



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:11 am BST

PDB ID : 4L71  
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-A on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-06-13  
Resolution : 3.90 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.

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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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

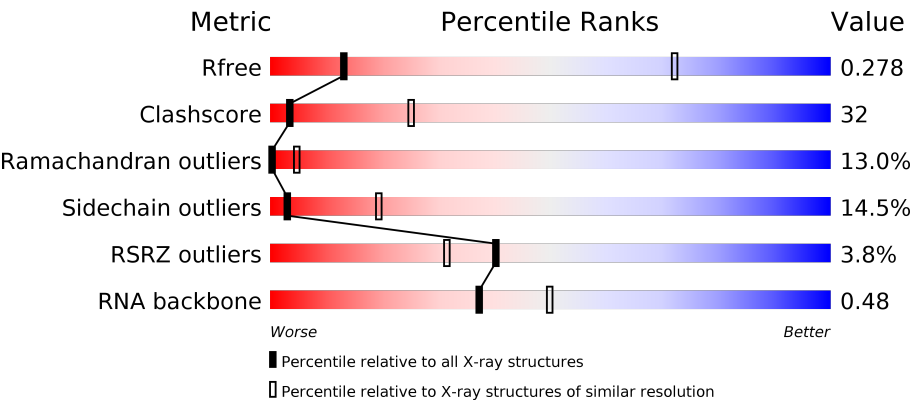


# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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 <sub>free</sub>	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

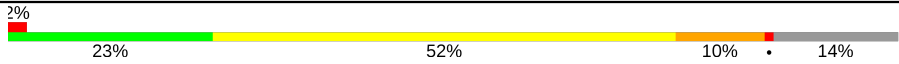
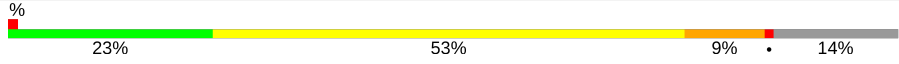
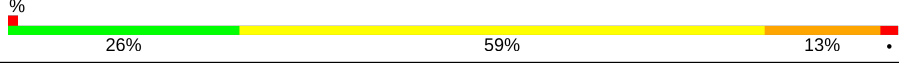
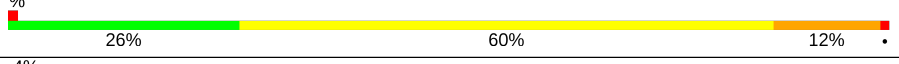
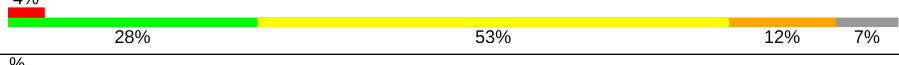
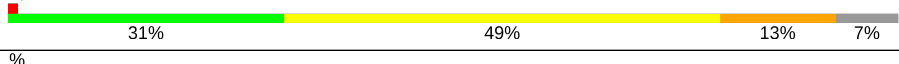
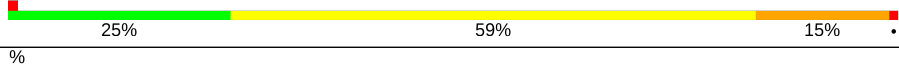
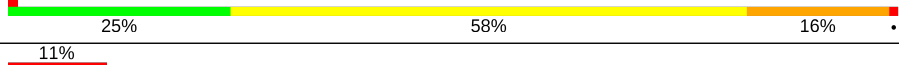
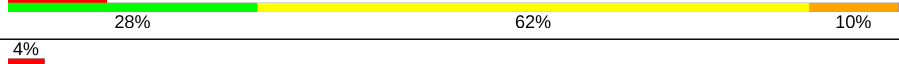
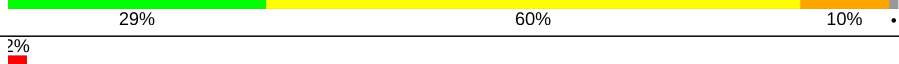

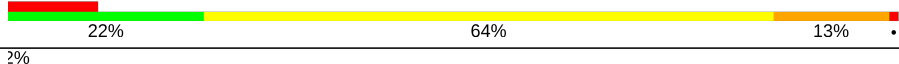
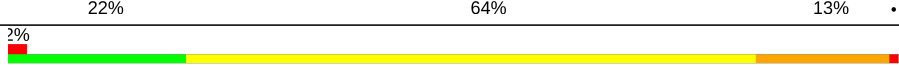
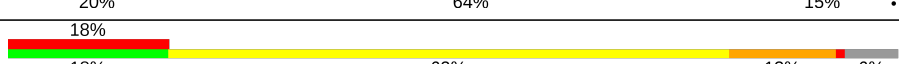
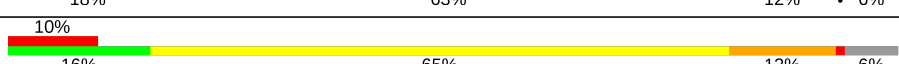
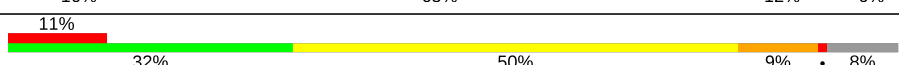
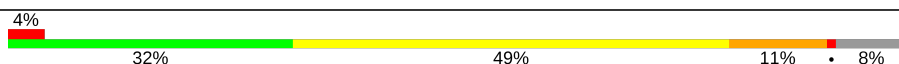
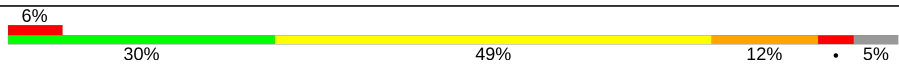
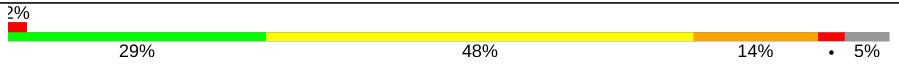
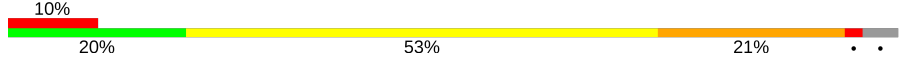
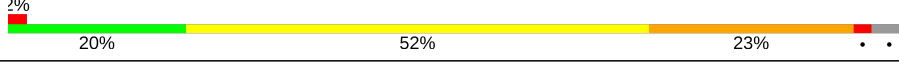
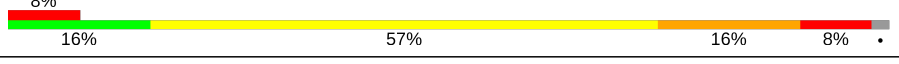

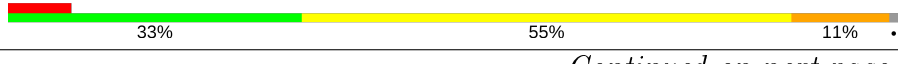

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	<div><div>2%</div><div><div></div><div>45%</div><div>42%</div><div>11%</div><div>..</div></div></div>
1	XA	1522	<div><div>%</div><div><div></div><div>43%</div><div>42%</div><div>12%</div><div>..</div></div></div>
2	QB	256	<div><div>6%</div><div><div></div><div>17%</div><div>59%</div><div>16%</div><div>7%</div></div></div>
2	XB	256	<div><div>4%</div><div><div></div><div>17%</div><div>59%</div><div>16%</div><div>7%</div></div></div>

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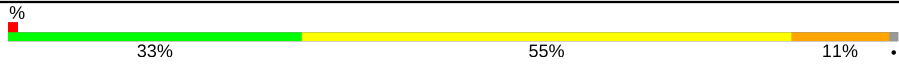
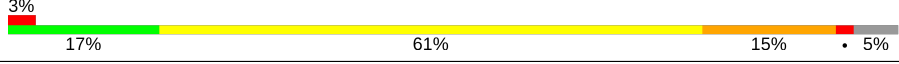
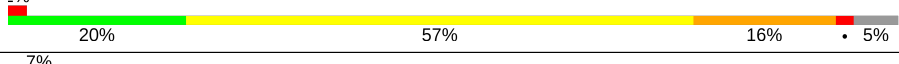
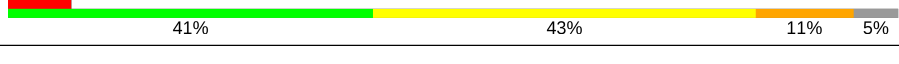
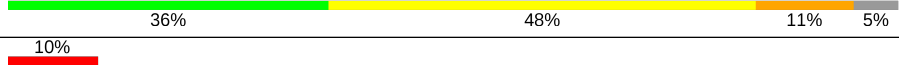
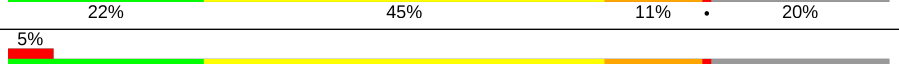
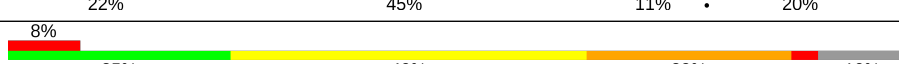
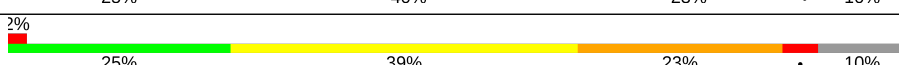
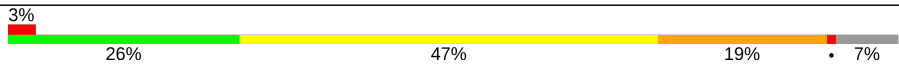
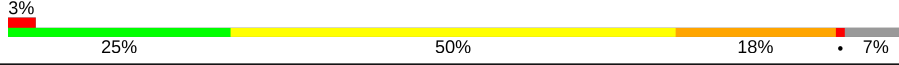
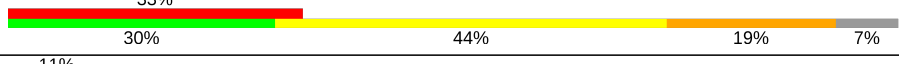
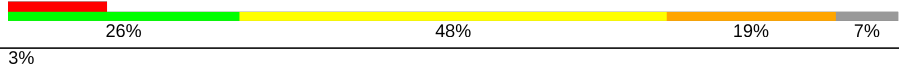
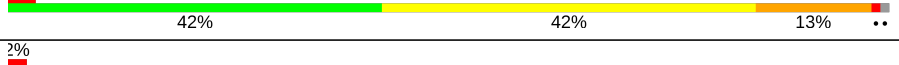

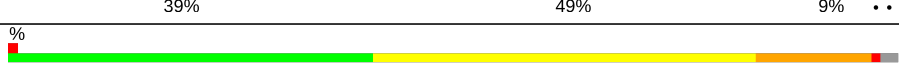
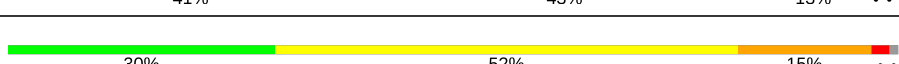
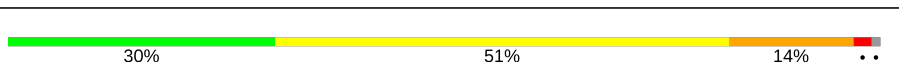
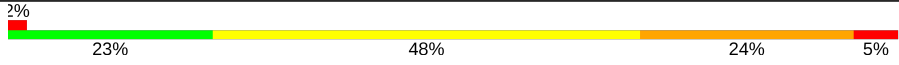
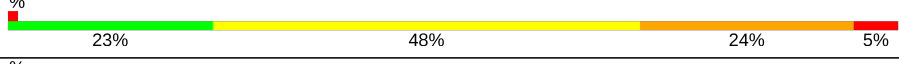


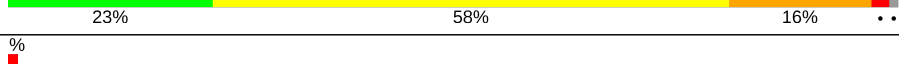
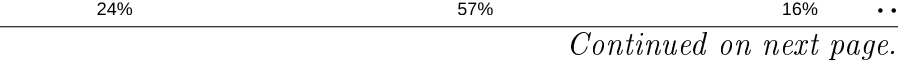


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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	RA	2916	
22	YA	2916	
23	RB	122	
23	YB	122	
24	RD	276	
24	YD	276	
25	RE	206	
25	YE	206	
26	RF	210	
26	YF	210	
27	RG	182	
27	YG	182	

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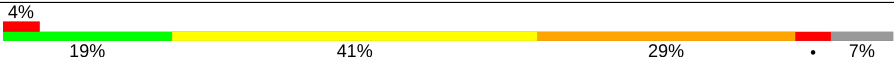
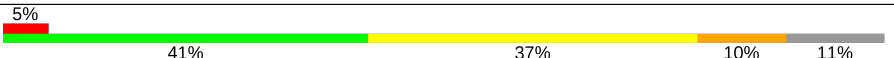
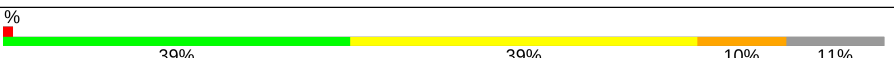

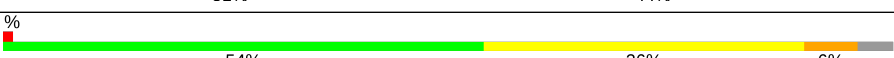
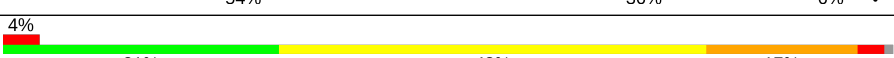
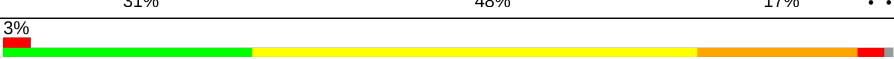
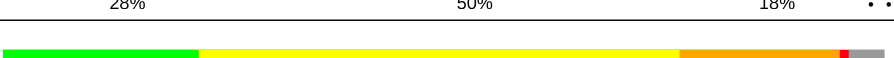
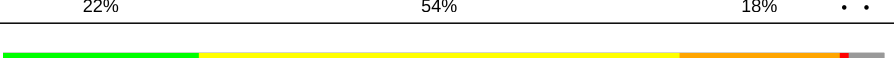
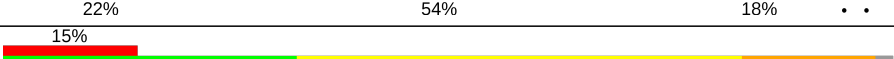




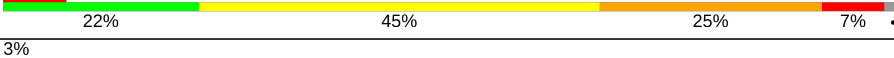
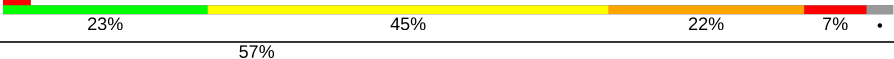



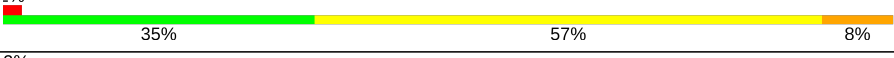
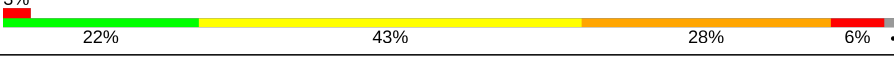


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Mol	Chain	Length	Quality of chain
28	RH	180	
28	YH	180	
29	RI	148	
29	YI	148	
30	RN	140	
30	YN	140	
31	RO	122	
31	YO	122	
32	RP	150	
32	YP	150	
33	RQ	141	
33	YQ	141	
34	RR	118	
34	YR	118	
35	RS	112	
35	YS	112	
36	RT	146	
36	YT	146	
37	RU	118	
37	YU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

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

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Mol	Chain	Length	Quality of chain
53	QV	77	
53	XV	77	
54	QX	25	
54	XX	25	
55	QY	18	
55	XY	18	
56	Z6	3	
56	Z8	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1602	-	-	-	X
57	MG	QA	1628	-	-	-	X
57	MG	QA	1665	-	-	-	X
57	MG	RA	3004	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3064	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3071	-	-	-	X
57	MG	RA	3123	-	-	-	X
57	MG	RA	3127	-	-	-	X
57	MG	RA	3164	-	-	-	X
57	MG	RA	3186	-	-	-	X
57	MG	RA	3205	-	-	-	X
57	MG	RA	3217	-	-	-	X
57	MG	RA	3219	-	-	-	X
57	MG	RA	3230	-	-	-	X
57	MG	XA	1601	-	-	-	X
57	MG	XA	1605	-	-	-	X
57	MG	XA	1635	-	-	-	X
57	MG	XA	1662	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3043	-	-	-	X
57	MG	YA	3053	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3079	-	-	-	X
57	MG	YA	3117	-	-	-	X
57	MG	YA	3150	-	-	-	X
57	MG	YA	3151	-	-	-	X
57	MG	YA	3223	-	-	-	X
57	MG	YA	3235	-	-	-	X
57	MG	YA	3245	-	-	-	X
57	MG	YA	3247	-	-	-	X
57	MG	YA	3250	-	-	-	X
57	MG	YA	3259	-	-	-	X
57	MG	YA	3261	-	-	-	X
59	ZN	R9	101	-	-	-	X
59	ZN	Y9	101	-	-	-	X



## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291950 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 Ribosomal RNA.

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
48	Y5	58	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

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

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

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

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

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

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

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

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

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



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

- Molecule 54 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	8	Total	C	N	O	P	0	0	0
			169	76	31	54	8			
54	XX	8	Total	C	N	O	P	0	0	0
			169	76	31	54	8			

- Molecule 55 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	QY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			
55	XY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	65	Total	Mg	0	0
			65	65		
57	RP	2	Total	Mg	0	0
			2	2		
57	QX	1	Total	Mg	0	0
			1	1		
57	YA	265	Total	Mg	0	0
			265	265		
57	QM	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XX	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	RU	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	244	Total 244	Mg 244	0	0
57	YP	2	Total 2	Mg 2	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	YB	3	Total 3	Mg 3	0	0
57	XV	2	Total 2	Mg 2	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0

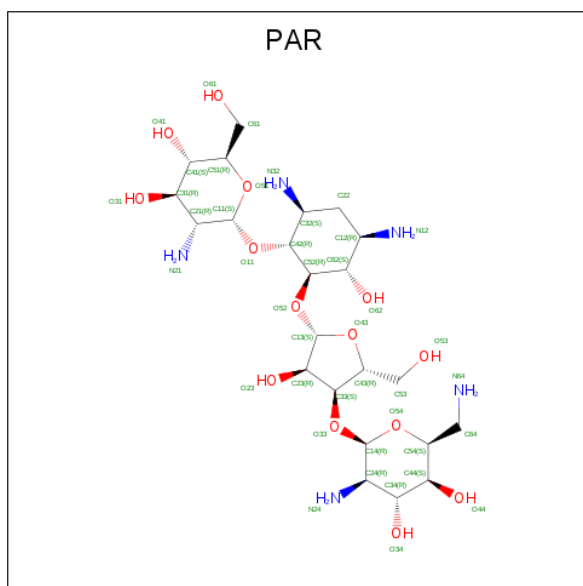
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YE	1	Total	Mg	0	0
			1	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total	C	N	O	0	0
			42	23	5	14		
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	Y9	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	QD	1	Total	Zn	0	0
			1	1		
59	XD	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		

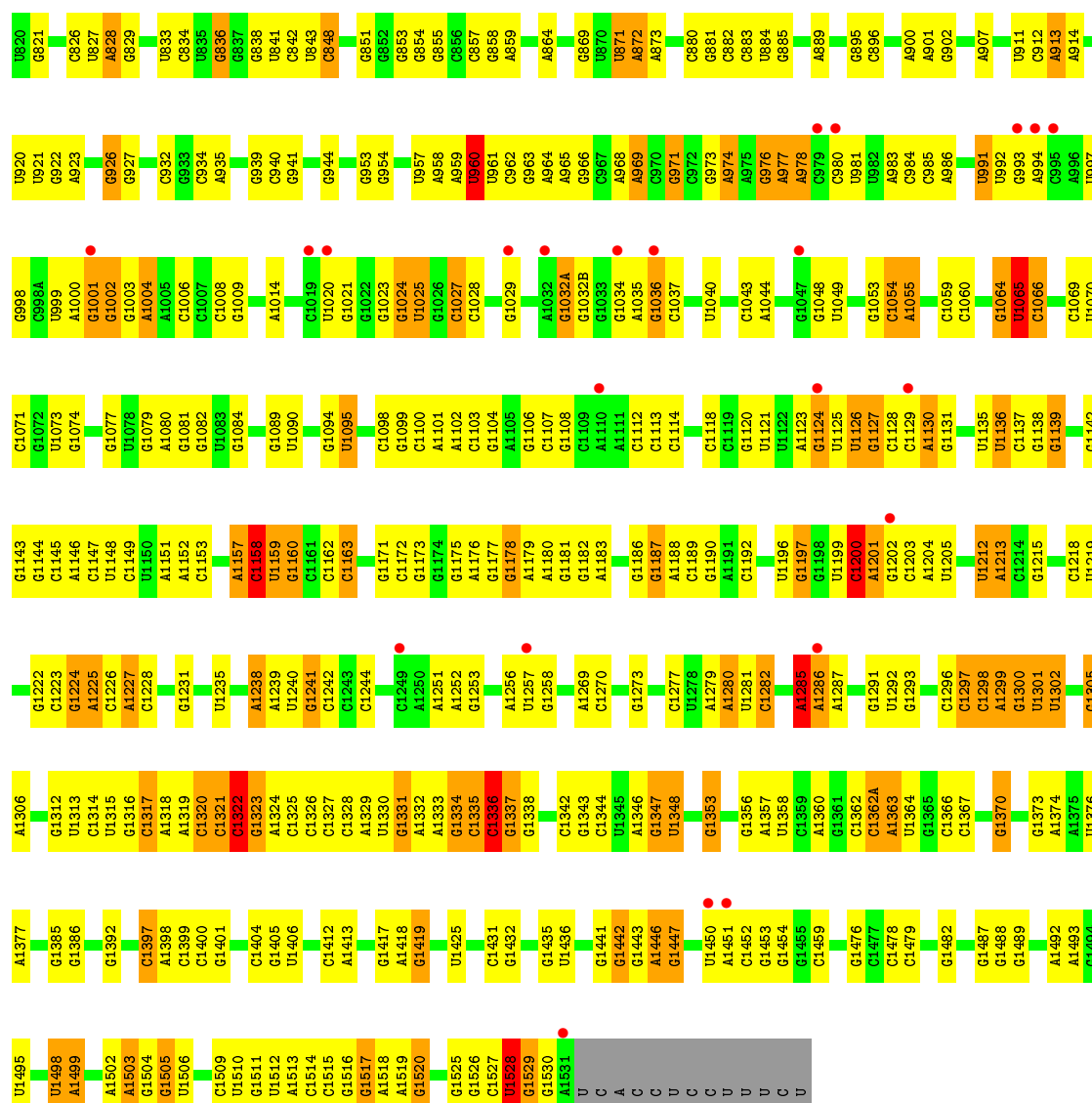


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

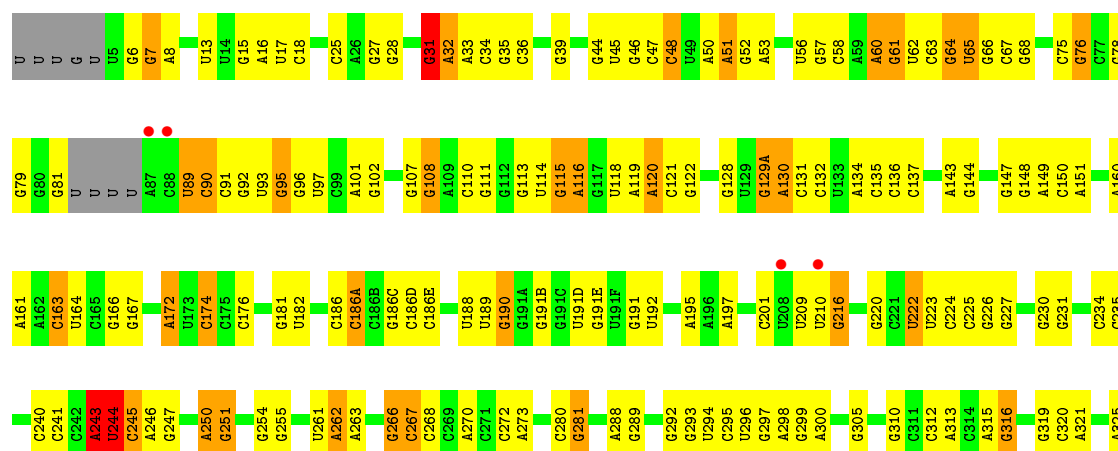
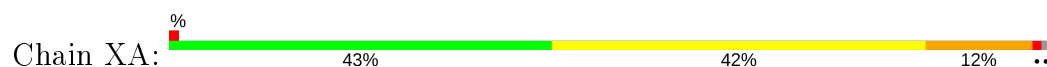
Chain QA:  45% 42% 11% ..

The visualization displays Chain QA results across a grid of colored squares, each containing a 3-letter code. The top bar chart shows a color gradient from red to purple, with percentage markers at 2%, 45%, 42%, and 11%. The grid is organized into rows and columns, with some cells highlighted in red or yellow. The bottom section contains a list of 3-letter codes corresponding to the grid cells.





