1.32	1.45
56	Z6	101	PPU	C-N3'	5.72	1.46	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z5	101	PPU	C3'-N3'-C	-8.59	110.26	123.21
56	Z6	101	PPU	C3'-N3'-C	-8.57	110.29	123.21
56	Z5	101	PPU	N3-C2-N1	-4.62	121.46	128.68
56	Z6	101	PPU	N3-C2-N1	-4.60	121.49	128.68
56	Z6	101	PPU	CA-C-N3'	4.03	121.75	116.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z5	101	PPU	14	0
56	Z6	101	PPU	11	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 891 ligands modelled in this entry, 889 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PAR	XA	1715	-	45,45,45	1.62	7 (15%)	64,67,67	1.37	6 (9%)
58	PAR	QA	1693	-	45,45,45	1.63	9 (20%)	64,67,67	1.32	7 (10%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	XA	1715	-	-	5/18/94/94	0/4/4/4
58	PAR	QA	1693	-	-	6/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1693	PAR	C64-C54	5.29	1.59	1.52
58	XA	1715	PAR	C64-C54	5.16	1.59	1.52
58	QA	1693	PAR	O54-C14	3.28	1.50	1.41
58	QA	1693	PAR	C52-C42	3.24	1.59	1.52
58	XA	1715	PAR	C52-C42	3.15	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1693	PAR	C14-O54-C54	5.05	123.59	113.69
58	XA	1715	PAR	O33-C14-C24	4.91	116.67	108.22
58	XA	1715	PAR	O52-C13-C23	4.14	116.54	107.96
58	XA	1715	PAR	C14-O54-C54	3.82	121.19	113.69
58	QA	1693	PAR	O52-C13-C23	3.59	115.40	107.96

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

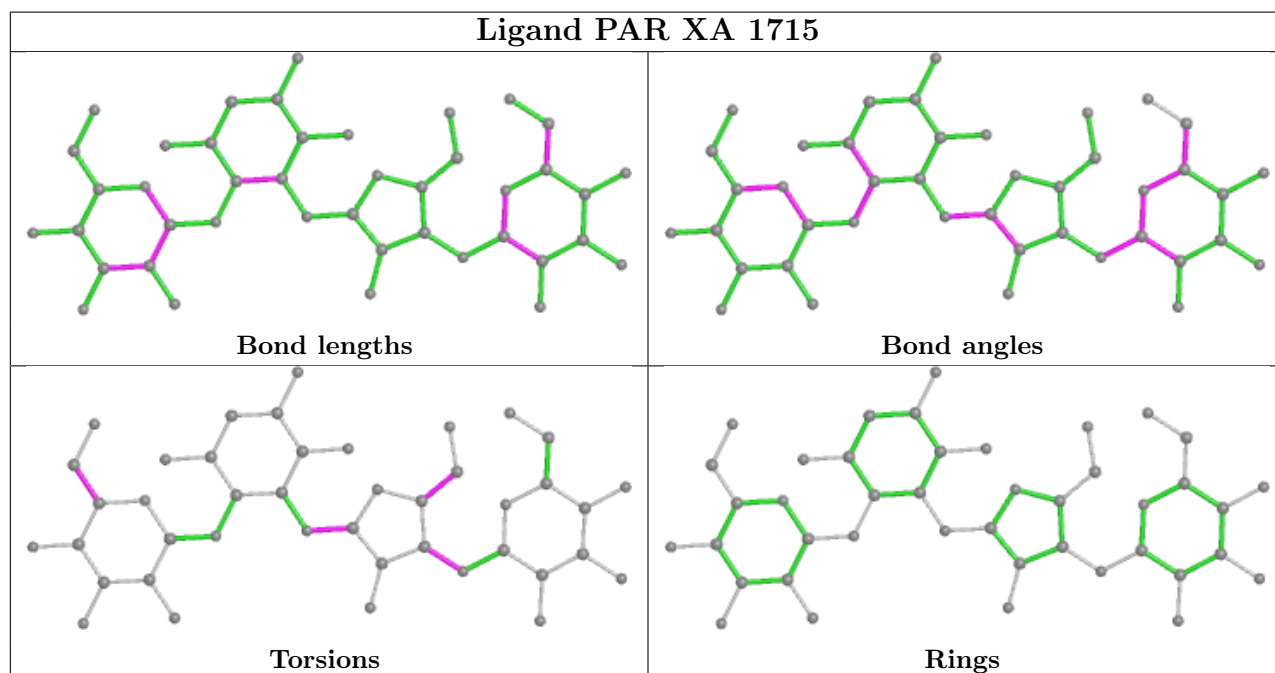
Mol	Chain	Res	Type	Atoms
58	XA	1715	PAR	O43-C43-C53-O53
58	XA	1715	PAR	C33-C43-C53-O53
58	QA	1693	PAR	O51-C51-C61-O61
58	QA	1693	PAR	C41-C51-C61-O61
58	QA	1693	PAR	C33-C43-C53-O53

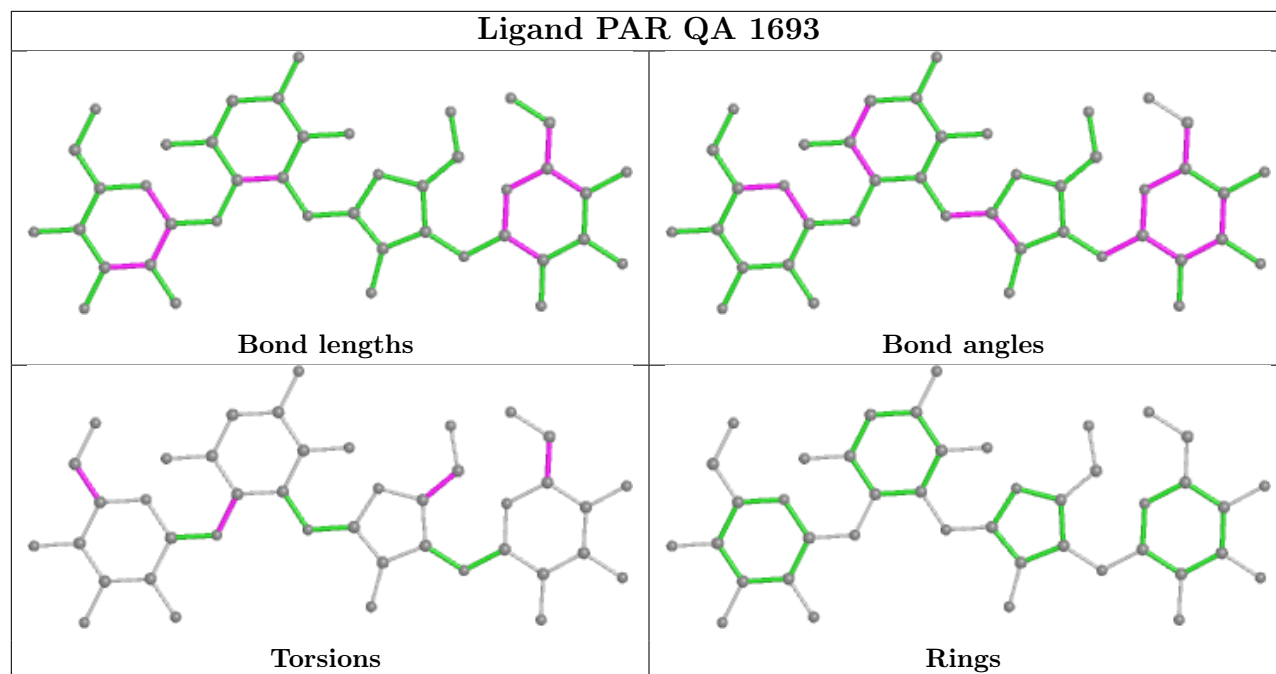
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1693	PAR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	QA	1500/1522 (98%)	0.42	85 (5%) 23 21	61, 101, 175, 382	0
1	XA	1500/1522 (98%)	0.44	75 (5%) 28 25	56, 98, 186, 365	0
2	QB	237/256 (92%)	0.43	22 (9%) 8 9	76, 148, 228, 296	0
2	XB	237/256 (92%)	0.39	17 (7%) 15 15	71, 139, 206, 252	0
3	QC	205/239 (85%)	0.25	9 (4%) 34 30	81, 128, 187, 266	0
3	XC	205/239 (85%)	0.14	8 (3%) 39 35	68, 116, 164, 239	0
4	QD	208/209 (99%)	-0.05	2 (0%) 82 77	68, 111, 160, 177	0
4	XD	208/209 (99%)	-0.11	2 (0%) 82 77	61, 99, 151, 202	0
5	QE	151/162 (93%)	0.08	0 100 100	73, 111, 156, 268	0
5	XE	151/162 (93%)	0.11	2 (1%) 77 71	58, 97, 154, 214	0
6	QF	101/101 (100%)	0.16	4 (3%) 38 33	59, 99, 140, 212	0
6	XF	101/101 (100%)	0.29	6 (5%) 22 20	58, 106, 157, 264	0
7	QG	155/156 (99%)	0.41	8 (5%) 27 24	83, 121, 173, 271	0
7	XG	155/156 (99%)	0.40	16 (10%) 6 7	86, 126, 175, 207	0
8	QH	138/138 (100%)	-0.31	0 100 100	71, 109, 148, 177	0
8	XH	138/138 (100%)	-0.19	0 100 100	70, 107, 143, 179	0
9	QI	127/128 (99%)	0.74	16 (12%) 3 5	81, 137, 188, 245	0
9	XI	127/128 (99%)	0.71	15 (11%) 4 5	79, 145, 214, 239	0
10	QJ	99/105 (94%)	1.16	29 (29%) 0 0	80, 157, 267, 320	0
10	XJ	99/105 (94%)	0.92	17 (17%) 1 1	86, 141, 200, 232	0
11	QK	119/129 (92%)	0.56	11 (9%) 9 9	64, 103, 161, 219	0
11	XK	119/129 (92%)	0.39	4 (3%) 45 40	62, 106, 166, 231	0
12	QL	125/132 (94%)	0.26	6 (4%) 30 27	63, 104, 160, 244	0
12	XL	125/132 (94%)	-0.00	4 (3%) 47 42	52, 87, 139, 275	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	0.08	9 (7%) 14 14	75, 120, 186, 312	0
13	XM	121/126 (96%)	0.09	4 (3%) 46 41	78, 124, 183, 300	0
14	QN	60/61 (98%)	0.27	3 (5%) 28 25	78, 123, 162, 173	0
14	XN	60/61 (98%)	0.34	4 (6%) 17 16	73, 108, 146, 156	0
15	QO	88/89 (98%)	-0.05	1 (1%) 80 75	61, 98, 155, 182	0
15	XO	88/89 (98%)	-0.03	1 (1%) 80 75	68, 100, 151, 178	0
16	QP	84/88 (95%)	0.25	0 100 100	62, 98, 138, 169	0
16	XP	84/88 (95%)	0.31	2 (2%) 59 53	75, 106, 155, 264	0
17	QQ	100/105 (95%)	0.14	2 (2%) 65 60	65, 106, 148, 180	0
17	XQ	100/105 (95%)	0.06	2 (2%) 65 60	66, 109, 150, 189	0
18	QR	70/88 (79%)	0.60	5 (7%) 16 15	56, 100, 161, 198	0
18	XR	70/88 (79%)	0.46	4 (5%) 23 21	67, 110, 147, 204	0
19	QS	84/93 (90%)	0.14	0 100 100	83, 135, 192, 210	0
19	XS	84/93 (90%)	-0.02	0 100 100	78, 126, 178, 234	0
20	QT	99/106 (93%)	0.28	5 (5%) 28 25	70, 112, 171, 201	0
20	XT	99/106 (93%)	-0.02	2 (2%) 65 60	70, 126, 177, 247	0
21	QU	25/27 (92%)	2.00	12 (48%) 0 0	95, 119, 177, 192	0
21	XU	25/27 (92%)	1.87	9 (36%) 0 0	101, 118, 187, 202	0
22	QV	77/77 (100%)	0.64	11 (14%) 2 3	63, 113, 184, 227	0
22	XV	77/77 (100%)	0.80	11 (14%) 2 3	57, 107, 161, 196	0
23	QX	9/25 (36%)	0.48	1 (11%) 5 6	78, 90, 122, 161	0
23	XX	11/25 (44%)	0.25	1 (9%) 9 9	70, 90, 176, 186	0
24	QY	15/18 (83%)	0.26	0 100 100	87, 111, 197, 245	0
24	XY	15/18 (83%)	0.09	0 100 100	89, 120, 198, 199	0
25	RA	2882/2915 (98%)	0.47	210 (7%) 15 15	50, 81, 218, 422	0
25	YA	2882/2915 (98%)	0.44	172 (5%) 21 19	41, 76, 207, 368	0
26	RB	120/122 (98%)	0.24	1 (0%) 86 81	79, 108, 146, 171	0
26	YB	120/122 (98%)	0.40	11 (9%) 9 9	78, 112, 152, 184	0
27	RD	272/276 (98%)	-0.13	1 (0%) 92 90	43, 74, 114, 213	0
27	YD	272/276 (98%)	-0.16	2 (0%) 87 83	36, 72, 111, 195	0
28	RE	205/206 (99%)	-0.01	0 100 100	52, 93, 160, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YE	205/206 (99%)	0.13	3 (1%) 73 68	46, 90, 159, 271	0
29	RF	202/210 (96%)	-0.01	0 100 100	46, 86, 147, 205	0
29	YF	202/210 (96%)	-0.12	0 100 100	40, 82, 142, 181	0
30	RG	181/182 (99%)	0.27	6 (3%) 46 41	74, 115, 172, 251	0
30	YG	181/182 (99%)	0.41	10 (5%) 25 22	74, 116, 169, 255	0
31	RH	170/180 (94%)	0.95	34 (20%) 1 1	92, 174, 251, 302	0
31	YH	170/180 (94%)	-0.01	5 (2%) 51 45	62, 108, 160, 215	0
32	RI	146/148 (98%)	0.31	4 (2%) 54 48	67, 122, 183, 277	0
32	YI	146/148 (98%)	0.49	10 (6%) 17 16	71, 128, 181, 218	0
33	RN	138/140 (98%)	-0.21	0 100 100	56, 99, 158, 202	0
33	YN	138/140 (98%)	-0.45	0 100 100	58, 94, 155, 189	0
34	RO	122/122 (100%)	-0.27	0 100 100	61, 86, 118, 161	0
34	YO	122/122 (100%)	-0.34	0 100 100	48, 74, 111, 137	0
35	RP	150/150 (100%)	0.06	2 (1%) 77 71	41, 98, 156, 283	0
35	YP	150/150 (100%)	0.32	9 (6%) 21 19	39, 93, 151, 270	0
36	RQ	141/141 (100%)	-0.01	3 (2%) 63 58	59, 101, 154, 239	0
36	YQ	141/141 (100%)	-0.08	3 (2%) 63 58	49, 91, 148, 280	0
