



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 10:58 PM UTC

PDB ID : 4L71 / pdb_00004l71
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

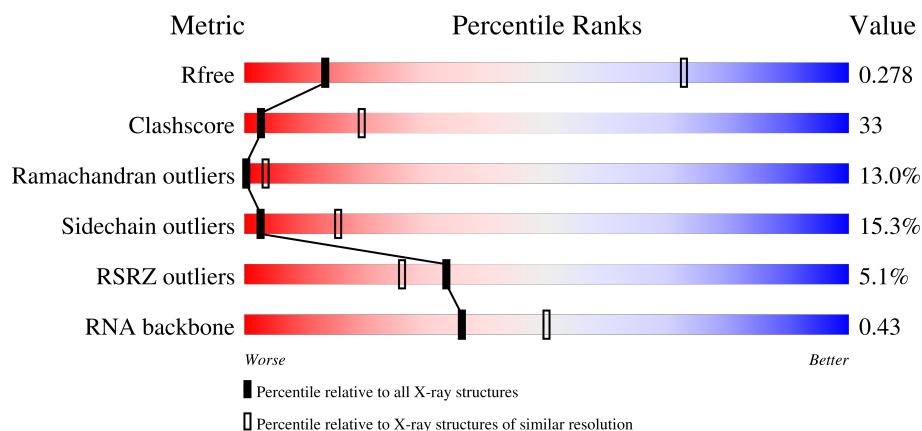
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	2% 45% 42% 11% .
1	XA	1522	% 43% 43% 12% .
2	QB	256	4% 16% 58% 17% . 7%
2	XB	256	% 16% 59% 16% . 7%

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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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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	

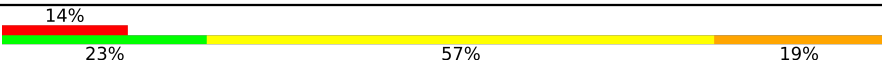
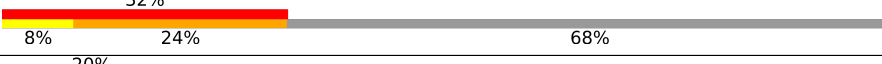
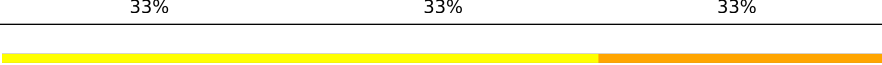
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Mol	Chain	Length	Quality of chain
40	YX	96	
41	RY	110	
41	YY	110	
42	RZ	206	
42	YZ	206	
43	R0	85	
43	Y0	85	
44	R1	98	
44	Y1	98	
45	R2	72	
45	Y2	72	
46	R3	60	
46	Y3	60	
47	R4	71	
47	Y4	71	
48	R5	60	
48	Y5	60	
49	R6	54	
49	Y6	54	
50	R7	49	
50	Y7	49	
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	1610	-	-	-	X
57	MG	RA	3003	-	-	-	X
57	MG	RA	3005	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3007	-	-	-	X
57	MG	RA	3014	-	-	-	X
57	MG	RA	3016	-	-	-	X
57	MG	RA	3019	-	-	-	X
57	MG	RA	3020	-	-	-	X
57	MG	RA	3021	-	-	-	X
57	MG	RA	3023	-	-	-	X
57	MG	RA	3027	-	-	-	X
57	MG	RA	3030	-	-	-	X
57	MG	RA	3031	-	-	-	X
57	MG	RA	3035	-	-	-	X
57	MG	RA	3038	-	-	-	X
57	MG	RA	3039	-	-	-	X
57	MG	RA	3041	-	-	-	X
57	MG	RA	3042	-	-	-	X
57	MG	RA	3043	-	-	-	X
57	MG	RA	3048	-	-	-	X
57	MG	RA	3051	-	-	-	X
57	MG	RA	3057	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3060	-	-	-	X
57	MG	RA	3064	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3071	-	-	-	X
57	MG	RA	3081	-	-	-	X
57	MG	RA	3093	-	-	-	X
57	MG	RA	3096	-	-	-	X
57	MG	RA	3099	-	-	-	X
57	MG	RA	3100	-	-	-	X
57	MG	RA	3123	-	-	-	X
57	MG	RA	3233	-	-	-	X
57	MG	RA	3234	-	-	-	X
57	MG	XA	1602	-	-	-	X
57	MG	XA	1606	-	-	-	X
57	MG	XA	1615	-	-	-	X
57	MG	XA	1616	-	-	-	X
57	MG	XA	1621	-	-	-	X
57	MG	XA	1635	-	-	-	X
57	MG	XA	1643	-	-	-	X
57	MG	XA	1662	-	-	-	X
57	MG	YA	3001	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3006	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3010	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3014	-	-	-	X
57	MG	YA	3018	-	-	-	X
57	MG	YA	3019	-	-	-	X
57	MG	YA	3021	-	-	-	X
57	MG	YA	3022	-	-	-	X
57	MG	YA	3024	-	-	-	X
57	MG	YA	3026	-	-	-	X
57	MG	YA	3030	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3040	-	-	-	X
57	MG	YA	3041	-	-	-	X
57	MG	YA	3043	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3053	-	-	-	X
57	MG	YA	3054	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3067	-	-	-	X
57	MG	YA	3072	-	-	-	X
57	MG	YA	3079	-	-	-	X
57	MG	YA	3080	-	-	-	X
57	MG	YA	3082	-	-	-	X
57	MG	YA	3085	-	-	-	X
57	MG	YA	3098	-	-	-	X
57	MG	YA	3099	-	-	-	X
57	MG	YA	3107	-	-	-	X
57	MG	YA	3113	-	-	-	X
57	MG	YA	3117	-	-	-	X
57	MG	YA	3134	-	-	-	X
57	MG	YA	3138	-	-	-	X
57	MG	YA	3151	-	-	-	X
57	MG	YA	3164	-	-	-	X
57	MG	YA	3197	-	-	-	X
57	MG	YA	3224	-	-	-	X
57	MG	YA	3250	-	-	-	X
57	MG	YA	3253	-	-	-	X
57	MG	YA	3255	-	-	-	X
57	MG	YA	3260	-	-	-	X
57	MG	YA	3261	-	-	-	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	65	Total	Mg	0	0
			65	65		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	RA	244	Total	Mg	0	0
			244	244		

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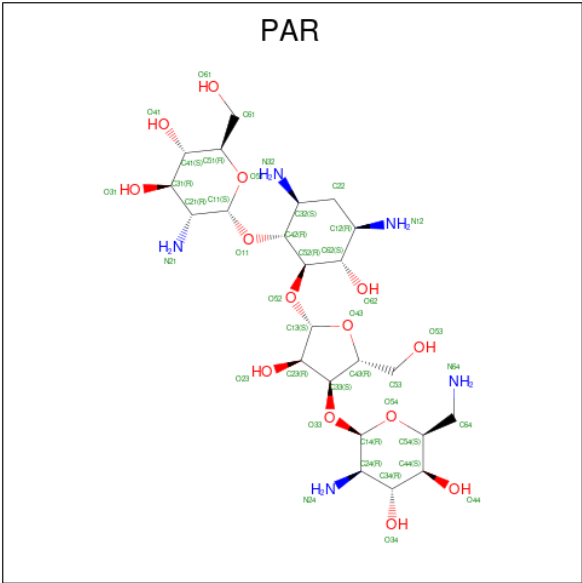
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RU	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	XM	1	Total 1	Mg 1	0	0
57	YA	265	Total 265	Mg 265	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YE	1	Total 1	Mg 1	0	0
57	YP	2	Total 2	Mg 2	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	QX	1	Total 1	Mg 1	0	0
57	XV	2	Total 2	Mg 2	0	0

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

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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		

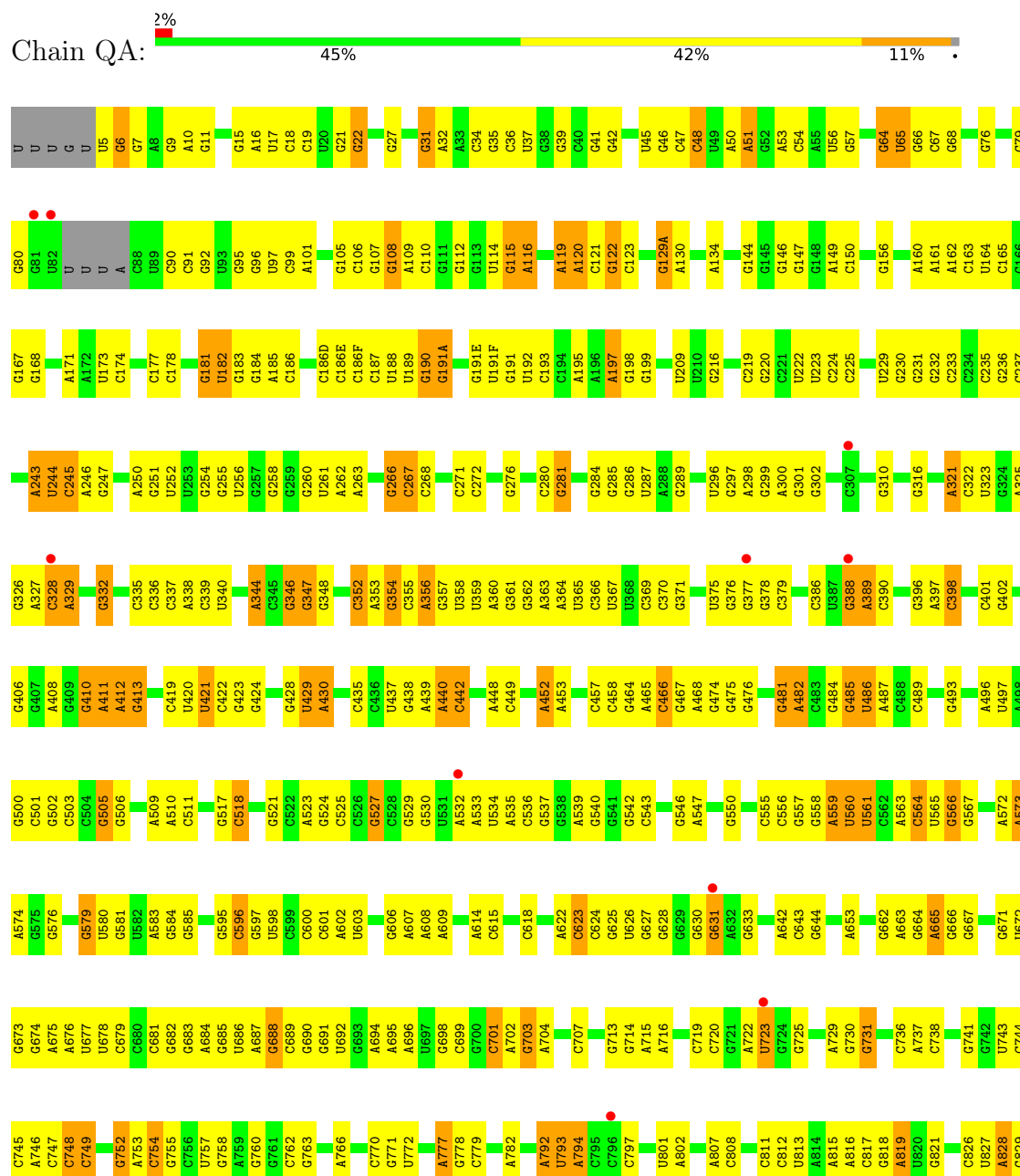
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