• Molecule 1: 16S Ribosomal RNA



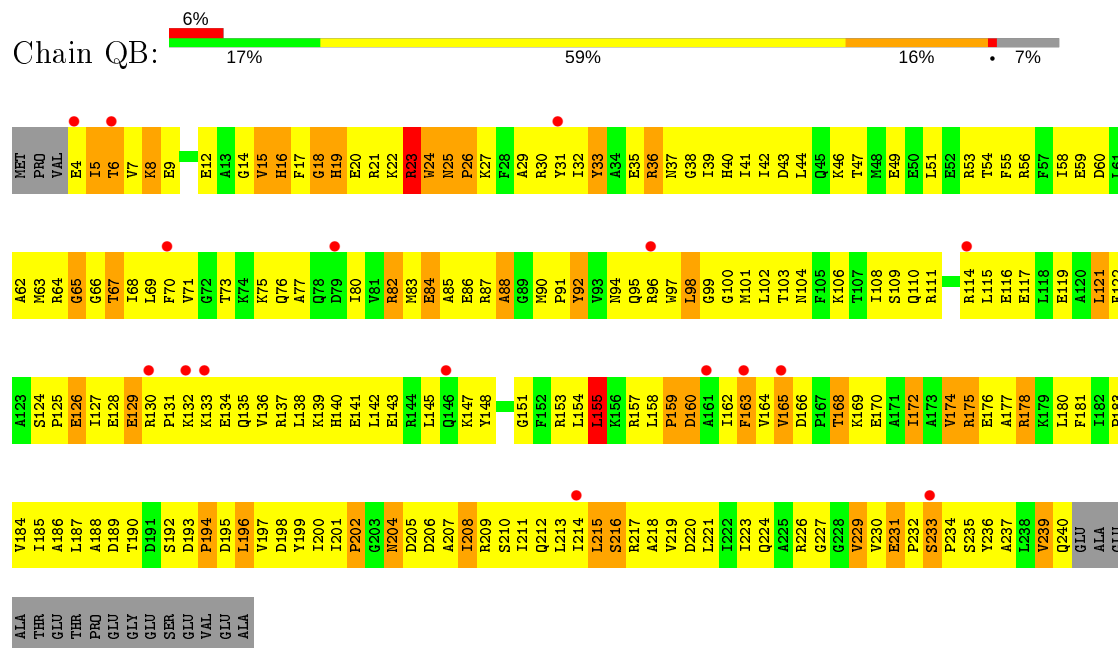


G1453	C1362A	G1294	G1215	G1142	G1064	C985	A909	U830	U743	G666	G566	C489	U405	C328
G1454	A1363	G1295	G1216	G1143	U1065	C986	C910	8821	C744	G667	G567	G493	G406	A329
G1455	C1296	C1297	G1217	G1144	C1066	9987	A913	C822	A746	G674	G568	G493	G407	A329
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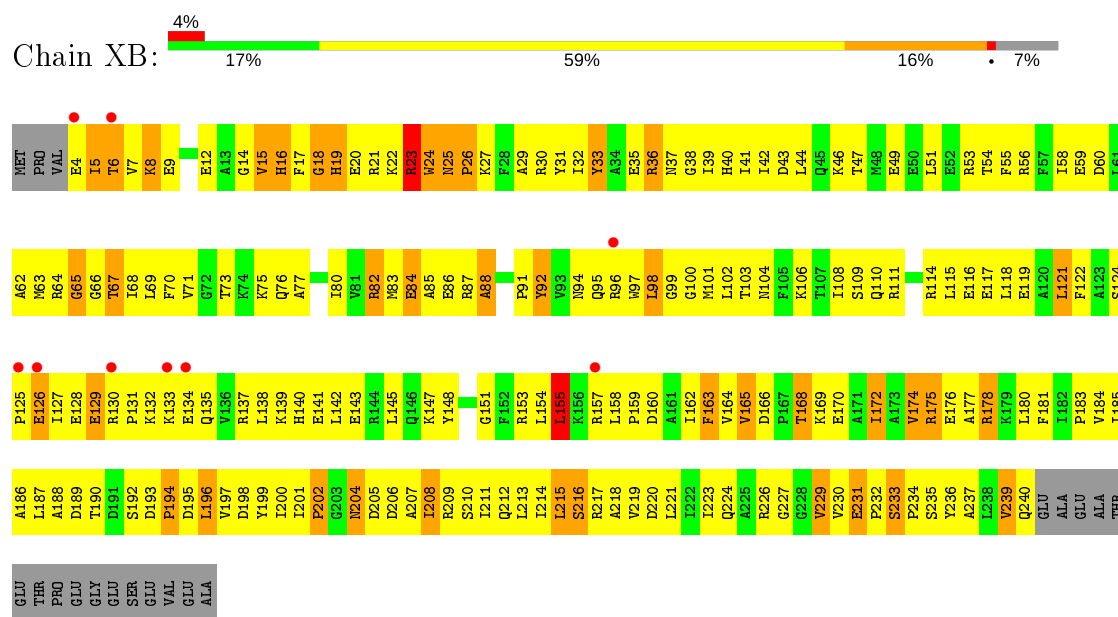


A  
C  
C  
U  
C  
C  
U  
U  
U  
C  
U

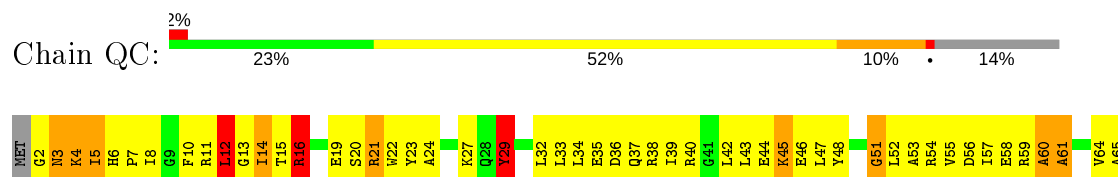
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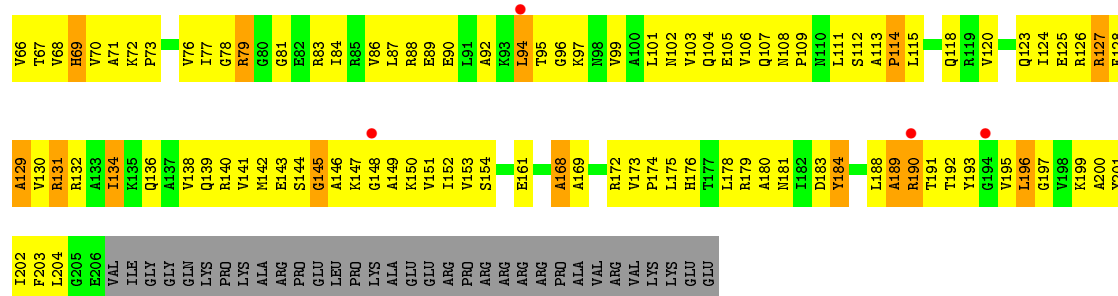
• Molecule 2: 30S ribosomal protein S2



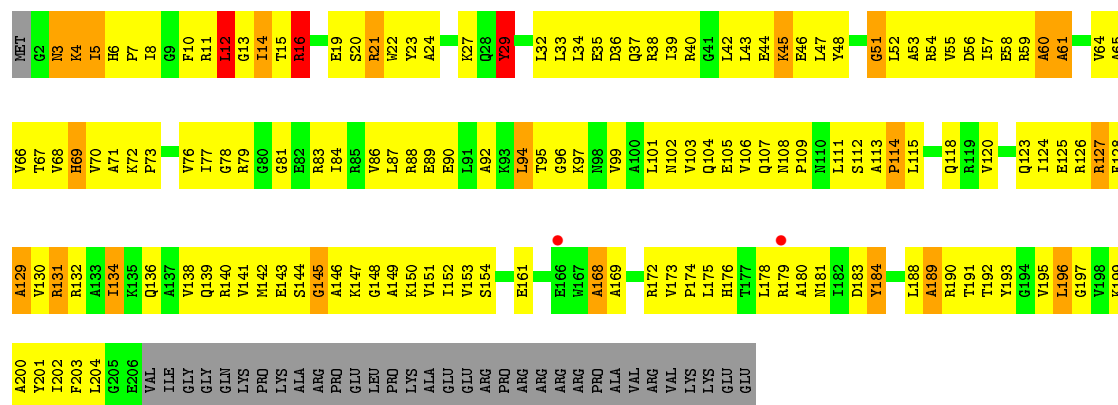
• Molecule 3: 30S ribosomal protein S3



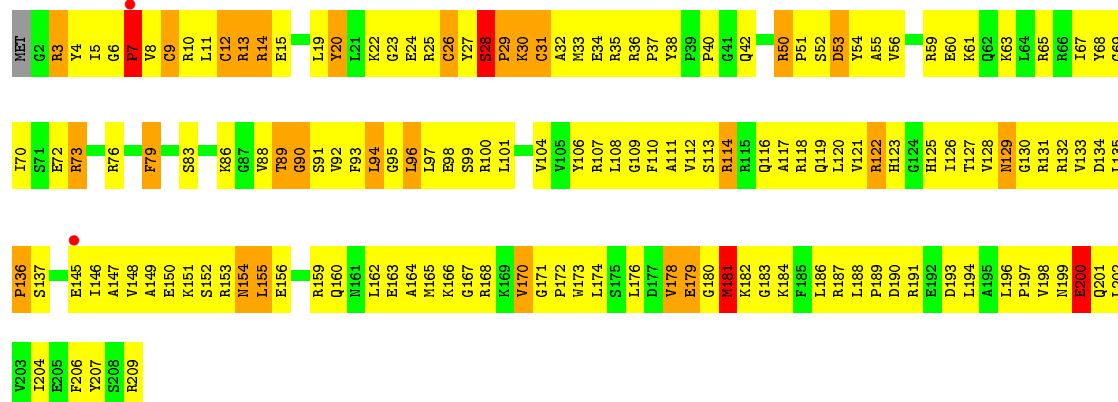




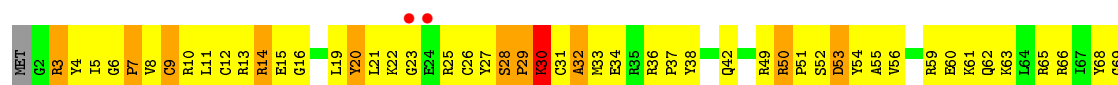
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



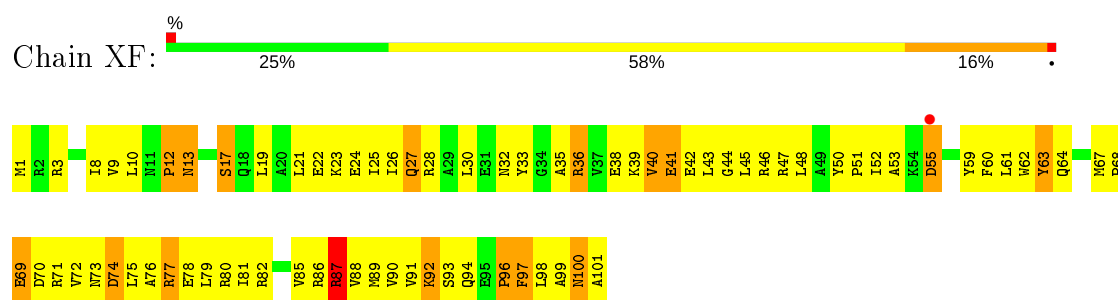
• Molecule 4: 30S ribosomal protein S4



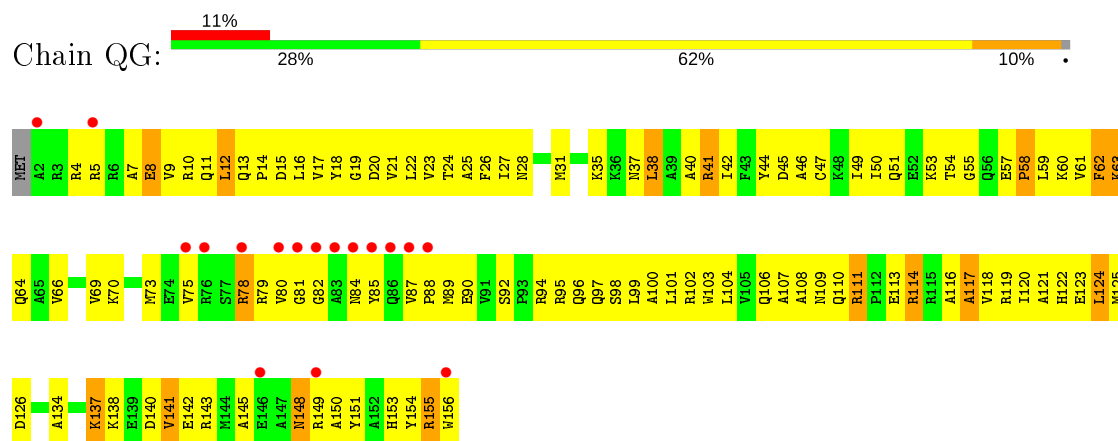




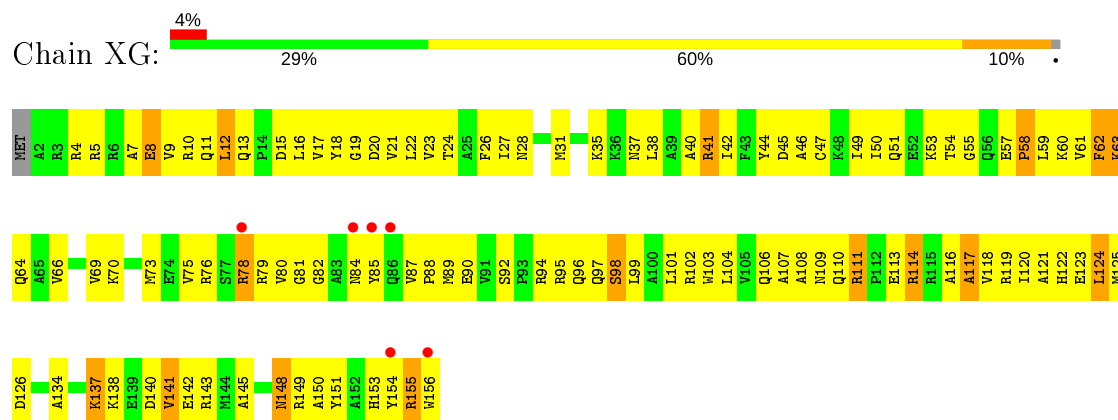




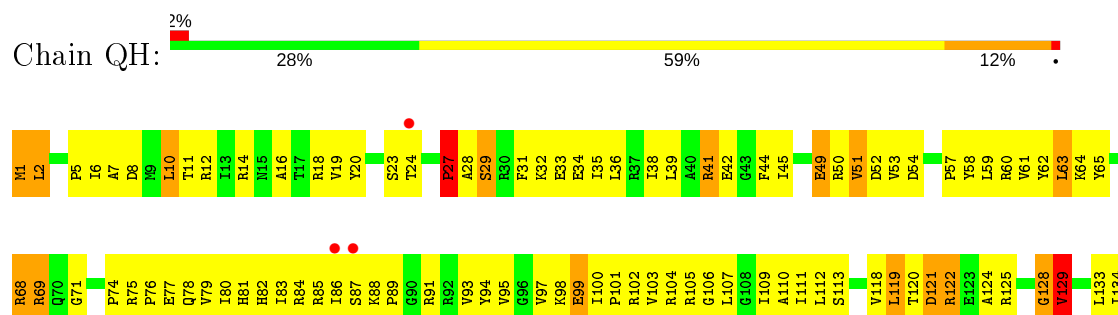
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

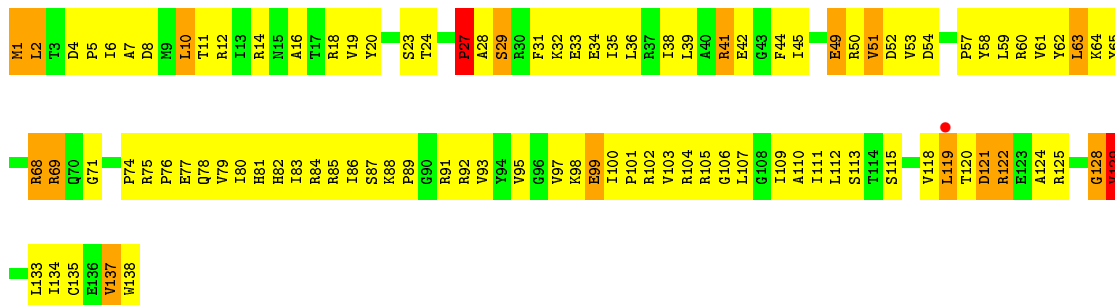




C135  
E136  
V137  
W138

• Molecule 8: 30S ribosomal protein S8

Chain XH: 



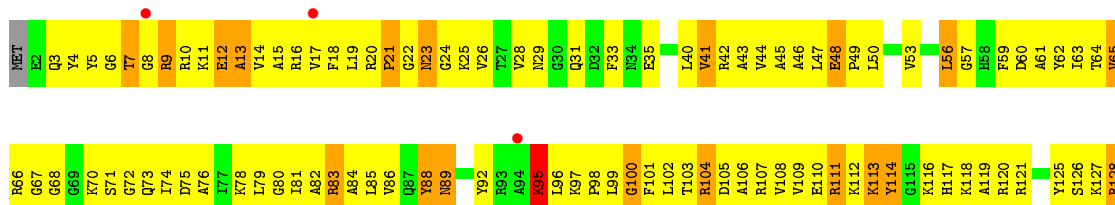
• Molecule 9: 30S ribosomal protein S9

Chain QI: 



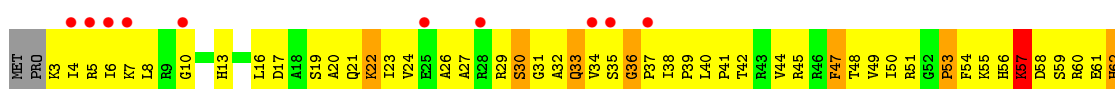
• Molecule 9: 30S ribosomal protein S9

Chain XI: 

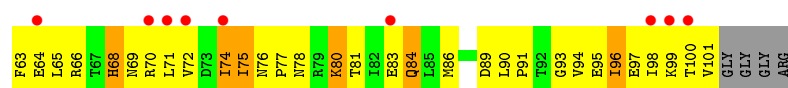


• Molecule 10: 30S ribosomal protein S10

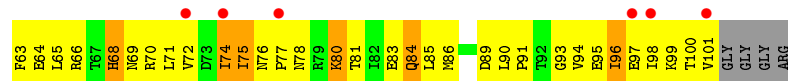
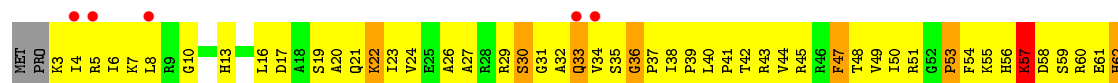
Chain QJ: 



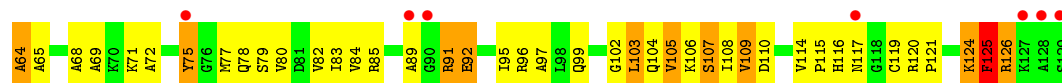
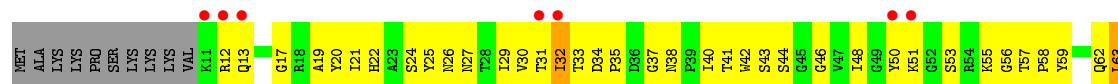




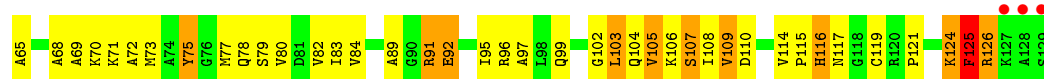
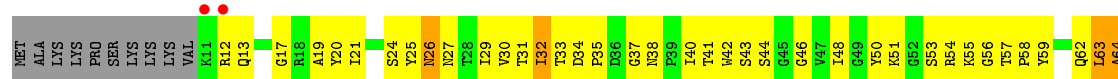
- Molecule 10: 30S ribosomal protein S10



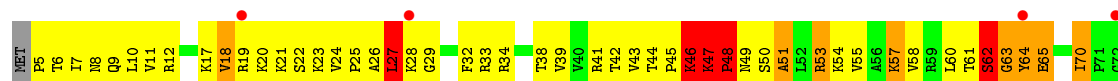
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

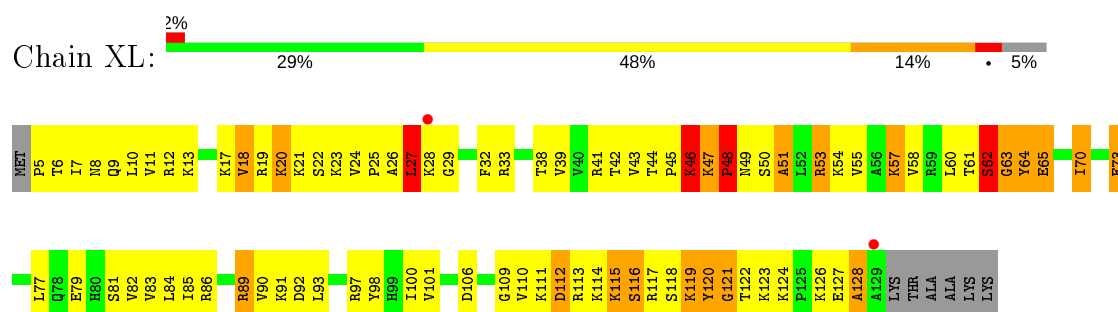


- Molecule 12: 30S ribosomal protein S12

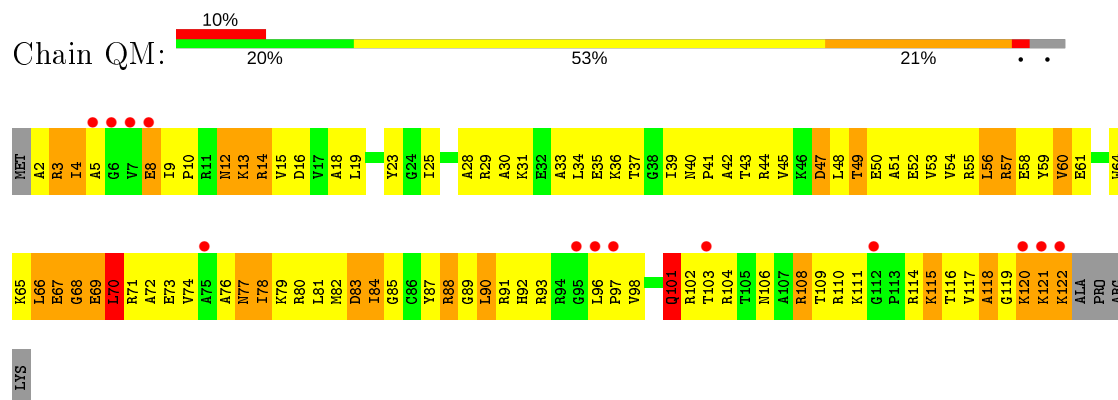


- Molecule 12: 30S ribosomal protein S12

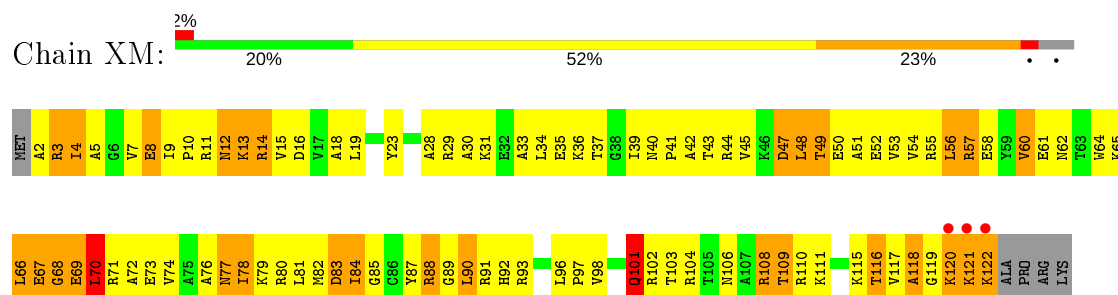




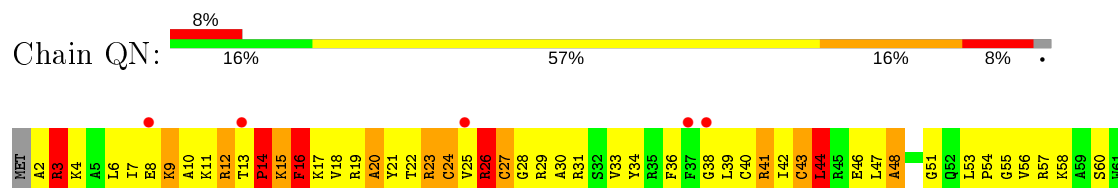
- Molecule 13: 30S ribosomal protein S13



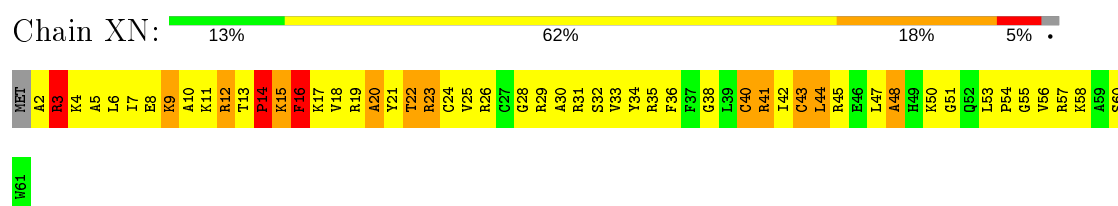
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

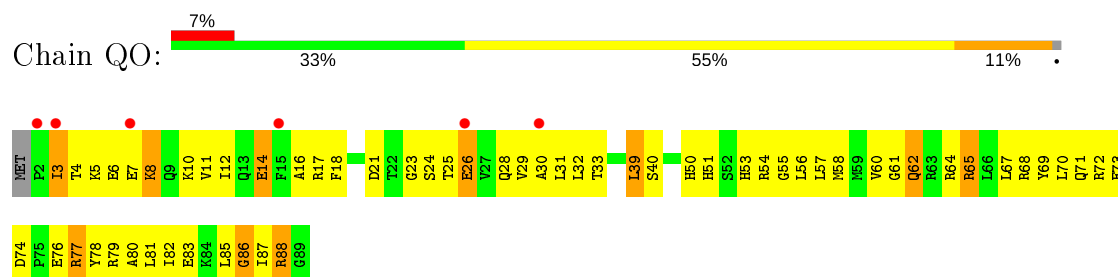


- Molecule 14: 30S ribosomal protein S14 type Z

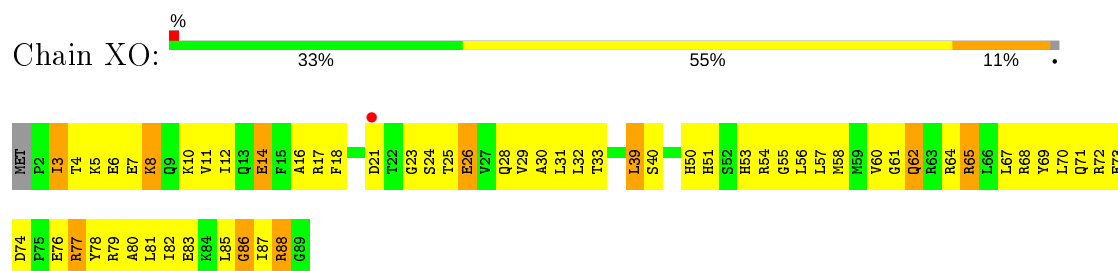




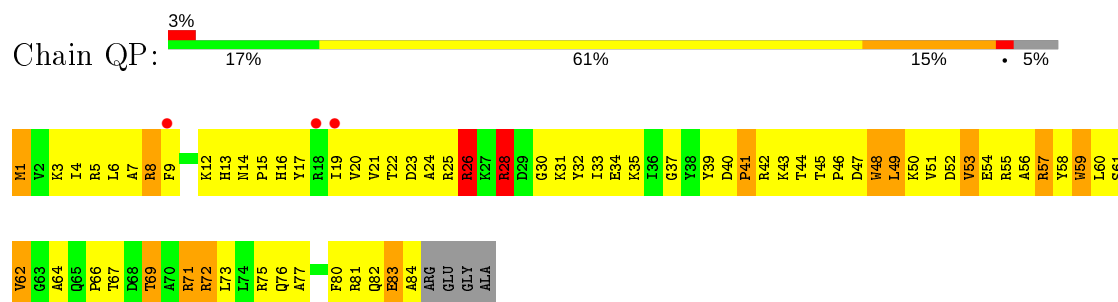
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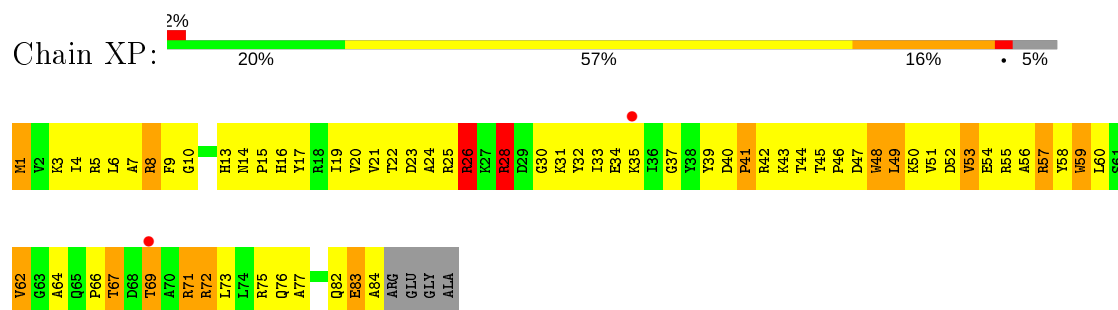
- Molecule 15: 30S ribosomal protein S15