37	RR	118/118 (100%)	-0.25	0 100 100	53, 82, 124, 141	0
37	YR	118/118 (100%)	-0.20	0 100 100	49, 83, 117, 163	0
38	RS	111/112 (99%)	0.19	3 (2%) 54 48	70, 111, 164, 217	0
38	YS	111/112 (99%)	0.57	11 (9%) 7 8	67, 120, 165, 230	0
39	RT	137/146 (93%)	0.11	5 (3%) 42 38	64, 100, 190, 286	0
39	YT	137/146 (93%)	-0.15	4 (2%) 51 45	56, 87, 187, 223	0
40	RU	117/118 (99%)	0.39	10 (8%) 10 11	51, 85, 143, 242	0
40	YU	117/118 (99%)	0.11	4 (3%) 45 40	47, 78, 131, 268	0
41	RV	101/101 (100%)	0.45	6 (5%) 22 20	63, 110, 170, 277	0
41	YV	101/101 (100%)	0.09	4 (3%) 38 33	50, 97, 158, 285	0
42	RW	113/113 (100%)	-0.31	0 100 100	50, 76, 131, 227	0
42	YW	113/113 (100%)	-0.09	1 (0%) 84 79	50, 75, 130, 218	0
43	RX	92/96 (95%)	-0.33	0 100 100	59, 85, 118, 154	0
43	YX	92/96 (95%)	-0.23	0 100 100	42, 77, 114, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RY	102/110 (92%)	1.04	21 (20%) 1 1	59, 118, 205, 341	0
44	YY	102/110 (92%)	0.05	5 (4%) 29 26	56, 102, 171, 280	0
45	RZ	183/206 (88%)	0.54	17 (9%) 8 9	74, 132, 209, 281	0
45	YZ	183/206 (88%)	0.43	11 (6%) 21 19	70, 123, 205, 357	0
46	R0	82/85 (96%)	-0.12	1 (1%) 79 73	60, 84, 114, 151	0
46	Y0	82/85 (96%)	-0.13	0 100 100	53, 88, 118, 144	0
47	R1	97/98 (98%)	0.22	3 (3%) 49 43	49, 85, 171, 230	0
47	Y1	97/98 (98%)	0.22	4 (4%) 37 33	54, 84, 162, 219	0
48	R2	69/72 (95%)	-0.01	0 100 100	74, 112, 167, 206	0
48	Y2	69/72 (95%)	0.00	3 (4%) 35 31	53, 90, 137, 228	0
49	R3	59/60 (98%)	0.19	2 (3%) 45 40	57, 96, 143, 190	0
49	Y3	59/60 (98%)	-0.05	0 100 100	58, 90, 144, 215	0
50	R4	71/71 (100%)	0.49	4 (5%) 24 22	103, 176, 301, 384	0
50	Y4	71/71 (100%)	0.16	3 (4%) 36 32	84, 167, 259, 304	0
51	R5	59/60 (98%)	0.59	8 (13%) 3 4	45, 95, 228, 264	0
51	Y5	58/60 (96%)	0.07	3 (5%) 27 24	45, 83, 227, 279	0
52	R6	49/54 (90%)	2.61	26 (53%) 0 0	104, 149, 204, 260	0
52	Y6	49/54 (90%)	2.16	24 (48%) 0 0	94, 152, 221, 246	0
53	R7	49/49 (100%)	0.42	1 (2%) 65 60	42, 67, 138, 176	0
53	Y7	49/49 (100%)	0.49	4 (8%) 11 12	32, 60, 135, 206	0
54	R8	64/65 (98%)	0.27	3 (4%) 31 28	47, 83, 140, 203	0
54	Y8	64/65 (98%)	-0.02	0 100 100	45, 78, 124, 214	0
55	R9	37/37 (100%)	3.22	25 (67%) 0 0	125, 171, 245, 278	0
55	Y9	37/37 (100%)	3.38	28 (75%) 0 0	102, 160, 211, 222	0
56	Z5	2/3 (66%)	0.68	0 100 100	79, 79, 79, 79	0
56	Z6	2/3 (66%)	0.53	0 100 100	59, 59, 59, 63	0
All	All	20877/21492 (97%)	0.31	1177 (5%) 24 22	32, 98, 188, 422	0

The worst 5 of 1177 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	1536	A	17.1
25	YA	1058	G	14.9

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Mol	Chain	Res	Type	RSRZ
40	RU	118	GLY	14.5
1	QA	1032	A	12.1
25	YA	2801	A	11.5

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	PPU	Z5	101	37/38	0.94	0.33	77,78,79,79	0
56	PPU	Z6	101	37/38	0.95	0.36	59,60,60,61	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
57	MG	XA	1702	1/1	-0.11	0.38	104,104,104,104	0
57	MG	R0	101	1/1	0.31	0.40	49,49,49,49	0
57	MG	QA	1662	1/1	0.33	1.33	88,88,88,88	0
57	MG	YA	3280	1/1	0.37	0.62	82,82,82,82	0
57	MG	XA	1694	1/1	0.43	0.73	55,55,55,55	0
57	MG	XF	201	1/1	0.47	0.29	86,86,86,86	0
57	MG	RA	3301	1/1	0.47	0.66	80,80,80,80	0
57	MG	Y0	101	1/1	0.47	0.49	62,62,62,62	0
57	MG	QK	201	1/1	0.49	0.33	106,106,106,106	0
57	MG	YA	3273	1/1	0.50	0.53	64,64,64,64	0
57	MG	XA	1646	1/1	0.52	0.25	95,95,95,95	0
57	MG	XA	1679	1/1	0.52	0.79	60,60,60,60	0
57	MG	QA	1673	1/1	0.52	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	RA	3205	1/1	0.52	0.15	48,48,48,48	0
57	MG	YA	3125	1/1	0.53	0.97	78,78,78,78	0
57	MG	XA	1682	1/1	0.53	0.38	88,88,88,88	0
57	MG	RA	3291	1/1	0.54	0.53	70,70,70,70	0
57	MG	YA	3266	1/1	0.55	0.37	46,46,46,46	0
57	MG	YA	3115	1/1	0.55	1.10	82,82,82,82	0
57	MG	YA	3268	1/1	0.56	0.69	72,72,72,72	0
57	MG	YA	3282	1/1	0.56	0.76	53,53,53,53	0
57	MG	RA	3178	1/1	0.56	1.25	58,58,58,58	0
57	MG	YA	3193	1/1	0.57	0.32	41,41,41,41	0
57	MG	RA	3179	1/1	0.58	0.40	39,39,39,39	0
57	MG	YA	3206	1/1	0.58	0.21	99,99,99,99	0
57	MG	RA	3221	1/1	0.59	0.27	61,61,61,61	0
57	MG	RA	3101	1/1	0.60	0.30	42,42,42,42	0
57	MG	QA	1686	1/1	0.60	0.49	73,73,73,73	0
57	MG	RA	3309	1/1	0.61	0.74	117,117,117,117	0
57	MG	YA	3157	1/1	0.62	0.62	56,56,56,56	0
57	MG	XA	1686	1/1	0.63	0.74	51,51,51,51	0
57	MG	YA	3185	1/1	0.64	0.36	46,46,46,46	0
57	MG	XA	1649	1/1	0.64	0.21	72,72,72,72	0
57	MG	YA	3204	1/1	0.64	0.60	97,97,97,97	0
57	MG	RA	3150	1/1	0.64	0.50	96,96,96,96	0
57	MG	YA	3184	1/1	0.64	0.15	66,66,66,66	0
57	MG	RA	3141	1/1	0.65	0.56	64,64,64,64	0
57	MG	XA	1632	1/1	0.66	0.38	84,84,84,84	0
57	MG	RA	3217	1/1	0.66	0.25	67,67,67,67	0
57	MG	RA	3068	1/1	0.66	0.17	52,52,52,52	0
57	MG	XA	1672	1/1	0.66	0.67	72,72,72,72	0
57	MG	YA	3214	1/1	0.67	0.41	34,34,34,34	0
57	MG	Y7	101	1/1	0.67	0.27	44,44,44,44	0
57	MG	YA	3272	1/1	0.68	0.39	81,81,81,81	0
57	MG	YA	3296	1/1	0.68	0.41	67,67,67,67	0
57	MG	RA	3287	1/1	0.68	0.54	55,55,55,55	0
57	MG	RA	3271	1/1	0.68	0.31	67,67,67,67	0
57	MG	RA	3139	1/1	0.69	0.23	62,62,62,62	0
57	MG	QA	1636	1/1	0.69	0.82	61,61,61,61	0
57	MG	RA	3294	1/1	0.70	0.82	63,63,63,63	0
57	MG	XA	1658	1/1	0.70	0.69	66,66,66,66	0
57	MG	RA	3069	1/1	0.70	0.29	25,25,25,25	0
57	MG	YA	3317	1/1	0.70	0.77	61,61,61,61	0
57	MG	YA	3323	1/1	0.70	1.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3281	1/1	0.70	0.58	57,57,57,57	0
57	MG	YA	3172	1/1	0.70	0.56	48,48,48,48	0
57	MG	YA	3306	1/1	0.71	0.12	41,41,41,41	0
57	MG	XA	1650	1/1	0.71	0.66	63,63,63,63	0
57	MG	YA	3197	1/1	0.71	0.36	58,58,58,58	0
57	MG	XA	1626	1/1	0.71	0.28	36,36,36,36	0
57	MG	XA	1692	1/1	0.71	0.49	65,65,65,65	0
57	MG	YA	3179	1/1	0.72	0.20	45,45,45,45	0
57	MG	YA	3137	1/1	0.72	0.18	47,47,47,47	0
57	MG	RA	3155	1/1	0.72	0.21	36,36,36,36	0
57	MG	YA	3164	1/1	0.72	0.32	76,76,76,76	0
57	MG	QA	1627	1/1	0.72	0.31	35,35,35,35	0
57	MG	YA	3160	1/1	0.73	0.30	61,61,61,61	0
57	MG	RA	3277	1/1	0.73	0.61	78,78,78,78	0
57	MG	YA	3071	1/1	0.73	0.27	25,25,25,25	0
57	MG	YA	3191	1/1	0.73	0.55	32,32,32,32	0
57	MG	YA	3192	1/1	0.73	0.25	58,58,58,58	0
57	MG	YA	3230	1/1	0.73	0.34	57,57,57,57	0
57	MG	YA	3321	1/1	0.74	0.77	67,67,67,67	0