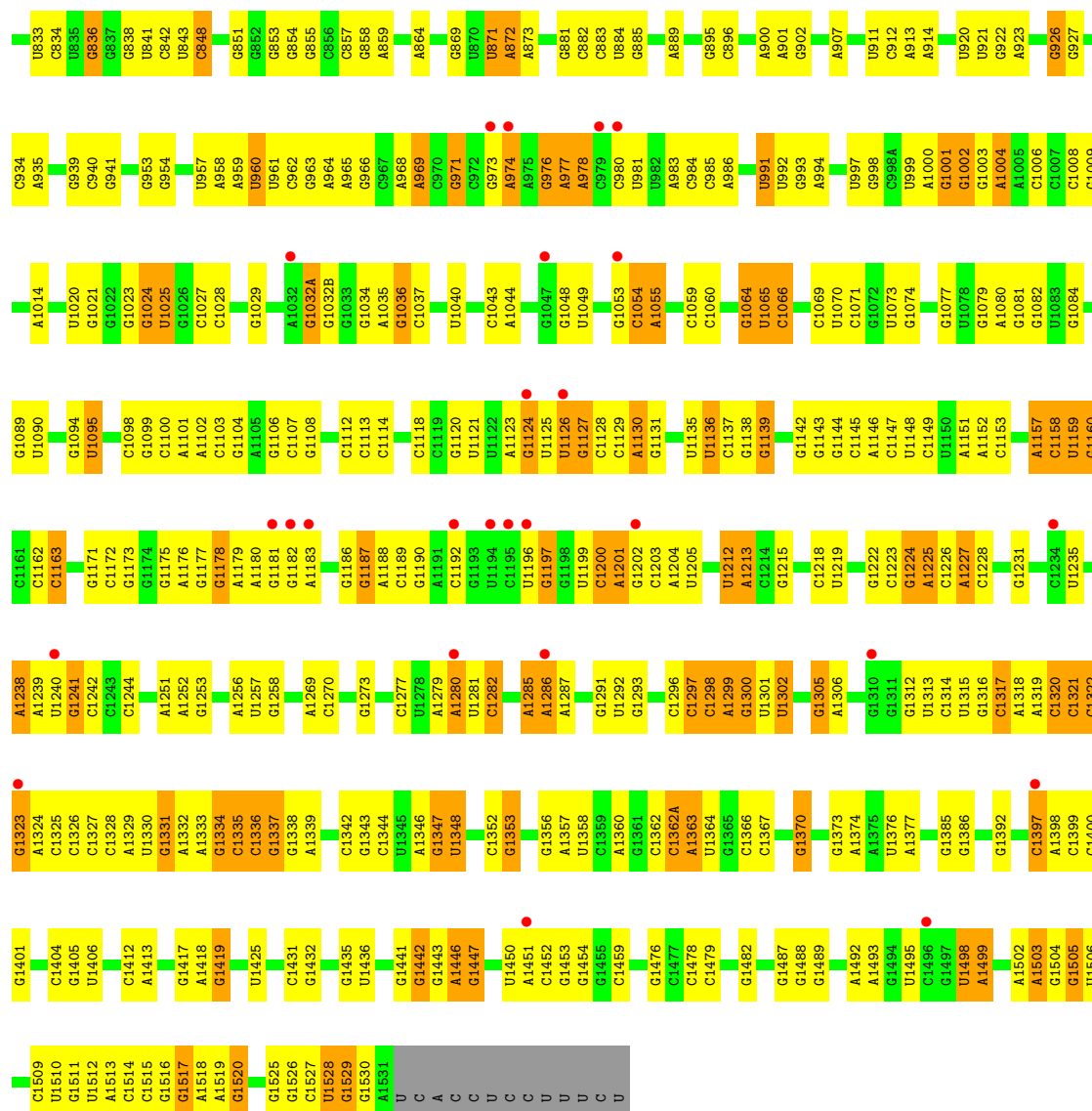
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QD	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	XD	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y9	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

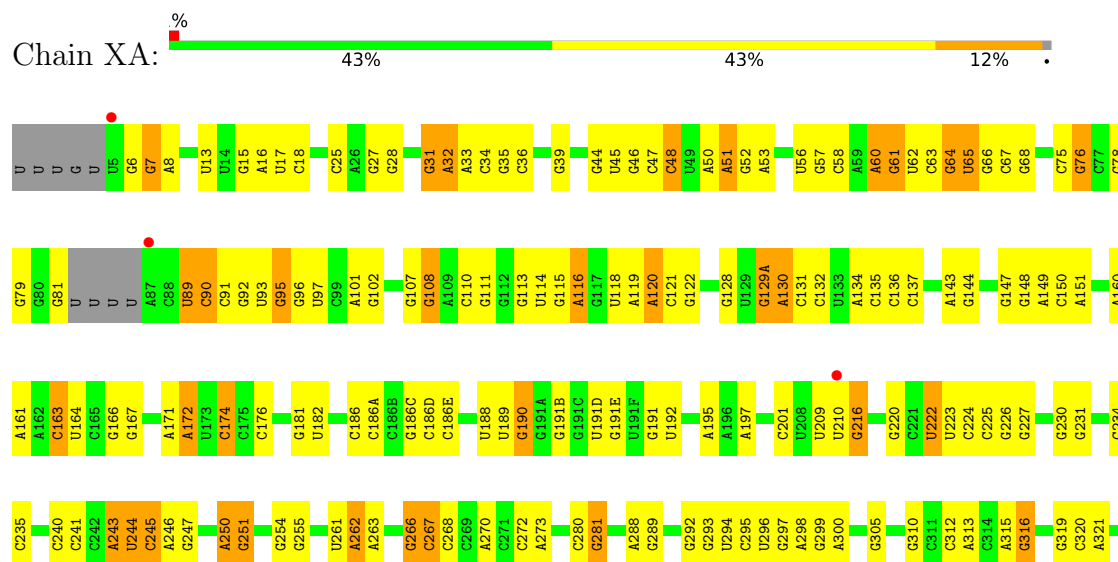
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S Ribosomal RNA