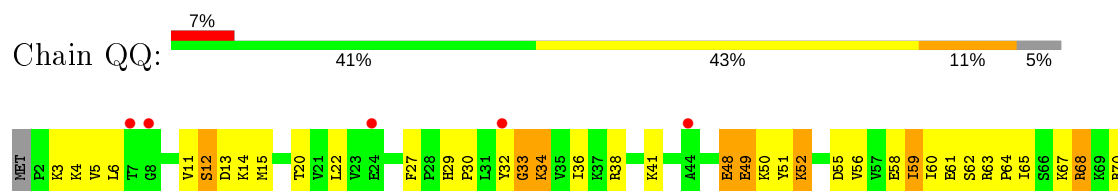
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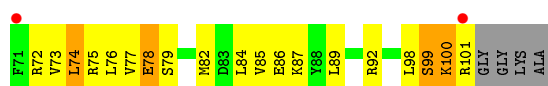
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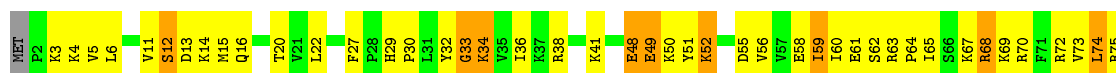
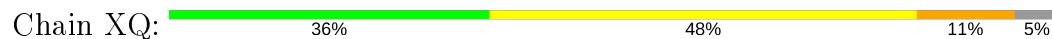
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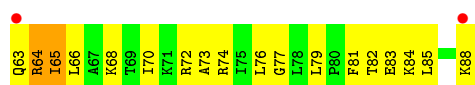
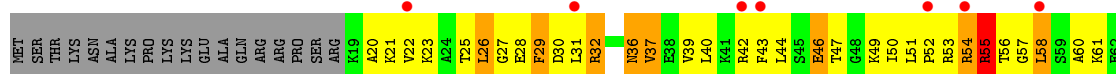
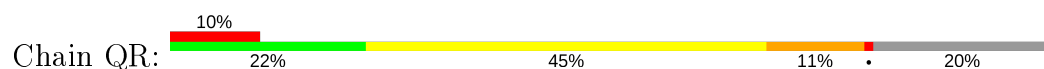




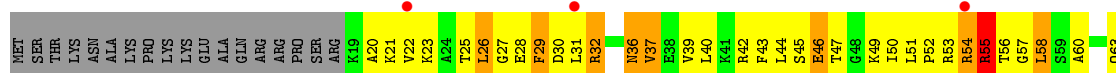
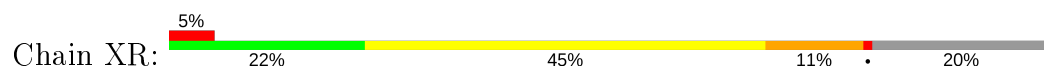
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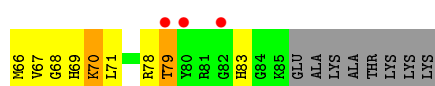
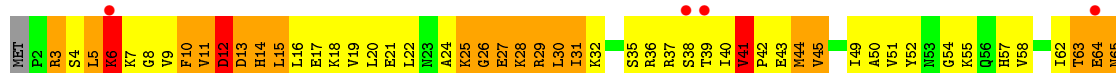
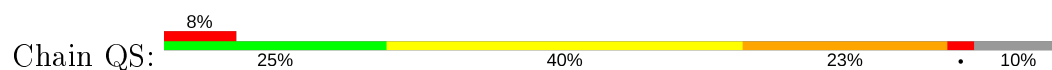
- Molecule 18: 30S ribosomal protein S18



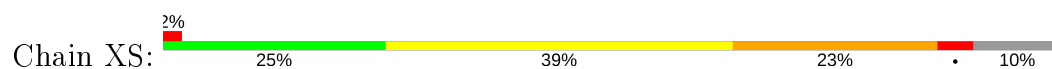
- Molecule 18: 30S ribosomal protein S18



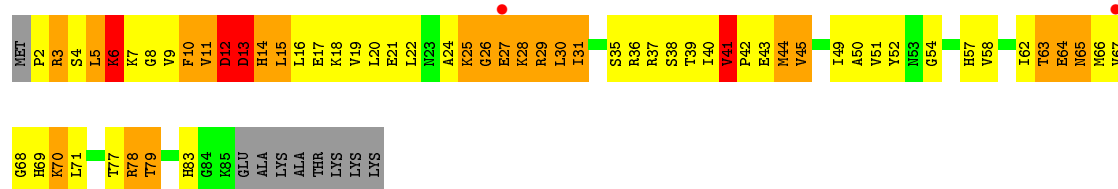
- Molecule 19: 30S ribosomal protein S19



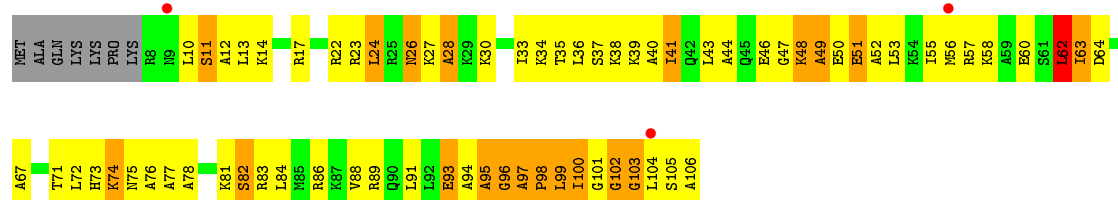
- Molecule 19: 30S ribosomal protein S19



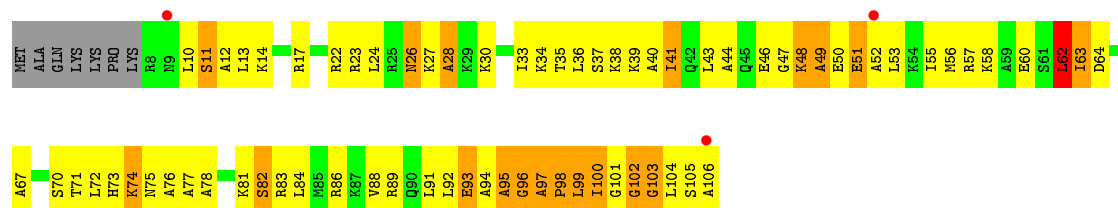




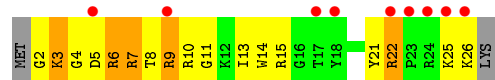
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



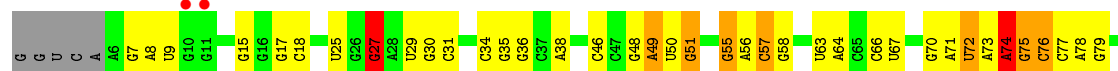
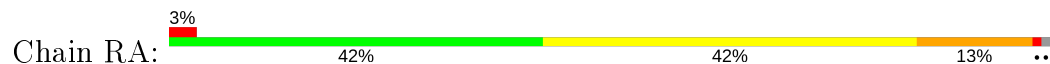
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: 23S Ribosomal RNA



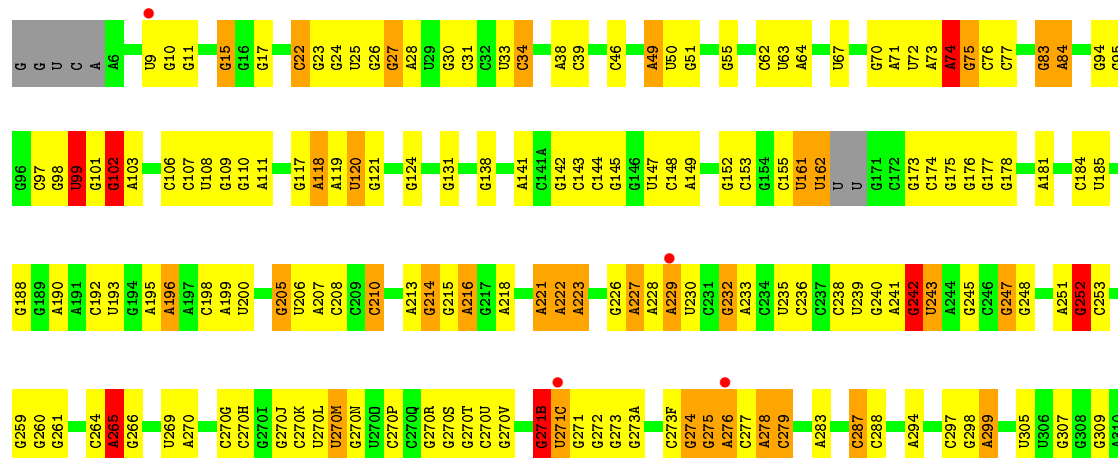


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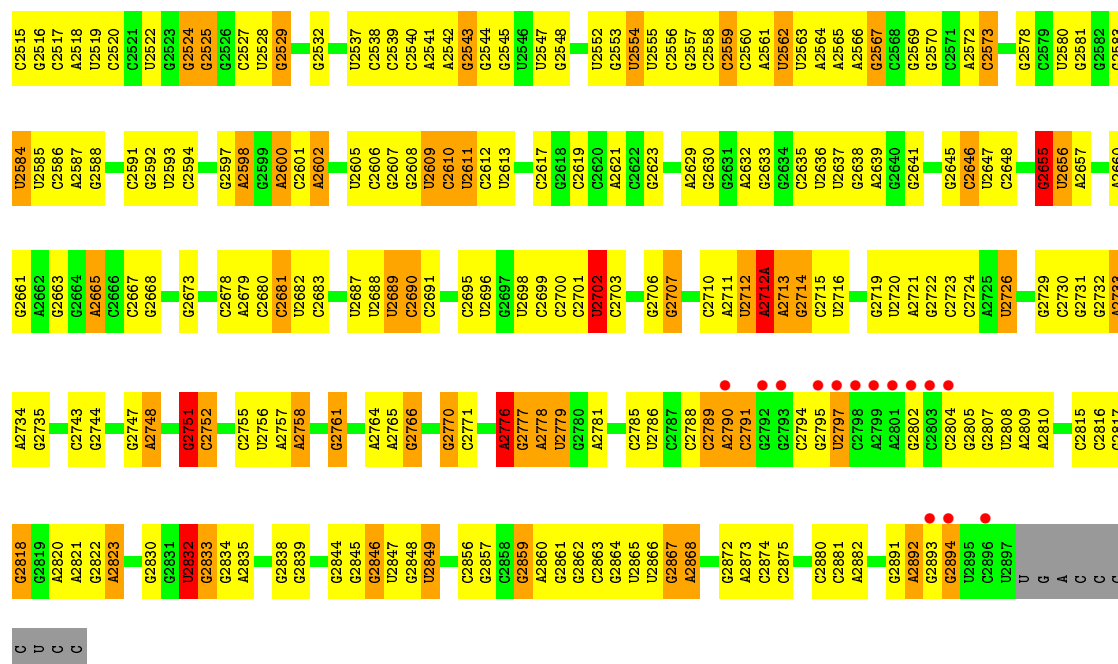


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G1328	U1187	C1109		A960	A887		G738	C658	A547	G467	C385
U1329	U1188			C962	C888	C817	G739	C659	A548	G468	G386
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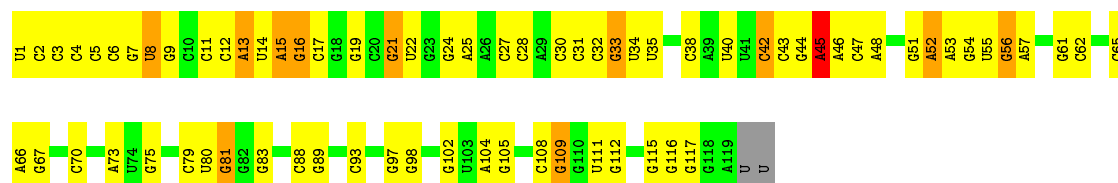
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G2446	G2372	G2299	A2211	G2052	A1966	C1894	U1805	U1730	C1637	C1545	A1545	A1472	C1404
G2447	G2373		G2212	G2053	G1967	C1895	A1812	U1731	U1637	U1473	U1473	A1473	U1405
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G2450	G2376	G2306	G2215	G2056	A1970	C1899	A1815		A1641	C1549	C1550		C1408
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C2504	A2426	G2348	G2280	U2115	U2028	G1949	G1869	C1788	G1696	A1529			U1455
C2505	G2429	G2349	G2281	G2116	A2030	U1950	C1870	C1789	A1698	G1530			G1456
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C2508	A2432	C2356	A2286	G2119	U2034	U1955	G1878	U1794	G1705	C1615			G1459
C2509	G2435	U2357	G2287	A2120	G2035	U1956	C1882	C1795	G1706	A1616			A1460
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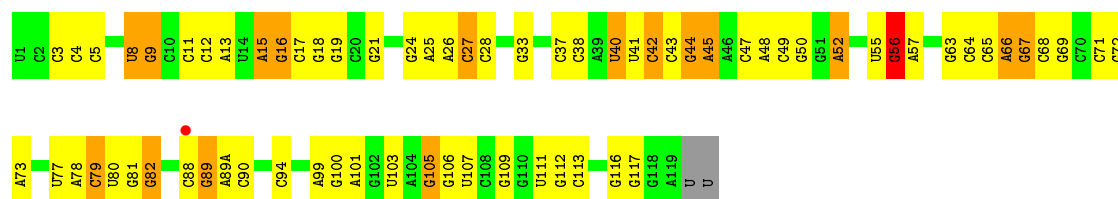
• Molecule 23: 5S Ribosomal RNA

Chain RB: 

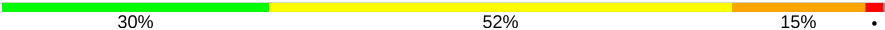


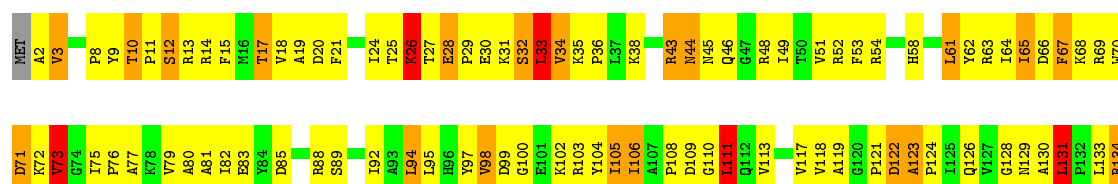
• Molecule 23: 5S Ribosomal RNA

Chain YB: 



• Molecule 24: 50S ribosomal protein L2

Chain RD: 

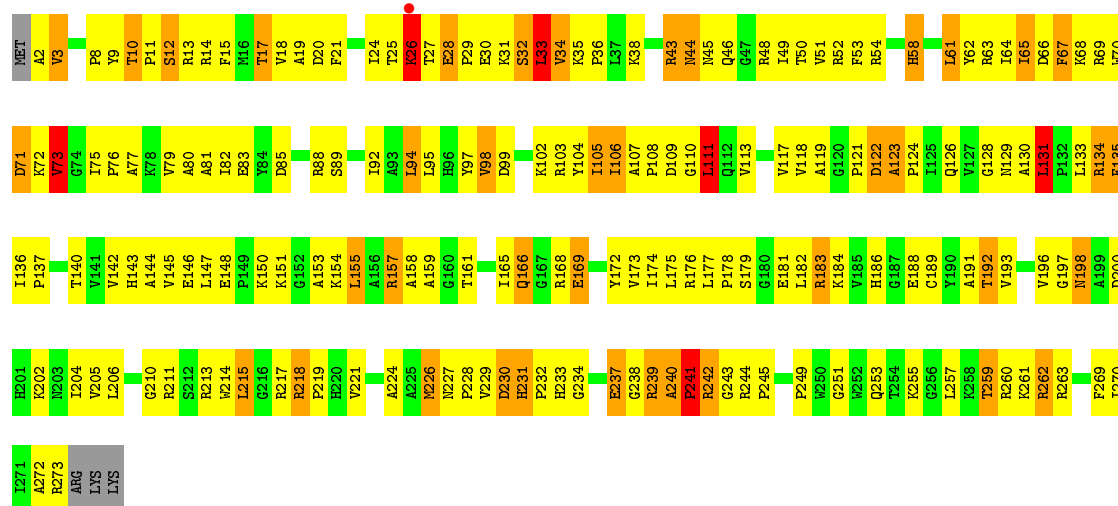






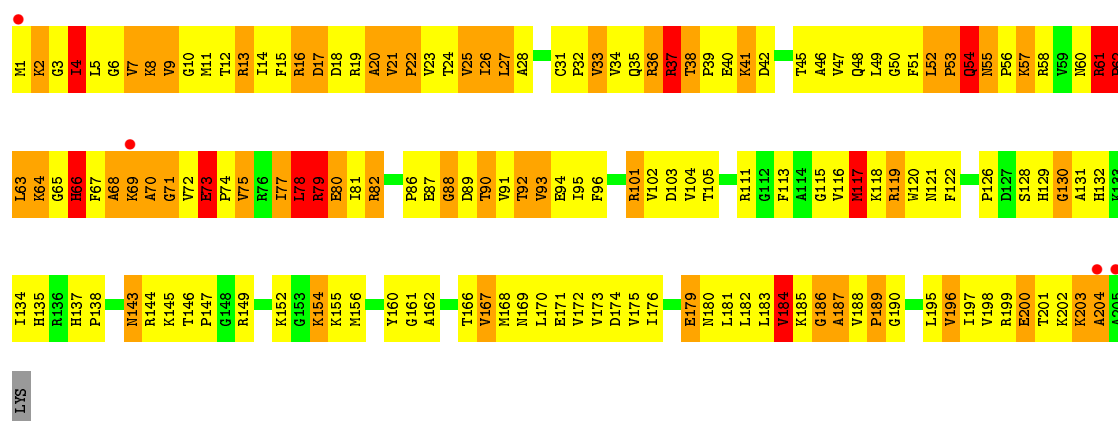
• Molecule 24: 50S ribosomal protein L2

Chain YD: 30% 51% 14% ..



• Molecule 25: 50S ribosomal protein L3

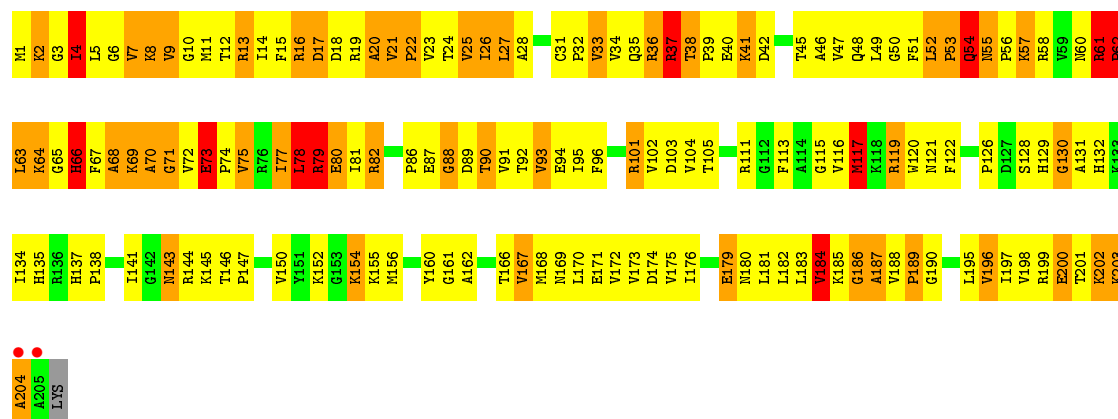
Chain RE: 2% 23% 48% 24% 5%



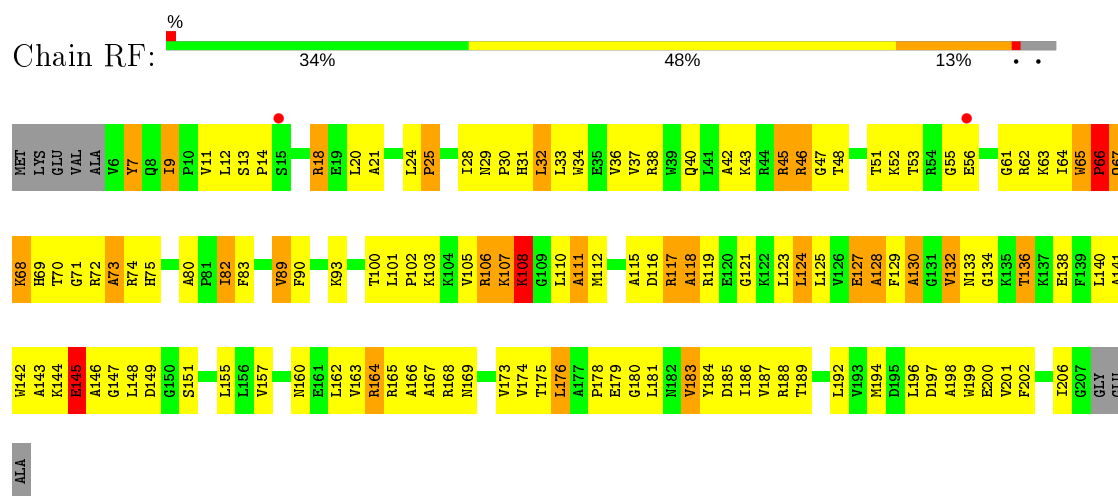
• Molecule 25: 50S ribosomal protein L3

Chain YE: 23% 48% 24% 5%

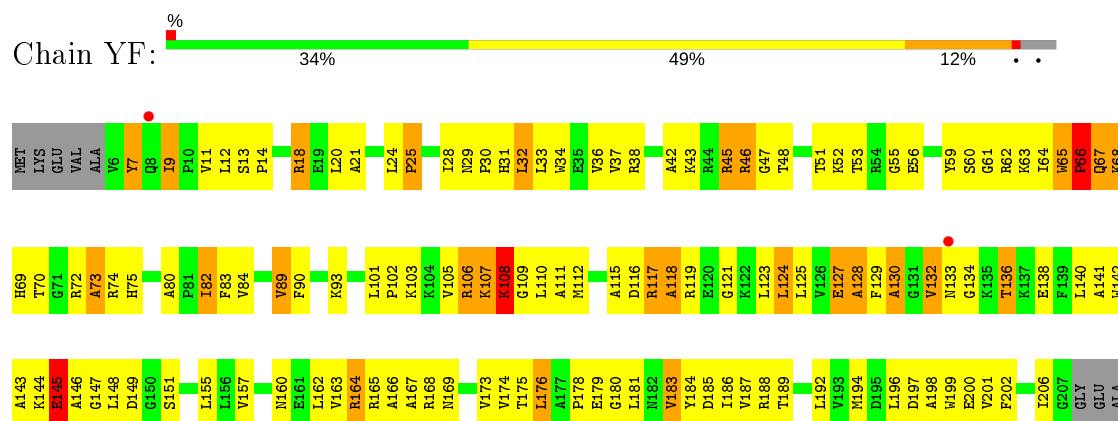




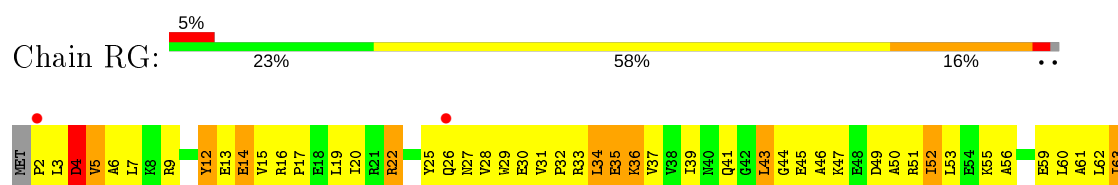
• Molecule 26: 50S ribosomal protein L4



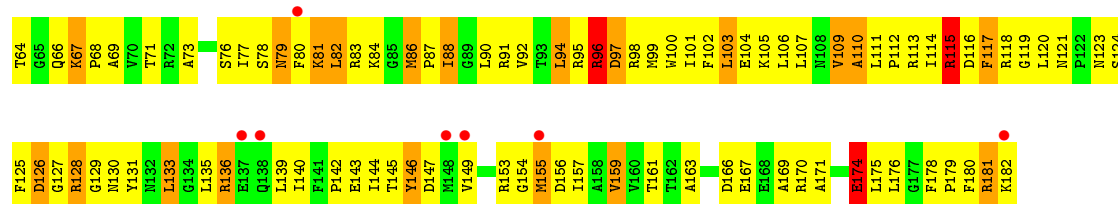
• Molecule 26: 50S ribosomal protein L4



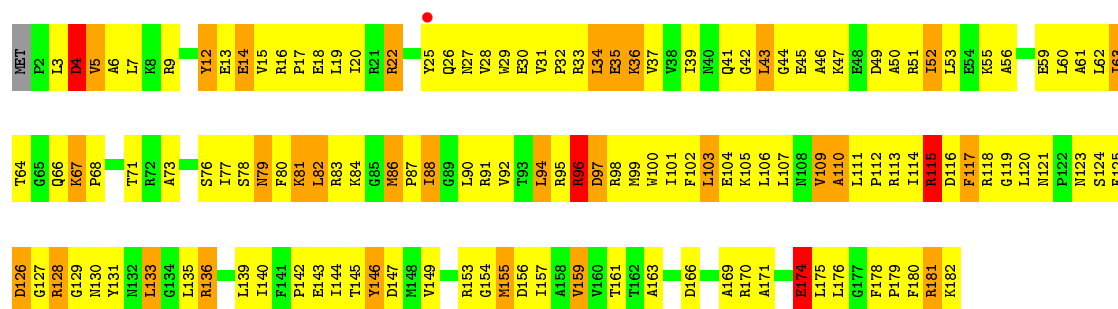
• Molecule 27: 50S ribosomal protein L5



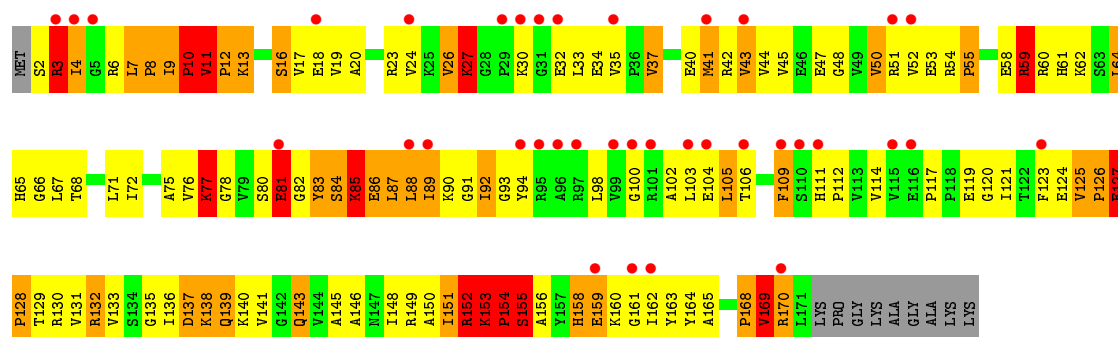
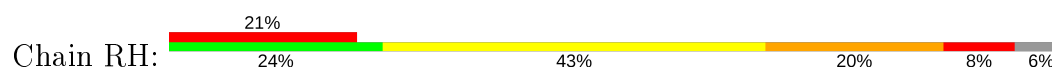