57	MG	YA	3119	1/1	0.74	0.51	63,63,63,63	0
57	MG	YA	3326	1/1	0.74	0.37	56,56,56,56	0
57	MG	RA	3194	1/1	0.74	0.22	33,33,33,33	0
57	MG	XA	1665	1/1	0.74	0.28	49,49,49,49	0
57	MG	RA	3181	1/1	0.75	0.42	55,55,55,55	0
57	MG	QA	1669	1/1	0.75	0.27	68,68,68,68	0
57	MG	RA	3303	1/1	0.75	0.44	75,75,75,75	0
57	MG	RA	3159	1/1	0.75	0.35	53,53,53,53	0
57	MG	YE	302	1/1	0.75	0.48	64,64,64,64	0
57	MG	QA	1626	1/1	0.75	0.20	76,76,76,76	0
57	MG	RA	3050	1/1	0.75	0.55	50,50,50,50	0
57	MG	YA	3313	1/1	0.76	0.56	68,68,68,68	0
57	MG	XA	1639	1/1	0.76	0.36	57,57,57,57	0
57	MG	RA	3292	1/1	0.76	0.55	73,73,73,73	0
57	MG	RF	301	1/1	0.76	0.34	87,87,87,87	0
57	MG	QA	1641	1/1	0.76	0.23	52,52,52,52	0
57	MG	XA	1617	1/1	0.76	0.30	40,40,40,40	0
57	MG	RA	3211	1/1	0.76	0.31	56,56,56,56	0
57	MG	RA	3198	1/1	0.76	0.38	81,81,81,81	0
57	MG	RA	3180	1/1	0.77	0.41	73,73,73,73	0
57	MG	QA	1629	1/1	0.77	0.34	96,96,96,96	0
57	MG	RA	3184	1/1	0.77	0.66	84,84,84,84	0
57	MG	RA	3185	1/1	0.77	0.28	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1658	1/1	0.77	0.59	55,55,55,55	0
57	MG	XA	1656	1/1	0.77	0.26	55,55,55,55	0
57	MG	RA	3241	1/1	0.77	0.44	47,47,47,47	0
57	MG	RA	3269	1/1	0.77	0.12	55,55,55,55	0
57	MG	YA	3165	1/1	0.77	1.16	52,52,52,52	0
57	MG	YA	3286	1/1	0.77	0.47	54,54,54,54	0
57	MG	RA	3286	1/1	0.78	0.86	74,74,74,74	0
57	MG	YA	3253	1/1	0.78	0.62	32,32,32,32	0
57	MG	YA	3261	1/1	0.78	0.52	45,45,45,45	0
57	MG	RP	201	1/1	0.78	0.48	117,117,117,117	0
57	MG	YA	3199	1/1	0.78	0.41	83,83,83,83	0
57	MG	QA	1679	1/1	0.79	0.37	48,48,48,48	0
57	MG	YA	3277	1/1	0.79	0.49	64,64,64,64	0
57	MG	YA	3143	1/1	0.79	0.58	58,58,58,58	0
57	MG	R5	101	1/1	0.79	0.29	61,61,61,61	0
57	MG	QA	1682	1/1	0.79	0.56	59,59,59,59	0
57	MG	RA	3222	1/1	0.79	0.61	78,78,78,78	0
57	MG	YA	3016	1/1	0.79	0.18	41,41,41,41	0
57	MG	RA	3304	1/1	0.79	0.25	51,51,51,51	0
57	MG	YA	3223	1/1	0.79	0.47	77,77,77,77	0
57	MG	YA	3176	1/1	0.79	1.28	60,60,60,60	0
57	MG	YA	3177	1/1	0.79	0.85	79,79,79,79	0
57	MG	RA	3138	1/1	0.79	0.24	30,30,30,30	0
57	MG	QA	1656	1/1	0.79	0.54	52,52,52,52	0
57	MG	RA	3170	1/1	0.79	0.24	62,62,62,62	0
57	MG	YA	3133	1/1	0.79	0.09	35,35,35,35	0
57	MG	XA	1703	1/1	0.80	0.22	57,57,57,57	0
57	MG	RA	3191	1/1	0.80	0.29	57,57,57,57	0
57	MG	XA	1680	1/1	0.80	0.68	48,48,48,48	0
57	MG	QA	1687	1/1	0.80	0.18	41,41,41,41	0
57	MG	XA	1661	1/1	0.80	0.30	56,56,56,56	0
57	MG	YA	3229	1/1	0.80	0.52	47,47,47,47	0
57	MG	XA	1664	1/1	0.80	0.35	78,78,78,78	0
57	MG	XA	1627	1/1	0.80	0.16	42,42,42,42	0
57	MG	RA	3197	1/1	0.80	0.27	63,63,63,63	0
57	MG	YA	3166	1/1	0.81	0.26	95,95,95,95	0
57	MG	RA	3296	1/1	0.81	0.70	54,54,54,54	0
57	MG	QA	1655	1/1	0.81	0.42	71,71,71,71	0
57	MG	RA	3189	1/1	0.81	0.50	72,72,72,72	0
57	MG	XA	1606	1/1	0.81	0.36	52,52,52,52	0
57	MG	RA	3116	1/1	0.81	0.17	34,34,34,34	0
57	MG	RA	3119	1/1	0.81	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	RA	3284	1/1	0.81	0.22	48,48,48,48	0
57	MG	XA	1628	1/1	0.81	0.23	41,41,41,41	0
57	MG	YA	3247	1/1	0.81	0.70	50,50,50,50	0
57	MG	QA	1685	1/1	0.82	0.21	91,91,91,91	0
57	MG	RA	3001	1/1	0.82	0.40	45,45,45,45	0
57	MG	RA	3114	1/1	0.82	0.21	48,48,48,48	0
57	MG	RA	3002	1/1	0.82	0.94	49,49,49,49	0
57	MG	RA	3117	1/1	0.82	0.19	57,57,57,57	0
57	MG	YA	3128	1/1	0.82	0.36	61,61,61,61	0
57	MG	RA	3188	1/1	0.82	0.33	56,56,56,56	0
57	MG	RA	3168	1/1	0.82	0.42	59,59,59,59	0
57	MG	YA	3196	1/1	0.82	0.30	55,55,55,55	0
57	MG	YA	3138	1/1	0.82	0.50	41,41,41,41	0
57	MG	YA	3142	1/1	0.82	0.47	55,55,55,55	0
57	MG	QA	1624	1/1	0.82	0.41	46,46,46,46	0
57	MG	XA	1698	1/1	0.82	0.44	67,67,67,67	0
57	MG	YA	3213	1/1	0.82	0.22	80,80,80,80	0
57	MG	RA	3247	1/1	0.82	0.98	73,73,73,73	0
57	MG	RA	3295	1/1	0.82	0.64	55,55,55,55	0
57	MG	XD	302	1/1	0.82	0.44	96,96,96,96	0
57	MG	QA	1603	1/1	0.82	0.45	60,60,60,60	0
57	MG	YA	3236	1/1	0.82	1.04	68,68,68,68	0
57	MG	YA	3001	1/1	0.82	0.29	35,35,35,35	0
57	MG	RA	3213	1/1	0.83	0.21	65,65,65,65	0
57	MG	YA	3218	1/1	0.83	0.17	74,74,74,74	0
57	MG	YA	3188	1/1	0.83	0.63	48,48,48,48	0
57	MG	YA	3283	1/1	0.83	0.52	62,62,62,62	0
57	MG	XA	1623	1/1	0.83	0.16	53,53,53,53	0
57	MG	XA	1643	1/1	0.83	0.19	43,43,43,43	0
57	MG	YA	3303	1/1	0.83	0.82	56,56,56,56	0
57	MG	RA	3062	1/1	0.83	0.21	97,97,97,97	0
57	MG	YA	3311	1/1	0.83	0.46	61,61,61,61	0
57	MG	YA	3195	1/1	0.83	0.36	55,55,55,55	0
57	MG	YA	3131	1/1	0.83	0.38	62,62,62,62	0
57	MG	XV	103	1/1	0.83	1.07	46,46,46,46	0
57	MG	XY	101	1/1	0.83	0.16	50,50,50,50	0
57	MG	QA	1667	1/1	0.83	1.06	66,66,66,66	0
57	MG	YA	3269	1/1	0.83	0.56	59,59,59,59	0
57	MG	YR	201	1/1	0.83	0.79	62,62,62,62	0
57	MG	RA	3293	1/1	0.83	0.54	50,50,50,50	0
57	MG	XA	1675	1/1	0.83	0.69	56,56,56,56	0
57	MG	RQ	201	1/1	0.84	0.66	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1688	1/1	0.84	0.50	61,61,61,61	0
57	MG	QA	1638	1/1	0.84	0.25	60,60,60,60	0
57	MG	YA	3291	1/1	0.84	0.34	43,43,43,43	0
57	MG	R0	102	1/1	0.84	0.37	40,40,40,40	0
57	MG	YA	3300	1/1	0.84	0.41	55,55,55,55	0
57	MG	QA	1646	1/1	0.84	0.30	36,36,36,36	0
57	MG	RA	3278	1/1	0.84	1.01	46,46,46,46	0
57	MG	RA	3218	1/1	0.84	0.30	116,116,116,116	0
57	MG	YA	3141	1/1	0.84	0.22	70,70,70,70	0
57	MG	RA	3176	1/1	0.84	0.15	56,56,56,56	0
57	MG	RA	3285	1/1	0.84	0.47	32,32,32,32	0
57	MG	RA	3200	1/1	0.84	0.81	61,61,61,61	0
57	MG	RA	3306	1/1	0.84	0.83	53,53,53,53	0
57	MG	RA	3160	1/1	0.84	0.83	54,54,54,54	0
57	MG	RA	3206	1/1	0.84	0.36	53,53,53,53	0
57	MG	RA	3192	1/1	0.84	0.47	64,64,64,64	0
57	MG	XA	1685	1/1	0.84	0.22	76,76,76,76	0
57	MG	QA	1618	1/1	0.85	1.11	67,67,67,67	0
57	MG	RA	3126	1/1	0.85	0.22	47,47,47,47	0
57	MG	RA	3290	1/1	0.85	1.25	79,79,79,79	0
57	MG	RA	3279	1/1	0.85	0.20	53,53,53,53	0
57	MG	YA	3150	1/1	0.85	0.56	67,67,67,67	0
57	MG	YA	3154	1/1	0.85	0.38	77,77,77,77	0
57	MG	YA	3238	1/1	0.85	0.36	48,48,48,48	0
57	MG	YA	3156	1/1	0.85	0.33	33,33,33,33	0
57	MG	XA	1604	1/1	0.85	0.56	51,51,51,51	0
57	MG	RA	3177	1/1	0.85	0.27	42,42,42,42	0
57	MG	YA	3315	1/1	0.85	0.42	56,56,56,56	0
57	MG	YA	3264	1/1	0.85	0.48	56,56,56,56	0
57	MG	YA	3162	1/1	0.85	0.13	40,40,40,40	0