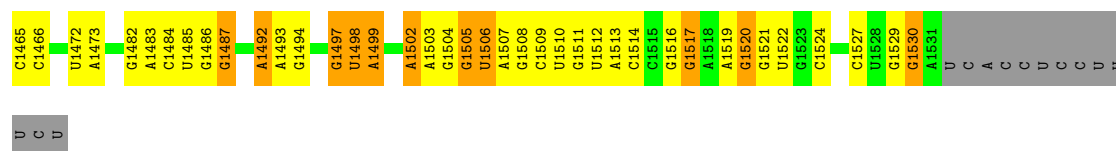




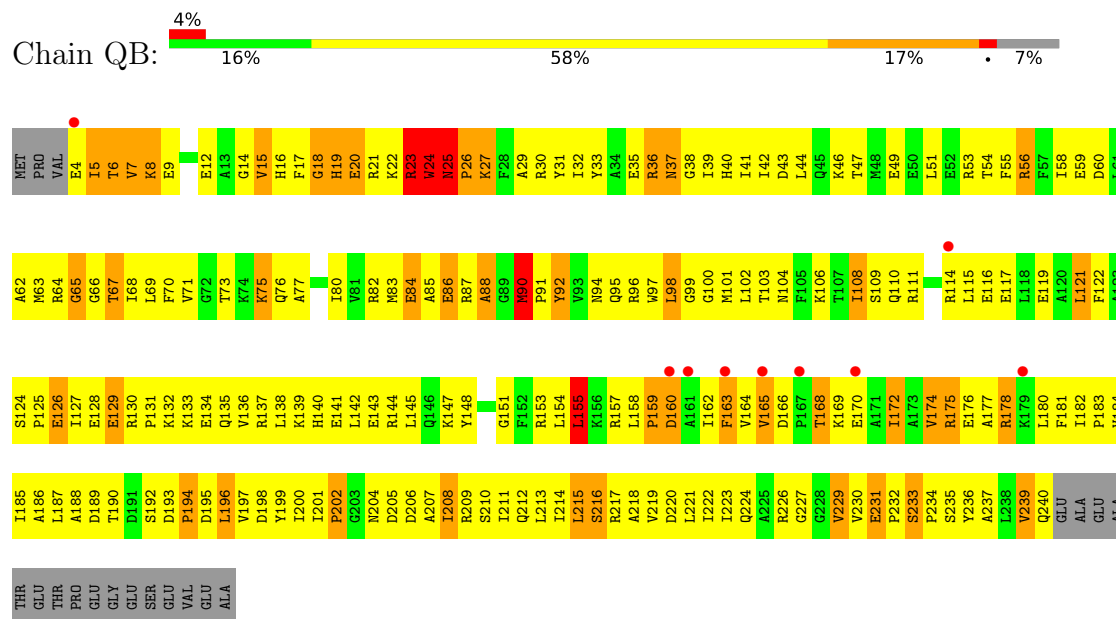
• Molecule 1: 16S Ribosomal RNA



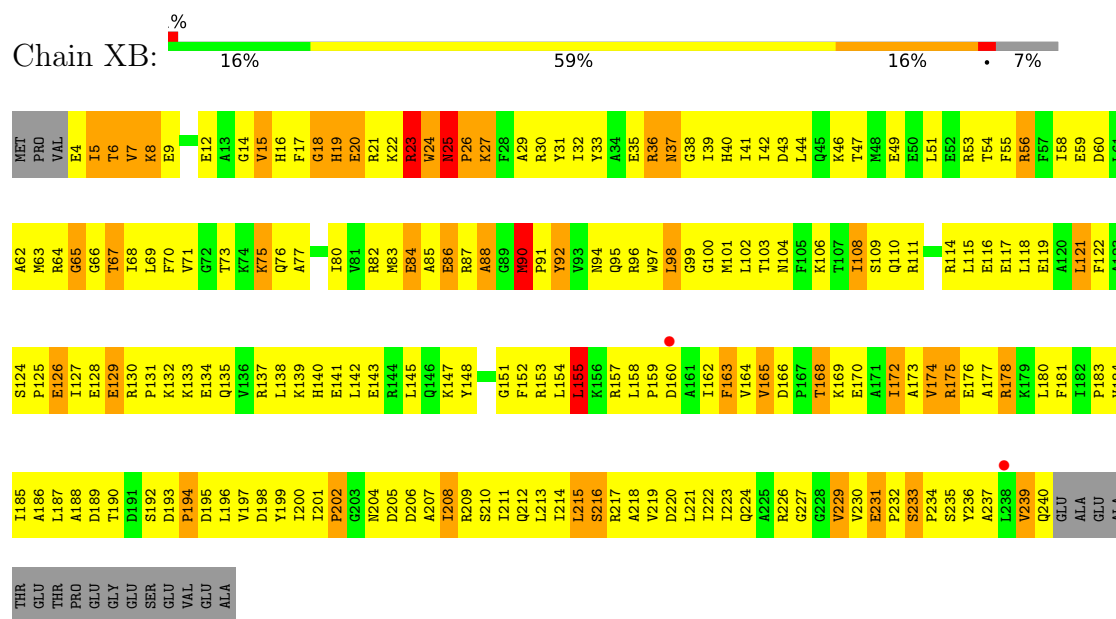
C1366	A1299	C1218	C1066	C985	C910	G821	C744	G406	A325
C1367	G1300	U1219	A1067	A986	A913	C822	C745	G407	A328
G1368	U1301	G1220	G1068	G987	A914	G825	A746	A408	A329
G1370	U1302	G1221	C1069	U991	A915	G826	C749	A409	G332
		G1222	U1070	U992	G916	U827	A676	A411	
A1374	G1305	G1223	C1071	U993	G917	A828	U677	A412	
A1375	A1306	G1224	C1072	U994	A918	G829	C679	G413	C337
U1376	U1307	A1225	U1073	G993			C678	A414	A338
A1377	G1309	C1226	G1074	A994	G922	G832	C754	A415	C339
A1378	G1310	G1155	C1075	A1000	G923	U833	G755	G416	
G1379	G1311	G1156	U1078	G1001	A923	U834	C756	C417	C345
		A1157	U1078	C924	C924	G836	U757	C418	C346
C1389	G1312	C1158	G1081	G1002	G1003	G837	A759		C347
U1390	U1313	U1159	U1086	A1004	A1005	G838	G760	U421	C348
U1391	C1314	C1161	U1086	A1006	C934	U841	G761	C422	A349
G1392	G1315	C1162	U1094	C1007	A935	G842	U765	G423	G350
		U1235	U1095	C936	C936	U843	A766	G424	G351
						U844	A767		C352
C1397	C1317	C1163	G1094	G1008	G939	U845	U692	U429	A353
A1398	A1318	U1095	U1095	G1009	G940	G853	G769	A430	C354
C1399	C1320	C1171	C1098	G1010	C941	G854	A774	A432	A356
C1400	C1321	C1172	G1099	A1014	G942	G855	G774	C433	
G1401	C1322	G1173	C1100	A1015	U943	G856	G775	U434	U359
		G1174	A1101	A1016	G944	G857	G776	U435	A360
		G1175	A1102	G1017	G945	G858	A777	C436	G361
G1405	C1244	C1245	C1103	G1017	G946	G859	G778	U437	U367
	C1246		C1104	U1020	A947	A859	G779	U438	U368
		A1251	A1105	G1021	C947	A860	A780	A439	C369
G1415	A1252	A1252	C1106	G1022	C948	A861	A781	A440	C370
G1416	G1253	C1254	G1107	G1023	G951	A862	A782	C442	G371
A1418	C1254	G1255	C1108	U1024	U952	C783	C783	G445	C372
G1419	G1336	G1256	C1109	U1025	G953	G784	C784	A448	A373
	G1337	U1257	C1112	G1026	G954	U871	A715		U375
	U1338	G1258	C1113	C1027	G955	A872	G786	A452	G376
G1422	C1339		C1114	C1028	A958	G873	C717		
G1430	A1340	G1264	C1118	G1029	A959	G874	G718	G464	G380
G1431	U1341	G1265	C1118		U960	C875	C719	A465	A383
G1432	C1342	G1265	C1118		U961	G876	C720	C466	G384
G1435	G1343	A1268	C1123	G1032A	C962	C877	G721	A467	
U1436	U1344	A1269	G1124	G1034	G963	G878	A722	G474	U387
	A1346	C1270	U1125	A1035	A964	C879	A794	G475	A388
C1439	G1347	G1273	U1126	G1036	G965	C880	C797	G476	C390
G1440	A1348		G1127	G1037	G966	G881	C808	A478	G391
G1441	A1349		C1128	C1037	C967	C882	C732	C479	G392
G1442	A1350	A1280	C1129	C1038	A968	C883	A733	U480	A393
G1443	U1281	U1197	A1130	C1039	G969	U884	C643	G481	A397
U1446	C1282	U1199	G1131	U1040	C970	G885	G644	U560	C398
G1447		G1200	C1132	G1048	G971	U891	U652	U561	G484
	A1285	A1201	G1133	U1049	C972	A892	A653	C562	G485
	A1286	A1287	U1136	G1053	A974	A900	C658	A563	U486
U1450	G1355		C1137	G1054	A975	A901	U659	C564	C403
A1451	U1356		G1138	A1055	G976	G902	C738	U565	U404
C1452	A1357	U1292	G1139	A1055	A977	G903	C739	G487	U405
G1453	U1358		C1140	C1059		C904	U740	C488	
G1454	C1359	U1212	C1141	G1064	C980	A908	G742	C489	
G1455		U1213	G1142	U1065	U981	A909	U820		
C1459	C1362A	C1214	G1143		U982				
	A1363	G1215	G1144						
	U1364	G1216							
G1462	G1365	C1217							