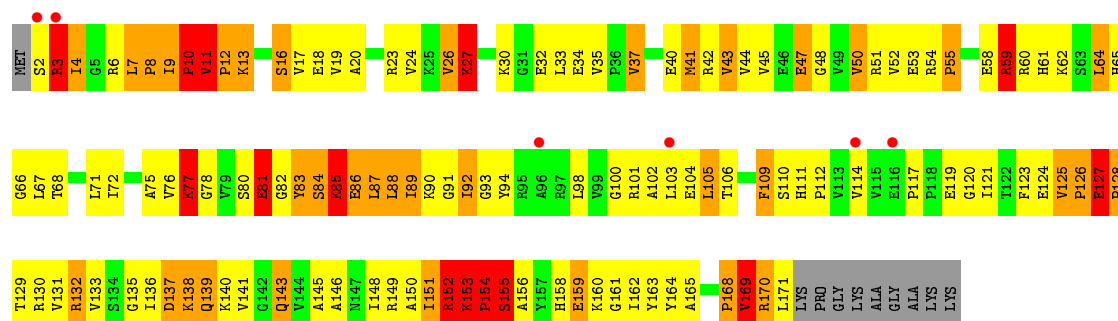
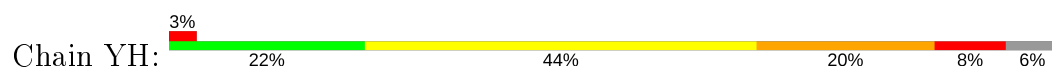
• Molecule 27: 50S ribosomal protein L5



• Molecule 28: 50S ribosomal protein L6

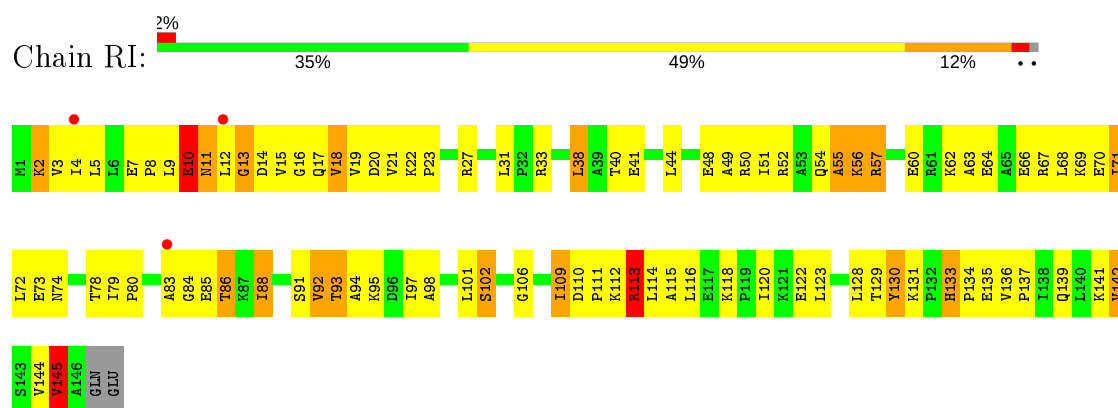


• Molecule 28: 50S ribosomal protein L6

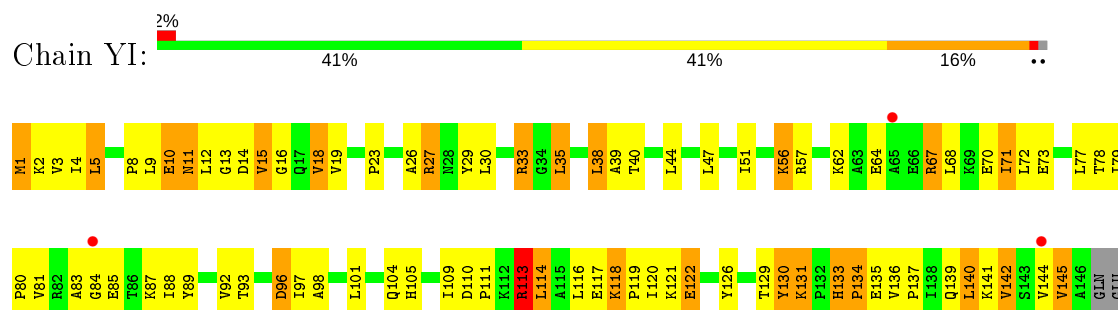


• Molecule 29: 50S ribosomal protein L9

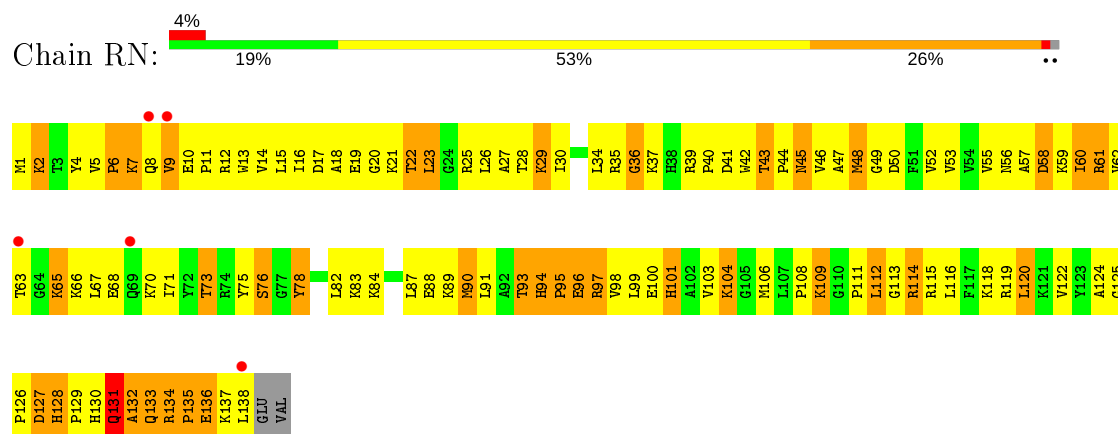




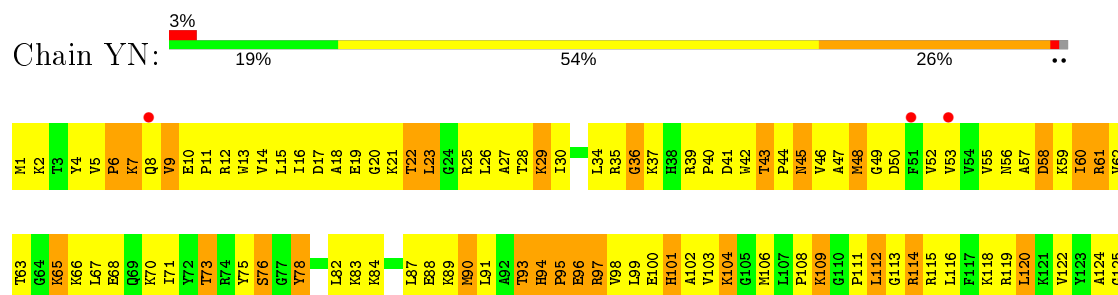
- Molecule 29: 50S ribosomal protein L9



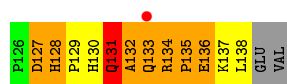
- Molecule 30: 50S ribosomal protein L13



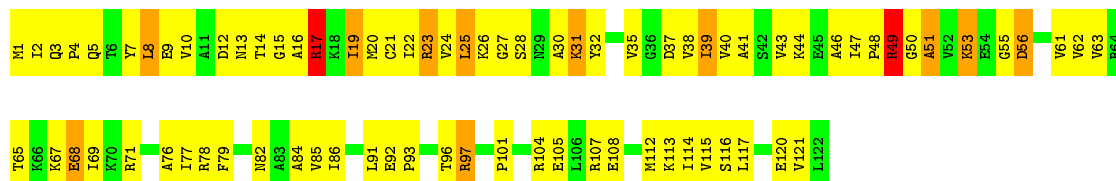
- Molecule 30: 50S ribosomal protein L13



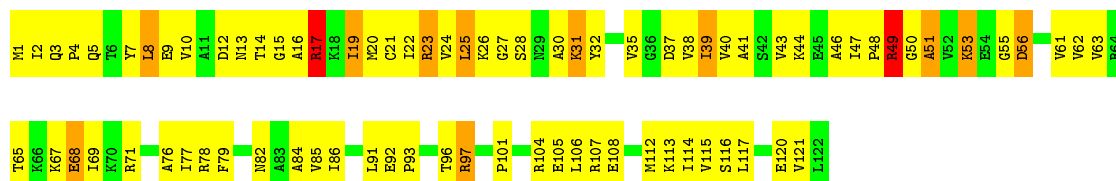




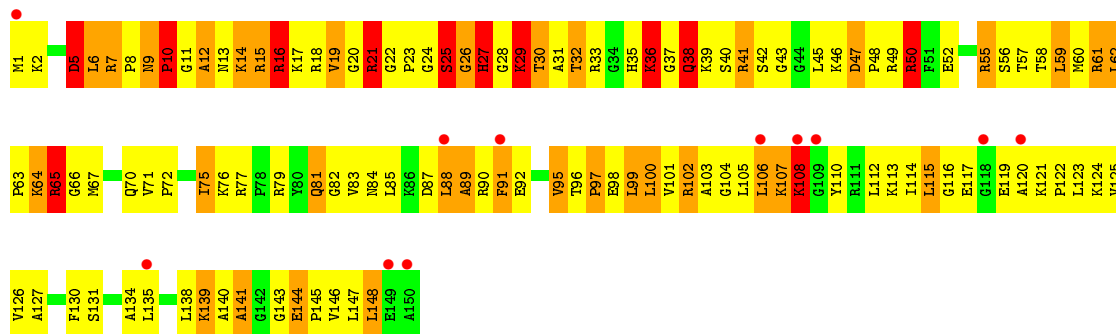
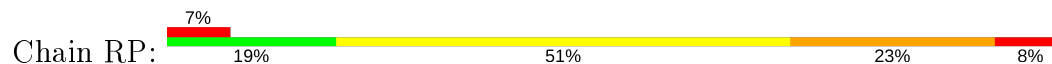
- Molecule 31: 50S ribosomal protein L14



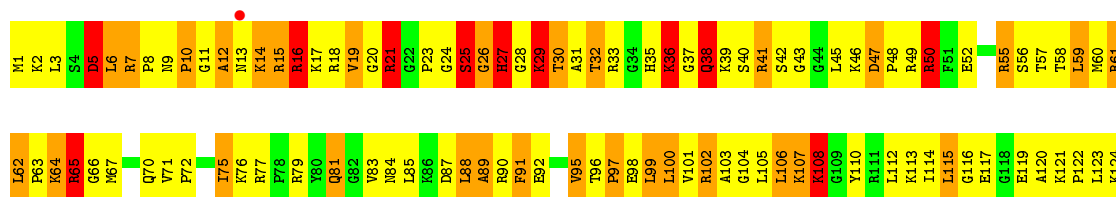
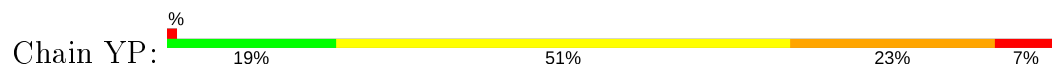
- Molecule 31: 50S ribosomal protein L14



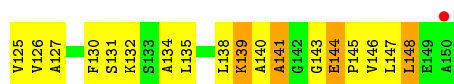
- Molecule 32: 50S ribosomal protein L15



- Molecule 32: 50S ribosomal protein L15



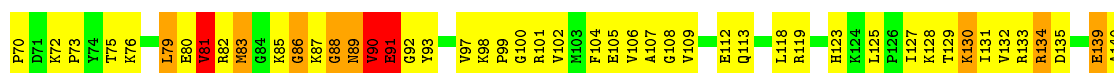




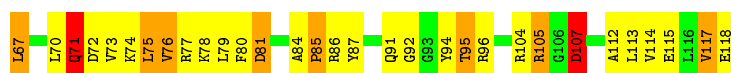
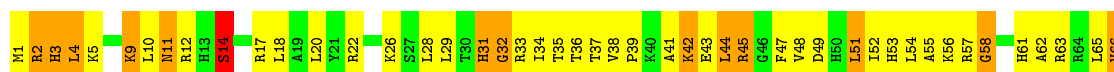
- Molecule 33: 50S ribosomal protein L16



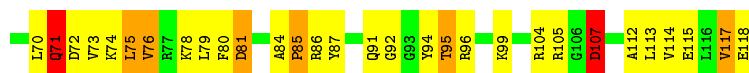
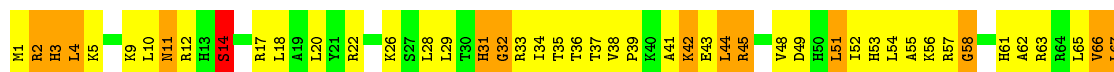
- Molecule 33: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L17

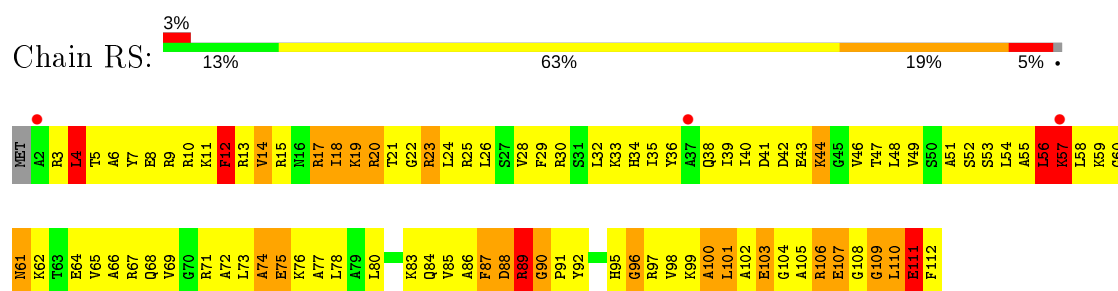


- Molecule 34: 50S ribosomal protein L17

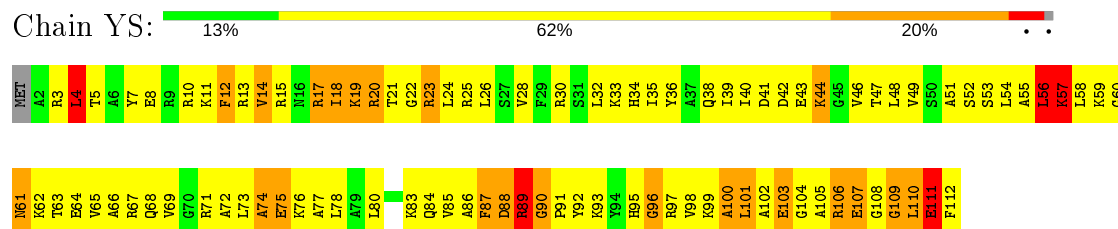


- Molecule 35: 50S ribosomal protein L18

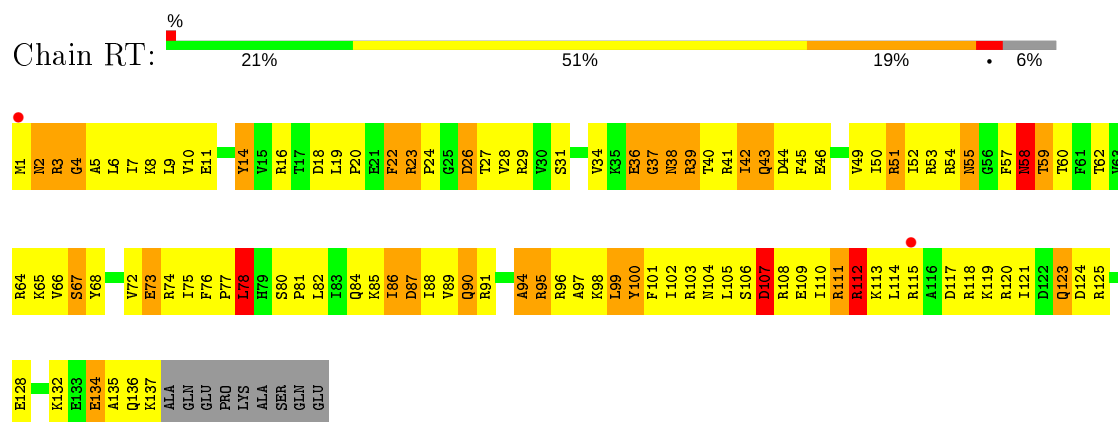




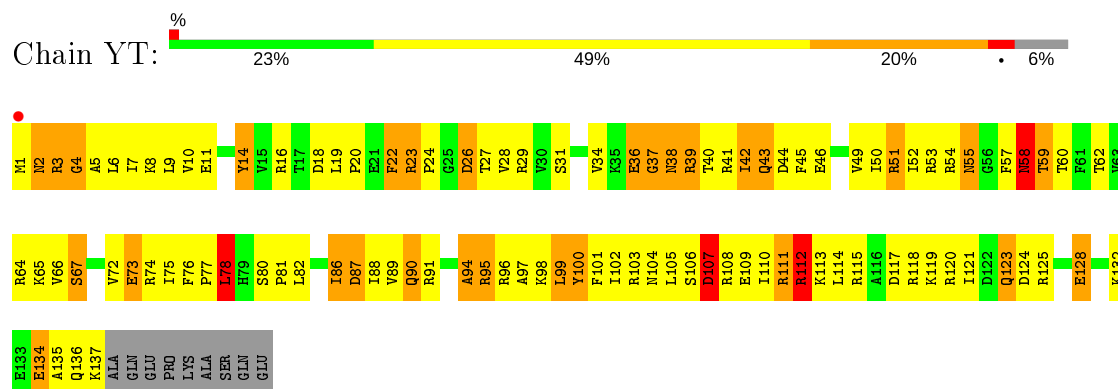
- Molecule 35: 50S ribosomal protein L18



- Molecule 36: 50S ribosomal protein L19



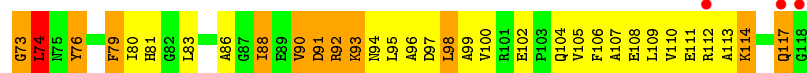
- Molecule 36: 50S ribosomal protein L19



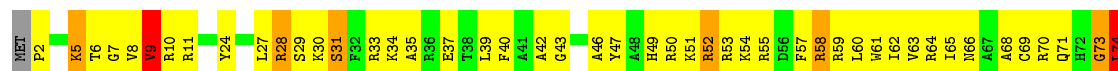
- Molecule 37: 50S ribosomal protein L20



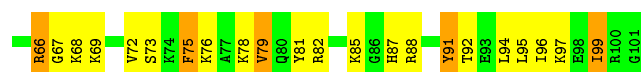
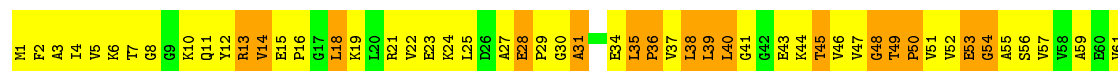




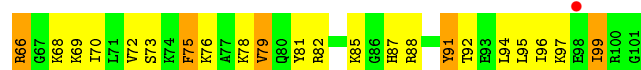
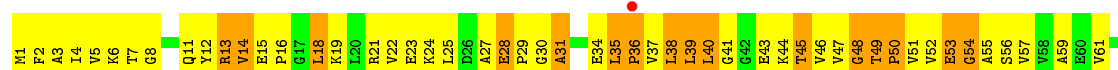
• Molecule 37: 50S ribosomal protein L20



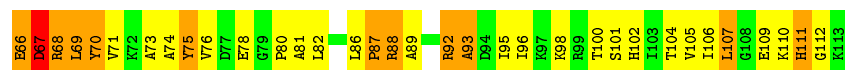
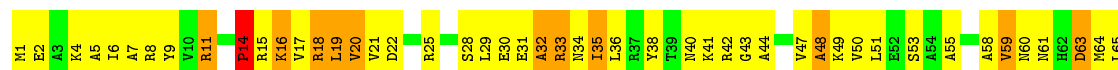
• Molecule 38: 50S ribosomal protein L21



• Molecule 38: 50S ribosomal protein L21

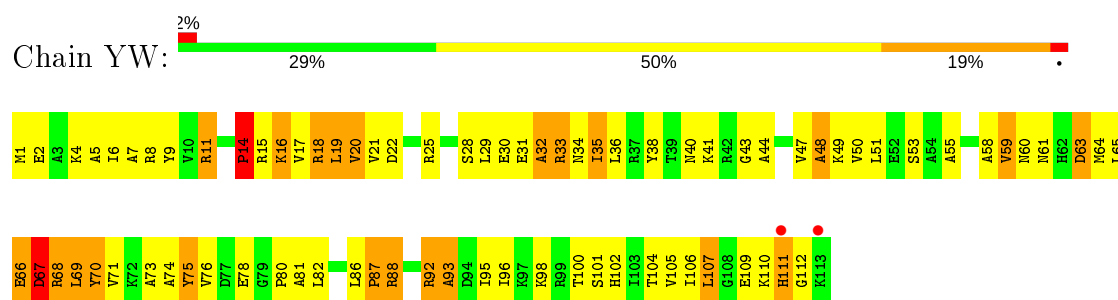


• Molecule 39: 50S ribosomal protein L22

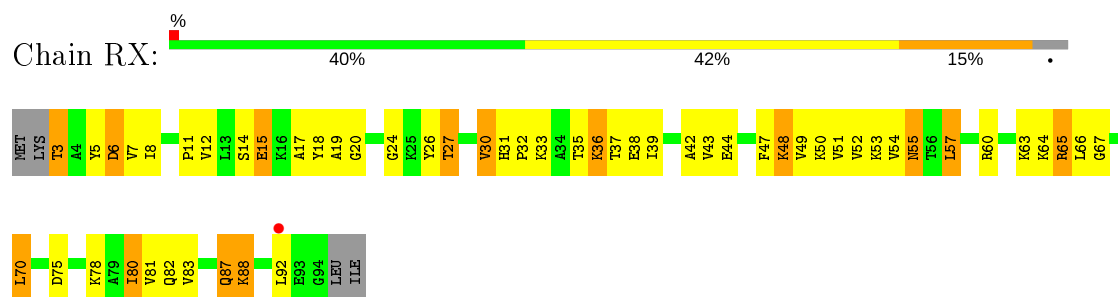


• Molecule 39: 50S ribosomal protein L22

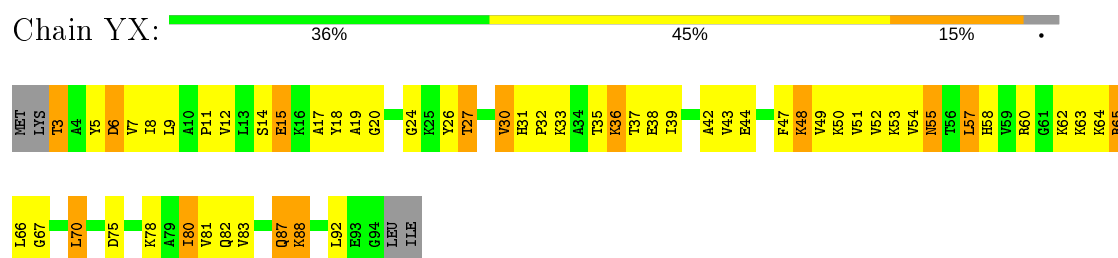




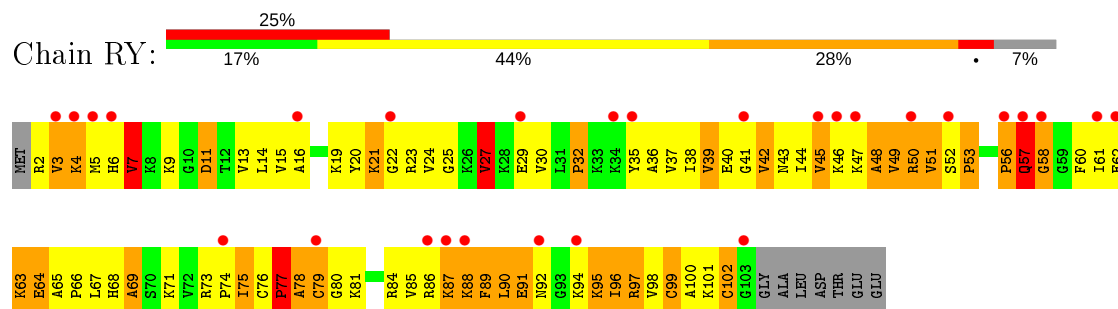
• Molecule 40: 50S ribosomal protein L23



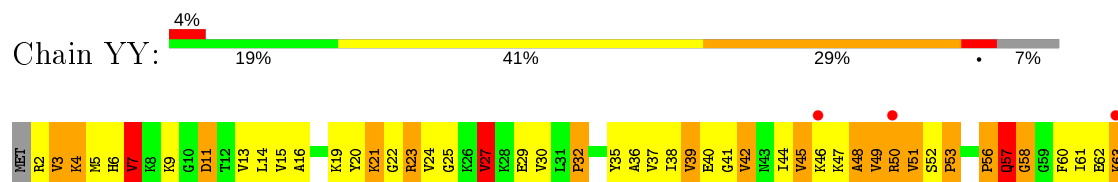
• Molecule 40: 50S ribosomal protein L23



• Molecule 41: 50S ribosomal protein L24



• Molecule 41: 50S ribosomal protein L24

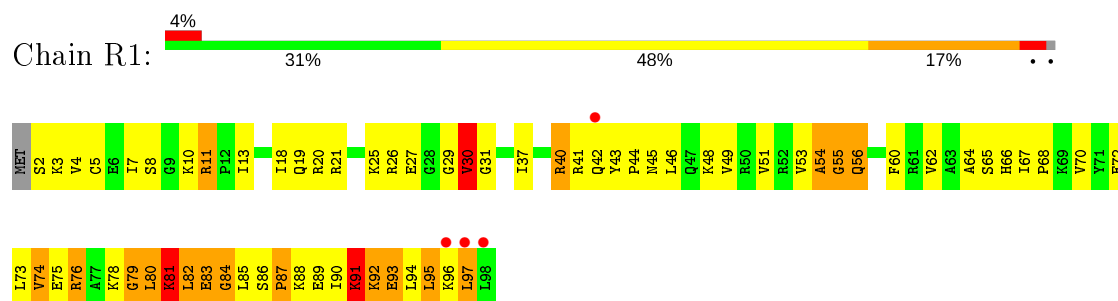




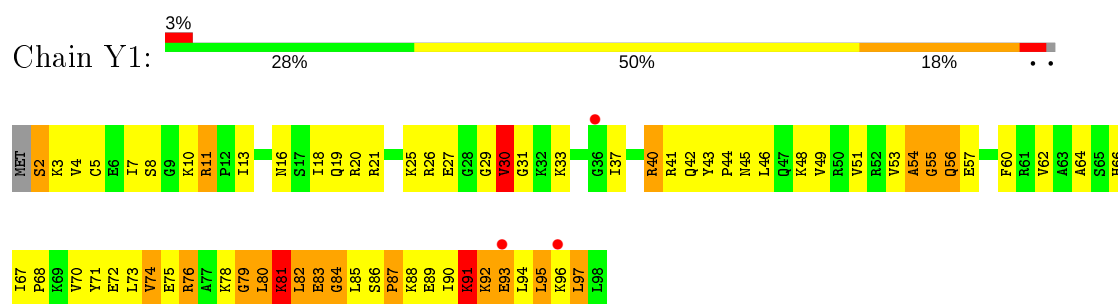




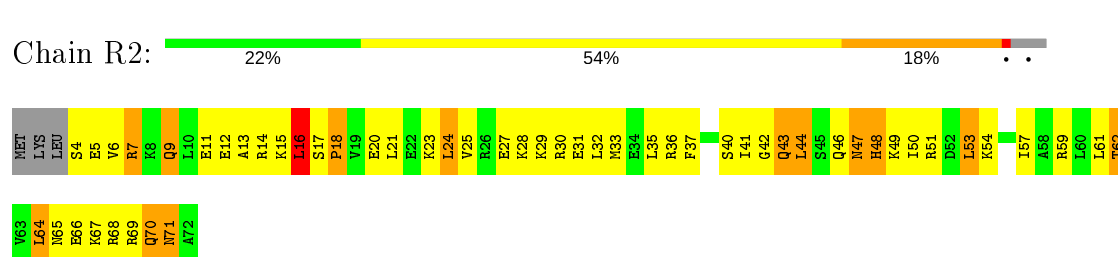
- Molecule 44: 50S ribosomal protein L28