57	MG	XA	1647	1/1	0.85	0.49	58,58,58,58	0
57	MG	XA	1713	1/1	0.85	0.70	50,50,50,50	0
57	MG	YD	301	1/1	0.85	0.32	40,40,40,40	0
57	MG	RA	3282	1/1	0.85	0.32	45,45,45,45	0
57	MG	RA	3216	1/1	0.85	0.80	49,49,49,49	0
57	MG	YU	201	1/1	0.85	0.35	61,61,61,61	0
57	MG	YY	201	1/1	0.85	0.20	56,56,56,56	0
57	MG	YA	3210	1/1	0.85	0.18	69,69,69,69	0
57	MG	RA	3276	1/1	0.85	0.34	53,53,53,53	0
59	ZN	QD	301	1/1	0.85	0.29	70,70,70,70	0
57	MG	XA	1660	1/1	0.86	0.19	59,59,59,59	0
57	MG	YA	3186	1/1	0.86	0.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3113	1/1	0.86	0.20	74,74,74,74	0
57	MG	YA	3063	1/1	0.86	0.23	40,40,40,40	0
57	MG	RA	3226	1/1	0.86	0.13	78,78,78,78	0
57	MG	YA	3083	1/1	0.86	0.35	55,55,55,55	0
57	MG	YA	3105	1/1	0.86	0.47	36,36,36,36	0
57	MG	XA	1697	1/1	0.86	0.48	48,48,48,48	0
57	MG	QA	1692	1/1	0.86	0.69	66,66,66,66	0
57	MG	RA	3133	1/1	0.86	0.22	51,51,51,51	0
57	MG	RA	3308	1/1	0.86	0.77	52,52,52,52	0
57	MG	RA	3267	1/1	0.86	0.40	69,69,69,69	0
57	MG	XA	1618	1/1	0.86	0.24	67,67,67,67	0
57	MG	YP	202	1/1	0.86	0.25	63,63,63,63	0
57	MG	YA	3135	1/1	0.86	0.30	56,56,56,56	0
57	MG	YA	3281	1/1	0.86	0.27	55,55,55,55	0
57	MG	QA	1609	1/1	0.86	0.12	50,50,50,50	0
57	MG	YA	3178	1/1	0.86	0.58	53,53,53,53	0
57	MG	QA	1690	1/1	0.86	0.25	35,35,35,35	0
57	MG	RA	3207	1/1	0.86	0.49	51,51,51,51	0
57	MG	RA	3146	1/1	0.87	0.41	63,63,63,63	0
57	MG	RA	3260	1/1	0.87	0.39	45,45,45,45	0
57	MG	RA	3262	1/1	0.87	0.89	49,49,49,49	0
57	MG	QF	201	1/1	0.87	0.28	78,78,78,78	0
57	MG	RA	3008	1/1	0.87	0.74	49,49,49,49	0
57	MG	RA	3026	1/1	0.87	0.29	48,48,48,48	0
57	MG	RA	3103	1/1	0.87	0.25	41,41,41,41	0
57	MG	RA	3167	1/1	0.87	0.21	74,74,74,74	0
57	MG	RA	3045	1/1	0.87	0.75	52,52,52,52	0
57	MG	YE	301	1/1	0.87	0.23	37,37,37,37	0
57	MG	YA	3226	1/1	0.87	0.31	64,64,64,64	0
57	MG	QA	1644	1/1	0.87	0.25	76,76,76,76	0
57	MG	YQ	201	1/1	0.87	0.15	75,75,75,75	0
57	MG	XA	1706	1/1	0.87	0.47	44,44,44,44	0
57	MG	YA	3232	1/1	0.87	0.31	40,40,40,40	0
57	MG	XA	1709	1/1	0.87	0.48	40,40,40,40	0
57	MG	RA	3238	1/1	0.87	0.46	42,42,42,42	0
57	MG	YA	3130	1/1	0.87	0.16	45,45,45,45	0
57	MG	QA	1619	1/1	0.87	0.63	48,48,48,48	0
57	MG	XA	1666	1/1	0.88	0.36	40,40,40,40	0
57	MG	RD	301	1/1	0.88	0.28	56,56,56,56	0
57	MG	RA	3091	1/1	0.88	0.34	65,65,65,65	0
57	MG	YA	3212	1/1	0.88	0.34	58,58,58,58	0
57	MG	XA	1629	1/1	0.88	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3294	1/1	0.88	0.59	51,51,51,51	0
57	MG	RA	3032	1/1	0.88	0.34	69,69,69,69	0
57	MG	YA	3217	1/1	0.88	0.19	35,35,35,35	0
57	MG	XA	1633	1/1	0.88	1.04	67,67,67,67	0
57	MG	XA	1636	1/1	0.88	0.10	54,54,54,54	0
57	MG	RA	3165	1/1	0.88	0.10	79,79,79,79	0
57	MG	YA	3111	1/1	0.88	0.34	53,53,53,53	0
57	MG	QX	101	1/1	0.88	0.22	48,48,48,48	0
57	MG	RA	3186	1/1	0.88	0.13	38,38,38,38	0
57	MG	YA	3235	1/1	0.88	0.47	60,60,60,60	0
57	MG	RA	3299	1/1	0.88	0.71	64,64,64,64	0
57	MG	QA	1637	1/1	0.88	0.30	63,63,63,63	0
57	MG	QA	1664	1/1	0.88	0.99	54,54,54,54	0
57	MG	XA	1652	1/1	0.88	1.19	64,64,64,64	0
57	MG	XA	1612	1/1	0.88	0.38	52,52,52,52	0
57	MG	YP	201	1/1	0.88	0.18	77,77,77,77	0
57	MG	XA	1704	1/1	0.88	0.27	59,59,59,59	0
57	MG	QA	1678	1/1	0.88	0.38	53,53,53,53	0
57	MG	RA	3149	1/1	0.88	0.52	65,65,65,65	0
57	MG	YA	3140	1/1	0.88	0.22	47,47,47,47	0
57	MG	XA	1712	1/1	0.88	0.60	66,66,66,66	0
57	MG	XA	1619	1/1	0.88	0.58	47,47,47,47	0
57	MG	Y0	102	1/1	0.88	0.73	56,56,56,56	0
57	MG	QA	1631	1/1	0.88	0.23	73,73,73,73	0
57	MG	RA	3084	1/1	0.88	0.27	42,42,42,42	0
57	MG	RA	3212	1/1	0.89	0.36	57,57,57,57	0
57	MG	RA	3268	1/1	0.89	0.20	48,48,48,48	0
57	MG	XA	1607	1/1	0.89	0.63	48,48,48,48	0
57	MG	RA	3086	1/1	0.89	0.27	17,17,17,17	0
57	MG	RA	3214	1/1	0.89	0.10	46,46,46,46	0
57	MG	YA	3293	1/1	0.89	0.35	61,61,61,61	0
57	MG	XA	1714	1/1	0.89	0.24	49,49,49,49	0
57	MG	RA	3273	1/1	0.89	0.30	92,92,92,92	0
57	MG	RA	3143	1/1	0.89	0.29	89,89,89,89	0
57	MG	RA	3302	1/1	0.89	0.70	60,60,60,60	0
57	MG	YA	3304	1/1	0.89	0.46	66,66,66,66	0
57	MG	XA	1669	1/1	0.89	0.35	58,58,58,58	0
57	MG	YA	3309	1/1	0.89	0.81	59,59,59,59	0
57	MG	YA	3310	1/1	0.89	0.25	63,63,63,63	0
57	MG	RA	3090	1/1	0.89	0.54	36,36,36,36	0
57	MG	YA	3007	1/1	0.89	0.40	20,20,20,20	0
57	MG	QA	1666	1/1	0.89	0.84	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	YA	3045	1/1	0.89	0.43	18,18,18,18	0
57	MG	QA	1683	1/1	0.89	0.28	59,59,59,59	0
57	MG	QA	1653	1/1	0.89	0.19	104,104,104,104	0
57	MG	RA	3158	1/1	0.89	0.30	40,40,40,40	0
57	MG	RA	3135	1/1	0.89	0.15	47,47,47,47	0
57	MG	RA	3137	1/1	0.89	0.28	31,31,31,31	0
57	MG	YA	3181	1/1	0.89	0.07	62,62,62,62	0
57	MG	QA	1648	1/1	0.89	0.17	81,81,81,81	0
57	MG	XA	1690	1/1	0.89	0.19	92,92,92,92	0
57	MG	XA	1691	1/1	0.89	0.19	108,108,108,108	0
57	MG	RA	3249	1/1	0.89	1.05	66,66,66,66	0
57	MG	XA	1645	1/1	0.89	0.88	87,87,87,87	0
57	MG	RR	201	1/1	0.89	0.95	40,40,40,40	0
57	MG	RA	3254	1/1	0.89	0.25	49,49,49,49	0
57	MG	RA	3049	1/1	0.89	0.15	23,23,23,23	0
57	MG	YA	3279	1/1	0.89	0.75	39,39,39,39	0
57	MG	RA	3187	1/1	0.89	0.80	58,58,58,58	0
57	MG	YA	3271	1/1	0.90	0.55	40,40,40,40	0
57	MG	QA	1676	1/1	0.90	1.26	55,55,55,55	0
57	MG	RA	3161	1/1	0.90	0.20	51,51,51,51	0
57	MG	RA	3100	1/1	0.90	0.19	65,65,65,65	0
57	MG	XA	1668	1/1	0.90	0.46	38,38,38,38	0
57	MG	QA	1632	1/1	0.90	0.52	45,45,45,45	0
57	MG	QA	1611	1/1	0.90	0.26	26,26,26,26	0
57	MG	RA	3106	1/1	0.90	0.19	23,23,23,23	0
57	MG	RA	3193	1/1	0.90	0.32	136,136,136,136	0
57	MG	YA	3285	1/1	0.90	0.53	51,51,51,51	0
57	MG	XX	101	1/1	0.90	0.47	80,80,80,80	0
57	MG	YA	3290	1/1	0.90	0.49	42,42,42,42	0
57	MG	RA	3142	1/1	0.90	0.22	60,60,60,60	0
57	MG	YA	3292	1/1	0.90	0.26	105,105,105,105	0
57	MG	YA	3202	1/1	0.90	0.30	60,60,60,60	0
57	MG	YA	3145	1/1	0.90	0.19	14,14,14,14	0
57	MG	YA	3149	1/1	0.90	0.92	38,38,38,38	0
57	MG	YA	3297	1/1	0.90	0.44	65,65,65,65	0
57	MG	QA	1620	1/1	0.90	0.13	63,63,63,63	0
57	MG	YA	3152	1/1	0.90	0.31	61,61,61,61	0
57	MG	YA	3153	1/1	0.90	0.17	48,48,48,48	0
57	MG	RA	3234	1/1	0.90	0.30	41,41,41,41	0
57	MG	QA	1628	1/1	0.90	0.23	80,80,80,80	0
57	MG	QA	1623	1/1	0.90	0.64	57,57,57,57	0