• Molecule 2: 30S ribosomal protein S2

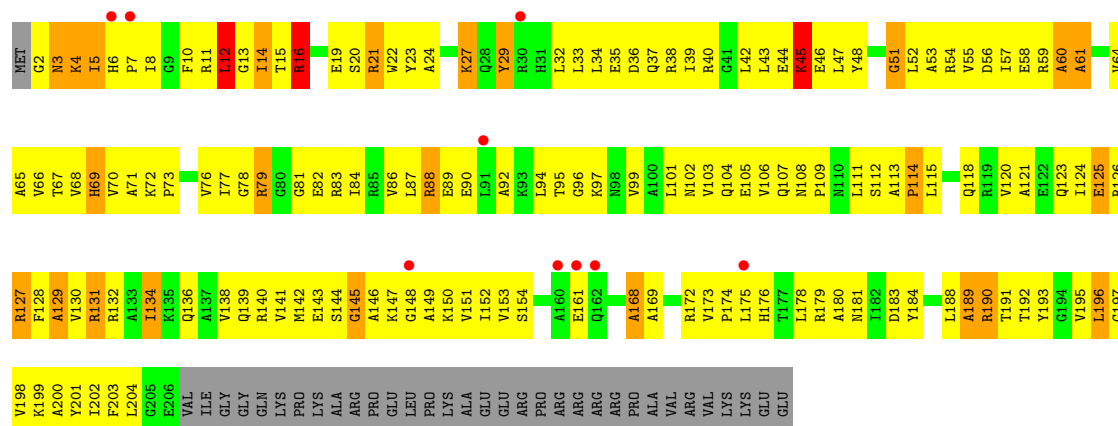


• Molecule 2: 30S ribosomal protein S2

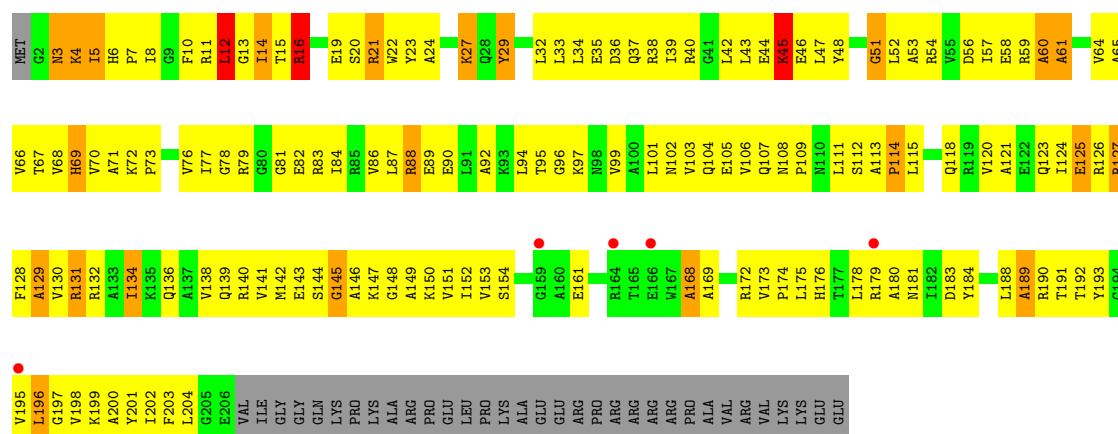


• Molecule 3: 30S ribosomal protein S3

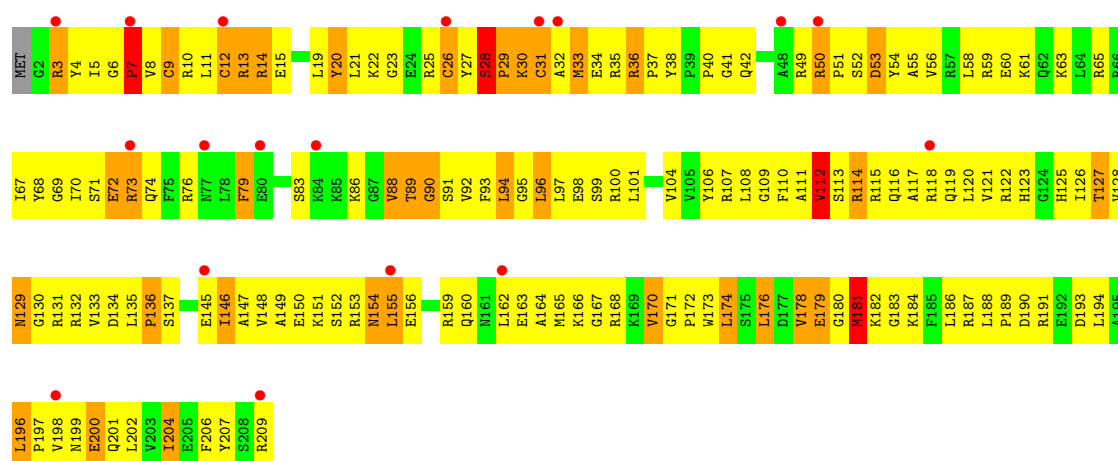




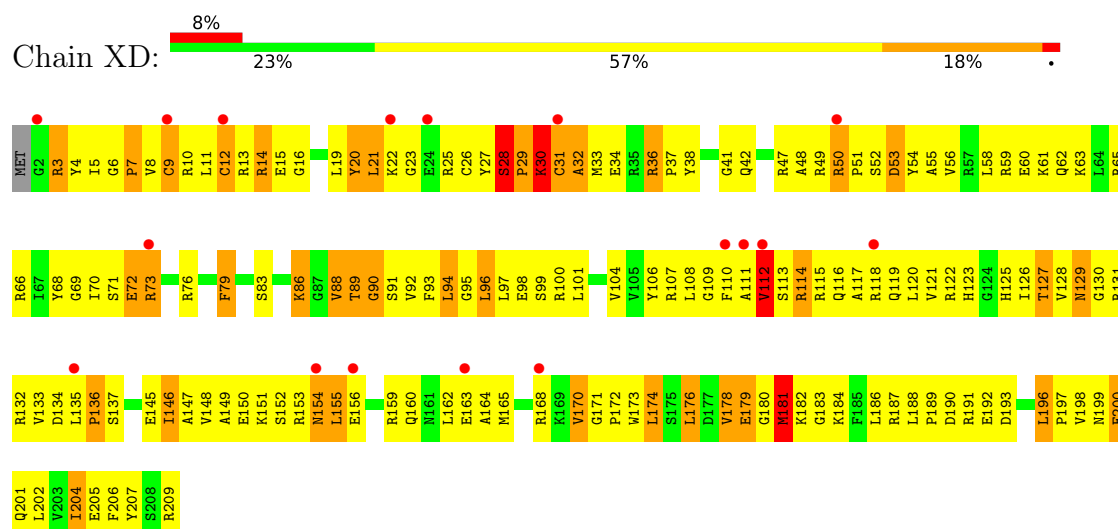
• Molecule 3: 30S ribosomal protein S3



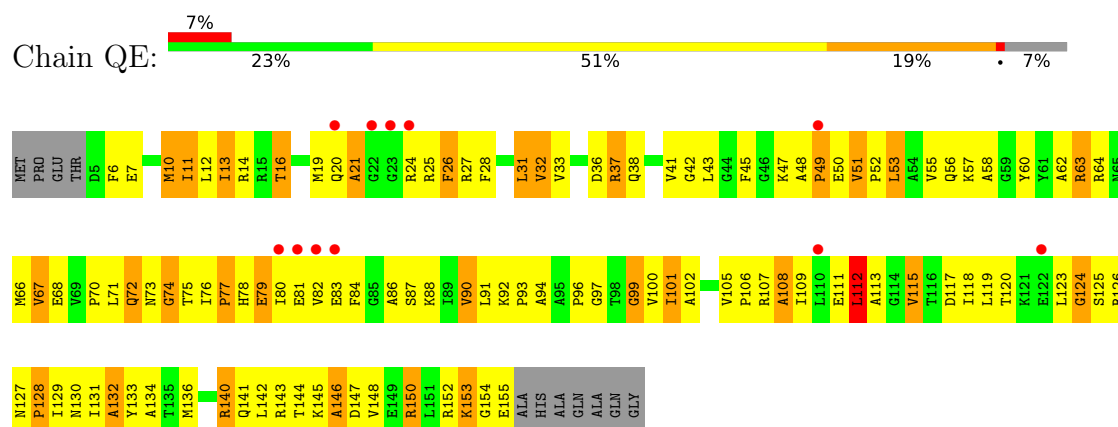
• Molecule 4: 30S ribosomal protein S4



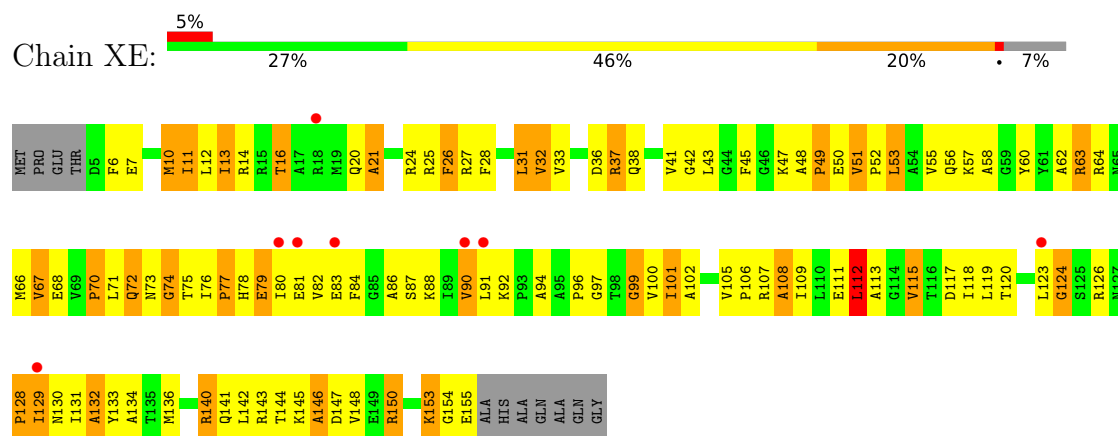
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

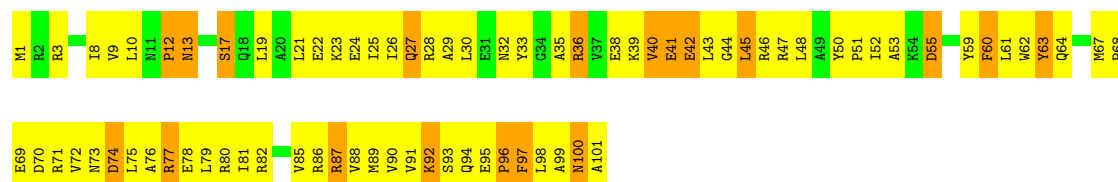


• Molecule 6: 30S ribosomal protein S6

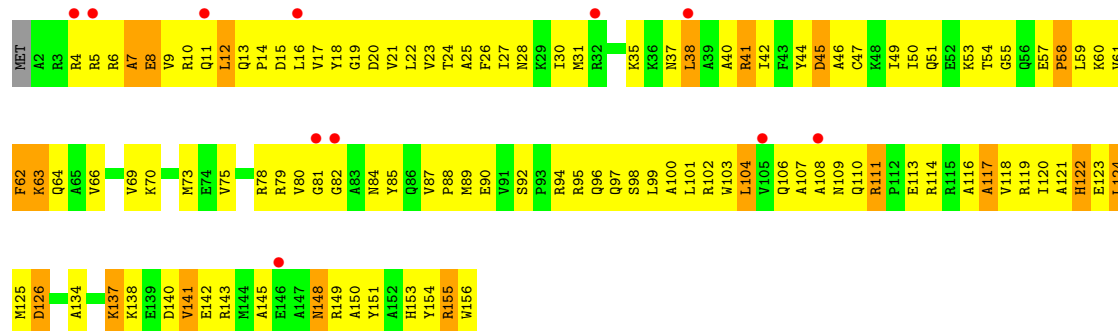




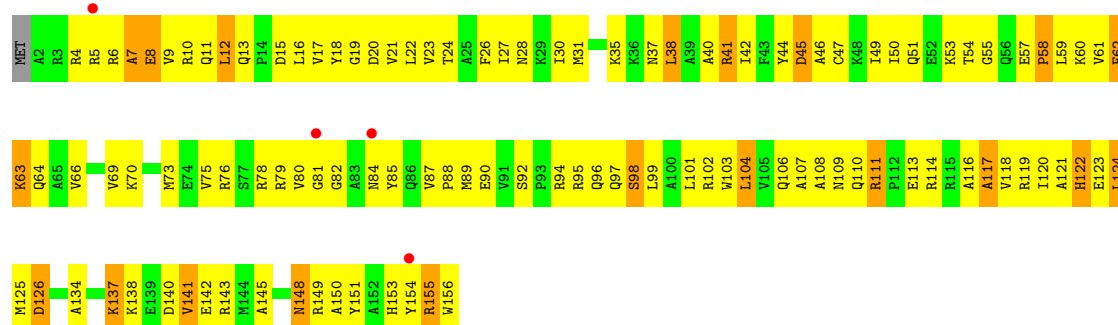
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