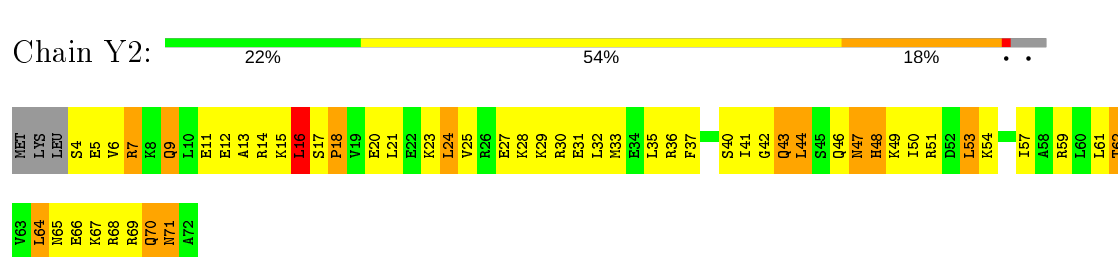
- Molecule 44: 50S ribosomal protein L28



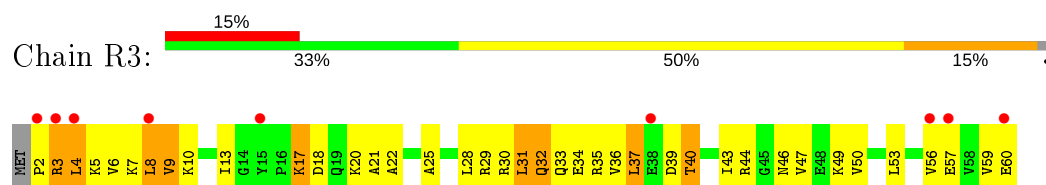
- Molecule 45: 50S ribosomal protein L29



- Molecule 45: 50S ribosomal protein L29

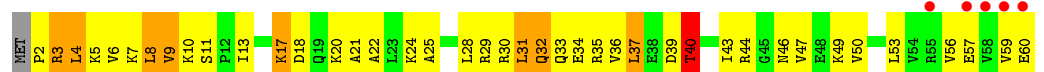


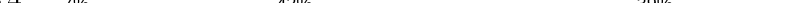
- Molecule 46: 50S ribosomal protein L30

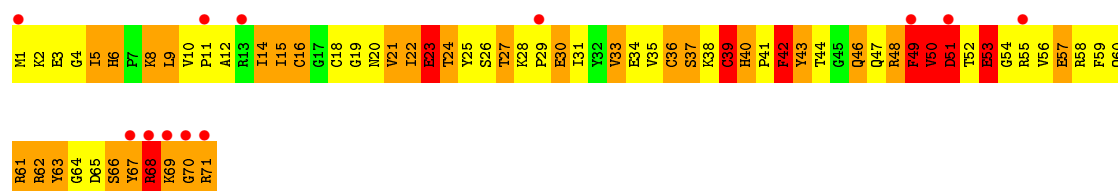


- Molecule 46: 50S ribosomal protein L30

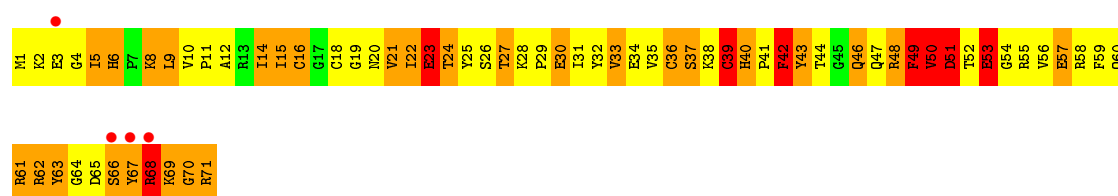




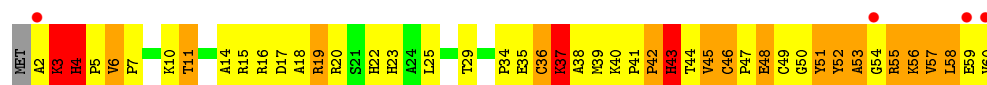
- Chain R4: 



- Chain Y4: 



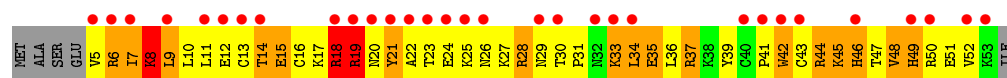
- Chain B5: 



- Chain Y5: 

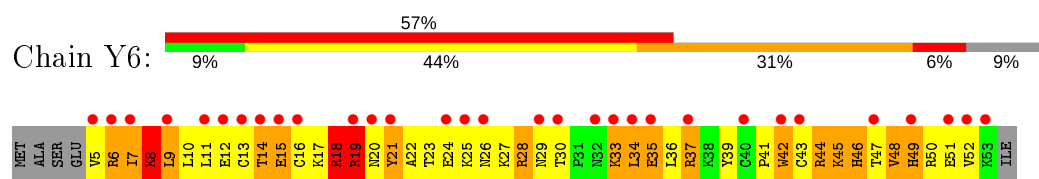


- Chain R6: 

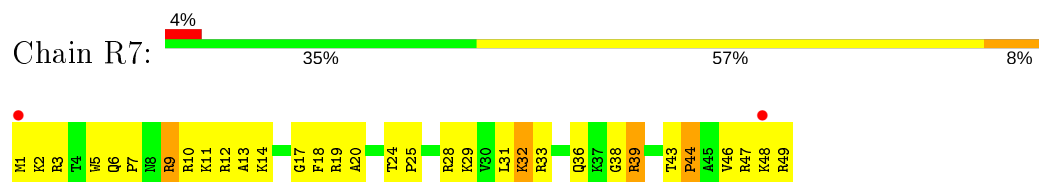


- 

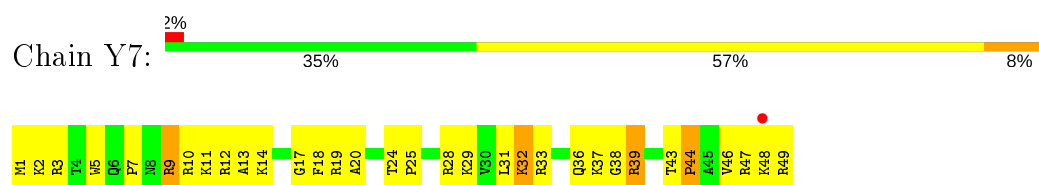




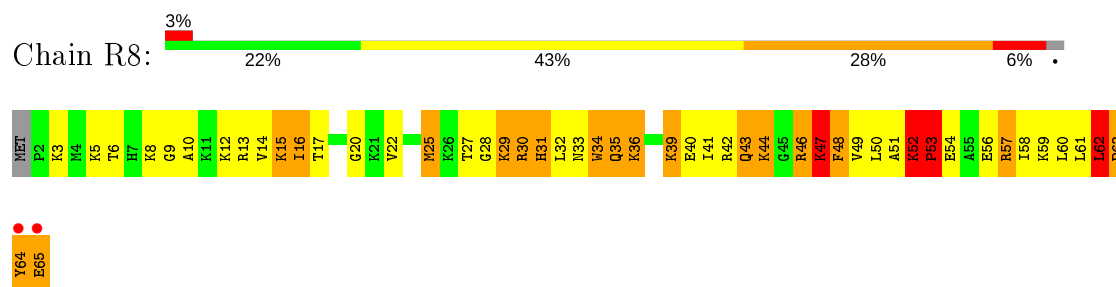
- Molecule 50: 50S ribosomal protein L34



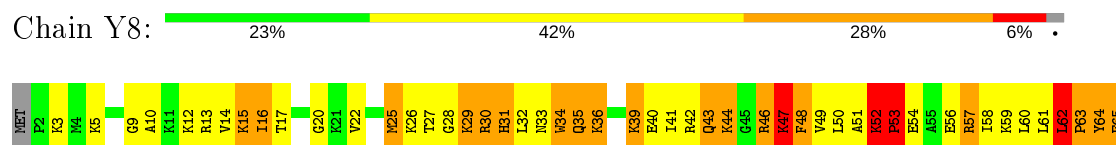
- Molecule 50: 50S ribosomal protein L34



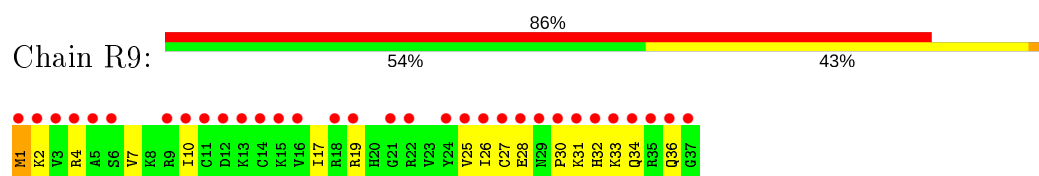
- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35



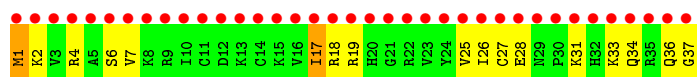
- Molecule 52: 50S ribosomal protein L36



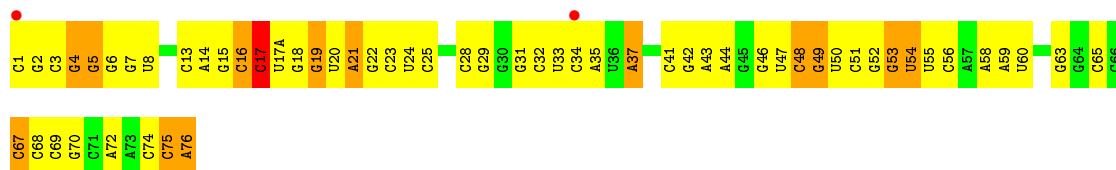
- Molecule 52: 50S ribosomal protein L36



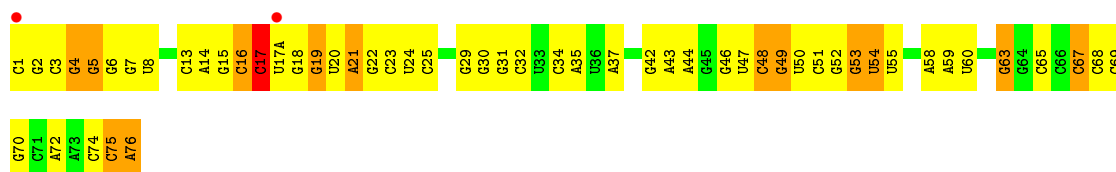




• Molecule 53: P-site tRNA fMet



• Molecule 53: P-site tRNA fMet



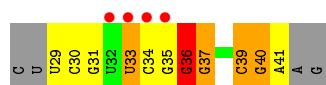
• Molecule 54: A-site ASL SufA6



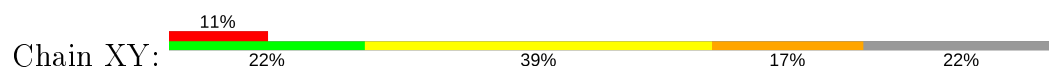
• Molecule 54: A-site ASL SufA6



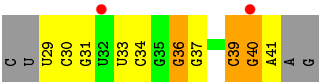
• Molecule 55: messenger RNA



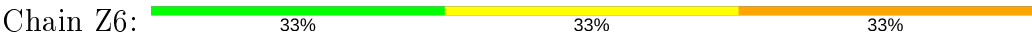
• Molecule 55: messenger RNA



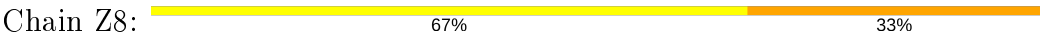




- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.24Å 446.10Å 623.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.90 49.68 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.68-3.90) 99.1 (49.68-3.70)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.235 , 0.278 0.235 , 0.278	Depositor DCC
$R_{free}$ test set	27641 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	291950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 1MG, PPU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	QA	0.43	0/36098	0.95	64/56341 (0.1%)
1	XA	0.48	0/36101	1.01	70/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.37	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.48	1/991 (0.1%)	0.79	2/1327 (0.2%)
12	XL	0.48	1/991 (0.1%)	0.79	2/1327 (0.2%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.34	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.66	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.69	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	RA	0.53	2/69521 (0.0%)	1.06	133/108529 (0.1%)
22	YA	0.59	2/69543 (0.0%)	1.12	219/108563 (0.2%)
23	RB	0.41	0/2878	0.95	4/4490 (0.1%)
23	YB	0.49	0/2878	1.04	4/4490 (0.1%)
24	RD	0.59	2/2165 (0.1%)	0.90	4/2919 (0.1%)
24	YD	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
25	RE	0.52	0/1601	0.91	2/2160 (0.1%)
25	YE	0.52	0/1601	0.91	2/2160 (0.1%)
26	RF	0.50	0/1620	0.76	0/2194
26	YF	0.50	0/1620	0.76	0/2194
27	RG	0.40	0/1499	0.66	0/2016
27	YG	0.40	0/1499	0.66	0/2016
28	RH	0.45	0/1332	0.85	3/1802 (0.2%)
28	YH	0.45	0/1332	0.85	4/1802 (0.2%)
29	RI	0.54	2/1151 (0.2%)	0.68	1/1558 (0.1%)
29	YI	0.34	0/1151	0.61	0/1558
30	RN	0.46	0/1131	0.78	1/1525 (0.1%)
30	YN	0.46	0/1131	0.78	1/1525 (0.1%)
31	RO	0.54	0/943	0.71	0/1269
31	YO	0.53	0/943	0.71	0/1269
32	RP	0.50	0/1162	0.94	3/1544 (0.2%)
32	YP	0.50	0/1162	0.95	3/1544 (0.2%)
33	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
33	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
34	RR	0.45	0/982	0.80	1/1312 (0.1%)
34	YR	0.45	0/982	0.80	1/1312 (0.1%)
35	RS	0.46	0/892	0.82	1/1187 (0.1%)
35	YS	0.45	0/892	0.83	1/1187 (0.1%)
36	RT	0.47	0/1155	0.73	2/1542 (0.1%)
36	YT	0.46	0/1155	0.73	2/1542 (0.1%)
37	RU	0.48	0/982	0.78	0/1306
37	YU	0.48	0/982	0.78	0/1306
38	RV	0.47	0/790	0.82	0/1057



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YV	0.47	0/790	0.82	0/1057
39	RW	0.45	0/911	0.75	0/1220
39	YW	0.45	0/911	0.75	0/1220
40	RX	0.56	0/739	0.77	0/993
40	YX	0.56	0/739	0.77	0/993
41	RY	0.52	0/798	0.80	0/1064
41	YY	0.52	0/798	0.80	0/1064
42	RZ	0.36	0/1493	0.58	0/2026
42	YZ	0.36	0/1493	0.62	0/2026
43	R0	0.42	0/657	0.63	0/874
43	Y0	0.42	0/657	0.65	0/874
44	R1	0.49	0/770	0.85	1/1022 (0.1%)
44	Y1	0.49	0/770	0.85	1/1022 (0.1%)
45	R2	0.50	0/583	0.84	1/771 (0.1%)
45	Y2	0.51	0/583	0.84	1/771 (0.1%)
46	R3	0.47	0/474	0.72	0/635
46	Y3	0.43	0/474	0.71	0/635
47	R4	0.38	0/594	0.78	1/795 (0.1%)
47	Y4	0.38	0/594	0.78	1/795 (0.1%)
48	R5	0.51	0/473	0.74	0/639
48	Y5	0.50	0/465	0.74	0/629
49	R6	0.42	0/431	0.76	0/575
49	Y6	0.43	0/431	0.76	0/575
50	R7	0.56	0/438	0.76	0/575
50	Y7	0.56	0/438	0.76	0/575
51	R8	0.62	0/525	0.93	1/691 (0.1%)
51	Y8	0.62	0/525	0.93	1/691 (0.1%)
52	R9	0.35	0/310	0.60	0/407
52	Y9	0.37	0/310	0.61	0/407
53	QV	0.51	0/1836	0.99	6/2859 (0.2%)
53	XV	0.51	0/1836	0.99	6/2859 (0.2%)
54	QX	0.74	0/188	0.84	0/290
54	XX	0.48	0/188	0.74	0/290
55	QY	0.78	1/311 (0.3%)	0.88	0/483
55	XY	0.51	0/311	0.88	0/483
56	Z6	0.79	0/40	1.79	1/60 (1.7%)
56	Z8	0.79	0/40	1.83	1/60 (1.7%)
All	All	0.50	12/316321 (0.0%)	0.98	568/472911 (0.1%)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	RD	236	GLY	C-N	8.53	1.53	1.34
29	RI	54	GLN	C-O	-7.01	1.10	1.23
55	QY	36	G	C2-N2	-6.93	1.27	1.34
22	YA	1142(A)	A	N9-C4	-6.45	1.33	1.37
29	RI	55	ALA	C-O	6.04	1.34	1.23

The worst 5 of 568 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	XV	17	C	C2-N1-C1'	11.79	131.77	118.80
53	QV	17	C	C2-N1-C1'	11.74	131.72	118.80
22	YA	761	A	N1-C6-N6	11.29	125.37	118.60
1	XA	328	C	C6-N1-C2	-10.26	116.19	120.30
25	YE	21	VAL	C-N-CD	-10.09	98.39	120.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	672	0
1	XA	32249	0	16278	742	1
2	QB	1924	0	1975	283	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	210	0
3	XC	1605	0	1668	210	0
4	QD	1703	0	1764	247	0
4	XD	1703	0	1765	215	1
5	QE	1155	0	1213	159	0
5	XE	1155	0	1213	133	0
6	QF	843	0	857	92	1
6	XF	843	0	857	96	0
7	QG	1257	0	1296	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1294	147	0
8	QH	1116	0	1175	151	0
8	XH	1116	0	1177	149	0
9	QI	1010	0	1037	140	0
9	XI	1010	0	1037	153	0
10	QJ	801	0	849	149	0
10	XJ	801	0	849	135	0
11	QK	885	0	904	103	0
11	XK	885	0	904	110	0
12	QL	975	0	1062	111	0
12	XL	975	0	1062	116	0
13	QM	964	0	1034	152	0
13	XM	964	0	1034	216	0
14	QN	492	0	529	103	0
14	XN	492	0	529	95	0
15	QO	734	0	771	78	0
15	XO	734	0	771	72	0
16	QP	705	0	725	115	0
16	XP	705	0	725	105	0
17	QQ	834	0	904	77	0
17	XQ	834	0	904	71	0
18	QR	574	0	644	69	0
18	XR	574	0	644	68	0
19	QS	674	0	699	117	0
19	XS	674	0	699	150	0
20	QT	763	0	860	109	0
20	XT	763	0	861	102	0
21	QU	217	0	234	25	0
21	XU	217	0	234	26	0
22	RA	62071	0	31286	1243	0
22	YA	62091	0	31295	1282	0
23	RB	2573	0	1306	68	0
23	YB	2573	0	1306	57	0
24	RD	2115	0	2195	320	0
24	YD	2115	0	2195	323	0
25	RE	1568	0	1634	268	0
25	YE	1568	0	1634	272	0
26	RF	1585	0	1632	178	0
26	YF	1585	0	1632	179	0
27	RG	1474	0	1535	202	0
27	YG	1474	0	1535	204	0
28	RH	1307	0	1382	220	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YH	1307	0	1382	227	3
29	RI	1136	0	1223	61	1
29	YI	1136	0	1223	57	0
30	RN	1104	0	1180	190	0
30	YN	1104	0	1180	186	0
31	RO	933	0	996	124	0
31	YO	933	0	996	131	0
32	RP	1145	0	1227	247	0
32	YP	1145	0	1228	239	0
33	RQ	1122	0	1179	150	0
33	YQ	1122	0	1178	149	0
34	RR	968	0	1033	110	0
34	YR	968	0	1033	114	0
35	RS	882	0	943	156	0
35	YS	882	0	943	159	0
36	RT	1141	0	1202	156	0
36	YT	1141	0	1202	152	0
37	RU	964	0	1022	128	0
37	YU	964	0	1022	134	0
38	RV	779	0	852	130	0
38	YV	779	0	852	128	0
39	RW	900	0	964	101	0
39	YW	900	0	964	102	0
40	RX	725	0	778	67	0
40	YX	725	0	778	67	0
41	RY	785	0	878	166	0
41	YY	785	0	878	154	3
42	RZ	1461	0	1493	63	0
42	YZ	1461	0	1493	70	0
43	R0	648	0	672	28	0
43	Y0	648	0	672	44	0
44	R1	763	0	848	143	0
44	Y1	763	0	848	140	0
45	R2	581	0	629	80	0
45	Y2	581	0	629	79	0
46	R3	469	0	518	41	0
46	Y3	469	0	518	44	0
47	R4	581	0	574	156	0
47	Y4	581	0	574	225	0
48	R5	459	0	480	74	0
48	Y5	451	0	471	68	0
49	R6	424	0	450	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y6	424	0	450	90	0
50	R7	430	0	480	42	0
50	Y7	430	0	480	44	0
51	R8	517	0	582	102	0
51	Y8	517	0	582	102	0
52	R9	307	0	335	16	0
52	Y9	307	0	336	20	0
53	QV	1644	0	836	63	0
53	XV	1644	0	836	56	0
54	QX	169	0	88	55	0
54	XX	169	0	88	17	0
55	QY	303	0	152	22	0
55	XY	303	0	154	30	0
56	Z6	74	0	51	24	0
56	Z8	74	0	51	14	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QX	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	244	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RR	1	0	0	0	0
57	RU	1	0	0	0	0
57	XA	72	0	0	0	0
57	XM	1	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	265	0	0	0	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	1	0	0	0	0
57	YX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QA	42	0	45	4	0
58	XA	42	0	45	2	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	291950	0	198321	15633	5

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 32.

The worst 5 of 15633 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)
1:XA:1400:C:N4	53:XV:34:C:C6	1.71	1.55
14:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.55
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.27	1.54
28:RH:127:GLU:CG	28:RH:128:PRO:HD3	1.35	1.53
28:YH:127:GLU:CG	28:YH:128:PRO:HD3	1.35	1.52

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:YH:45:VAL:O	41:YY:24:VAL:N[4_445]	1.97	0.23
29:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.05	0.15
28:YH:44:VAL:CG2	41:YY:23:ARG:CD[4_445]	2.08	0.12
6:QF:15:ASP:OD2	4:XD:27:TYR:OH[4_555]	2.14	0.06
28:YH:47:GLU:OE2	41:YY:79:CYS:CB[4_445]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	5
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	5
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	12
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	12
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	11
4	XD	206/209 (99%)	135 (66%)	48 (23%)	23 (11%)	0	7
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	10
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	8
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
7	QG	153/156 (98%)	101 (66%)	37 (24%)	15 (10%)	0	10
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	12
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	12
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	9
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	18
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	18
12	QL	123/132 (93%)	84 (68%)	23 (19%)	16 (13%)	0	5
12	XL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	0	6
13	QM	119/126 (94%)	71 (60%)	29 (24%)	19 (16%)	0	3
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	3
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	2
14	XN	58/61 (95%)	33 (57%)	13 (22%)	12 (21%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	17
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	17
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	6
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
19	QS	82/93 (88%)	47 (57%)	17 (21%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	2
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	3
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	3
24	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	17
24	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	17
25	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
25	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
26	RF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	10
26	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	10
27	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
27	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
28	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
28	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
29	RI	144/148 (97%)	106 (74%)	21 (15%)	17 (12%)	0	6
29	YI	144/148 (97%)	100 (69%)	27 (19%)	17 (12%)	0	6
30	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
30	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
31	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16
31	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16
32	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
32	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
33	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	10
33	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	10
34	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
35	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
35	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
36	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
36	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
37	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	15
37	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	15
38	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
38	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
39	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
39	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
40	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
40	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
41	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	1
41	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	1
42	RZ	181/206 (88%)	131 (72%)	28 (16%)	22 (12%)	0	6
42	YZ	181/206 (88%)	128 (71%)	35 (19%)	18 (10%)	0	10
43	R0	80/85 (94%)	67 (84%)	12 (15%)	1 (1%)	12	48
43	Y0	80/85 (94%)	67 (84%)	11 (14%)	2 (2%)	5	36
44	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
44	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
45	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	4
45	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	4
46	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
46	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
47	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
47	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
48	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
48	Y5	56/60 (93%)	32 (57%)	9 (16%)	15 (27%)	0	0
49	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
49	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19
50	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19
51	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
51	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
52	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
52	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11469/12128 (95%)	7649 (67%)	2333 (20%)	1487 (13%)	0	5