57	MG	YA	3219	1/1	0.90	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3220	1/1	0.90	0.28	72,72,72,72	0
57	MG	RA	3202	1/1	0.90	1.72	71,71,71,71	0
57	MG	RA	3204	1/1	0.90	0.43	56,56,56,56	0
57	MG	YA	3074	1/1	0.90	0.95	50,50,50,50	0
57	MG	QA	1606	1/1	0.90	0.72	40,40,40,40	0
57	MG	YA	3324	1/1	0.90	0.62	63,63,63,63	0
57	MG	YA	3103	1/1	0.90	0.17	21,21,21,21	0
57	MG	YA	3234	1/1	0.90	0.56	31,31,31,31	0
57	MG	YA	3167	1/1	0.90	0.23	86,86,86,86	0
57	MG	YA	3171	1/1	0.90	0.12	55,55,55,55	0
57	MG	RA	3255	1/1	0.90	1.12	66,66,66,66	0
57	MG	YA	3242	1/1	0.90	0.59	14,14,14,14	0
57	MG	QA	1674	1/1	0.90	0.62	80,80,80,80	0
57	MG	YA	3251	1/1	0.90	0.54	48,48,48,48	0
57	MG	RA	3011	1/1	0.90	0.62	49,49,49,49	0
57	MG	RA	3263	1/1	0.90	0.23	38,38,38,38	0
57	MG	YA	3123	1/1	0.90	0.33	34,34,34,34	0
57	MG	YA	3180	1/1	0.90	0.62	39,39,39,39	0
57	MG	RA	3209	1/1	0.90	0.32	67,67,67,67	0
57	MG	QA	1689	1/1	0.90	0.41	36,36,36,36	0
57	MG	RA	3164	1/1	0.91	0.58	36,36,36,36	0
57	MG	RA	3252	1/1	0.91	0.24	50,50,50,50	0
57	MG	RA	3289	1/1	0.91	0.56	64,64,64,64	0
57	MG	XA	1663	1/1	0.91	0.21	70,70,70,70	0
57	MG	RA	3120	1/1	0.91	0.30	64,64,64,64	0
57	MG	QA	1670	1/1	0.91	0.22	32,32,32,32	0
57	MG	RA	3256	1/1	0.91	0.10	48,48,48,48	0
57	MG	RA	3075	1/1	0.91	0.14	34,34,34,34	0
57	MG	QA	1677	1/1	0.91	0.15	57,57,57,57	0
57	MG	RA	3172	1/1	0.91	0.23	47,47,47,47	0
57	MG	YA	3010	1/1	0.91	0.49	33,33,33,33	0
57	MG	RA	3266	1/1	0.91	0.49	43,43,43,43	0
57	MG	YA	3225	1/1	0.91	0.11	37,37,37,37	0
57	MG	YA	3301	1/1	0.91	0.22	58,58,58,58	0
57	MG	RA	3297	1/1	0.91	0.50	69,69,69,69	0
57	MG	RA	3174	1/1	0.91	0.27	63,63,63,63	0
57	MG	XA	1681	1/1	0.91	0.22	80,80,80,80	0
57	MG	QV	101	1/1	0.91	0.48	42,42,42,42	0
57	MG	RA	3156	1/1	0.91	0.65	71,71,71,71	0
57	MG	RA	3195	1/1	0.91	0.57	52,52,52,52	0
57	MG	XA	1687	1/1	0.91	0.23	90,90,90,90	0
57	MG	RA	3272	1/1	0.91	0.59	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3219	1/1	0.91	0.40	53,53,53,53	0
57	MG	RA	3055	1/1	0.91	0.21	59,59,59,59	0
57	MG	YA	3249	1/1	0.91	0.29	48,48,48,48	0
57	MG	YA	3122	1/1	0.91	0.41	32,32,32,32	0
57	MG	QA	1665	1/1	0.91	0.45	73,73,73,73	0
57	MG	YB	201	1/1	0.91	0.34	52,52,52,52	0
57	MG	YA	3258	1/1	0.91	0.30	21,21,21,21	0
57	MG	YD	302	1/1	0.91	0.21	55,55,55,55	0
57	MG	RB	203	1/1	0.91	0.33	45,45,45,45	0
57	MG	RA	3225	1/1	0.91	0.38	21,21,21,21	0
57	MG	YA	3265	1/1	0.91	0.11	99,99,99,99	0
57	MG	RA	3093	1/1	0.91	0.44	37,37,37,37	0
57	MG	XA	1699	1/1	0.91	0.15	90,90,90,90	0
57	MG	XA	1701	1/1	0.91	0.40	45,45,45,45	0
57	MG	RA	3201	1/1	0.91	1.06	85,85,85,85	0
57	MG	QA	1643	1/1	0.91	0.80	48,48,48,48	0
57	MG	XA	1651	1/1	0.91	0.21	40,40,40,40	0
57	MG	YA	3139	1/1	0.91	0.47	71,71,71,71	0
57	MG	RA	3182	1/1	0.91	0.54	71,71,71,71	0
57	MG	RA	3162	1/1	0.91	0.32	51,51,51,51	0
57	MG	XA	1705	1/1	0.92	1.12	52,52,52,52	0
57	MG	YA	3032	1/1	0.92	0.29	22,22,22,22	0
57	MG	YA	3158	1/1	0.92	0.22	42,42,42,42	0
57	MG	YA	3312	1/1	0.92	0.81	54,54,54,54	0
57	MG	RA	3240	1/1	0.92	0.11	55,55,55,55	0
57	MG	RA	3131	1/1	0.92	0.38	47,47,47,47	0
57	MG	RA	3173	1/1	0.92	0.27	54,54,54,54	0
57	MG	RA	3115	1/1	0.92	0.52	41,41,41,41	0
57	MG	YA	3079	1/1	0.92	0.44	19,19,19,19	0
57	MG	YA	3081	1/1	0.92	0.37	40,40,40,40	0
57	MG	RA	3059	1/1	0.92	0.34	11,11,11,11	0
57	MG	QA	1602	1/1	0.92	0.57	29,29,29,29	0
57	MG	YA	3245	1/1	0.92	0.31	28,28,28,28	0
57	MG	YA	3287	1/1	0.92	0.35	48,48,48,48	0
57	MG	YA	3174	1/1	0.92	0.46	53,53,53,53	0
57	MG	YA	3208	1/1	0.92	0.46	66,66,66,66	0
57	MG	XA	1677	1/1	0.92	0.45	34,34,34,34	0
57	MG	XA	1657	1/1	0.92	0.11	62,62,62,62	0
57	MG	RA	3111	1/1	0.92	0.70	37,37,37,37	0
57	MG	YA	3259	1/1	0.92	0.54	39,39,39,39	0
57	MG	YA	3118	1/1	0.92	0.27	64,64,64,64	0
57	MG	YA	3262	1/1	0.92	0.24	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	RA	3040	1/1	0.92	0.21	25,25,25,25	0
57	MG	RA	3300	1/1	0.92	0.31	55,55,55,55	0
57	MG	RA	3121	1/1	0.92	0.51	38,38,38,38	0
57	MG	QA	1652	1/1	0.92	0.32	43,43,43,43	0
57	MG	QA	1633	1/1	0.93	0.16	78,78,78,78	0
57	MG	YA	3046	1/1	0.93	0.35	15,15,15,15	0
57	MG	YA	3054	1/1	0.93	0.36	49,49,49,49	0
57	MG	YA	3305	1/1	0.93	1.06	45,45,45,45	0
57	MG	YA	3216	1/1	0.93	0.29	57,57,57,57	0
57	MG	YA	3307	1/1	0.93	0.56	46,46,46,46	0
57	MG	YA	3308	1/1	0.93	0.48	63,63,63,63	0
57	MG	YA	3056	1/1	0.93	0.11	13,13,13,13	0
57	MG	RA	3023	1/1	0.93	0.21	25,25,25,25	0
57	MG	YA	3065	1/1	0.93	0.26	32,32,32,32	0
57	MG	QA	1635	1/1	0.93	0.23	55,55,55,55	0
57	MG	YA	3222	1/1	0.93	0.78	51,51,51,51	0
57	MG	XA	1640	1/1	0.93	0.23	38,38,38,38	0
57	MG	XA	1642	1/1	0.93	0.73	88,88,88,88	0
57	MG	YA	3278	1/1	0.93	0.21	32,32,32,32	0
57	MG	QA	1642	1/1	0.93	0.56	70,70,70,70	0
57	MG	RA	3230	1/1	0.93	0.74	39,39,39,39	0
57	MG	QA	1615	1/1	0.93	0.21	39,39,39,39	0
57	MG	XA	1693	1/1	0.93	0.50	54,54,54,54	0
57	MG	YB	202	1/1	0.93	0.09	49,49,49,49	0
57	MG	RA	3236	1/1	0.93	0.43	17,17,17,17	0
57	MG	YA	3284	1/1	0.93	0.80	69,69,69,69	0
57	MG	YA	3114	1/1	0.93	0.29	40,40,40,40	0
57	MG	RA	3265	1/1	0.93	0.44	47,47,47,47	0
57	MG	QA	1612	1/1	0.93	0.31	20,20,20,20	0
57	MG	YA	3289	1/1	0.93	0.40	50,50,50,50	0
57	MG	RA	3203	1/1	0.93	0.24	67,67,67,67	0
57	MG	XA	1700	1/1	0.93	0.17	48,48,48,48	0
57	MG	RA	3009	1/1	0.93	0.40	59,59,59,59	0
57	MG	RA	3010	1/1	0.93	0.48	67,67,67,67	0
57	MG	YA	3019	1/1	0.93	0.32	19,19,19,19	0
57	MG	YA	3030	1/1	0.93	0.24	16,16,16,16	0
57	MG	RA	3125	1/1	0.93	0.23	38,38,38,38	0
58	PAR	QA	1693	42/42	0.93	0.23	81,81,81,81	0
57	MG	YA	3168	1/1	0.93	0.16	46,46,46,46	0
57	MG	RA	3275	1/1	0.94	0.24	55,55,55,55	0
57	MG	QA	1663	1/1	0.94	0.42	52,52,52,52	0
57	MG	QA	1616	1/1	0.94	0.14	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3018	1/1	0.94	0.36	28,28,28,28	0
57	MG	RA	3231	1/1	0.94	0.49	44,44,44,44	0
57	MG	YA	3024	1/1	0.94	0.19	14,14,14,14	0
57	MG	RA	3232	1/1	0.94	0.70	34,34,34,34	0
57	MG	YA	3169	1/1	0.94	0.21	49,49,49,49	0
57	MG	QA	1605	1/1	0.94	0.44	25,25,25,25	0
57	MG	YA	3041	1/1	0.94	0.34	14,14,14,14	0
57	MG	XA	1605	1/1	0.94	0.78	39,39,39,39	0
57	MG	XA	1676	1/1	0.94	0.30	38,38,38,38	0
57	MG	YA	3274	1/1	0.94	0.50	30,30,30,30	0
57	MG	YA	3050	1/1	0.94	0.44	24,24,24,24	0