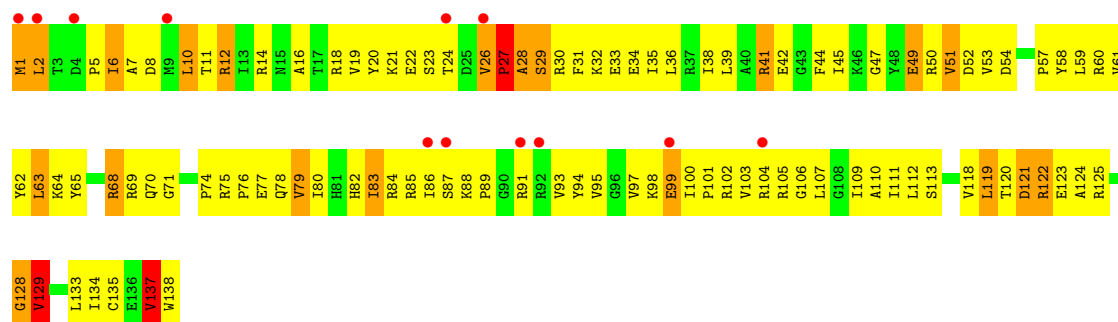


• Molecule 7: 30S ribosomal protein S7

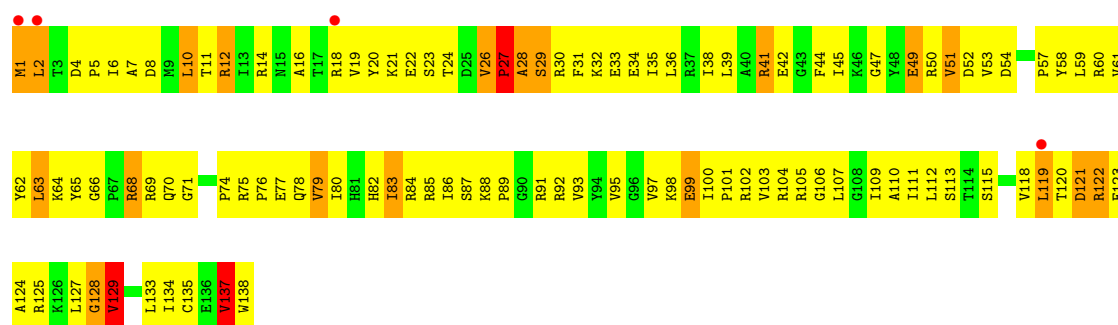


• Molecule 8: 30S ribosomal protein S8

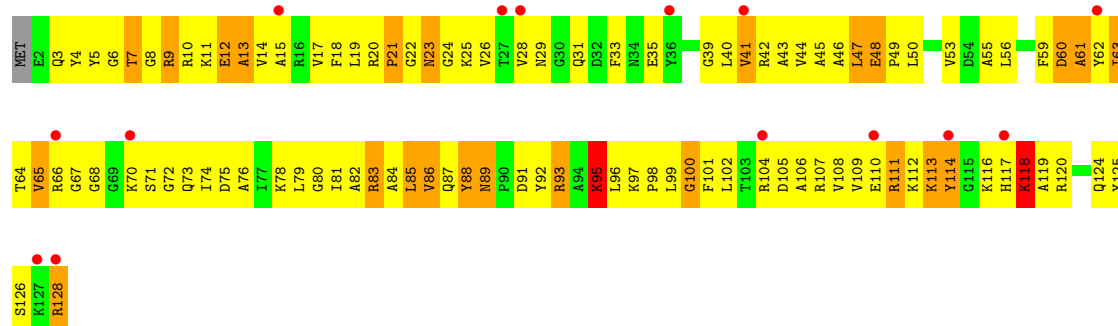




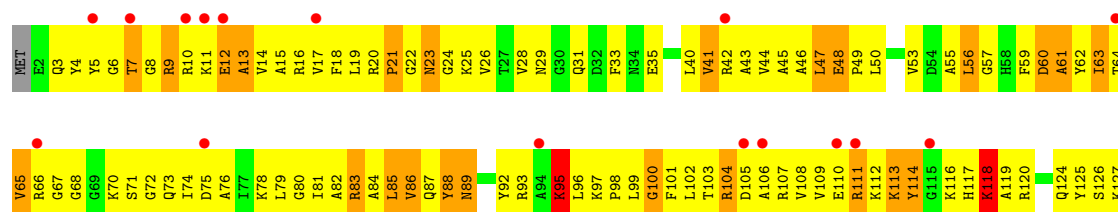
• Molecule 8: 30S ribosomal protein S8

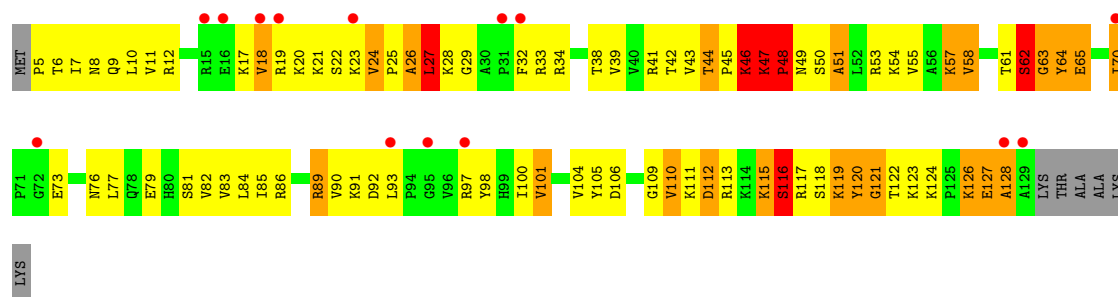


• Molecule 9: 30S ribosomal protein S9

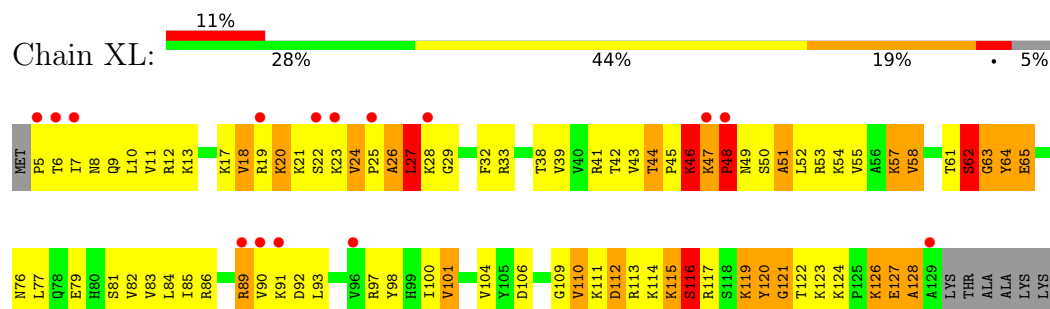


• Molecule 9: 30S ribosomal protein S9

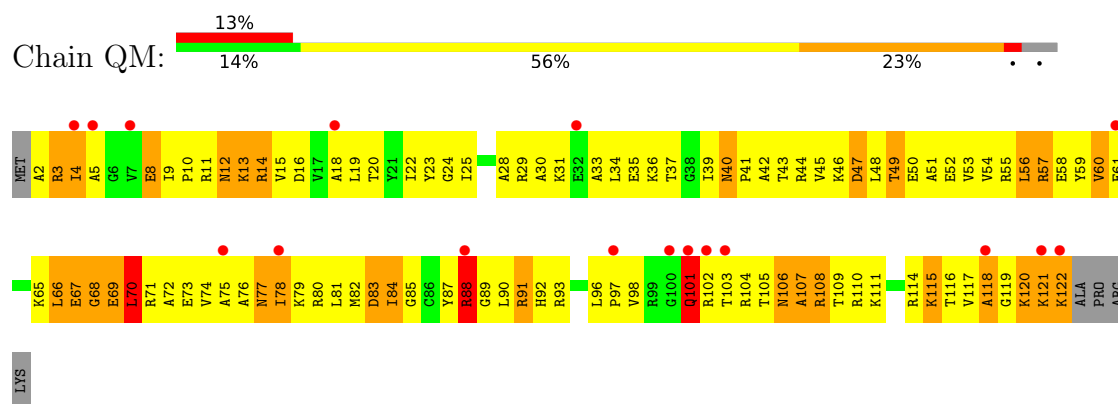




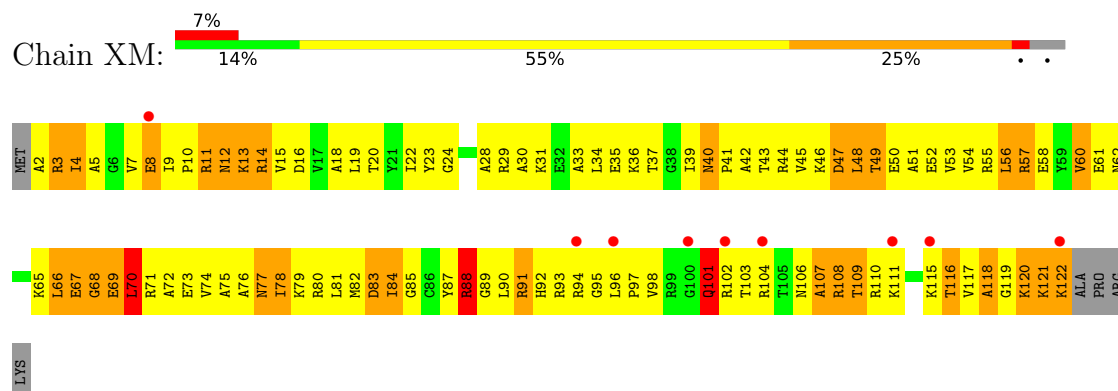
- Molecule 12: 30S ribosomal protein S12



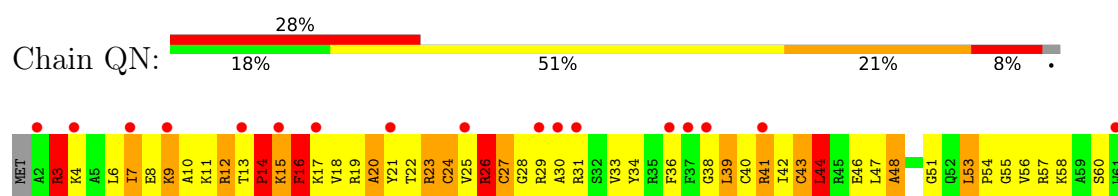
- Molecule 13: 30S ribosomal protein S13



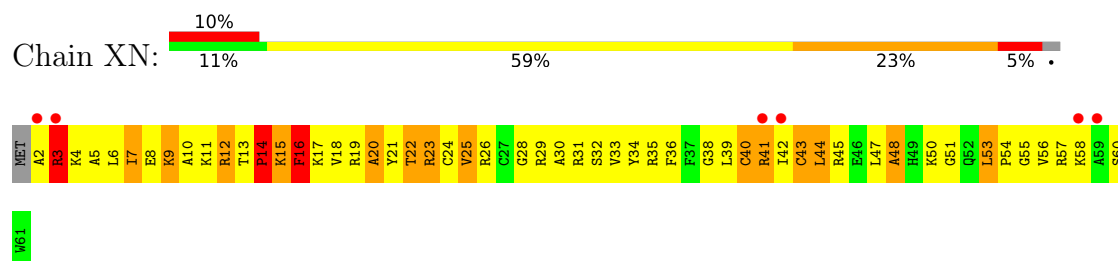
- Molecule 13: 30S ribosomal protein S13



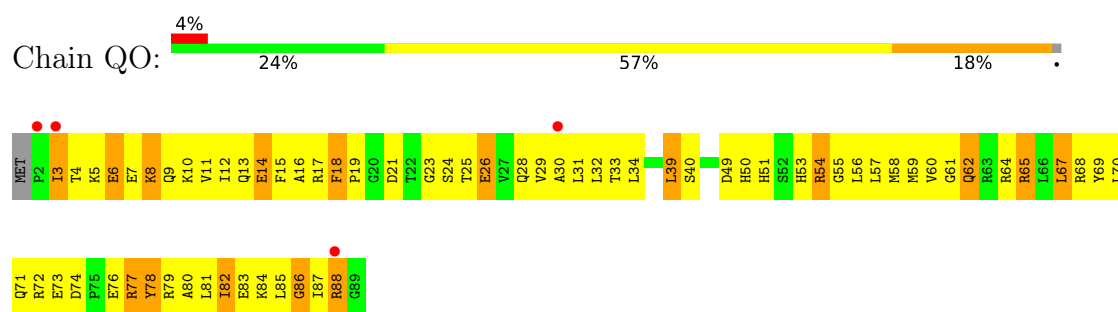
- Molecule 14: 30S ribosomal protein S14 type Z



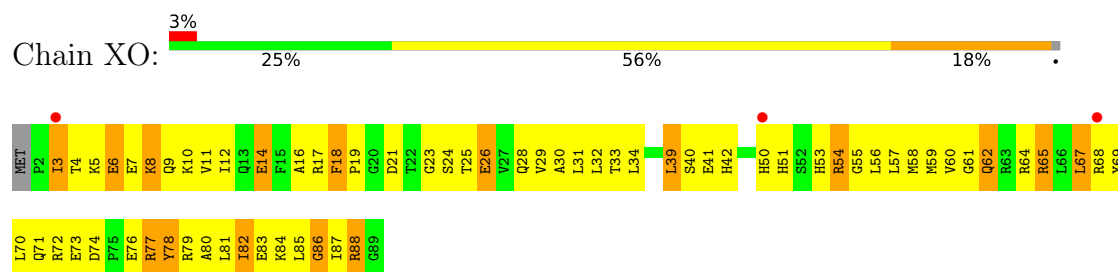
- Molecule 14: 30S ribosomal protein S14 type Z



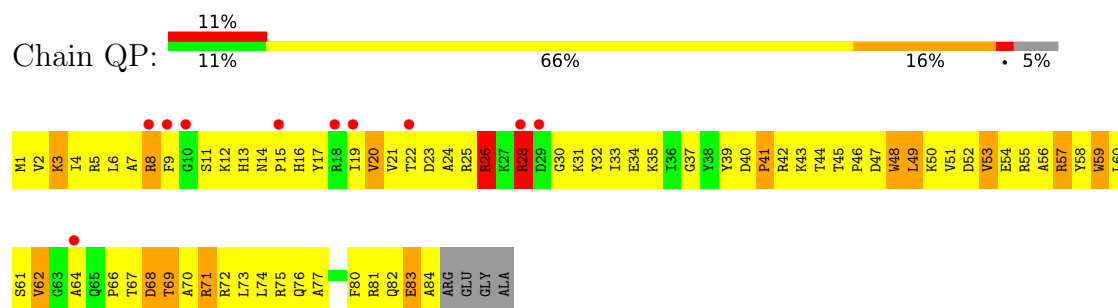
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