5 of 1487 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	6	THR
2	QB	15	VAL
2	QB	26	PRO
2	QB	84	GLU
2	QB	88	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	5	26
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5	26
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7	30
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7	30
4	QD	180/181 (99%)	160 (89%)	20 (11%)	6	27
4	XD	180/181 (99%)	165 (92%)	15 (8%)	11	39
5	QE	116/123 (94%)	107 (92%)	9 (8%)	12	41
5	XE	116/123 (94%)	107 (92%)	9 (8%)	12	41
6	QF	90/90 (100%)	76 (84%)	14 (16%)	2	17
6	XF	90/90 (100%)	76 (84%)	14 (16%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8	33
7	XG	126/127 (99%)	115 (91%)	11 (9%)	10	37
8	QH	119/119 (100%)	106 (89%)	13 (11%)	6	28
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	28
9	QI	98/99 (99%)	87 (89%)	11 (11%)	6	27
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	27
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	36
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	9	36
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	30
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	30
12	QL	104/109 (95%)	88 (85%)	16 (15%)	2	17
12	XL	104/109 (95%)	89 (86%)	15 (14%)	3	20
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	15
13	XM	97/101 (96%)	81 (84%)	16 (16%)	2	15
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	11
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	30
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	42
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	42
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	23
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	23
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	26
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	26
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	18
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	18
20	QT	76/82 (93%)	68 (90%)	8 (10%)	7	29
20	XT	76/82 (93%)	69 (91%)	7 (9%)	9	34
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	53
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	53
24	RD	214/218 (98%)	177 (83%)	37 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	YD	214/218 (98%)	178 (83%)	36 (17%)	2	15
25	RE	165/166 (99%)	127 (77%)	38 (23%)	1	6
25	YE	165/166 (99%)	127 (77%)	38 (23%)	1	6
26	RF	161/166 (97%)	140 (87%)	21 (13%)	4	23
26	YF	161/166 (97%)	140 (87%)	21 (13%)	4	23
27	RG	155/156 (99%)	130 (84%)	25 (16%)	2	16
27	YG	155/156 (99%)	131 (84%)	24 (16%)	2	17
28	RH	142/148 (96%)	114 (80%)	28 (20%)	1	9
28	YH	142/148 (96%)	114 (80%)	28 (20%)	1	9
29	RI	122/124 (98%)	100 (82%)	22 (18%)	1	12
29	YI	122/124 (98%)	101 (83%)	21 (17%)	2	14
30	RN	117/119 (98%)	98 (84%)	19 (16%)	2	16
30	YN	117/119 (98%)	98 (84%)	19 (16%)	2	16
31	RO	100/100 (100%)	90 (90%)	10 (10%)	7	30
31	YO	100/100 (100%)	90 (90%)	10 (10%)	7	30
32	RP	116/116 (100%)	89 (77%)	27 (23%)	1	5
32	YP	116/116 (100%)	89 (77%)	27 (23%)	1	5
33	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
33	YQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
34	RR	101/101 (100%)	84 (83%)	17 (17%)	2	15
34	YR	101/101 (100%)	84 (83%)	17 (17%)	2	15
35	RS	87/88 (99%)	74 (85%)	13 (15%)	3	18
35	YS	87/88 (99%)	74 (85%)	13 (15%)	3	18
36	RT	120/127 (94%)	97 (81%)	23 (19%)	1	10
36	YT	120/127 (94%)	97 (81%)	23 (19%)	1	10
37	RU	93/94 (99%)	80 (86%)	13 (14%)	3	21
37	YU	93/94 (99%)	80 (86%)	13 (14%)	3	21
38	RV	82/82 (100%)	71 (87%)	11 (13%)	4	22
38	YV	82/82 (100%)	71 (87%)	11 (13%)	4	22
39	RW	92/92 (100%)	77 (84%)	15 (16%)	2	16
39	YW	92/92 (100%)	77 (84%)	15 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	RX	74/78 (95%)	63 (85%)	11 (15%)	3	18
40	YX	74/78 (95%)	63 (85%)	11 (15%)	3	18
41	RY	85/91 (93%)	70 (82%)	15 (18%)	2	13
41	YY	85/91 (93%)	70 (82%)	15 (18%)	2	13
42	RZ	162/179 (90%)	141 (87%)	21 (13%)	4	23
42	YZ	162/179 (90%)	139 (86%)	23 (14%)	3	20
43	R0	65/67 (97%)	57 (88%)	8 (12%)	4	24
43	Y0	65/67 (97%)	60 (92%)	5 (8%)	13	42
44	R1	82/83 (99%)	67 (82%)	15 (18%)	1	11
44	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	11
45	R2	64/67 (96%)	57 (89%)	7 (11%)	6	28
45	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	28
46	R3	51/52 (98%)	40 (78%)	11 (22%)	1	7
46	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	7
47	R4	63/63 (100%)	44 (70%)	19 (30%)	0	2
47	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
48	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
48	Y5	50/52 (96%)	38 (76%)	12 (24%)	0	5
49	R6	48/52 (92%)	38 (79%)	10 (21%)	1	7
49	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
50	R7	42/42 (100%)	39 (93%)	3 (7%)	14	44
50	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	44
51	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
51	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	3
52	R9	34/34 (100%)	32 (94%)	2 (6%)	19	49
52	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	49
All	All	9701/10066 (96%)	8295 (86%)	1406 (14%)	3	19

5 of 1406 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	R2	53	LEU
6	XF	97	PHE

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Mol	Chain	Res	Type
42	YZ	139	VAL
47	R4	23	GLU
2	XB	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
45	R2	47	ASN
6	XF	64	GLN
42	YZ	32	HIS
46	R3	32	GLN
2	XB	204	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	281 (18%)	47 (3%)
1	XA	1498/1522 (98%)	299 (19%)	52 (3%)
22	RA	2879/2916 (98%)	658 (22%)	65 (2%)
22	YA	2880/2916 (98%)	639 (22%)	65 (2%)
23	RB	119/122 (97%)	20 (16%)	2 (1%)
23	YB	119/122 (97%)	25 (21%)	1 (0%)
53	QV	76/77 (98%)	30 (39%)	1 (1%)
53	XV	76/77 (98%)	30 (39%)	1 (1%)
54	QX	7/25 (28%)	5 (71%)	2 (28%)
54	XX	7/25 (28%)	4 (57%)	1 (14%)
55	QY	13/18 (72%)	6 (46%)	2 (15%)
55	XY	13/18 (72%)	5 (38%)	1 (7%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9188/9366 (98%)	2002 (21%)	240 (2%)

5 of 2002 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G



5 of 240 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	RA	2776	A
1	XA	530	G
22	YA	2566	A
22	RA	2867	G
1	XA	243	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	PPU	Z8	76	56,22	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z6	76	56,22	32,40,41	2.56	6 (18%)	33,57,60	2.16	5 (15%)
55	1MG	QY	37	55	18,26,27	1.86	2 (11%)	19,39,42	1.70	4 (21%)
55	1MG	XY	37	55	18,26,27	2.79	3 (16%)	19,39,42	1.48	4 (21%)

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	Z8	76	56,22	-	2/21/43/44	0/4/4/4
56	PPU	Z6	76	56,22	-	2/21/43/44	0/4/4/4
55	1MG	QY	37	55	-	0/3/25/26	0/3/3/3
55	1MG	XY	37	55	-	0/3/25/26	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.30	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.27	1.41	1.23
55	XY	37	1MG	C4-N3	8.62	1.49	1.35
55	XY	37	1MG	C2-N2	7.15	1.48	1.33
55	QY	37	1MG	C6-C5	6.37	1.51	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.63	110.20	123.21
56	Z8	76	PPU	C3'-N3'-C	-8.59	110.25	123.21
55	QY	37	1MG	C5-C6-N1	-4.96	112.91	118.20
56	Z8	76	PPU	N3-C2-N1	-4.69	121.34	128.68
56	Z6	76	PPU	N3-C2-N1	-4.64	121.42	128.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	11	0
56	Z6	76	PPU	14	0
55	QY	37	1MG	2	0
55	XY	37	1MG	7	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 684 ligands modelled in this entry, 682 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	QA	1666	-	45,45,45	1.48	7 (15%)	64,67,67	1.39	8 (12%)
58	PAR	XA	1673	-	45,45,45	1.51	7 (15%)	64,67,67	1.34	5 (7%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C64-C54	5.19	1.59	1.52
58	XA	1673	PAR	C64-C54	4.99	1.58	1.52
58	QA	1666	PAR	C52-C42	3.07	1.58	1.52
58	XA	1673	PAR	C52-C42	2.95	1.58	1.52
58	XA	1673	PAR	O54-C14	2.92	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1673	PAR	O33-C14-C24	4.73	116.36	108.22
58	XA	1673	PAR	C14-O54-C54	4.31	122.15	113.69
58	QA	1666	PAR	O52-C13-C23	3.86	115.96	107.96
58	QA	1666	PAR	C14-O54-C54	3.83	121.21	113.69
58	QA	1666	PAR	O33-C14-C24	3.75	114.67	108.22

There are no chirality outliers.

5 of 14 torsion outliers are listed below:



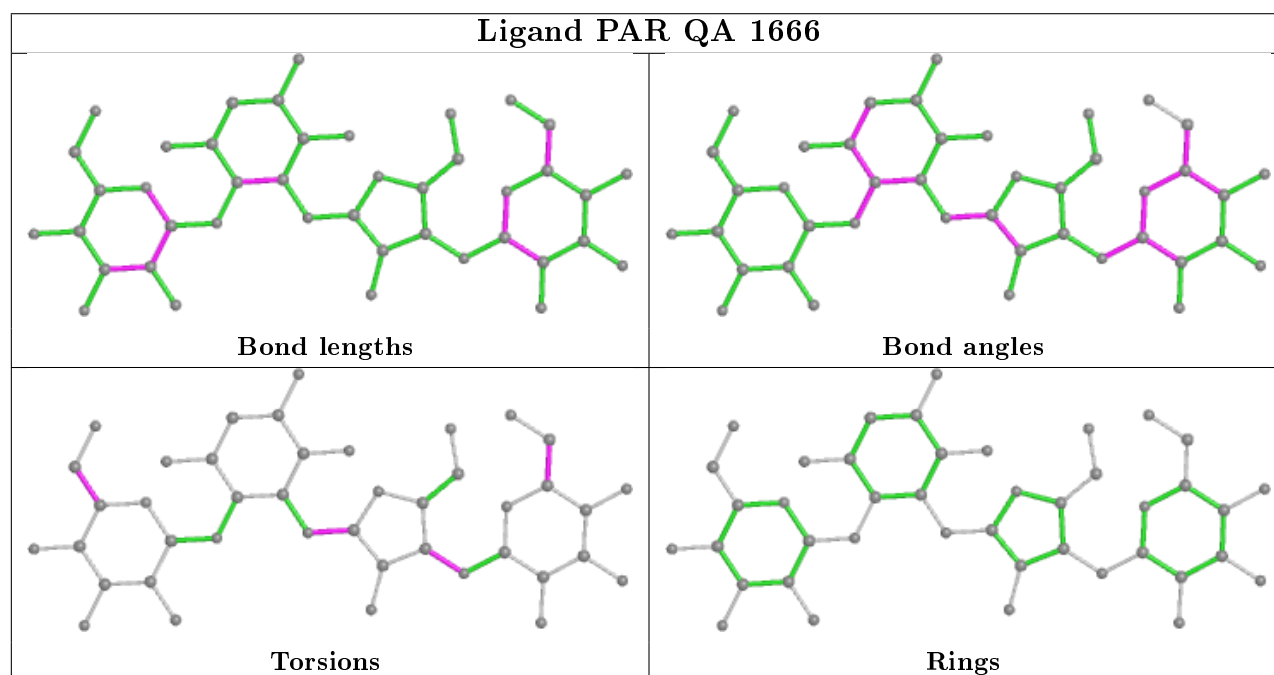
Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	QA	1666	PAR	O51-C51-C61-O61
58	XA	1673	PAR	O51-C51-C61-O61
58	QA	1666	PAR	C41-C51-C61-O61

There are no ring outliers.

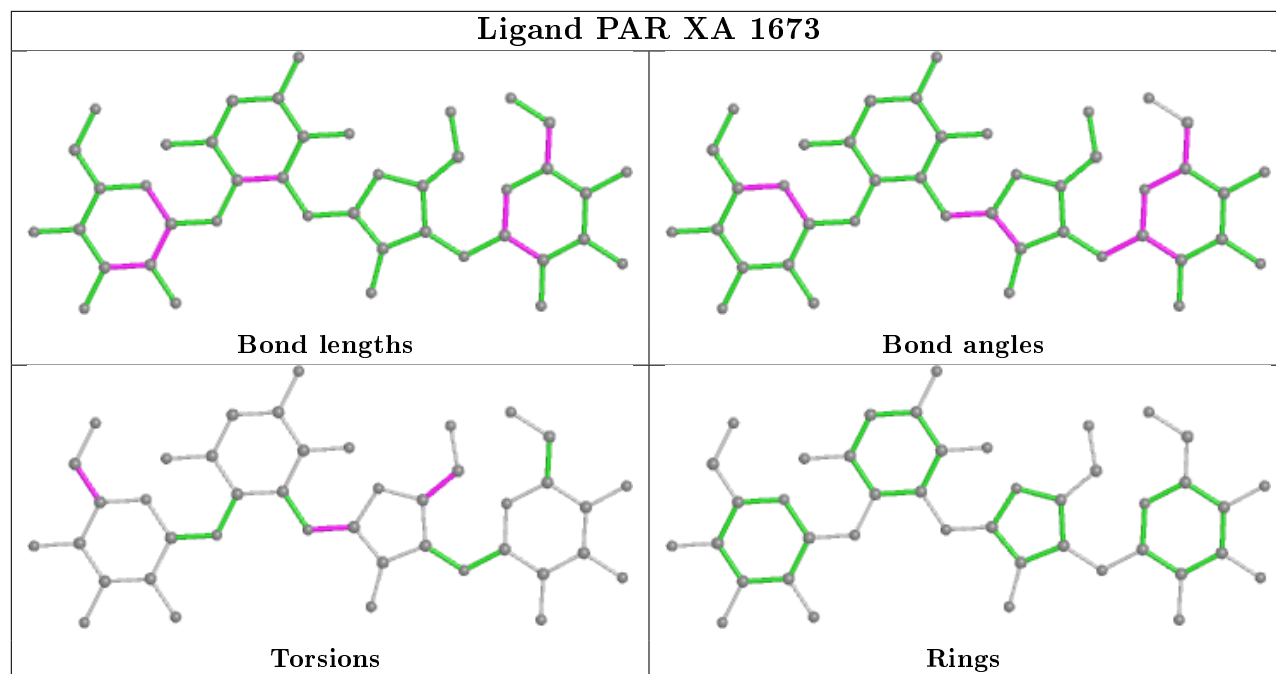
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1666	PAR	4	0
58	XA	1673	PAR	2	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.09	27 (1%) 68 59	22, 75, 152, 231	0
1	XA	1500/1522 (98%)	-0.25	9 (0%) 89 84	7, 55, 142, 232	0
2	QB	237/256 (92%)	0.39	16 (6%) 17 12	47, 109, 145, 182	0
2	XB	237/256 (92%)	0.18	9 (3%) 40 31	38, 88, 133, 159	0
3	QC	205/239 (85%)	0.14	4 (1%) 65 55	39, 98, 133, 150	0
3	XC	205/239 (85%)	-0.18	2 (0%) 82 75	20, 67, 110, 138	0
4	QD	208/209 (99%)	0.14	2 (0%) 82 75	29, 79, 128, 167	0
4	XD	208/209 (99%)	0.05	2 (0%) 82 75	10, 72, 110, 139	0
5	QE	151/162 (93%)	0.28	6 (3%) 38 30	25, 85, 122, 159	0
5	XE	151/162 (93%)	-0.03	2 (1%) 77 68	1, 62, 104, 134	0
6	QF	101/101 (100%)	0.15	1 (0%) 82 75	16, 74, 116, 131	0
6	XF	101/101 (100%)	-0.03	1 (0%) 82 75	16, 65, 110, 133	0
7	QG	155/156 (99%)	0.48	17 (10%) 5 5	30, 84, 125, 149	0
7	XG	155/156 (99%)	0.18	6 (3%) 39 30	20, 71, 109, 131	0
8	QH	138/138 (100%)	0.32	3 (2%) 62 51	45, 88, 124, 156	0
8	XH	138/138 (100%)	0.10	1 (0%) 87 82	19, 70, 102, 125	0
9	QI	127/128 (99%)	0.71	13 (10%) 6 6	46, 97, 137, 144	0
9	XI	127/128 (99%)	0.20	3 (2%) 59 48	16, 79, 119, 129	0
10	QJ	99/105 (94%)	1.05	19 (19%) 1 1	44, 108, 142, 161	0
10	XJ	99/105 (94%)	0.56	11 (11%) 5 5	9, 83, 129, 147	0
11	QK	119/129 (92%)	0.40	14 (11%) 4 4	18, 71, 123, 149	0
11	XK	119/129 (92%)	0.26	5 (4%) 36 29	15, 63, 110, 147	0
12	QL	125/132 (94%)	0.45	8 (6%) 19 14	20, 72, 108, 139	0
12	XL	125/132 (94%)	-0.02	2 (1%) 72 62	0, 48, 91, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	0.52	13 (10%) 6 5	39, 96, 131, 170	0
13	XM	121/126 (96%)	-0.00	3 (2%) 57 47	4, 68, 125, 149	0
14	QN	60/61 (98%)	0.64	5 (8%) 11 9	52, 98, 137, 146	0
14	XN	60/61 (98%)	-0.07	0 100 100	4, 60, 100, 120	0
15	QO	88/89 (98%)	0.14	6 (6%) 17 12	30, 79, 120, 136	0
15	XO	88/89 (98%)	0.01	1 (1%) 80 73	10, 64, 93, 107	0
16	QP	84/88 (95%)	0.32	3 (3%) 42 33	12, 68, 103, 138	0
16	XP	84/88 (95%)	0.45	2 (2%) 59 48	30, 70, 106, 135	0
17	QQ	100/105 (95%)	0.56	7 (7%) 16 12	33, 82, 115, 141	0
17	XQ	100/105 (95%)	0.21	0 100 100	14, 64, 102, 124	0
18	QR	70/88 (79%)	0.53	9 (12%) 3 3	18, 78, 119, 147	0
18	XR	70/88 (79%)	0.38	4 (5%) 23 19	22, 67, 109, 135	0
19	QS	84/93 (90%)	0.67	7 (8%) 11 9	60, 102, 132, 147	0
19	XS	84/93 (90%)	0.21	2 (2%) 59 48	15, 73, 112, 164	0
20	QT	99/106 (93%)	0.19	3 (3%) 50 38	3, 77, 111, 131	0
20	XT	99/106 (93%)	0.29	3 (3%) 50 38	19, 77, 117, 126	0
21	QU	25/27 (92%)	1.78	9 (36%) 0 0	37, 85, 131, 145	0
21	XU	25/27 (92%)	0.97	3 (12%) 4 4	30, 75, 103, 134	0
22	RA	2882/2916 (98%)	-0.17	97 (3%) 45 35	2, 45, 174, 236	0
22	YA	2883/2916 (98%)	-0.27	71 (2%) 57 47	1, 35, 165, 227	0
23	RB	120/122 (98%)	-0.17	0 100 100	46, 89, 131, 153	0
23	YB	120/122 (98%)	-0.48	1 (0%) 86 79	18, 58, 93, 139	0
24	RD	272/276 (98%)	-0.11	0 100 100	4, 41, 81, 123	0
24	YD	272/276 (98%)	-0.05	1 (0%) 92 87	1, 33, 74, 140	0
25	RE	205/206 (99%)	0.13	4 (1%) 65 55	7, 62, 112, 141	0
25	YE	205/206 (99%)	0.04	2 (0%) 82 75	6, 56, 103, 125	0
26	RF	202/210 (96%)	-0.04	2 (0%) 82 75	1, 64, 110, 129	0
26	YF	202/210 (96%)	-0.06	2 (0%) 82 75	1, 47, 95, 112	0
27	RG	181/182 (99%)	0.37	9 (4%) 28 24	34, 99, 142, 166	0
27	YG	181/182 (99%)	-0.06	1 (0%) 89 84	9, 66, 115, 163	0
28	RH	170/180 (94%)	1.11	37 (21%) 0 1	32, 108, 152, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YH	170/180 (94%)	0.20	6 (3%) 44 34	14, 68, 110, 133	0
29	RI	146/148 (98%)	0.36	3 (2%) 63 53	16, 78, 122, 154	0
29	YI	146/148 (98%)	0.17	3 (2%) 63 53	8, 72, 119, 159	0
30	RN	138/140 (98%)	0.31	5 (3%) 42 33	14, 70, 110, 124	0
30	YN	138/140 (98%)	0.03	4 (2%) 51 40	8, 55, 103, 128	0
31	RO	122/122 (100%)	0.15	0 100 100	5, 56, 97, 126	0
31	YO	122/122 (100%)	-0.01	0 100 100	0, 42, 79, 94	0
32	RP	150/150 (100%)	0.49	11 (7%) 15 11	6, 65, 126, 159	0
32	YP	150/150 (100%)	0.04	2 (1%) 77 68	5, 53, 105, 154	0
33	RQ	141/141 (100%)	0.18	3 (2%) 63 53	2, 62, 106, 142	0
33	YQ	141/141 (100%)	-0.12	0 100 100	3, 42, 94, 132	0
34	RR	118/118 (100%)	-0.05	0 100 100	8, 50, 92, 118	0
34	YR	118/118 (100%)	-0.07	0 100 100	7, 43, 89, 109	0
35	RS	111/112 (99%)	0.37	3 (2%) 54 43	35, 78, 114, 141	0
35	YS	111/112 (99%)	0.01	0 100 100	7, 61, 94, 111	0
36	RT	137/146 (93%)	0.11	2 (1%) 73 64	13, 64, 125, 165	0
36	YT	137/146 (93%)	-0.10	1 (0%) 87 82	10, 58, 111, 158	0
37	RU	117/118 (99%)	-0.06	3 (2%) 56 45	10, 61, 104, 147	0
37	YU	117/118 (99%)	-0.16	2 (1%) 70 60	0, 44, 108, 129	0
38	RV	101/101 (100%)	0.07	0 100 100	20, 75, 116, 144	0
38	YV	101/101 (100%)	0.19	2 (1%) 65 55	11, 65, 104, 156	0
39	RW	113/113 (100%)	0.10	0 100 100	3, 43, 93, 149	0
39	YW	113/113 (100%)	-0.09	2 (1%) 68 59	2, 42, 91, 144	0
40	RX	92/96 (95%)	-0.09	1 (1%) 80 73	15, 52, 96, 125	0
40	YX	92/96 (95%)	-0.11	0 100 100	3, 37, 76, 96	0
41	RY	102/110 (92%)	1.27	28 (27%) 0 0	26, 88, 132, 159	0
41	YY	102/110 (92%)	0.34	4 (3%) 39 30	9, 63, 120, 140	0
42	RZ	183/206 (88%)	0.39	10 (5%) 25 20	21, 88, 133, 152	0
42	YZ	183/206 (88%)	0.01	3 (1%) 72 62	20, 70, 123, 155	0
43	R0	82/85 (96%)	0.36	3 (3%) 41 32	14, 48, 79, 112	0
43	Y0	82/85 (96%)	0.18	1 (1%) 79 70	3, 36, 66, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	R1	97/98 (98%)	0.47	4 (4%) 37 29	5, 53, 126, 159	0
44	Y1	97/98 (98%)	0.29	3 (3%) 49 38	5, 43, 104, 139	0
45	R2	69/72 (95%)	0.05	0 100 100	13, 72, 111, 129	0
45	Y2	69/72 (95%)	-0.20	0 100 100	5, 50, 104, 121	0
46	R3	59/60 (98%)	1.17	9 (15%) 2 2	12, 63, 111, 139	0
46	Y3	59/60 (98%)	0.47	5 (8%) 10 8	2, 44, 101, 174	0
47	R4	71/71 (100%)	0.89	12 (16%) 1 1	75, 131, 170, 189	0
47	Y4	71/71 (100%)	0.27	4 (5%) 24 19	46, 102, 154, 161	0
48	R5	59/60 (98%)	0.11	4 (6%) 17 12	6, 55, 133, 141	0
48	Y5	58/60 (96%)	0.14	2 (3%) 45 35	10, 59, 143, 162	0
49	R6	49/54 (90%)	3.21	31 (63%) 0 0	83, 118, 150, 157	0
49	Y6	49/54 (90%)	2.67	31 (63%) 0 0	51, 109, 141, 149	0
50	R7	49/49 (100%)	0.07	2 (4%) 37 29	8, 35, 87, 146	0
50	Y7	49/49 (100%)	0.08	1 (2%) 65 55	1, 29, 71, 121	0
51	R8	64/65 (98%)	0.23	2 (3%) 49 38	1, 52, 96, 158	0
51	Y8	64/65 (98%)	0.01	0 100 100	5, 40, 81, 149	0
52	R9	37/37 (100%)	3.91	32 (86%) 0 0	66, 110, 156, 168	0
52	Y9	37/37 (100%)	4.48	37 (100%) 0 0	78, 107, 132, 166	0
53	QV	77/77 (100%)	0.14	2 (2%) 56 45	46, 99, 145, 169	0
53	XV	77/77 (100%)	0.04	2 (2%) 56 45	28, 72, 119, 180	0
54	QX	8/25 (32%)	3.09	6 (75%) 0 0	103, 130, 144, 183	0
54	XX	8/25 (32%)	1.62	2 (25%) 0 0	56, 75, 115, 190	0
55	QY	13/18 (72%)	1.53	4 (30%) 0 0	112, 161, 199, 206	0
55	XY	13/18 (72%)	1.16	2 (15%) 2 2	72, 116, 180, 193	0
56	Z6	2/3 (66%)	0.35	0 100 100	52, 52, 52, 57	0
56	Z8	2/3 (66%)	0.56	0 100 100	46, 46, 46, 46	0
All	All	20870/21494 (97%)	0.06	789 (3%) 40 31	0, 61, 135, 236	0

The worst 5 of 789 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R9	11	CYS	11.7
52	Y9	34	GLN	9.8

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Mol	Chain	Res	Type	RSRZ
49	R6	22	ALA	9.7
52	R9	14	CYS	9.5
13	QM	121	LYS	8.4