57	MG	RA	3199	1/1	0.94	0.39	37,37,37,37	0
57	MG	XA	1678	1/1	0.94	0.41	20,20,20,20	0
57	MG	YA	3058	1/1	0.94	0.43	38,38,38,38	0
57	MG	RA	3054	1/1	0.94	0.34	26,26,26,26	0
57	MG	YA	3183	1/1	0.94	0.18	66,66,66,66	0
57	MG	XA	1611	1/1	0.94	0.16	39,39,39,39	0
57	MG	RA	3175	1/1	0.94	0.41	44,44,44,44	0
57	MG	QA	1613	1/1	0.94	0.21	31,31,31,31	0
57	MG	YA	3187	1/1	0.94	0.17	37,37,37,37	0
57	MG	XA	1683	1/1	0.94	0.14	41,41,41,41	0
57	MG	YA	3190	1/1	0.94	0.11	58,58,58,58	0
57	MG	XA	1684	1/1	0.94	0.89	41,41,41,41	0
57	MG	RA	3243	1/1	0.94	0.33	31,31,31,31	0
57	MG	YA	3101	1/1	0.94	0.08	50,50,50,50	0
57	MG	YA	3194	1/1	0.94	0.61	73,73,73,73	0
57	MG	RA	3288	1/1	0.94	0.47	50,50,50,50	0
57	MG	YA	3295	1/1	0.94	0.43	45,45,45,45	0
57	MG	RA	3246	1/1	0.94	0.32	62,62,62,62	0
57	MG	RA	3112	1/1	0.94	0.21	58,58,58,58	0
57	MG	YA	3299	1/1	0.94	0.68	49,49,49,49	0
57	MG	YA	3198	1/1	0.94	0.30	44,44,44,44	0
57	MG	QA	1691	1/1	0.94	0.35	60,60,60,60	0
57	MG	QA	1604	1/1	0.94	0.66	38,38,38,38	0
57	MG	RA	3015	1/1	0.94	0.18	35,35,35,35	0
57	MG	XA	1631	1/1	0.94	0.31	46,46,46,46	0
57	MG	YA	3207	1/1	0.94	0.14	58,58,58,58	0
57	MG	YA	3121	1/1	0.94	0.28	38,38,38,38	0
57	MG	RA	3016	1/1	0.94	0.56	19,19,19,19	0
57	MG	QA	1659	1/1	0.94	0.51	26,26,26,26	0
57	MG	YA	3124	1/1	0.94	0.20	55,55,55,55	0
57	MG	RA	3257	1/1	0.94	0.30	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	XA	1637	1/1	0.94	0.18	86,86,86,86	0
57	MG	RA	3259	1/1	0.94	0.20	29,29,29,29	0
57	MG	RA	3183	1/1	0.94	0.24	54,54,54,54	0
57	MG	RA	3261	1/1	0.94	0.46	55,55,55,55	0
57	MG	YA	3319	1/1	0.94	0.35	53,53,53,53	0
57	MG	YA	3134	1/1	0.94	0.34	33,33,33,33	0
57	MG	RA	3118	1/1	0.94	0.11	44,44,44,44	0
57	MG	RA	3077	1/1	0.94	0.36	12,12,12,12	0
57	MG	RA	3264	1/1	0.94	0.70	47,47,47,47	0
57	MG	QA	1661	1/1	0.94	0.62	50,50,50,50	0
57	MG	XA	1708	1/1	0.94	0.61	47,47,47,47	0
57	MG	RA	3305	1/1	0.94	0.33	66,66,66,66	0
57	MG	XA	1711	1/1	0.94	0.59	93,93,93,93	0
57	MG	YA	3233	1/1	0.94	0.44	32,32,32,32	0
57	MG	RA	3029	1/1	0.94	0.22	23,23,23,23	0
57	MG	RA	3307	1/1	0.94	0.07	71,71,71,71	0
57	MG	RA	3123	1/1	0.94	0.15	52,52,52,52	0
57	MG	QA	1684	1/1	0.94	0.81	63,63,63,63	0
57	MG	RB	202	1/1	0.94	0.13	52,52,52,52	0
57	MG	YA	3244	1/1	0.94	0.39	24,24,24,24	0
57	MG	XV	101	1/1	0.94	0.42	35,35,35,35	0
57	MG	RA	3039	1/1	0.94	0.28	27,27,27,27	0
57	MG	RA	3130	1/1	0.94	0.35	78,78,78,78	0
57	MG	QA	1621	1/1	0.94	0.14	62,62,62,62	0
57	MG	YA	3252	1/1	0.94	0.51	32,32,32,32	0
57	MG	RA	3095	1/1	0.94	0.47	32,32,32,32	0
59	ZN	XD	301	1/1	0.94	0.32	65,65,65,65	0
57	MG	YA	3275	1/1	0.95	0.35	30,30,30,30	0
57	MG	YA	3126	1/1	0.95	0.35	21,21,21,21	0
57	MG	YA	3127	1/1	0.95	0.15	38,38,38,38	0
57	MG	RA	3153	1/1	0.95	0.05	54,54,54,54	0
57	MG	RA	3274	1/1	0.95	0.41	61,61,61,61	0
57	MG	QV	102	1/1	0.95	0.22	24,24,24,24	0
57	MG	QA	1647	1/1	0.95	0.33	40,40,40,40	0
57	MG	YA	3006	1/1	0.95	0.19	29,29,29,29	0
57	MG	XA	1635	1/1	0.95	0.18	59,59,59,59	0
57	MG	RA	3242	1/1	0.95	0.33	27,27,27,27	0
57	MG	RA	3124	1/1	0.95	0.16	49,49,49,49	0
57	MG	XA	1638	1/1	0.95	0.38	36,36,36,36	0
57	MG	QY	101	1/1	0.95	0.21	54,54,54,54	0
57	MG	RA	3210	1/1	0.95	0.34	34,34,34,34	0
57	MG	RA	3041	1/1	0.95	0.30	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3283	1/1	0.95	0.14	45,45,45,45	0
57	MG	RA	3104	1/1	0.95	0.17	30,30,30,30	0
57	MG	YA	3146	1/1	0.95	0.27	37,37,37,37	0
57	MG	RA	3070	1/1	0.95	0.41	22,22,22,22	0
57	MG	RA	3163	1/1	0.95	0.41	54,54,54,54	0
57	MG	YA	3151	1/1	0.95	0.15	61,61,61,61	0
57	MG	XA	1648	1/1	0.95	0.48	61,61,61,61	0
57	MG	YA	3221	1/1	0.95	0.32	60,60,60,60	0
57	MG	RA	3110	1/1	0.95	0.38	39,39,39,39	0
57	MG	YA	3302	1/1	0.95	0.85	71,71,71,71	0
57	MG	XA	1695	1/1	0.95	0.23	35,35,35,35	0
57	MG	YA	3155	1/1	0.95	0.57	54,54,54,54	0
57	MG	RA	3072	1/1	0.95	0.47	35,35,35,35	0
57	MG	YA	3228	1/1	0.95	0.23	31,31,31,31	0
57	MG	RA	3258	1/1	0.95	0.32	45,45,45,45	0
57	MG	RA	3044	1/1	0.95	0.55	51,51,51,51	0
57	MG	XA	1655	1/1	0.95	0.22	77,77,77,77	0
57	MG	YA	3161	1/1	0.95	0.28	62,62,62,62	0
57	MG	YA	3073	1/1	0.95	0.19	28,28,28,28	0
57	MG	QA	1622	1/1	0.95	0.32	70,70,70,70	0
57	MG	YA	3078	1/1	0.95	0.14	36,36,36,36	0
57	MG	RA	3080	1/1	0.95	0.69	39,39,39,39	0
57	MG	YA	3316	1/1	0.95	0.19	40,40,40,40	0
57	MG	YA	3239	1/1	0.95	0.45	14,14,14,14	0
57	MG	YA	3318	1/1	0.95	0.26	38,38,38,38	0
57	MG	RA	3083	1/1	0.95	0.28	29,29,29,29	0
57	MG	RA	3048	1/1	0.95	0.46	19,19,19,19	0
57	MG	YA	3322	1/1	0.95	0.76	48,48,48,48	0
57	MG	YA	3085	1/1	0.95	0.46	25,25,25,25	0
57	MG	YA	3087	1/1	0.95	0.27	20,20,20,20	0
57	MG	YA	3092	1/1	0.95	0.66	26,26,26,26	0
57	MG	YA	3250	1/1	0.95	0.57	28,28,28,28	0
57	MG	YA	3098	1/1	0.95	0.51	24,24,24,24	0
57	MG	QA	1688	1/1	0.95	0.32	65,65,65,65	0
57	MG	XA	1615	1/1	0.95	0.19	39,39,39,39	0
57	MG	YA	3104	1/1	0.95	0.48	44,44,44,44	0
57	MG	XA	1707	1/1	0.95	0.43	70,70,70,70	0
57	MG	RA	3228	1/1	0.95	0.23	35,35,35,35	0
57	MG	YA	3112	1/1	0.95	0.23	54,54,54,54	0
57	MG	QA	1650	1/1	0.95	0.17	70,70,70,70	0
57	MG	XA	1710	1/1	0.95	0.18	45,45,45,45	0
57	MG	RA	3148	1/1	0.95	0.41	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	YA	3267	1/1	0.95	0.13	62,62,62,62	0
57	MG	RA	3027	1/1	0.95	0.29	17,17,17,17	0
57	MG	XA	1624	1/1	0.95	0.10	32,32,32,32	0
57	MG	Y5	101	1/1	0.95	0.18	39,39,39,39	0
57	MG	RA	3233	1/1	0.95	0.49	48,48,48,48	0
57	MG	XA	1674	1/1	0.95	0.47	46,46,46,46	0
58	PAR	XA	1715	42/42	0.95	0.21	66,66,67,67	0
57	MG	QA	1630	1/1	0.95	0.14	75,75,75,75	0
59	ZN	QN	101	1/1	0.95	0.12	105,105,105,105	0
57	MG	RA	3152	1/1	0.95	0.52	49,49,49,49	0
57	MG	RA	3071	1/1	0.96	0.49	52,52,52,52	0
57	MG	YA	3256	1/1	0.96	0.21	33,33,33,33	0
57	MG	XA	1620	1/1	0.96	0.10	63,63,63,63	0
57	MG	RA	3157	1/1	0.96	0.37	46,46,46,46	0
57	MG	YA	3053	1/1	0.96	0.33	17,17,17,17	0
57	MG	RA	3128	1/1	0.96	0.28	50,50,50,50	0
57	MG	YA	3055	1/1	0.96	0.23	13,13,13,13	0
57	MG	YA	3163	1/1	0.96	0.36	34,34,34,34	0
57	MG	RA	3215	1/1	0.96	0.69	35,35,35,35	0
57	MG	QA	1614	1/1	0.96	0.49	58,58,58,58	0
57	MG	YA	3061	1/1	0.96	0.40	31,31,31,31	0
57	MG	RA	3074	1/1	0.96	0.21	16,16,16,16	0
57	MG	YA	3270	1/1	0.96	0.34	33,33,33,33	0