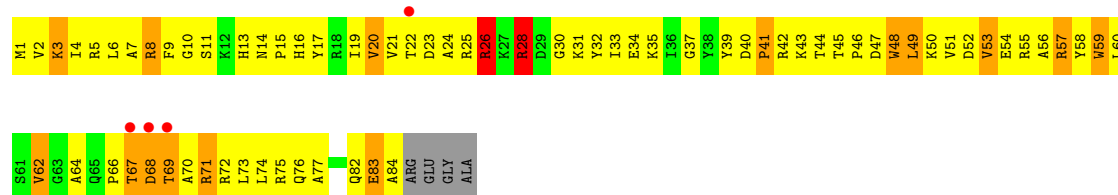


- Molecule 16: 30S ribosomal protein S16

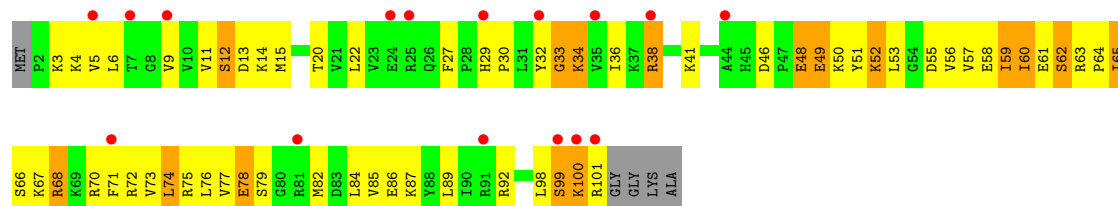


- Molecule 16: 30S ribosomal protein S16

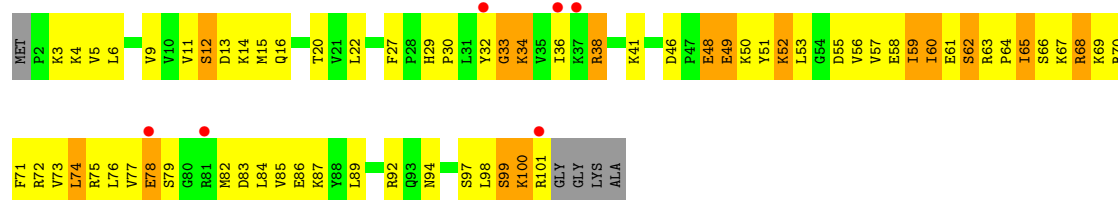




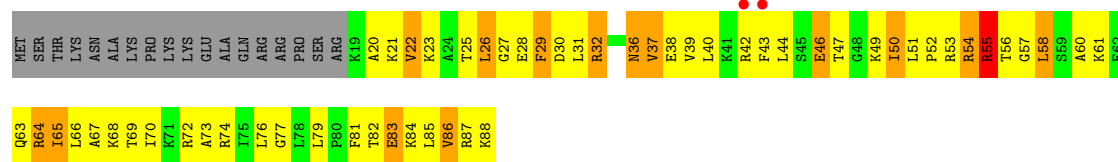
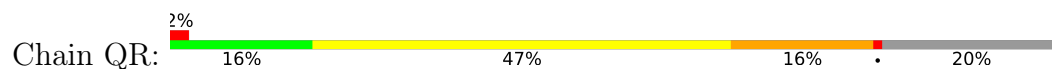
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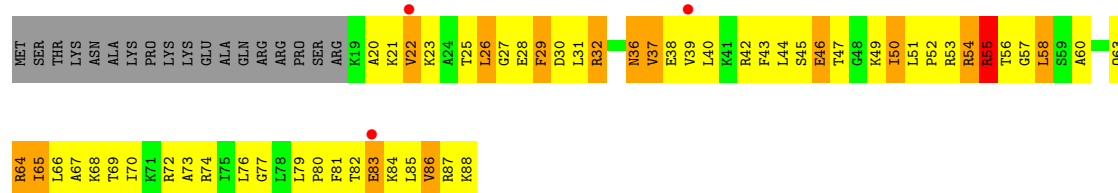
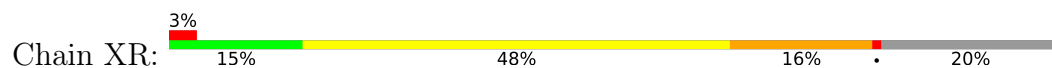
• Molecule 17: 30S ribosomal protein S17



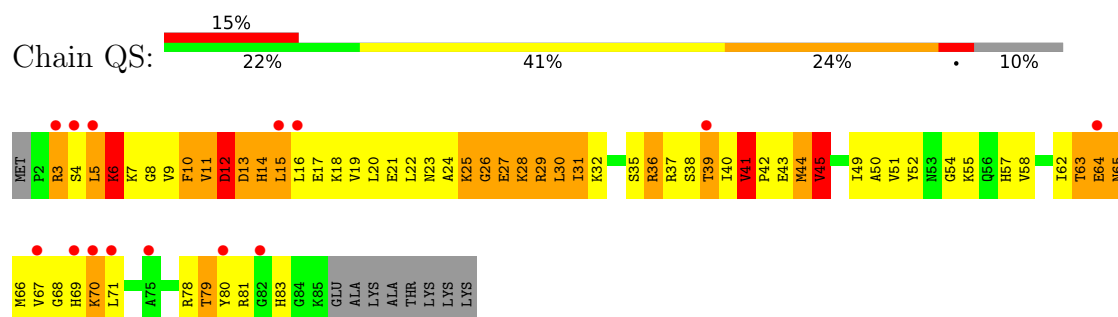
• Molecule 18: 30S ribosomal protein S18



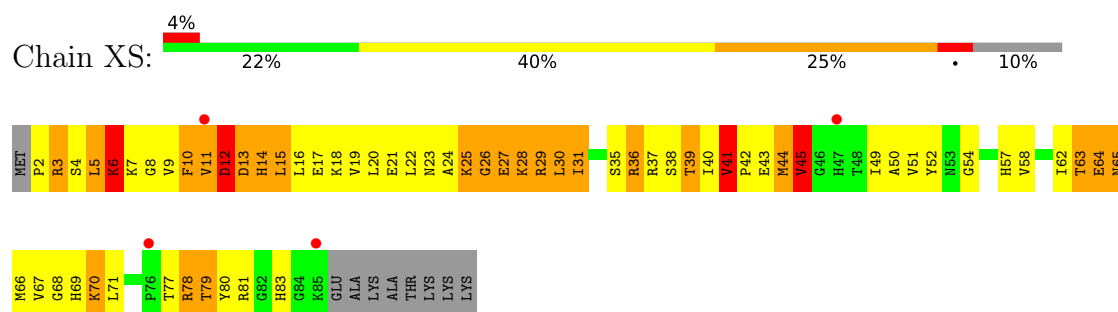
• Molecule 18: 30S ribosomal protein S18



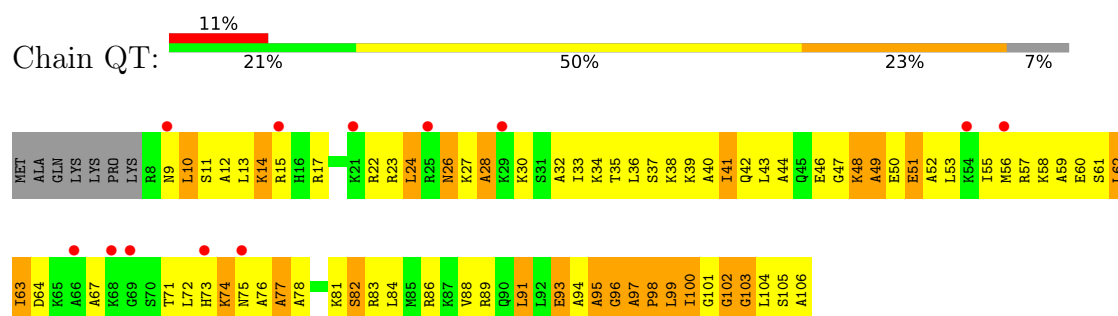
- Molecule 19: 30S ribosomal protein S19



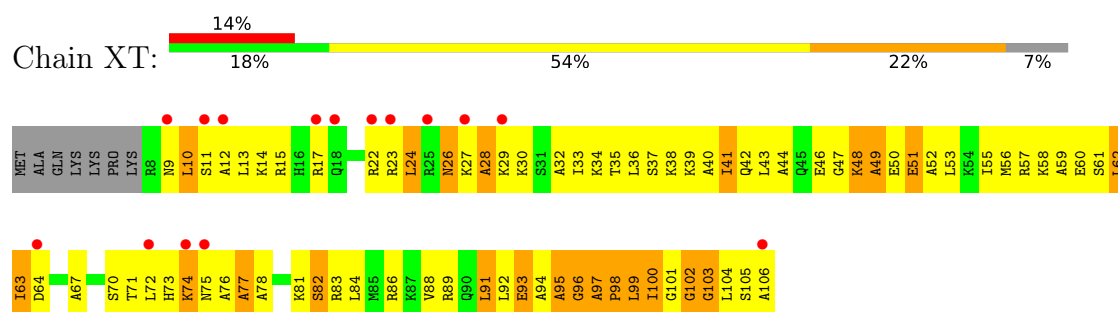
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

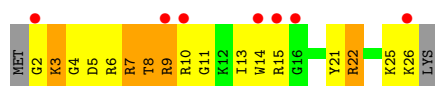


- Molecule 20: 30S ribosomal protein S20

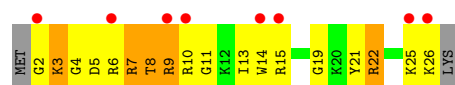


- Molecule 21: 30S ribosomal protein Thx

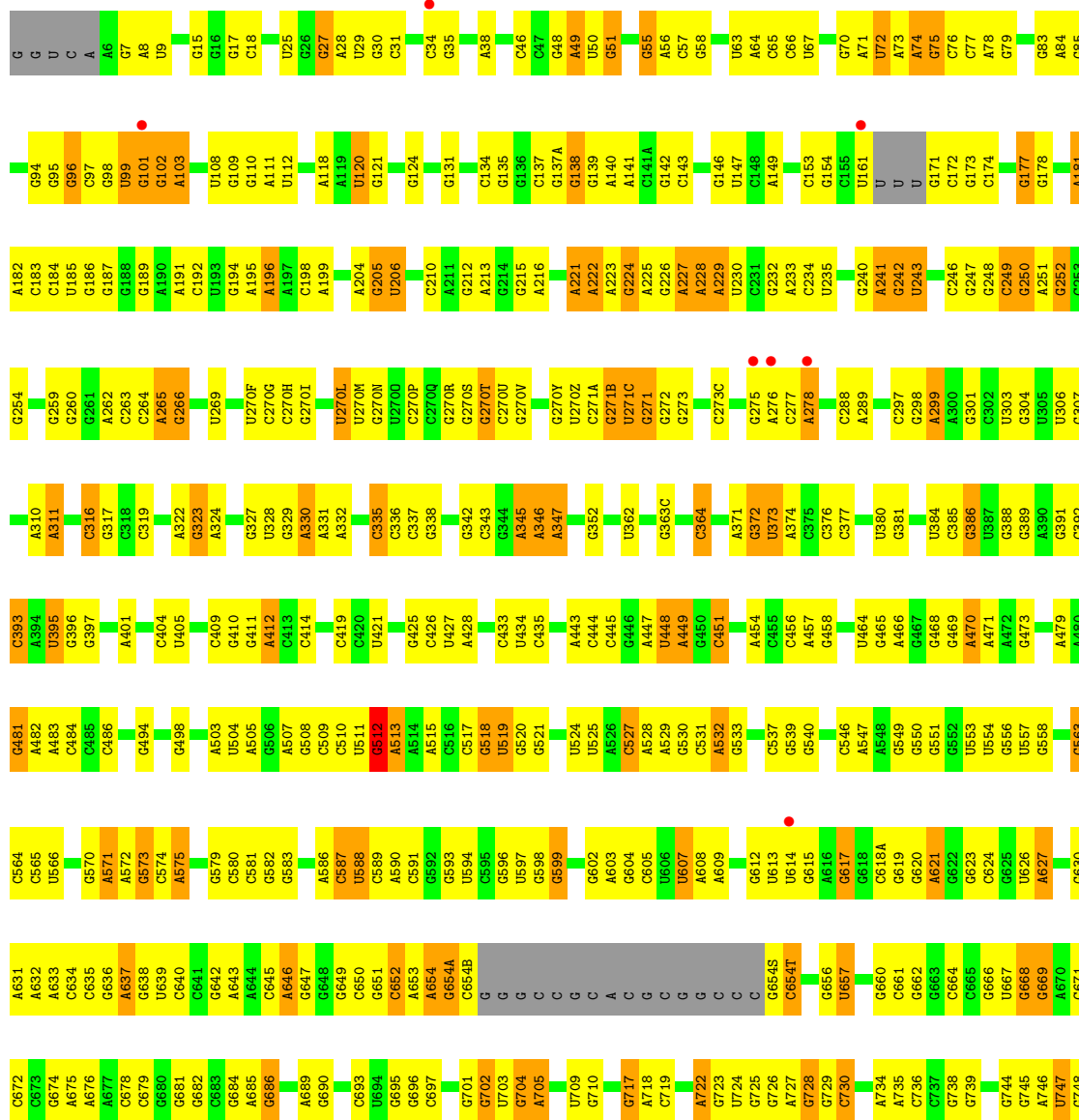
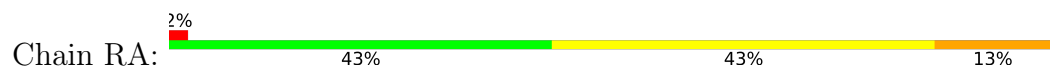




- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: 23S Ribosomal RNA

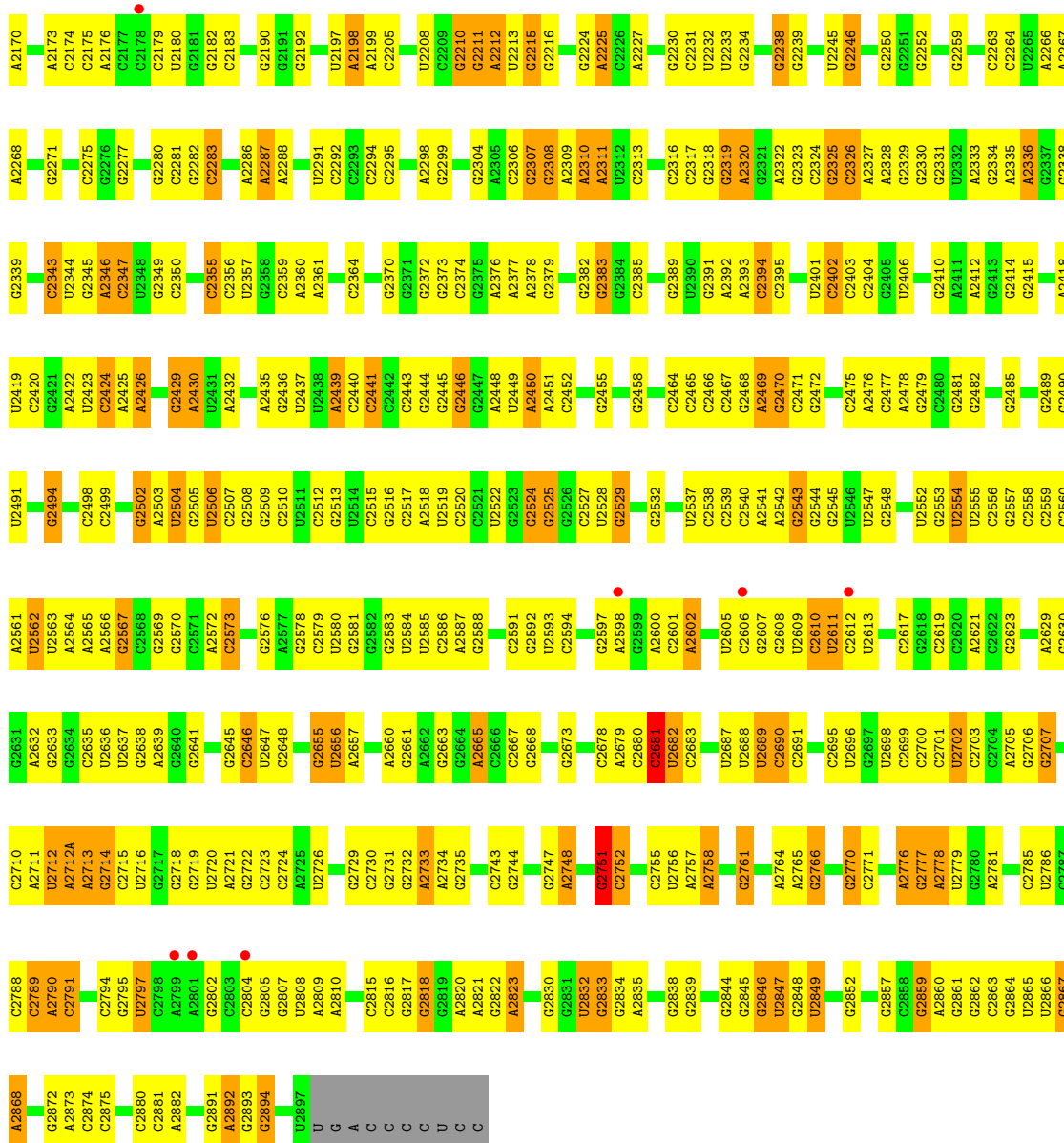


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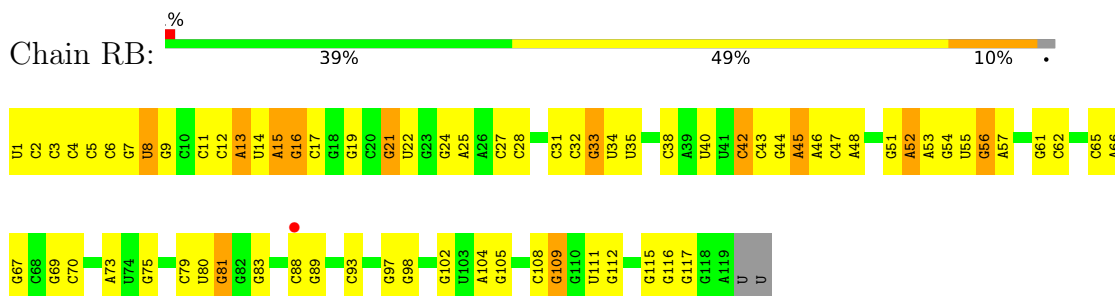
- Molecule 22: 23S Ribosomal RNA



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			C1350	G1417	G1488	A1566	G1653	G1757	A1827	U1918	U1993	U2074	
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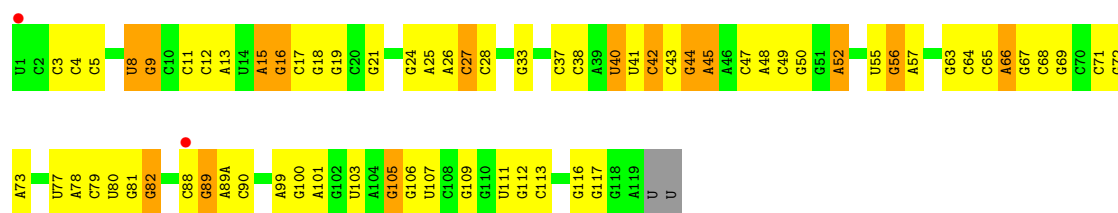