## 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
55	1MG	QY	37	24/25	0.84	0.31	125,125,125,125	0
55	1MG	XY	37	24/25	0.89	0.20	64,64,64,64	0
56	PPU	Z8	76	37/38	0.93	0.33	48,48,48,48	0
56	PPU	Z6	76	37/38	0.93	0.32	51,51,51,51	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
59	ZN	R9	101	1/1	0.30	0.76	177,177,177,177	0
57	MG	QH	201	1/1	0.31	0.27	27,27,27,27	0
57	MG	RA	3230	1/1	0.47	0.48	45,45,45,45	0
57	MG	YA	3148	1/1	0.49	0.23	38,38,38,38	0
57	MG	QA	1631	1/1	0.50	0.24	63,63,63,63	0
57	MG	RA	3229	1/1	0.52	0.33	50,50,50,50	0
57	MG	YA	3012	1/1	0.55	1.42	50,50,50,50	0
57	MG	YA	3163	1/1	0.57	0.31	9,9,9,9	0
57	MG	RA	3071	1/1	0.57	0.89	50,50,50,50	0
57	MG	QA	1628	1/1	0.61	0.43	21,21,21,21	0
57	MG	XA	1662	1/1	0.62	0.74	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	YA	3235	1/1	0.63	0.47	34,34,34,34	0
57	MG	YA	3156	1/1	0.65	0.24	8,8,8,8	0
57	MG	RA	3217	1/1	0.67	0.91	16,16,16,16	0
57	MG	RA	3186	1/1	0.68	0.72	51,51,51,51	0
57	MG	QA	1640	1/1	0.69	0.23	6,6,6,6	0
57	MG	QF	201	1/1	0.69	0.32	40,40,40,40	0
57	MG	RA	3116	1/1	0.70	0.32	0,0,0,0	0
59	ZN	Y9	101	1/1	0.70	0.53	158,158,158,158	0
57	MG	YA	3150	1/1	0.71	0.59	16,16,16,16	0
57	MG	RA	3004	1/1	0.72	0.44	9,9,9,9	0
57	MG	RA	3127	1/1	0.72	0.52	15,15,15,15	0
57	MG	RA	3065	1/1	0.72	1.22	50,50,50,50	0
57	MG	YA	3117	1/1	0.72	0.80	50,50,50,50	0
57	MG	XA	1650	1/1	0.73	0.31	22,22,22,22	0
57	MG	RA	3205	1/1	0.73	0.46	33,33,33,33	0
57	MG	XA	1635	1/1	0.73	1.57	50,50,50,50	0
57	MG	YA	3151	1/1	0.73	0.55	50,50,50,50	0
57	MG	QA	1638	1/1	0.73	0.20	8,8,8,8	0
57	MG	RA	3181	1/1	0.73	0.33	9,9,9,9	0
57	MG	YA	3153	1/1	0.73	0.28	16,16,16,16	0
57	MG	XA	1601	1/1	0.74	1.10	50,50,50,50	0
57	MG	YA	3070	1/1	0.74	0.30	33,33,33,33	0
57	MG	YA	3247	1/1	0.74	0.59	16,16,16,16	0
57	MG	QA	1665	1/1	0.75	0.48	37,37,37,37	0
57	MG	RA	3212	1/1	0.75	0.26	33,33,33,33	0
57	MG	RA	3064	1/1	0.75	1.71	50,50,50,50	0
57	MG	YA	3126	1/1	0.75	0.33	50,50,50,50	0
57	MG	RA	3223	1/1	0.75	0.33	16,16,16,16	0
57	MG	RA	3140	1/1	0.75	0.24	61,61,61,61	0
57	MG	YA	3250	1/1	0.76	1.15	50,50,50,50	0
57	MG	QA	1643	1/1	0.76	0.14	20,20,20,20	0
57	MG	YA	3223	1/1	0.76	0.93	11,11,11,11	0
57	MG	YA	3043	1/1	0.77	1.09	50,50,50,50	0
57	MG	XA	1649	1/1	0.77	0.39	16,16,16,16	0
57	MG	XA	1605	1/1	0.77	0.61	16,16,16,16	0
57	MG	YA	3053	1/1	0.78	1.01	50,50,50,50	0
57	MG	QA	1602	1/1	0.78	1.00	11,11,11,11	0
57	MG	YA	3261	1/1	0.78	0.96	50,50,50,50	0
57	MG	YA	3259	1/1	0.78	0.67	2,2,2,2	0
57	MG	RA	3034	1/1	0.78	1.60	50,50,50,50	0
57	MG	RA	3164	1/1	0.78	0.55	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1664	1/1	0.78	0.35	10,10,10,10	0
57	MG	YA	3137	1/1	0.79	0.28	22,22,22,22	0
57	MG	RA	3219	1/1	0.79	0.56	40,40,40,40	0
57	MG	RA	3201	1/1	0.79	0.36	41,41,41,41	0
57	MG	XA	1634	1/1	0.79	0.21	11,11,11,11	0
57	MG	YA	3079	1/1	0.79	1.26	50,50,50,50	0
57	MG	RA	3123	1/1	0.79	0.94	50,50,50,50	0
57	MG	QA	1601	1/1	0.79	0.40	21,21,21,21	0
57	MG	QA	1655	1/1	0.80	0.39	66,66,66,66	0
58	PAR	QA	1666	42/42	0.80	0.38	104,104,104,104	0
57	MG	XA	1615	1/1	0.80	0.48	50,50,50,50	0
57	MG	YA	3245	1/1	0.80	0.57	3,3,3,3	0
57	MG	YA	3119	1/1	0.80	0.41	66,66,66,66	0
57	MG	QA	1603	1/1	0.80	0.52	10,10,10,10	0
57	MG	RA	3041	1/1	0.80	0.64	50,50,50,50	0
57	MG	RA	3050	1/1	0.81	0.14	8,8,8,8	0
57	MG	QA	1622	1/1	0.81	0.45	52,52,52,52	0
57	MG	RA	3225	1/1	0.81	0.29	47,47,47,47	0
57	MG	RA	3231	1/1	0.81	0.35	3,3,3,3	0
57	MG	RA	3184	1/1	0.81	0.36	40,40,40,40	0
57	MG	RA	3063	1/1	0.81	0.11	19,19,19,19	0
57	MG	RA	3007	1/1	0.81	1.30	50,50,50,50	0
57	MG	YA	3171	1/1	0.81	0.22	7,7,7,7	0
57	MG	YA	3193	1/1	0.82	0.74	7,7,7,7	0
57	MG	RA	3157	1/1	0.82	0.25	39,39,39,39	0
57	MG	RA	3027	1/1	0.82	0.97	50,50,50,50	0
57	MG	R8	101	1/1	0.82	0.39	6,6,6,6	0
57	MG	YA	3187	1/1	0.82	0.21	47,47,47,47	0
57	MG	XA	1664	1/1	0.82	0.40	27,27,27,27	0
57	MG	YA	3253	1/1	0.82	1.86	50,50,50,50	0
57	MG	YA	3041	1/1	0.82	0.85	50,50,50,50	0
57	MG	YA	3105	1/1	0.83	0.74	8,8,8,8	0
57	MG	YA	3204	1/1	0.83	0.16	11,11,11,11	0
57	MG	RA	3128	1/1	0.83	0.23	10,10,10,10	0
57	MG	QA	1651	1/1	0.83	0.43	16,16,16,16	0
57	MG	RA	3001	1/1	0.83	0.78	1,1,1,1	0
57	MG	XA	1653	1/1	0.83	0.15	29,29,29,29	0
57	MG	XA	1607	1/1	0.83	0.32	17,17,17,17	0
57	MG	YA	3185	1/1	0.84	0.16	74,74,74,74	0
57	MG	YA	3157	1/1	0.84	0.32	8,8,8,8	0
57	MG	XA	1665	1/1	0.84	0.19	18,18,18,18	0
57	MG	YA	3024	1/1	0.84	0.53	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	YA	3154	1/1	0.84	0.26	5,5,5,5	0
57	MG	QX	101	1/1	0.84	0.15	6,6,6,6	0
57	MG	YA	3047	1/1	0.84	1.00	50,50,50,50	0
57	MG	YA	3206	1/1	0.84	0.29	20,20,20,20	0
57	MG	YA	3191	1/1	0.84	0.39	14,14,14,14	0
57	MG	QA	1610	1/1	0.85	0.57	50,50,50,50	0
57	MG	RA	3051	1/1	0.85	0.83	50,50,50,50	0
57	MG	YA	3198	1/1	0.85	0.28	2,2,2,2	0
57	MG	RA	3194	1/1	0.85	0.15	82,82,82,82	0
57	MG	RA	3119	1/1	0.85	0.25	88,88,88,88	0
57	MG	QA	1639	1/1	0.85	0.26	27,27,27,27	0
57	MG	YA	3217	1/1	0.85	0.62	52,52,52,52	0
57	MG	XM	201	1/1	0.85	0.17	78,78,78,78	0
57	MG	QA	1637	1/1	0.85	0.26	3,3,3,3	0
57	MG	RA	3043	1/1	0.85	0.70	50,50,50,50	0
57	MG	YA	3202	1/1	0.85	0.42	13,13,13,13	0
57	MG	YB	201	1/1	0.85	0.29	14,14,14,14	0
57	MG	YA	3125	1/1	0.85	0.45	15,15,15,15	0
57	MG	RA	3136	1/1	0.85	0.24	14,14,14,14	0
57	MG	YA	3168	1/1	0.85	0.16	13,13,13,13	0
57	MG	RA	3078	1/1	0.85	0.83	50,50,50,50	0
57	MG	RA	3023	1/1	0.86	0.49	50,50,50,50	0
57	MG	RA	3146	1/1	0.86	0.41	7,7,7,7	0
57	MG	YA	3262	1/1	0.86	0.33	9,9,9,9	0
57	MG	XA	1638	1/1	0.86	0.17	27,27,27,27	0
57	MG	RA	3085	1/1	0.86	0.22	27,27,27,27	0
57	MG	YA	3031	1/1	0.86	1.04	50,50,50,50	0
57	MG	RA	3166	1/1	0.86	0.94	9,9,9,9	0
57	MG	QA	1658	1/1	0.86	0.42	46,46,46,46	0
57	MG	QA	1623	1/1	0.86	0.52	13,13,13,13	0
57	MG	YA	3242	1/1	0.86	0.20	5,5,5,5	0
57	MG	RA	3131	1/1	0.86	0.18	25,25,25,25	0
57	MG	XA	1606	1/1	0.86	0.64	13,13,13,13	0
57	MG	XA	1652	1/1	0.86	0.26	50,50,50,50	0
57	MG	YA	3176	1/1	0.86	0.31	11,11,11,11	0
57	MG	RP	202	1/1	0.86	0.31	75,75,75,75	0
57	MG	YA	3006	1/1	0.86	0.86	50,50,50,50	0
57	MG	XA	1616	1/1	0.86	0.77	50,50,50,50	0
57	MG	YB	202	1/1	0.86	0.43	5,5,5,5	0
57	MG	YA	3134	1/1	0.86	0.66	50,50,50,50	0
57	MG	YA	3083	1/1	0.86	0.21	16,16,16,16	0
57	MG	YA	3030	1/1	0.86	0.89	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	1628	1/1	0.86	0.14	2,2,2,2	0
57	MG	RA	3021	1/1	0.86	1.12	50,50,50,50	0
57	MG	XA	1609	1/1	0.87	0.55	8,8,8,8	0
57	MG	YA	3264	1/1	0.87	0.53	14,14,14,14	0
57	MG	RA	3003	1/1	0.87	1.15	50,50,50,50	0
57	MG	RA	3206	1/1	0.87	0.25	11,11,11,11	0
57	MG	RA	3180	1/1	0.87	0.36	1,1,1,1	0
57	MG	RA	3039	1/1	0.87	0.66	50,50,50,50	0
57	MG	XA	1641	1/1	0.87	0.33	14,14,14,14	0
57	MG	RA	3175	1/1	0.87	0.28	12,12,12,12	0
57	MG	RA	3121	1/1	0.87	0.15	0,0,0,0	0
57	MG	XA	1671	1/1	0.87	0.18	28,28,28,28	0
57	MG	YA	3074	1/1	0.87	0.61	4,4,4,4	0
57	MG	RA	3211	1/1	0.87	0.25	11,11,11,11	0
57	MG	YA	3115	1/1	0.87	0.29	15,15,15,15	0
57	MG	RA	3160	1/1	0.87	0.33	2,2,2,2	0
57	MG	YA	3162	1/1	0.87	0.29	30,30,30,30	0
57	MG	RA	3174	1/1	0.87	0.15	40,40,40,40	0
57	MG	RA	3151	1/1	0.87	0.35	37,37,37,37	0
57	MG	RA	3005	1/1	0.87	0.80	50,50,50,50	0
57	MG	YA	3169	1/1	0.87	0.86	7,7,7,7	0
58	PAR	XA	1673	42/42	0.87	0.32	132,132,132,132	0
57	MG	RA	3241	1/1	0.87	0.38	0,0,0,0	0
57	MG	RA	3237	1/1	0.87	0.23	4,4,4,4	0
57	MG	RA	3222	1/1	0.87	0.37	4,4,4,4	0
57	MG	YA	3234	1/1	0.87	0.09	2,2,2,2	0
57	MG	YA	3249	1/1	0.87	0.70	5,5,5,5	0
57	MG	RA	3228	1/1	0.88	0.15	7,7,7,7	0
57	MG	YA	3220	1/1	0.88	0.15	26,26,26,26	0
57	MG	RA	3196	1/1	0.88	0.33	22,22,22,22	0
57	MG	YA	3113	1/1	0.88	0.48	50,50,50,50	0
57	MG	RA	3020	1/1	0.88	0.71	50,50,50,50	0
57	MG	XA	1625	1/1	0.88	0.48	50,50,50,50	0
57	MG	YA	3183	1/1	0.88	0.19	17,17,17,17	0
57	MG	XA	1656	1/1	0.88	0.89	12,12,12,12	0
57	MG	YA	3170	1/1	0.88	0.28	8,8,8,8	0
57	MG	RA	3069	1/1	0.88	0.26	9,9,9,9	0
57	MG	RA	3139	1/1	0.88	0.54	18,18,18,18	0
57	MG	YA	3254	1/1	0.88	0.37	0,0,0,0	0
57	MG	YA	3045	1/1	0.88	0.55	0,0,0,0	0
57	MG	YA	3236	1/1	0.88	0.20	12,12,12,12	0
57	MG	Y7	101	1/1	0.88	0.27	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3138	1/1	0.88	0.49	4,4,4,4	0
57	MG	QA	1618	1/1	0.88	0.42	8,8,8,8	0
57	MG	YA	3131	1/1	0.88	0.50	17,17,17,17	0
57	MG	YA	3128	1/1	0.88	0.23	0,0,0,0	0
57	MG	YA	3197	1/1	0.88	1.38	50,50,50,50	0
57	MG	YA	3085	1/1	0.89	0.81	50,50,50,50	0
57	MG	RA	3122	1/1	0.89	0.30	19,19,19,19	0
57	MG	RA	3091	1/1	0.89	0.49	2,2,2,2	0
57	MG	XX	101	1/1	0.89	0.17	88,88,88,88	0
57	MG	RA	3156	1/1	0.89	0.16	7,7,7,7	0
57	MG	YA	3215	1/1	0.89	0.25	2,2,2,2	0
57	MG	YA	3130	1/1	0.89	0.10	3,3,3,3	0
57	MG	YA	3062	1/1	0.89	0.23	0,0,0,0	0
57	MG	RA	3207	1/1	0.89	0.25	5,5,5,5	0
57	MG	YA	3232	1/1	0.89	0.22	15,15,15,15	0
57	MG	YA	3180	1/1	0.89	0.71	5,5,5,5	0
57	MG	QA	1657	1/1	0.89	0.10	19,19,19,19	0
57	MG	RA	3114	1/1	0.89	0.18	3,3,3,3	0
57	MG	QA	1612	1/1	0.89	0.38	4,4,4,4	0
57	MG	YA	3103	1/1	0.89	0.15	31,31,31,31	0
57	MG	RA	3178	1/1	0.89	0.37	5,5,5,5	0
57	MG	YA	3027	1/1	0.89	0.17	1,1,1,1	0
57	MG	YA	3116	1/1	0.89	0.40	11,11,11,11	0
57	MG	YA	3040	1/1	0.89	0.69	50,50,50,50	0
57	MG	QA	1608	1/1	0.89	0.23	63,63,63,63	0
57	MG	YA	3005	1/1	0.89	0.21	2,2,2,2	0
57	MG	YA	3001	1/1	0.89	1.16	50,50,50,50	0
57	MG	RA	3202	1/1	0.89	0.31	2,2,2,2	0
57	MG	YA	3178	1/1	0.89	0.52	32,32,32,32	0
57	MG	RA	3240	1/1	0.89	0.67	12,12,12,12	0
57	MG	YA	3207	1/1	0.89	0.25	0,0,0,0	0
57	MG	RA	3054	1/1	0.89	0.31	4,4,4,4	0
57	MG	YA	3246	1/1	0.89	0.51	2,2,2,2	0
57	MG	RA	3221	1/1	0.89	0.69	79,79,79,79	0
57	MG	RD	301	1/1	0.89	0.28	15,15,15,15	0
57	MG	YA	3055	1/1	0.90	0.19	24,24,24,24	0
57	MG	YA	3145	1/1	0.90	0.22	25,25,25,25	0
57	MG	RA	3203	1/1	0.90	0.20	34,34,34,34	0
57	MG	XA	1659	1/1	0.90	0.16	15,15,15,15	0
57	MG	YA	3112	1/1	0.90	0.21	19,19,19,19	0
57	MG	YA	3226	1/1	0.90	0.23	10,10,10,10	0
57	MG	RA	3220	1/1	0.90	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3190	1/1	0.90	0.51	17,17,17,17	0
57	MG	YA	3213	1/1	0.90	0.31	15,15,15,15	0
57	MG	YA	3173	1/1	0.90	0.20	14,14,14,14	0
57	MG	RA	3153	1/1	0.90	0.41	36,36,36,36	0
57	MG	YA	3073	1/1	0.90	0.29	4,4,4,4	0
57	MG	RA	3072	1/1	0.90	0.35	0,0,0,0	0
57	MG	RA	3149	1/1	0.90	0.62	17,17,17,17	0
57	MG	RA	3197	1/1	0.90	0.16	9,9,9,9	0
57	MG	RA	3010	1/1	0.90	0.31	56,56,56,56	0
57	MG	RA	3038	1/1	0.90	0.73	50,50,50,50	0
57	MG	RA	3093	1/1	0.90	0.71	50,50,50,50	0
57	MG	RA	3167	1/1	0.90	0.09	26,26,26,26	0
57	MG	RA	3092	1/1	0.90	0.23	59,59,59,59	0
57	MG	QA	1633	1/1	0.90	0.43	1,1,1,1	0
57	MG	RA	3216	1/1	0.90	0.29	1,1,1,1	0
57	MG	RA	3030	1/1	0.90	0.73	50,50,50,50	0
57	MG	YA	3075	1/1	0.90	1.18	50,50,50,50	0
57	MG	XA	1629	1/1	0.90	0.14	32,32,32,32	0
57	MG	XA	1603	1/1	0.90	0.95	50,50,50,50	0
57	MG	RA	3006	1/1	0.90	1.06	50,50,50,50	0
57	MG	YA	3221	1/1	0.91	0.24	7,7,7,7	0
57	MG	RA	3239	1/1	0.91	0.79	10,10,10,10	0
57	MG	YA	3214	1/1	0.91	0.24	23,23,23,23	0
57	MG	RA	3210	1/1	0.91	0.15	11,11,11,11	0
57	MG	YA	3248	1/1	0.91	0.87	15,15,15,15	0
57	MG	QA	1611	1/1	0.91	0.27	4,4,4,4	0
57	MG	YA	3143	1/1	0.91	0.23	11,11,11,11	0
57	MG	YA	3179	1/1	0.91	0.27	20,20,20,20	0
57	MG	YA	3244	1/1	0.91	0.48	6,6,6,6	0
57	MG	YA	3098	1/1	0.91	0.84	50,50,50,50	0
57	MG	YA	3020	1/1	0.91	0.58	6,6,6,6	0
57	MG	RA	3190	1/1	0.91	0.14	4,4,4,4	0
57	MG	YA	3080	1/1	0.91	0.83	50,50,50,50	0
57	MG	RA	3026	1/1	0.91	0.17	13,13,13,13	0
57	MG	XA	1660	1/1	0.91	0.10	19,19,19,19	0
57	MG	RA	3087	1/1	0.91	0.43	0,0,0,0	0
57	MG	RA	3188	1/1	0.91	0.13	16,16,16,16	0
57	MG	RA	3090	1/1	0.91	0.45	4,4,4,4	0
57	MG	RA	3014	1/1	0.91	0.90	50,50,50,50	0
57	MG	RA	3118	1/1	0.91	0.20	1,1,1,1	0
57	MG	RA	3134	1/1	0.91	0.09	23,23,23,23	0
57	MG	RA	3035	1/1	0.91	0.81	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	RA	3148	1/1	0.91	0.13	0,0,0,0	0
57	MG	RA	3011	1/1	0.91	0.38	7,7,7,7	0
57	MG	QA	1617	1/1	0.91	0.44	2,2,2,2	0
57	MG	YA	3172	1/1	0.91	0.14	19,19,19,19	0
57	MG	YA	3081	1/1	0.91	0.28	7,7,7,7	0
57	MG	RA	3028	1/1	0.91	0.23	23,23,23,23	0
57	MG	XA	1667	1/1	0.91	0.14	4,4,4,4	0
57	MG	XA	1648	1/1	0.91	0.19	10,10,10,10	0
57	MG	YA	3019	1/1	0.91	0.80	50,50,50,50	0
57	MG	YA	3205	1/1	0.91	0.24	40,40,40,40	0
57	MG	RA	3182	1/1	0.91	0.50	10,10,10,10	0
57	MG	YA	3016	1/1	0.91	0.20	8,8,8,8	0
57	MG	RA	3218	1/1	0.91	0.35	10,10,10,10	0
57	MG	YA	3035	1/1	0.91	0.80	50,50,50,50	0
57	MG	QA	1627	1/1	0.91	0.15	1,1,1,1	0
57	MG	YA	3189	1/1	0.91	0.42	7,7,7,7	0
57	MG	RA	3142	1/1	0.92	0.43	8,8,8,8	0
57	MG	RA	3056	1/1	0.92	0.20	0,0,0,0	0
57	MG	RA	3162	1/1	0.92	0.21	18,18,18,18	0
57	MG	YA	3258	1/1	0.92	0.52	4,4,4,4	0
57	MG	XA	1630	1/1	0.92	0.31	1,1,1,1	0
57	MG	XA	1631	1/1	0.92	0.18	10,10,10,10	0
57	MG	YA	3086	1/1	0.92	0.42	19,19,19,19	0
57	MG	RA	3045	1/1	0.92	0.28	0,0,0,0	0
57	MG	RA	3185	1/1	0.92	0.19	3,3,3,3	0
57	MG	QA	1614	1/1	0.92	0.24	21,21,21,21	0
57	MG	XA	1643	1/1	0.92	0.75	50,50,50,50	0
57	MG	QA	1626	1/1	0.92	0.17	17,17,17,17	0
57	MG	YA	3194	1/1	0.92	0.19	15,15,15,15	0
57	MG	XA	1646	1/1	0.92	0.17	8,8,8,8	0
57	MG	XV	101	1/1	0.92	0.39	1,1,1,1	0
57	MG	RA	3214	1/1	0.92	0.21	43,43,43,43	0
57	MG	RA	3195	1/1	0.92	0.14	23,23,23,23	0
57	MG	RA	3101	1/1	0.92	0.27	9,9,9,9	0
57	MG	YA	3188	1/1	0.92	0.12	36,36,36,36	0
57	MG	YA	3099	1/1	0.92	0.79	50,50,50,50	0
57	MG	QA	1656	1/1	0.92	0.09	63,63,63,63	0
57	MG	YA	3182	1/1	0.92	0.63	14,14,14,14	0
57	MG	XA	1657	1/1	0.92	0.26	4,4,4,4	0
57	MG	RA	3238	1/1	0.92	0.71	3,3,3,3	0
57	MG	RA	3224	1/1	0.92	0.17	16,16,16,16	0
57	MG	RA	3244	1/1	0.92	0.20	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3054	1/1	0.92	0.59	50,50,50,50	0
57	MG	XA	1651	1/1	0.92	0.17	84,84,84,84	0
57	MG	YA	3032	1/1	0.92	0.52	50,50,50,50	0
57	MG	YA	3227	1/1	0.92	0.17	15,15,15,15	0
57	MG	YA	3071	1/1	0.92	0.32	6,6,6,6	0
57	MG	XA	1621	1/1	0.92	0.57	6,6,6,6	0
57	MG	XA	1666	1/1	0.92	0.21	34,34,34,34	0
57	MG	RA	3013	1/1	0.92	0.35	0,0,0,0	0
57	MG	YA	3160	1/1	0.92	0.38	4,4,4,4	0
57	MG	YA	3140	1/1	0.92	0.22	19,19,19,19	0
57	MG	XA	1669	1/1	0.92	0.08	15,15,15,15	0
57	MG	QA	1646	1/1	0.92	0.58	11,11,11,11	0
57	MG	XA	1602	1/1	0.92	0.92	50,50,50,50	0
57	MG	YA	3149	1/1	0.92	0.76	7,7,7,7	0
57	MG	RA	3233	1/1	0.93	1.47	50,50,50,50	0
57	MG	YA	3219	1/1	0.93	0.10	22,22,22,22	0
57	MG	YA	3211	1/1	0.93	0.13	3,3,3,3	0
57	MG	YA	3056	1/1	0.93	0.88	50,50,50,50	0
57	MG	RA	3031	1/1	0.93	0.77	50,50,50,50	0
57	MG	YA	3090	1/1	0.93	0.22	17,17,17,17	0
57	MG	XA	1614	1/1	0.93	0.31	25,25,25,25	0
57	MG	XA	1654	1/1	0.93	0.43	17,17,17,17	0
57	MG	RA	3154	1/1	0.93	0.45	6,6,6,6	0
57	MG	RA	3104	1/1	0.93	0.13	5,5,5,5	0
57	MG	YA	3048	1/1	0.93	0.46	50,50,50,50	0
57	MG	RA	3234	1/1	0.93	0.85	50,50,50,50	0
57	MG	RA	3215	1/1	0.93	0.28	14,14,14,14	0
57	MG	QA	1642	1/1	0.93	0.16	9,9,9,9	0
57	MG	RA	3226	1/1	0.93	0.32	29,29,29,29	0
57	MG	RA	3108	1/1	0.93	0.24	5,5,5,5	0
57	MG	QA	1650	1/1	0.93	0.23	8,8,8,8	0
57	MG	RA	3171	1/1	0.93	0.44	15,15,15,15	0
57	MG	YA	3265	1/1	0.93	0.65	11,11,11,11	0
57	MG	QA	1659	1/1	0.93	0.19	4,4,4,4	0
57	MG	YA	3142	1/1	0.93	0.27	9,9,9,9	0
57	MG	XA	1608	1/1	0.93	0.18	50,50,50,50	0
57	MG	RA	3016	1/1	0.93	0.65	50,50,50,50	0
57	MG	RA	3172	1/1	0.93	0.27	17,17,17,17	0
57	MG	YA	3158	1/1	0.93	0.24	6,6,6,6	0
57	MG	YA	3199	1/1	0.93	0.18	11,11,11,11	0
57	MG	YA	3036	1/1	0.93	0.19	3,3,3,3	0
57	MG	RA	3187	1/1	0.93	0.16	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3255	1/1	0.93	1.37	50,50,50,50	0
57	MG	YA	3102	1/1	0.93	0.84	6,6,6,6	0
57	MG	YA	3072	1/1	0.93	0.49	50,50,50,50	0
57	MG	YA	3132	1/1	0.93	0.37	26,26,26,26	0
57	MG	XA	1670	1/1	0.93	0.19	44,44,44,44	0
57	MG	YA	3243	1/1	0.93	0.77	50,50,50,50	0
57	MG	RA	3147	1/1	0.93	0.24	6,6,6,6	0
57	MG	QA	1605	1/1	0.93	0.52	4,4,4,4	0
57	MG	YA	3100	1/1	0.93	0.71	0,0,0,0	0
57	MG	XA	1633	1/1	0.93	0.18	13,13,13,13	0
57	MG	RA	3008	1/1	0.93	0.28	0,0,0,0	0
57	MG	RA	3046	1/1	0.93	0.45	0,0,0,0	0
57	MG	YA	3166	1/1	0.94	0.13	14,14,14,14	0
57	MG	YA	3222	1/1	0.94	0.11	2,2,2,2	0
57	MG	YA	3241	1/1	0.94	0.27	13,13,13,13	0
57	MG	QA	1661	1/1	0.94	0.10	44,44,44,44	0
57	MG	YA	3007	1/1	0.94	0.22	1,1,1,1	0
57	MG	QA	1630	1/1	0.94	0.13	14,14,14,14	0
57	MG	YA	3141	1/1	0.94	0.10	18,18,18,18	0
57	MG	YA	3003	1/1	0.94	0.46	50,50,50,50	0
57	MG	RA	3189	1/1	0.94	0.17	16,16,16,16	0
57	MG	YA	3109	1/1	0.94	0.20	9,9,9,9	0
57	MG	RA	3213	1/1	0.94	0.31	10,10,10,10	0
57	MG	RA	3232	1/1	0.94	0.30	5,5,5,5	0
57	MG	XA	1640	1/1	0.94	0.14	119,119,119,119	0
57	MG	YA	3181	1/1	0.94	0.57	5,5,5,5	0
57	MG	RU	201	1/1	0.94	0.16	86,86,86,86	0
59	ZN	XD	301	1/1	0.94	0.39	50,50,50,50	0
57	MG	RA	3200	1/1	0.94	0.20	31,31,31,31	0
57	MG	YA	3195	1/1	0.94	0.19	21,21,21,21	0
57	MG	YA	3186	1/1	0.94	0.18	10,10,10,10	0
57	MG	RA	3052	1/1	0.94	0.48	50,50,50,50	0
57	MG	RF	301	1/1	0.94	0.27	10,10,10,10	0
57	MG	RA	3144	1/1	0.94	0.18	29,29,29,29	0
57	MG	XA	1619	1/1	0.94	0.41	8,8,8,8	0
57	MG	RA	3048	1/1	0.94	1.15	50,50,50,50	0
57	MG	YA	3065	1/1	0.94	0.75	8,8,8,8	0
57	MG	YA	3018	1/1	0.94	0.82	50,50,50,50	0
57	MG	YA	3133	1/1	0.94	0.08	12,12,12,12	0
57	MG	RA	3113	1/1	0.94	0.30	1,1,1,1	0
57	MG	YA	3049	1/1	0.94	1.10	50,50,50,50	0
57	MG	XA	1658	1/1	0.94	0.28	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3002	1/1	0.94	0.19	8,8,8,8	0
57	MG	YA	3147	1/1	0.94	0.17	0,0,0,0	0
57	MG	RA	3130	1/1	0.94	0.17	19,19,19,19	0
57	MG	YA	3251	1/1	0.94	1.32	50,50,50,50	0
57	MG	RA	3075	1/1	0.94	0.36	37,37,37,37	0
57	MG	RA	3173	1/1	0.94	0.35	3,3,3,3	0
57	MG	RA	3243	1/1	0.94	0.38	18,18,18,18	0
57	MG	RA	3176	1/1	0.94	0.28	30,30,30,30	0
57	MG	YA	3093	1/1	0.94	0.48	4,4,4,4	0
57	MG	RA	3168	1/1	0.94	0.23	10,10,10,10	0
57	MG	YE	301	1/1	0.94	0.24	1,1,1,1	0
57	MG	QA	1621	1/1	0.94	0.19	35,35,35,35	0
57	MG	RA	3120	1/1	0.94	0.20	31,31,31,31	0
57	MG	RE	302	1/1	0.94	0.20	15,15,15,15	0
57	MG	YA	3111	1/1	0.94	0.24	7,7,7,7	0
57	MG	YA	3260	1/1	0.94	0.57	50,50,50,50	0
57	MG	YA	3026	1/1	0.94	1.28	50,50,50,50	0
57	MG	RA	3037	1/1	0.94	0.43	0,0,0,0	0
57	MG	YA	3084	1/1	0.94	0.28	2,2,2,2	0
57	MG	RA	3019	1/1	0.94	1.19	50,50,50,50	0
57	MG	RA	3061	1/1	0.94	0.77	50,50,50,50	0
57	MG	RA	3193	1/1	0.94	0.15	17,17,17,17	0
57	MG	RA	3103	1/1	0.94	0.22	8,8,8,8	0
57	MG	XV	102	1/1	0.94	0.16	16,16,16,16	0
57	MG	RA	3242	1/1	0.94	0.61	8,8,8,8	0
57	MG	QA	1649	1/1	0.95	0.10	19,19,19,19	0
57	MG	XA	1668	1/1	0.95	0.27	6,6,6,6	0
57	MG	YA	3039	1/1	0.95	0.23	0,0,0,0	0
57	MG	YA	3044	1/1	0.95	0.53	16,16,16,16	0
57	MG	RP	201	1/1	0.95	0.43	85,85,85,85	0
57	MG	RA	3107	1/1	0.95	0.27	9,9,9,9	0
57	MG	RA	3161	1/1	0.95	0.14	8,8,8,8	0
57	MG	QA	1652	1/1	0.95	0.21	24,24,24,24	0
57	MG	R5	101	1/1	0.95	0.15	14,14,14,14	0
57	MG	YA	3203	1/1	0.95	0.40	29,29,29,29	0
57	MG	YA	3229	1/1	0.95	0.13	5,5,5,5	0
57	MG	RA	3076	1/1	0.95	0.17	3,3,3,3	0
57	MG	YA	3124	1/1	0.95	0.27	13,13,13,13	0
59	ZN	XN	101	1/1	0.95	0.18	59,59,59,59	0
57	MG	YA	3034	1/1	0.95	0.34	7,7,7,7	0
57	MG	XA	1632	1/1	0.95	0.41	2,2,2,2	0
57	MG	YA	3033	1/1	0.95	0.73	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	1642	1/1	0.95	0.23	11,11,11,11	0
57	MG	RA	3179	1/1	0.95	0.24	10,10,10,10	0
57	MG	RA	3155	1/1	0.95	0.19	9,9,9,9	0
57	MG	YA	3092	1/1	0.95	0.40	2,2,2,2	0
57	MG	YA	3135	1/1	0.95	0.39	9,9,9,9	0
57	MG	YA	3037	1/1	0.95	0.34	3,3,3,3	0
57	MG	RA	3080	1/1	0.95	0.16	5,5,5,5	0
57	MG	YA	3089	1/1	0.95	0.24	13,13,13,13	0
57	MG	RA	3057	1/1	0.95	0.77	50,50,50,50	0
57	MG	RA	3177	1/1	0.95	0.27	30,30,30,30	0
57	MG	Y5	101	1/1	0.95	0.14	2,2,2,2	0
57	MG	YA	3059	1/1	0.95	0.30	3,3,3,3	0
57	MG	RA	3077	1/1	0.95	0.39	50,50,50,50	0
57	MG	XA	1624	1/1	0.95	0.60	8,8,8,8	0
57	MG	RA	3143	1/1	0.95	0.08	12,12,12,12	0
57	MG	QA	1625	1/1	0.95	0.08	74,74,74,74	0
57	MG	YX	101	1/1	0.95	0.41	50,50,50,50	0
57	MG	YA	3008	1/1	0.95	0.21	1,1,1,1	0
57	MG	YA	3002	1/1	0.95	0.73	50,50,50,50	0
57	MG	XA	1645	1/1	0.95	0.45	8,8,8,8	0
57	MG	QA	1624	1/1	0.95	0.29	16,16,16,16	0
57	MG	YA	3209	1/1	0.95	0.20	9,9,9,9	0
57	MG	XA	1647	1/1	0.95	0.34	11,11,11,11	0
57	MG	RA	3132	1/1	0.95	0.38	7,7,7,7	0
57	MG	RA	3089	1/1	0.95	0.38	0,0,0,0	0
57	MG	RA	3047	1/1	0.95	0.16	2,2,2,2	0
57	MG	RA	3208	1/1	0.95	0.14	50,50,50,50	0
57	MG	QA	1613	1/1	0.95	0.42	1,1,1,1	0
57	MG	QA	1619	1/1	0.95	0.25	29,29,29,29	0
57	MG	RA	3100	1/1	0.95	1.01	50,50,50,50	0
57	MG	YA	3021	1/1	0.95	0.56	50,50,50,50	0
57	MG	RA	3133	1/1	0.95	0.14	4,4,4,4	0
57	MG	RA	3126	1/1	0.95	0.22	14,14,14,14	0
57	MG	QA	1604	1/1	0.95	0.37	7,7,7,7	0
57	MG	RA	3165	1/1	0.95	0.25	3,3,3,3	0
57	MG	YA	3144	1/1	0.95	0.54	6,6,6,6	0
57	MG	YA	3233	1/1	0.95	0.10	3,3,3,3	0
57	MG	YA	3097	1/1	0.95	0.70	50,50,50,50	0
57	MG	RA	3135	1/1	0.95	0.13	28,28,28,28	0
57	MG	RA	3169	1/1	0.95	0.12	19,19,19,19	0
57	MG	RA	3098	1/1	0.95	0.40	4,4,4,4	0
57	MG	YA	3057	1/1	0.95	0.50	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3064	1/1	0.95	0.17	4,4,4,4	0
57	MG	YA	3082	1/1	0.95	0.58	50,50,50,50	0
57	MG	QA	1653	1/1	0.95	0.11	6,6,6,6	0
57	MG	RA	3102	1/1	0.95	0.13	10,10,10,10	0
57	MG	YA	3106	1/1	0.95	0.49	50,50,50,50	0
57	MG	YA	3091	1/1	0.95	0.58	12,12,12,12	0
57	MG	RA	3158	1/1	0.95	0.26	15,15,15,15	0
57	MG	XA	1672	1/1	0.95	0.26	5,5,5,5	0
57	MG	RA	3097	1/1	0.96	0.60	11,11,11,11	0
57	MG	QA	1641	1/1	0.96	0.08	3,3,3,3	0
57	MG	RA	3192	1/1	0.96	0.16	27,27,27,27	0
57	MG	YA	3155	1/1	0.96	0.18	8,8,8,8	0
57	MG	YA	3061	1/1	0.96	0.49	9,9,9,9	0
57	MG	RA	3012	1/1	0.96	0.27	1,1,1,1	0
57	MG	XA	1655	1/1	0.96	0.22	7,7,7,7	0
57	MG	XA	1611	1/1	0.96	0.33	1,1,1,1	0
57	MG	RE	301	1/1	0.96	0.13	2,2,2,2	0
57	MG	RA	3081	1/1	0.96	0.34	10,10,10,10	0
57	MG	XA	1604	1/1	0.96	1.07	50,50,50,50	0
57	MG	XA	1663	1/1	0.96	0.17	3,3,3,3	0
57	MG	RA	3083	1/1	0.96	0.39	3,3,3,3	0
57	MG	YA	3152	1/1	0.96	0.39	7,7,7,7	0
57	MG	YA	3212	1/1	0.96	0.24	8,8,8,8	0
57	MG	YA	3200	1/1	0.96	0.15	35,35,35,35	0
57	MG	XA	1610	1/1	0.96	0.26	1,1,1,1	0
57	MG	QA	1620	1/1	0.96	0.12	21,21,21,21	0
57	MG	YA	3069	1/1	0.96	0.10	8,8,8,8	0
57	MG	YB	203	1/1	0.96	0.18	17,17,17,17	0
57	MG	YA	3225	1/1	0.96	0.36	23,23,23,23	0
57	MG	YA	3013	1/1	0.96	0.37	1,1,1,1	0
57	MG	RA	3073	1/1	0.96	0.28	36,36,36,36	0
57	MG	RA	3235	1/1	0.96	0.14	2,2,2,2	0
57	MG	YA	3094	1/1	0.96	0.38	8,8,8,8	0
57	MG	RA	3141	1/1	0.96	0.45	5,5,5,5	0
57	MG	QA	1648	1/1	0.96	0.19	16,16,16,16	0
57	MG	YA	3146	1/1	0.96	0.21	6,6,6,6	0
57	MG	RA	3060	1/1	0.96	0.70	13,13,13,13	0
57	MG	YA	3210	1/1	0.96	0.30	30,30,30,30	0
57	MG	QA	1615	1/1	0.96	0.18	54,54,54,54	0
57	MG	YA	3175	1/1	0.96	0.12	2,2,2,2	0
57	MG	YA	3050	1/1	0.96	0.50	50,50,50,50	0
57	MG	QA	1662	1/1	0.96	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3227	1/1	0.96	0.14	39,39,39,39	0
57	MG	YA	3256	1/1	0.96	0.14	9,9,9,9	0
57	MG	YA	3121	1/1	0.96	0.15	8,8,8,8	0
57	MG	RA	3105	1/1	0.96	0.21	1,1,1,1	0
57	MG	RA	3022	1/1	0.96	0.25	5,5,5,5	0
57	MG	YA	3017	1/1	0.96	0.28	7,7,7,7	0
57	MG	RA	3042	1/1	0.96	0.58	50,50,50,50	0
57	MG	YA	3015	1/1	0.96	0.77	50,50,50,50	0
57	MG	RA	3033	1/1	0.96	0.60	16,16,16,16	0
57	MG	RA	3138	1/1	0.96	0.37	8,8,8,8	0
57	MG	RA	3170	1/1	0.96	0.41	2,2,2,2	0
59	ZN	QN	101	1/1	0.96	0.13	56,56,56,56	0
57	MG	RA	3111	1/1	0.96	0.44	4,4,4,4	0
57	MG	QA	1644	1/1	0.96	0.29	24,24,24,24	0
57	MG	RA	3018	1/1	0.96	0.28	3,3,3,3	0
57	MG	YA	3120	1/1	0.96	0.16	16,16,16,16	0
57	MG	YA	3201	1/1	0.96	0.16	10,10,10,10	0
57	MG	RA	3152	1/1	0.96	0.16	26,26,26,26	0
57	MG	XA	1617	1/1	0.96	0.26	2,2,2,2	0
57	MG	RA	3124	1/1	0.96	0.29	19,19,19,19	0
57	MG	XA	1620	1/1	0.96	0.15	0,0,0,0	0
57	MG	YA	3014	1/1	0.96	0.39	1,1,1,1	0
57	MG	YA	3192	1/1	0.96	0.15	15,15,15,15	0
57	MG	YA	3139	1/1	0.96	0.27	13,13,13,13	0
57	MG	RA	3009	1/1	0.96	0.57	7,7,7,7	0
57	MG	YA	3123	1/1	0.96	0.18	0,0,0,0	0
57	MG	RA	3163	1/1	0.96	0.18	38,38,38,38	0
57	MG	YA	3237	1/1	0.96	0.20	38,38,38,38	0
57	MG	YA	3076	1/1	0.96	0.39	1,1,1,1	0
57	MG	RA	3112	1/1	0.96	0.38	2,2,2,2	0
57	MG	YA	3114	1/1	0.96	0.29	16,16,16,16	0
57	MG	XA	1644	1/1	0.96	0.30	11,11,11,11	0
57	MG	QA	1647	1/1	0.96	0.15	55,55,55,55	0
57	MG	RA	3086	1/1	0.96	0.30	50,50,50,50	0
57	MG	YQ	201	1/1	0.96	0.20	79,79,79,79	0
57	MG	YA	3009	1/1	0.96	0.74	50,50,50,50	0
57	MG	YA	3029	1/1	0.97	0.32	6,6,6,6	0
57	MG	YA	3068	1/1	0.97	0.27	1,1,1,1	0
57	MG	RA	3015	1/1	0.97	0.29	15,15,15,15	0
57	MG	YA	3122	1/1	0.97	0.58	50,50,50,50	0
57	MG	QA	1632	1/1	0.97	0.11	71,71,71,71	0
57	MG	RA	3088	1/1	0.97	0.25	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3183	1/1	0.97	0.49	11,11,11,11	0
57	MG	RA	3040	1/1	0.97	0.23	11,11,11,11	0
57	MG	RR	201	1/1	0.97	0.27	9,9,9,9	0
57	MG	RA	3032	1/1	0.97	0.68	50,50,50,50	0
57	MG	XA	1613	1/1	0.97	0.08	16,16,16,16	0
57	MG	XA	1627	1/1	0.97	0.35	9,9,9,9	0
57	MG	YA	3046	1/1	0.97	0.27	12,12,12,12	0
57	MG	RA	3017	1/1	0.97	0.30	0,0,0,0	0
57	MG	RA	3145	1/1	0.97	0.42	3,3,3,3	0
57	MG	YA	3165	1/1	0.97	0.20	42,42,42,42	0
57	MG	YA	3263	1/1	0.97	0.29	2,2,2,2	0
57	MG	YA	3052	1/1	0.97	0.33	5,5,5,5	0
57	MG	YA	3078	1/1	0.97	0.26	10,10,10,10	0
57	MG	XA	1618	1/1	0.97	0.31	4,4,4,4	0
57	MG	YA	3110	1/1	0.97	0.16	5,5,5,5	0
57	MG	RA	3062	1/1	0.97	0.49	2,2,2,2	0
57	MG	YA	3129	1/1	0.97	0.11	1,1,1,1	0
57	MG	QM	201	1/1	0.97	0.10	34,34,34,34	0
57	MG	YA	3177	1/1	0.97	0.07	92,92,92,92	0
57	MG	YA	3208	1/1	0.97	0.16	0,0,0,0	0
57	MG	XA	1637	1/1	0.97	0.27	13,13,13,13	0
57	MG	YA	3164	1/1	0.97	0.76	97,97,97,97	0
57	MG	RA	3236	1/1	0.97	0.49	2,2,2,2	0
57	MG	XA	1612	1/1	0.97	0.22	23,23,23,23	0
57	MG	XA	1636	1/1	0.97	0.23	9,9,9,9	0
57	MG	YP	202	1/1	0.97	0.33	5,5,5,5	0
57	MG	QA	1616	1/1	0.97	0.28	10,10,10,10	0
57	MG	YA	3095	1/1	0.97	0.32	8,8,8,8	0
57	MG	YA	3088	1/1	0.97	0.26	3,3,3,3	0
57	MG	YA	3216	1/1	0.97	0.25	30,30,30,30	0
57	MG	RA	3115	1/1	0.97	0.16	8,8,8,8	0
57	MG	YA	3196	1/1	0.97	0.27	76,76,76,76	0
57	MG	YA	3184	1/1	0.97	0.32	50,50,50,50	0
57	MG	RA	3084	1/1	0.97	0.31	6,6,6,6	0
57	MG	YA	3022	1/1	0.97	0.75	50,50,50,50	0
57	MG	YA	3159	1/1	0.97	0.19	22,22,22,22	0
57	MG	RA	3117	1/1	0.97	0.35	4,4,4,4	0
57	MG	YA	3224	1/1	0.97	0.80	50,50,50,50	0
57	MG	YA	3231	1/1	0.97	0.35	11,11,11,11	0
57	MG	YA	3257	1/1	0.97	0.78	50,50,50,50	0
57	MG	RA	3059	1/1	0.97	0.50	50,50,50,50	0
57	MG	XA	1639	1/1	0.97	0.06	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3125	1/1	0.97	0.08	14,14,14,14	0
57	MG	YA	3252	1/1	0.97	0.15	4,4,4,4	0
57	MG	RA	3095	1/1	0.97	0.42	24,24,24,24	0
57	MG	RA	3025	1/1	0.97	0.25	7,7,7,7	0
57	MG	YA	3077	1/1	0.97	0.22	0,0,0,0	0
57	MG	YA	3004	1/1	0.97	0.43	5,5,5,5	0
57	MG	RA	3198	1/1	0.97	0.06	35,35,35,35	0
57	MG	YA	3010	1/1	0.97	0.60	50,50,50,50	0
57	MG	QA	1663	1/1	0.98	0.09	19,19,19,19	0
57	MG	XA	1622	1/1	0.98	0.11	6,6,6,6	0
57	MG	RB	202	1/1	0.98	0.20	15,15,15,15	0
57	MG	RA	3067	1/1	0.98	0.17	6,6,6,6	0
57	MG	YP	201	1/1	0.98	0.05	83,83,83,83	0
57	MG	RA	3068	1/1	0.98	0.48	4,4,4,4	0
57	MG	YA	3167	1/1	0.98	0.18	39,39,39,39	0
57	MG	RA	3209	1/1	0.98	0.12	44,44,44,44	0
57	MG	QA	1635	1/1	0.98	0.14	11,11,11,11	0
57	MG	QA	1645	1/1	0.98	0.27	37,37,37,37	0
57	MG	YA	3161	1/1	0.98	0.35	14,14,14,14	0
57	MG	RA	3036	1/1	0.98	0.40	0,0,0,0	0
57	MG	QA	1654	1/1	0.98	0.12	17,17,17,17	0
57	MG	YA	3127	1/1	0.98	0.10	12,12,12,12	0
57	MG	QA	1609	1/1	0.98	0.12	10,10,10,10	0
57	MG	RA	3082	1/1	0.98	0.14	5,5,5,5	0
57	MG	QA	1606	1/1	0.98	0.06	23,23,23,23	0
57	MG	RA	3096	1/1	0.98	0.48	11,11,11,11	0
57	MG	RA	3029	1/1	0.98	0.24	5,5,5,5	0
57	MG	RA	3129	1/1	0.98	0.10	19,19,19,19	0
57	MG	RA	3074	1/1	0.98	0.19	20,20,20,20	0
57	MG	YA	3118	1/1	0.98	0.46	12,12,12,12	0
57	MG	RA	3110	1/1	0.98	0.10	15,15,15,15	0
57	MG	YA	3042	1/1	0.98	0.46	50,50,50,50	0
57	MG	RA	3191	1/1	0.98	0.26	38,38,38,38	0
57	MG	YA	3218	1/1	0.98	0.27	5,5,5,5	0
57	MG	RA	3066	1/1	0.98	0.24	23,23,23,23	0
57	MG	XA	1626	1/1	0.98	0.21	1,1,1,1	0
57	MG	RA	3094	1/1	0.98	0.36	3,3,3,3	0
57	MG	YA	3025	1/1	0.98	0.27	3,3,3,3	0
59	ZN	QD	301	1/1	0.98	0.19	12,12,12,12	0
57	MG	RA	3024	1/1	0.98	0.36	15,15,15,15	0
57	MG	YA	3136	1/1	0.98	0.12	1,1,1,1	0
57	MG	YA	3101	1/1	0.98	0.12	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3204	1/1	0.98	0.53	15,15,15,15	0
57	MG	YA	3239	1/1	0.98	0.12	13,13,13,13	0
57	MG	QA	1636	1/1	0.98	0.18	11,11,11,11	0
57	MG	RA	3099	1/1	0.98	0.33	20,20,20,20	0
57	MG	YA	3108	1/1	0.98	0.12	10,10,10,10	0
57	MG	RA	3044	1/1	0.98	0.23	8,8,8,8	0
57	MG	RA	3053	1/1	0.98	0.63	50,50,50,50	0
57	MG	RA	3070	1/1	0.98	0.15	21,21,21,21	0
57	MG	RA	3109	1/1	0.98	0.25	11,11,11,11	0
57	MG	YA	3060	1/1	0.98	0.09	9,9,9,9	0
57	MG	RB	201	1/1	0.98	0.08	38,38,38,38	0
57	MG	YA	3028	1/1	0.98	0.22	8,8,8,8	0
57	MG	YA	3023	1/1	0.98	0.46	5,5,5,5	0
57	MG	YA	3104	1/1	0.98	0.14	11,11,11,11	0
57	MG	YA	3107	1/1	0.98	0.45	2,2,2,2	0
57	MG	YA	3096	1/1	0.99	0.24	17,17,17,17	0
57	MG	YA	3240	1/1	0.99	0.14	15,15,15,15	0
57	MG	QA	1634	1/1	0.99	0.12	44,44,44,44	0
57	MG	YA	3038	1/1	0.99	0.25	5,5,5,5	0
57	MG	XA	1623	1/1	0.99	0.22	23,23,23,23	0
57	MG	RA	3106	1/1	0.99	0.26	3,3,3,3	0
57	MG	YA	3238	1/1	0.99	0.10	33,33,33,33	0
57	MG	YA	3067	1/1	0.99	0.45	7,7,7,7	0
57	MG	RA	3079	1/1	0.99	0.40	0,0,0,0	0
57	MG	RA	3199	1/1	0.99	0.16	1,1,1,1	0
57	MG	YA	3087	1/1	0.99	0.37	6,6,6,6	0
57	MG	RA	3137	1/1	0.99	0.10	3,3,3,3	0
57	MG	YA	3011	1/1	0.99	0.41	3,3,3,3	0
57	MG	YA	3066	1/1	0.99	0.19	9,9,9,9	0
57	MG	YA	3230	1/1	0.99	0.20	19,19,19,19	0
57	MG	RA	3159	1/1	0.99	0.14	18,18,18,18	0
57	MG	YA	3058	1/1	0.99	0.20	13,13,13,13	0
57	MG	RA	3058	1/1	0.99	0.29	0,0,0,0	0
57	MG	QA	1607	1/1	0.99	0.06	30,30,30,30	0
57	MG	YA	3174	1/1	0.99	0.37	3,3,3,3	0
57	MG	YA	3228	1/1	0.99	0.17	67,67,67,67	0
57	MG	RA	3055	1/1	0.99	0.28	12,12,12,12	0
57	MG	QA	1629	1/1	0.99	0.08	38,38,38,38	0
57	MG	YA	3051	1/1	0.99	0.21	5,5,5,5	0
57	MG	YA	3063	1/1	0.99	0.29	15,15,15,15	0
57	MG	QA	1660	1/1	0.99	0.33	16,16,16,16	0
57	MG	RA	3150	1/1	0.99	0.26	4,4,4,4	0