57	MG	RA	3046	1/1	0.96	0.31	43,43,43,43	0
57	MG	YA	3066	1/1	0.96	0.75	41,41,41,41	0
57	MG	XA	1630	1/1	0.96	0.45	55,55,55,55	0
57	MG	RA	3134	1/1	0.96	0.32	83,83,83,83	0
57	MG	RA	3190	1/1	0.96	0.10	46,46,46,46	0
57	MG	YA	3276	1/1	0.96	0.41	41,41,41,41	0
57	MG	YA	3077	1/1	0.96	0.22	28,28,28,28	0
57	MG	RA	3003	1/1	0.96	0.29	27,27,27,27	0
57	MG	XA	1634	1/1	0.96	0.23	30,30,30,30	0
57	MG	RA	3223	1/1	0.96	0.31	25,25,25,25	0
57	MG	YA	3082	1/1	0.96	0.45	59,59,59,59	0
57	MG	RA	3079	1/1	0.96	0.28	41,41,41,41	0
57	MG	YA	3182	1/1	0.96	0.43	50,50,50,50	0
57	MG	YA	3084	1/1	0.96	0.28	35,35,35,35	0
57	MG	RA	3024	1/1	0.96	0.23	27,27,27,27	0
57	MG	YA	3086	1/1	0.96	0.27	32,32,32,32	0
57	MG	RA	3166	1/1	0.96	0.19	61,61,61,61	0
57	MG	RA	3229	1/1	0.96	0.69	43,43,43,43	0
57	MG	YA	3097	1/1	0.96	0.37	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3189	1/1	0.96	0.30	26,26,26,26	0
57	MG	RA	3081	1/1	0.96	0.15	36,36,36,36	0
57	MG	YA	3099	1/1	0.96	0.50	19,19,19,19	0
57	MG	RA	3270	1/1	0.96	0.47	48,48,48,48	0
57	MG	YA	3102	1/1	0.96	0.44	25,25,25,25	0
57	MG	RA	3140	1/1	0.96	0.39	31,31,31,31	0
57	MG	RA	3169	1/1	0.96	0.60	48,48,48,48	0
57	MG	YA	3298	1/1	0.96	0.90	53,53,53,53	0
57	MG	RA	3006	1/1	0.96	0.45	31,31,31,31	0
57	MG	YA	3109	1/1	0.96	0.27	36,36,36,36	0
57	MG	RA	3007	1/1	0.96	0.46	18,18,18,18	0
57	MG	RA	3235	1/1	0.96	0.38	44,44,44,44	0
57	MG	YA	3201	1/1	0.96	0.16	40,40,40,40	0
57	MG	QA	1601	1/1	0.96	0.88	57,57,57,57	0
57	MG	RA	3237	1/1	0.96	0.61	23,23,23,23	0
57	MG	RA	3144	1/1	0.96	0.54	29,29,29,29	0
57	MG	QA	1645	1/1	0.96	0.10	60,60,60,60	0
57	MG	YA	3120	1/1	0.96	0.19	34,34,34,34	0
57	MG	XA	1654	1/1	0.96	0.22	43,43,43,43	0
57	MG	YA	3211	1/1	0.96	0.30	65,65,65,65	0
57	MG	RA	3280	1/1	0.96	0.32	58,58,58,58	0
57	MG	QA	1657	1/1	0.96	0.33	61,61,61,61	0
57	MG	XA	1601	1/1	0.96	0.55	21,21,21,21	0
57	MG	XA	1602	1/1	0.96	0.47	29,29,29,29	0
57	MG	XA	1659	1/1	0.96	0.23	58,58,58,58	0
57	MG	RA	3063	1/1	0.96	0.45	17,17,17,17	0
57	MG	QA	1608	1/1	0.96	0.13	47,47,47,47	0
57	MG	RA	3012	1/1	0.96	0.28	22,22,22,22	0
57	MG	QA	1671	1/1	0.96	0.49	43,43,43,43	0
57	MG	YA	3132	1/1	0.96	0.58	52,52,52,52	0
57	MG	XA	1609	1/1	0.96	0.32	29,29,29,29	0
57	MG	YA	3224	1/1	0.96	0.16	76,76,76,76	0
57	MG	XA	1610	1/1	0.96	0.23	50,50,50,50	0
57	MG	YA	3004	1/1	0.96	0.34	27,27,27,27	0
57	MG	YA	3005	1/1	0.96	0.18	5,5,5,5	0
57	MG	XA	1667	1/1	0.96	0.24	38,38,38,38	0
57	MG	RA	3248	1/1	0.96	0.29	77,77,77,77	0
57	MG	YA	3231	1/1	0.96	0.23	36,36,36,36	0
57	MG	RA	3154	1/1	0.96	0.17	46,46,46,46	0
57	MG	YA	3015	1/1	0.96	0.39	27,27,27,27	0
57	MG	XA	1670	1/1	0.96	0.34	46,46,46,46	0
57	MG	XA	1613	1/1	0.96	0.31	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1614	1/1	0.96	0.28	23,23,23,23	0
57	MG	YA	3237	1/1	0.96	0.41	36,36,36,36	0
57	MG	RA	3251	1/1	0.96	0.58	42,42,42,42	0
57	MG	YA	3147	1/1	0.96	0.17	47,47,47,47	0
57	MG	YA	3148	1/1	0.96	0.08	57,57,57,57	0
57	MG	YA	3026	1/1	0.96	0.89	34,34,34,34	0
57	MG	XA	1616	1/1	0.96	0.44	35,35,35,35	0
57	MG	YA	3031	1/1	0.96	0.36	13,13,13,13	0
57	MG	RA	3102	1/1	0.96	0.51	33,33,33,33	0
57	MG	YA	3039	1/1	0.96	0.11	18,18,18,18	0
57	MG	RA	3253	1/1	0.96	0.17	35,35,35,35	0
57	MG	YA	3044	1/1	0.96	0.23	7,7,7,7	0
57	MG	YA	3255	1/1	0.97	0.34	46,46,46,46	0
57	MG	RA	3013	1/1	0.97	0.30	27,27,27,27	0
57	MG	YA	3075	1/1	0.97	0.51	24,24,24,24	0
57	MG	RA	3042	1/1	0.97	0.15	22,22,22,22	0
57	MG	XA	1653	1/1	0.97	0.48	43,43,43,43	0
57	MG	QA	1660	1/1	0.97	0.39	33,33,33,33	0
57	MG	QA	1640	1/1	0.97	0.17	62,62,62,62	0
57	MG	YA	3170	1/1	0.97	0.72	37,37,37,37	0
57	MG	RA	3196	1/1	0.97	0.19	35,35,35,35	0
57	MG	XA	1608	1/1	0.97	0.30	32,32,32,32	0
57	MG	RA	3004	1/1	0.97	0.34	21,21,21,21	0
57	MG	YA	3175	1/1	0.97	0.14	47,47,47,47	0
57	MG	RA	3047	1/1	0.97	0.46	16,16,16,16	0
57	MG	QA	1651	1/1	0.97	0.18	30,30,30,30	0
57	MG	RA	3122	1/1	0.97	0.29	46,46,46,46	0
57	MG	YA	3089	1/1	0.97	0.39	36,36,36,36	0
57	MG	XA	1662	1/1	0.97	0.67	49,49,49,49	0
57	MG	YA	3094	1/1	0.97	0.51	20,20,20,20	0
57	MG	YA	3095	1/1	0.97	0.46	22,22,22,22	0
57	MG	RA	3025	1/1	0.97	0.29	50,50,50,50	0
57	MG	RA	3085	1/1	0.97	0.30	26,26,26,26	0
57	MG	QM	201	1/1	0.97	0.17	79,79,79,79	0
57	MG	YA	3100	1/1	0.97	0.62	42,42,42,42	0
57	MG	XV	102	1/1	0.97	0.27	21,21,21,21	0
57	MG	RA	3088	1/1	0.97	0.31	38,38,38,38	0
57	MG	RA	3089	1/1	0.97	0.35	24,24,24,24	0
57	MG	RA	3051	1/1	0.97	0.40	21,21,21,21	0
57	MG	RA	3053	1/1	0.97	0.63	27,27,27,27	0
57	MG	YA	3107	1/1	0.97	0.55	36,36,36,36	0
57	MG	RA	3132	1/1	0.97	0.23	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3288	1/1	0.97	0.35	39,39,39,39	0
57	MG	XA	1622	1/1	0.97	0.47	29,29,29,29	0
57	MG	XA	1673	1/1	0.97	0.35	59,59,59,59	0
57	MG	QA	1625	1/1	0.97	0.34	62,62,62,62	0
57	MG	YA	3008	1/1	0.97	0.15	23,23,23,23	0
57	MG	YA	3117	1/1	0.97	0.40	25,25,25,25	0
57	MG	RA	3094	1/1	0.97	0.14	27,27,27,27	0
57	MG	YA	3200	1/1	0.97	0.11	28,28,28,28	0
57	MG	YA	3011	1/1	0.97	0.28	28,28,28,28	0
57	MG	QA	1634	1/1	0.97	0.15	30,30,30,30	0
57	MG	RA	3136	1/1	0.97	0.24	51,51,51,51	0
57	MG	YA	3205	1/1	0.97	0.34	70,70,70,70	0
57	MG	RA	3057	1/1	0.97	0.45	50,50,50,50	0
57	MG	RA	3058	1/1	0.97	0.38	22,22,22,22	0
57	MG	YA	3022	1/1	0.97	0.51	26,26,26,26	0
57	MG	YA	3209	1/1	0.97	0.09	70,70,70,70	0
57	MG	RA	3030	1/1	0.97	0.32	19,19,19,19	0
57	MG	QA	1681	1/1	0.97	0.28	72,72,72,72	0
57	MG	YA	3029	1/1	0.97	0.32	33,33,33,33	0
57	MG	RA	3033	1/1	0.97	0.43	8,8,8,8	0
57	MG	RA	3105	1/1	0.97	0.26	28,28,28,28	0
57	MG	RA	3220	1/1	0.97	0.32	47,47,47,47	0
57	MG	YA	3036	1/1	0.97	0.25	38,38,38,38	0
57	MG	RA	3066	1/1	0.97	0.39	13,13,13,13	0
57	MG	RA	3107	1/1	0.97	0.08	34,34,34,34	0
57	MG	YA	3042	1/1	0.97	0.42	38,38,38,38	0
57	MG	YA	3314	1/1	0.97	0.37	46,46,46,46	0
57	MG	YA	3043	1/1	0.97	0.42	15,15,15,15	0
57	MG	RA	3145	1/1	0.97	0.19	37,37,37,37	0
57	MG	RA	3224	1/1	0.97	0.48	20,20,20,20	0
57	MG	RA	3109	1/1	0.97	0.30	63,63,63,63	0
57	MG	YA	3048	1/1	0.97	0.27	24,24,24,24	0
57	MG	RE	302	1/1	0.97	0.21	17,17,17,17	0
57	MG	YA	3227	1/1	0.97	0.23	80,80,80,80	0
57	MG	YA	3051	1/1	0.97	0.23	19,19,19,19	0
57	MG	YA	3144	1/1	0.97	0.55	51,51,51,51	0
57	MG	YA	3052	1/1	0.97	0.22	22,22,22,22	0
57	MG	XA	1641	1/1	0.97	0.30	46,46,46,46	0
57	MG	RA	3147	1/1	0.97	0.20	56,56,56,56	0
57	MG	RA	3227	1/1	0.97	0.66	39,39,39,39	0
57	MG	XA	1644	1/1	0.97	0.15	59,59,59,59	0
57	MG	YA	3057	1/1	0.97	0.46	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1696	1/1	0.97	0.24	50,50,50,50	0
57	MG	YA	3060	1/1	0.97	0.25	26,26,26,26	0
57	MG	RA	3034	1/1	0.97	0.53	33,33,33,33	0
57	MG	RA	3035	1/1	0.97	0.47	23,23,23,23	0
57	MG	YA	3240	1/1	0.97	0.68	26,26,26,26	0
57	MG	YA	3064	1/1	0.97	0.40	40,40,40,40	0
57	MG	RA	3037	1/1	0.97	0.38	17,17,17,17	0
57	MG	RA	3151	1/1	0.97	0.07	53,53,53,53	0
57	MG	YA	3246	1/1	0.97	0.36	25,25,25,25	0
57	MG	YA	3069	1/1	0.97	0.35	27,27,27,27	0
57	MG	YA	3248	1/1	0.97	0.40	36,36,36,36	0
57	MG	YA	3159	1/1	0.97	0.78	55,55,55,55	0
57	MG	YA	3070	1/1	0.97	0.17	34,34,34,34	0
57	MG	QA	1672	1/1	0.97	0.15	48,48,48,48	0
57	MG	YA	3072	1/1	0.97	0.42	27,27,27,27	0
57	MG	QA	1654	1/1	0.97	0.16	107,107,107,107	0
59	ZN	XN	101	1/1	0.97	0.14	100,100,100,100	0
57	MG	YA	3037	1/1	0.98	0.48	16,16,16,16	0
57	MG	RA	3298	1/1	0.98	0.20	52,52,52,52	0
57	MG	RA	3171	1/1	0.98	0.51	35,35,35,35	0
57	MG	RA	3245	1/1	0.98	0.11	75,75,75,75	0
57	MG	RA	3060	1/1	0.98	0.49	19,19,19,19	0
57	MG	RA	3127	1/1	0.98	0.30	47,47,47,47	0
57	MG	RA	3061	1/1	0.98	0.49	29,29,29,29	0
57	MG	RA	3082	1/1	0.98	0.31	34,34,34,34	0
57	MG	YA	3047	1/1	0.98	0.52	26,26,26,26	0
57	MG	YA	3110	1/1	0.98	0.13	30,30,30,30	0
57	MG	RA	3250	1/1	0.98	0.20	45,45,45,45	0
57	MG	YA	3049	1/1	0.98	0.52	22,22,22,22	0
57	MG	RA	3018	1/1	0.98	0.23	32,32,32,32	0
57	MG	YA	3173	1/1	0.98	0.05	46,46,46,46	0
57	MG	RA	3022	1/1	0.98	0.28	22,22,22,22	0
57	MG	QA	1649	1/1	0.98	0.10	121,121,121,121	0
57	MG	RA	3067	1/1	0.98	0.42	36,36,36,36	0
57	MG	RB	201	1/1	0.98	0.07	72,72,72,72	0
57	MG	RA	3087	1/1	0.98	0.32	37,37,37,37	0
57	MG	XA	1621	1/1	0.98	0.34	44,44,44,44	0
57	MG	YA	3003	1/1	0.98	0.41	30,30,30,30	0
57	MG	XA	1689	1/1	0.98	0.56	52,52,52,52	0
57	MG	RA	3036	1/1	0.98	0.40	24,24,24,24	0
57	MG	YA	3243	1/1	0.98	0.28	25,25,25,25	0
57	MG	RA	3005	1/1	0.98	0.45	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	RE	301	1/1	0.98	0.23	28,28,28,28	0
57	MG	XA	1625	1/1	0.98	0.32	27,27,27,27	0
57	MG	RA	3038	1/1	0.98	0.41	42,42,42,42	0
57	MG	QA	1675	1/1	0.98	0.32	53,53,53,53	0
57	MG	YA	3012	1/1	0.98	0.25	13,13,13,13	0
57	MG	YA	3013	1/1	0.98	0.50	12,12,12,12	0
57	MG	YA	3014	1/1	0.98	0.34	17,17,17,17	0
57	MG	RA	3208	1/1	0.98	0.17	57,57,57,57	0
57	MG	QA	1680	1/1	0.98	0.21	60,60,60,60	0
57	MG	YA	3254	1/1	0.98	0.43	29,29,29,29	0
57	MG	YA	3136	1/1	0.98	0.32	20,20,20,20	0
57	MG	YA	3320	1/1	0.98	0.22	38,38,38,38	0
57	MG	RA	3014	1/1	0.98	0.54	14,14,14,14	0
57	MG	QA	1639	1/1	0.98	0.10	41,41,41,41	0
57	MG	YA	3076	1/1	0.98	0.24	28,28,28,28	0
57	MG	YA	3260	1/1	0.98	0.14	32,32,32,32	0
57	MG	YA	3325	1/1	0.98	0.07	47,47,47,47	0
57	MG	YA	3020	1/1	0.98	0.54	16,16,16,16	0
57	MG	YA	3021	1/1	0.98	0.53	36,36,36,36	0
57	MG	YA	3263	1/1	0.98	0.57	33,33,33,33	0
57	MG	RA	3096	1/1	0.98	0.78	29,29,29,29	0
57	MG	YA	3023	1/1	0.98	0.36	18,18,18,18	0
57	MG	RA	3099	1/1	0.98	0.40	21,21,21,21	0
57	MG	YA	3025	1/1	0.98	0.36	24,24,24,24	0
57	MG	YA	3203	1/1	0.98	0.61	60,60,60,60	0
57	MG	R8	101	1/1	0.98	0.81	53,53,53,53	0
57	MG	YA	3028	1/1	0.98	0.20	20,20,20,20	0
57	MG	RA	3076	1/1	0.98	0.23	25,25,25,25	0
57	MG	RA	3239	1/1	0.98	0.12	37,37,37,37	0
57	MG	YA	3088	1/1	0.98	0.35	28,28,28,28	0
57	MG	QA	1610	1/1	0.98	0.21	46,46,46,46	0
57	MG	YA	3090	1/1	0.98	0.25	60,60,60,60	0
57	MG	RA	3078	1/1	0.98	0.45	24,24,24,24	0
57	MG	YA	3093	1/1	0.98	0.33	43,43,43,43	0
57	MG	YA	3033	1/1	0.98	0.52	19,19,19,19	0
57	MG	YA	3034	1/1	0.98	0.34	18,18,18,18	0
57	MG	YA	3215	1/1	0.98	0.39	24,24,24,24	0
57	MG	YA	3096	1/1	0.98	0.32	39,39,39,39	0
57	MG	YA	3035	1/1	0.98	0.31	18,18,18,18	0
57	MG	RA	3017	1/1	0.98	0.27	23,23,23,23	0
57	MG	RA	3028	1/1	0.99	0.19	11,11,11,11	0
57	MG	YA	3116	1/1	0.99	0.17	27,27,27,27	0

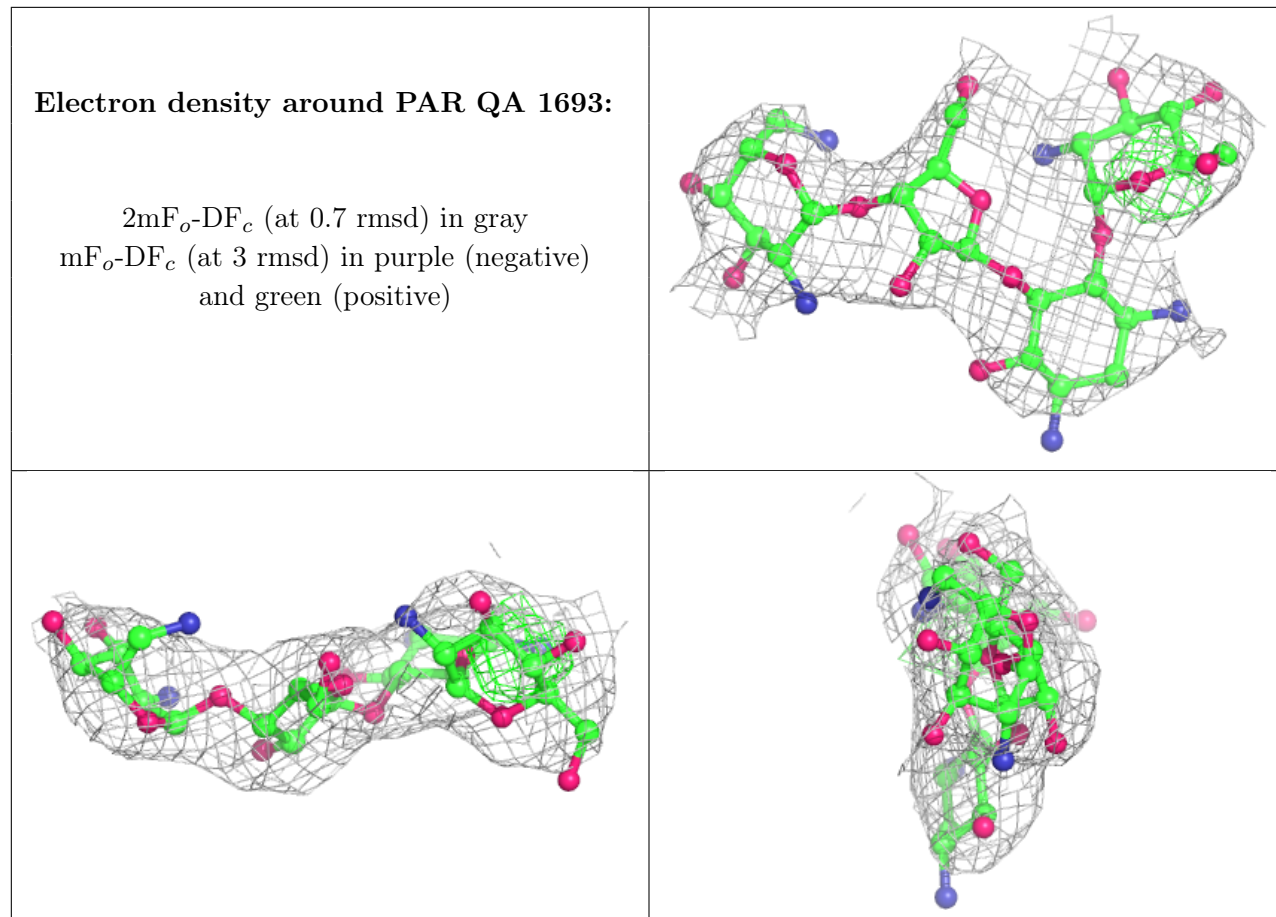
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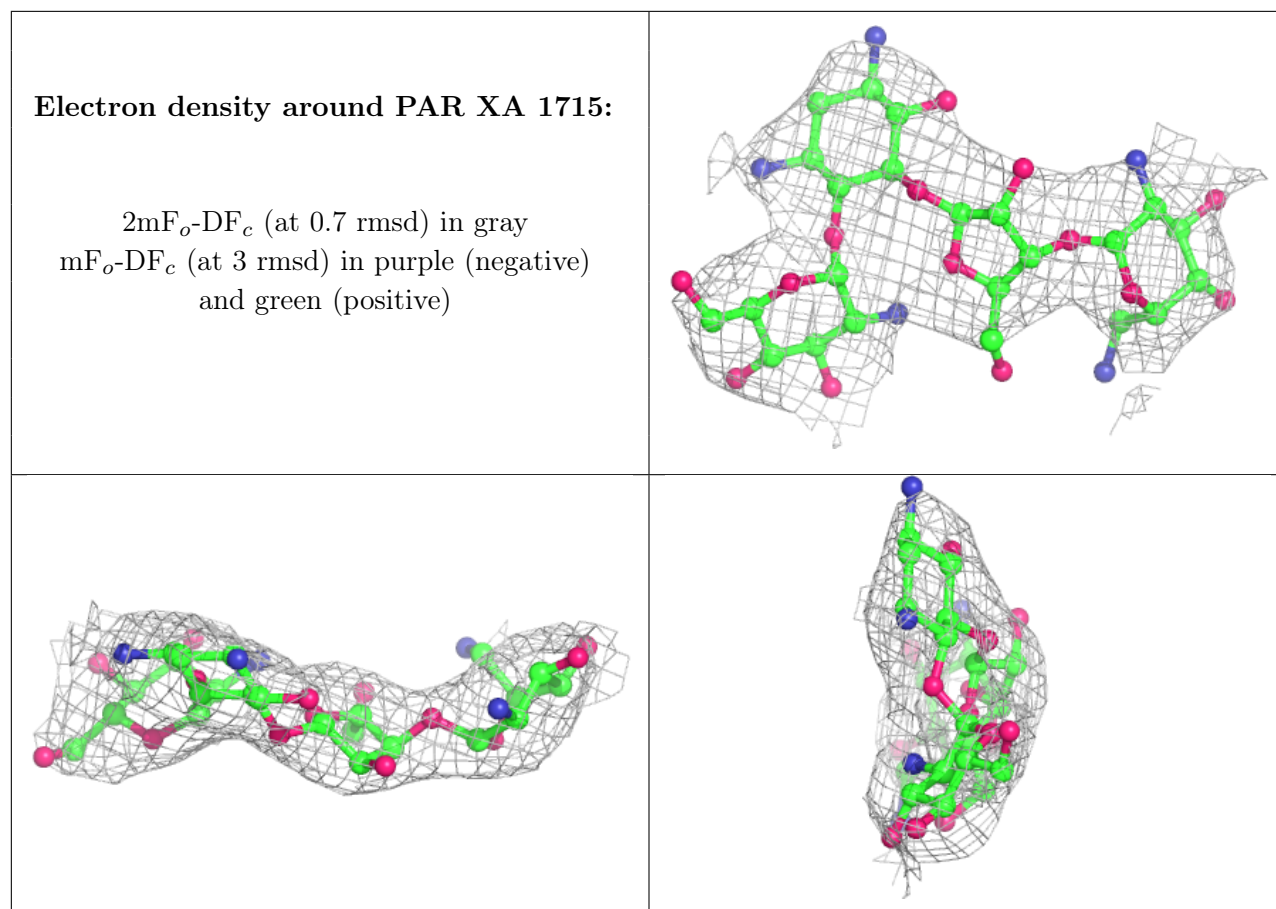
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3080	1/1	0.99	0.21	17,17,17,17	0
57	MG	RA	3056	1/1	0.99	0.56	28,28,28,28	0
57	MG	QA	1617	1/1	0.99	0.28	34,34,34,34	0
57	MG	QA	1668	1/1	0.99	0.21	52,52,52,52	0
57	MG	RA	3031	1/1	0.99	0.38	22,22,22,22	0
57	MG	RA	3073	1/1	0.99	0.18	52,52,52,52	0
57	MG	YA	3027	1/1	0.99	0.29	21,21,21,21	0
57	MG	YA	3002	1/1	0.99	0.51	12,12,12,12	0
57	MG	QA	1607	1/1	0.99	0.16	44,44,44,44	0
57	MG	RA	3019	1/1	0.99	0.58	24,24,24,24	0
57	MG	YA	3241	1/1	0.99	0.57	40,40,40,40	0
57	MG	RA	3020	1/1	0.99	0.27	12,12,12,12	0
57	MG	YA	3091	1/1	0.99	0.41	19,19,19,19	0
57	MG	YA	3129	1/1	0.99	0.12	46,46,46,46	0
57	MG	YA	3059	1/1	0.99	0.14	40,40,40,40	0
57	MG	RA	3108	1/1	0.99	0.21	11,11,11,11	0
57	MG	RA	3052	1/1	0.99	0.34	14,14,14,14	0
57	MG	YA	3062	1/1	0.99	0.20	10,10,10,10	0
57	MG	RA	3092	1/1	0.99	0.20	20,20,20,20	0
57	MG	RA	3129	1/1	0.99	0.18	55,55,55,55	0
57	MG	RA	3244	1/1	0.99	0.30	48,48,48,48	0
57	MG	RA	3064	1/1	0.99	0.64	26,26,26,26	0
57	MG	YA	3067	1/1	0.99	0.11	28,28,28,28	0
57	MG	YA	3068	1/1	0.99	0.33	29,29,29,29	0
57	MG	YA	3038	1/1	0.99	0.28	29,29,29,29	0
57	MG	XA	1603	1/1	0.99	0.56	27,27,27,27	0
57	MG	YA	3257	1/1	0.99	0.27	21,21,21,21	0
57	MG	YA	3040	1/1	0.99	0.32	8,8,8,8	0
57	MG	RA	3065	1/1	0.99	0.30	36,36,36,36	0
57	MG	YA	3106	1/1	0.99	0.33	7,7,7,7	0
57	MG	RA	3043	1/1	0.99	0.23	39,39,39,39	0
57	MG	YA	3108	1/1	0.99	0.29	51,51,51,51	0
57	MG	RA	3021	1/1	0.99	0.37	6,6,6,6	0
57	MG	YA	3017	1/1	0.99	0.30	28,28,28,28	0
57	MG	RA	3097	1/1	0.99	0.26	13,13,13,13	0
57	MG	XA	1671	1/1	0.99	0.54	37,37,37,37	0
57	MG	YA	3113	1/1	0.99	0.41	18,18,18,18	0
57	MG	RA	3098	1/1	0.99	0.46	15,15,15,15	0
57	MG	YA	3009	1/1	1.00	0.23	26,26,26,26	0

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

orientation to approximate a three-dimensional view.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.