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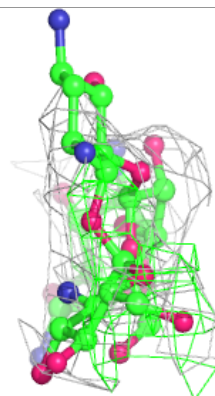
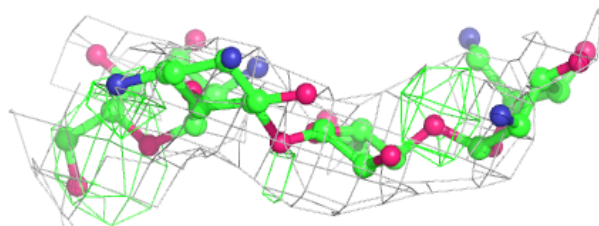
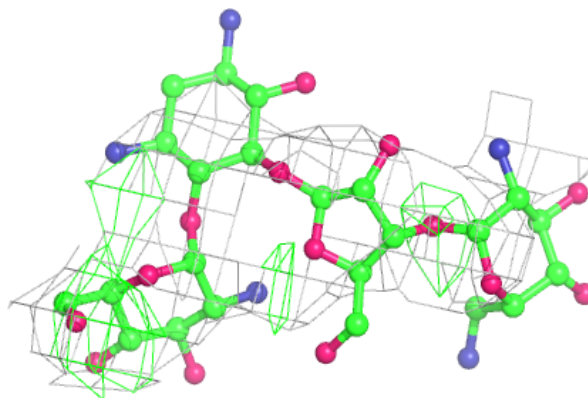
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1661	1/1	0.99	0.07	14,14,14,14	0
57	MG	RA	3049	1/1	0.99	0.34	1,1,1,1	0

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

**Electron density around PAR QA 1666:**

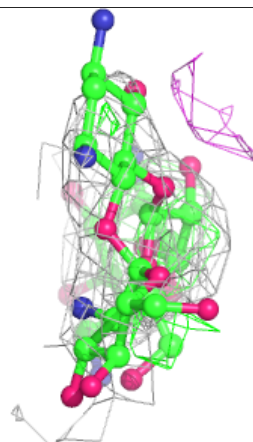
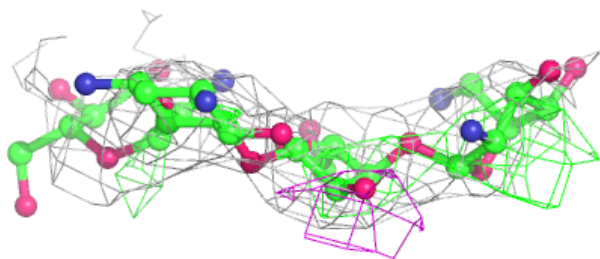
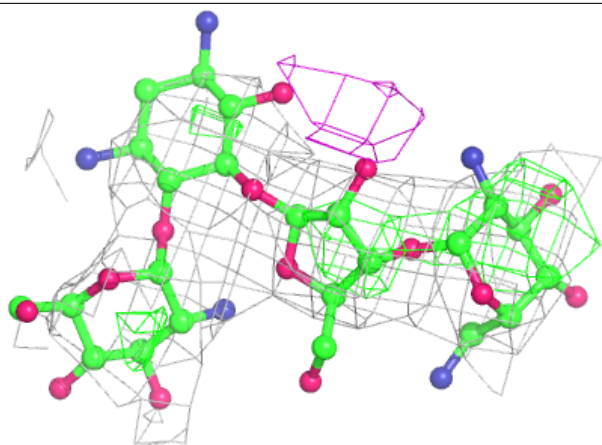
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PAR XA 1673:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.