• Molecule 23: 5S Ribosomal RNA

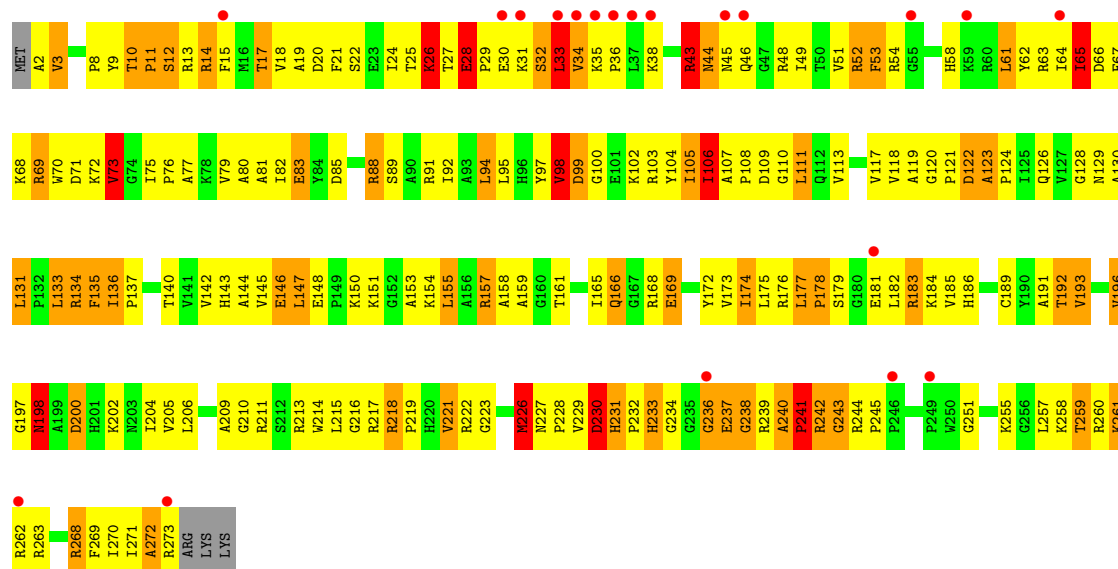


• Molecule 23: 5S Ribosomal RNA

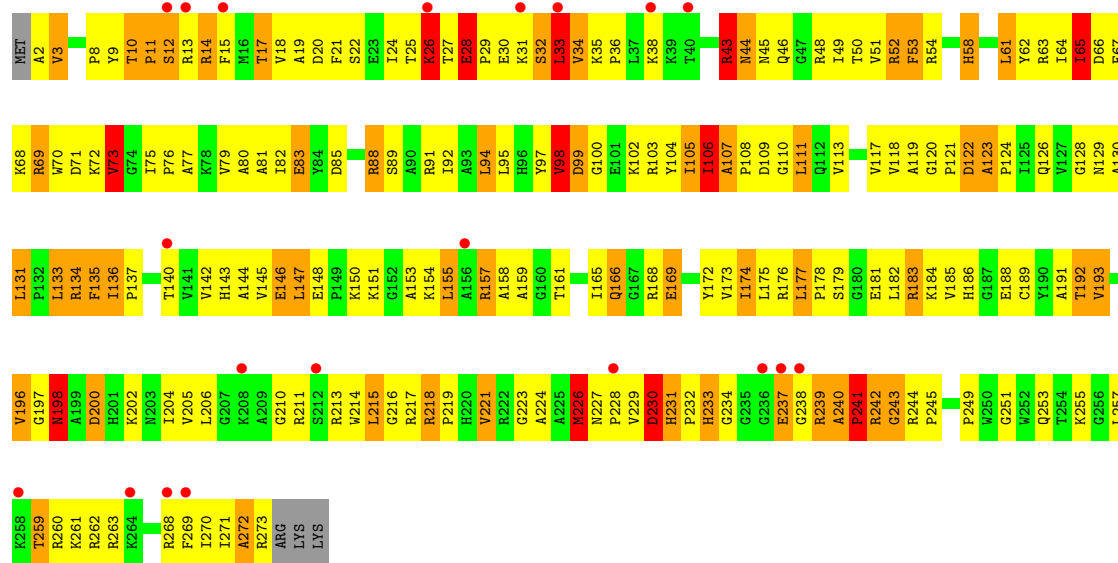




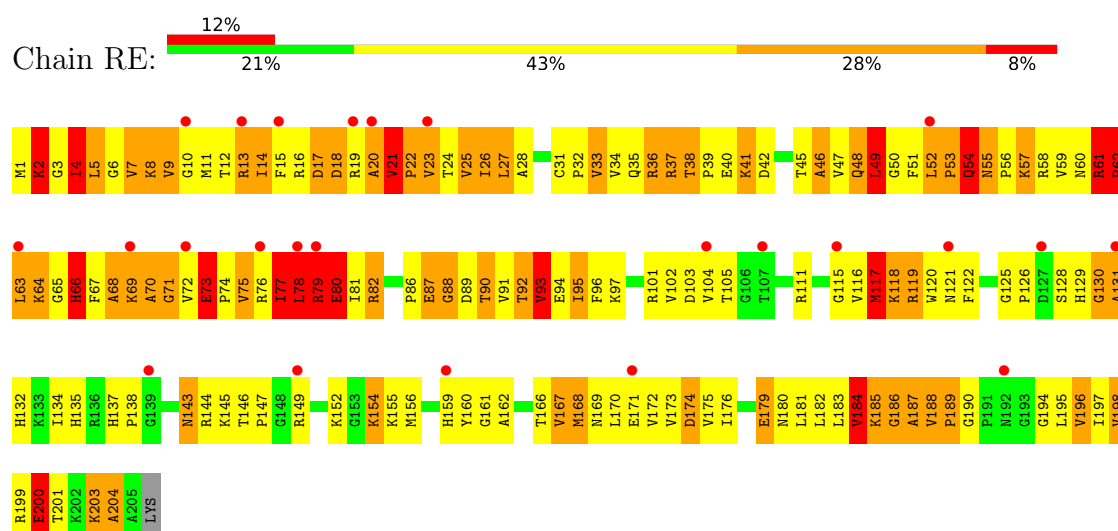
• Molecule 24: 50S ribosomal protein L2



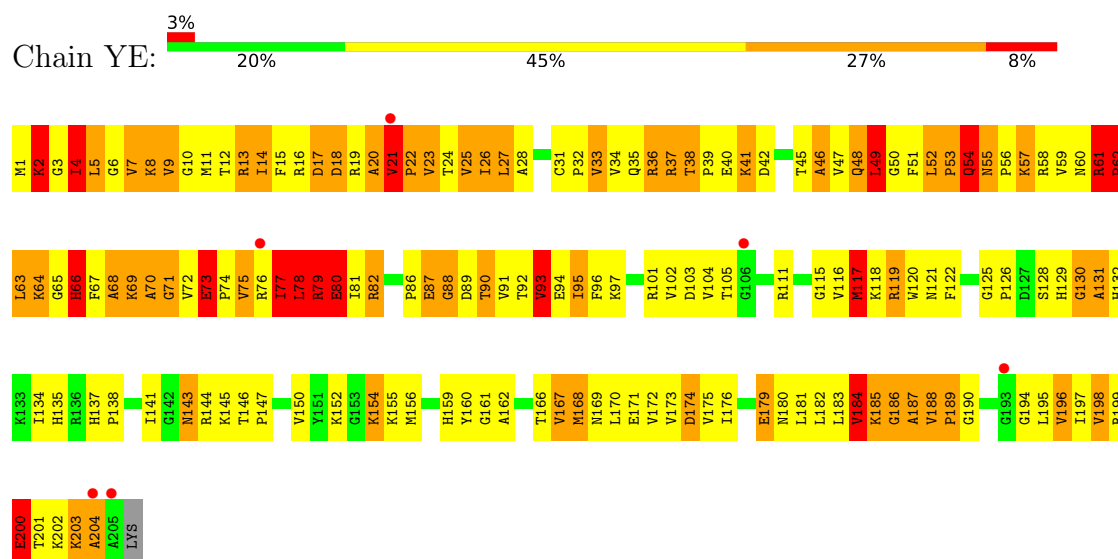
• Molecule 24: 50S ribosomal protein L2



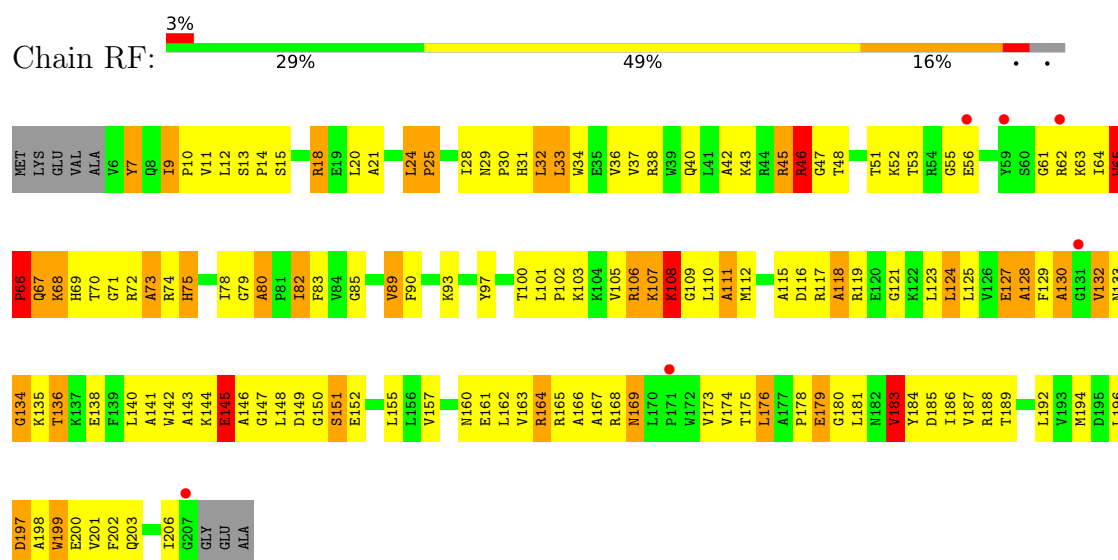
• Molecule 25: 50S ribosomal protein L3



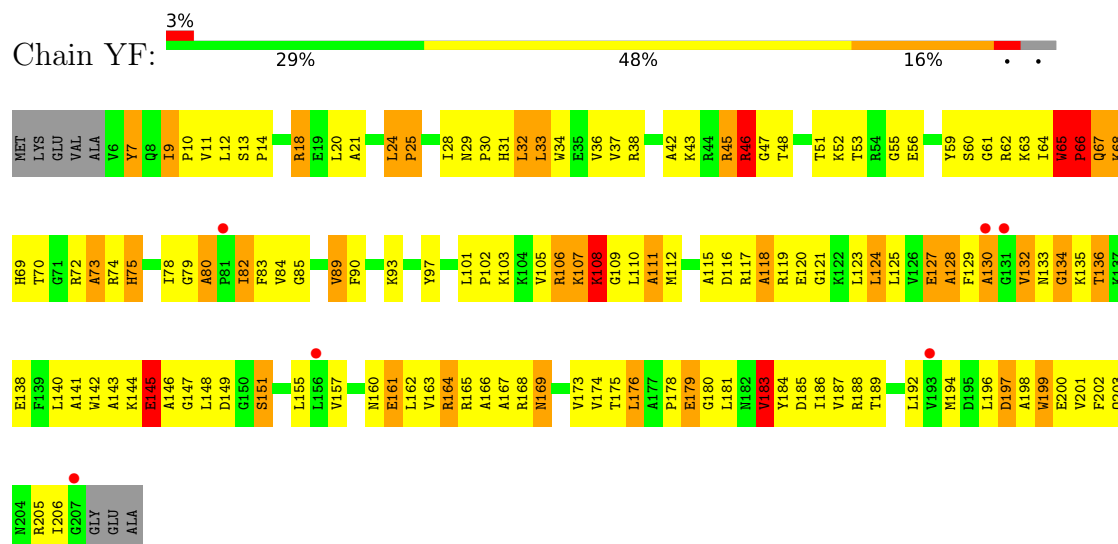
• Molecule 25: 50S ribosomal protein L3



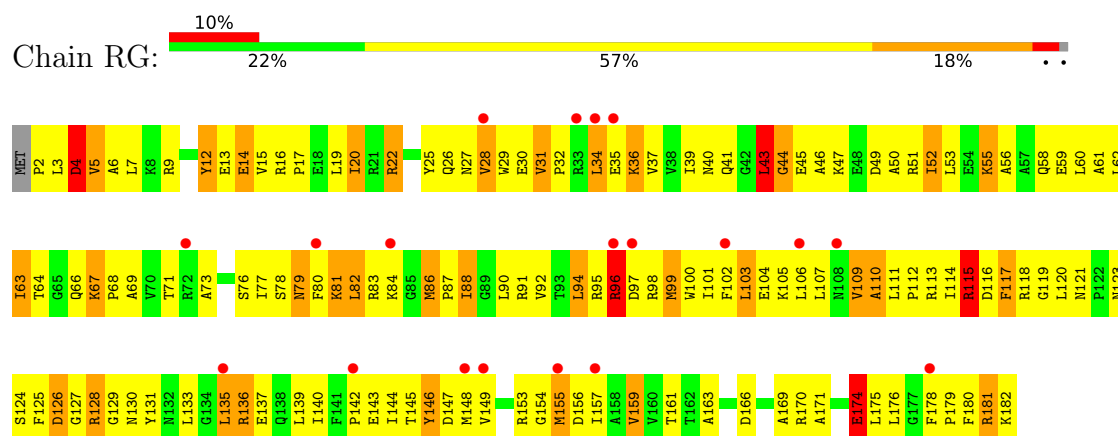
• Molecule 26: 50S ribosomal protein L4



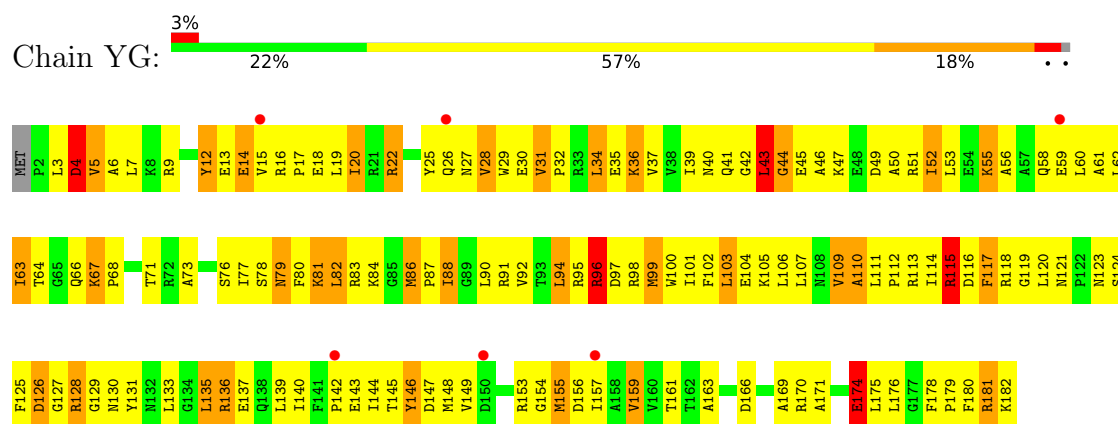
- Molecule 26: 50S ribosomal protein L4



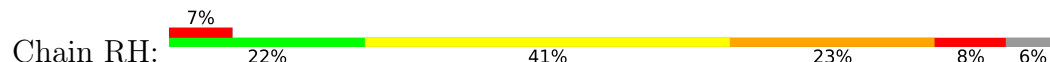
- Molecule 27: 50S ribosomal protein L5

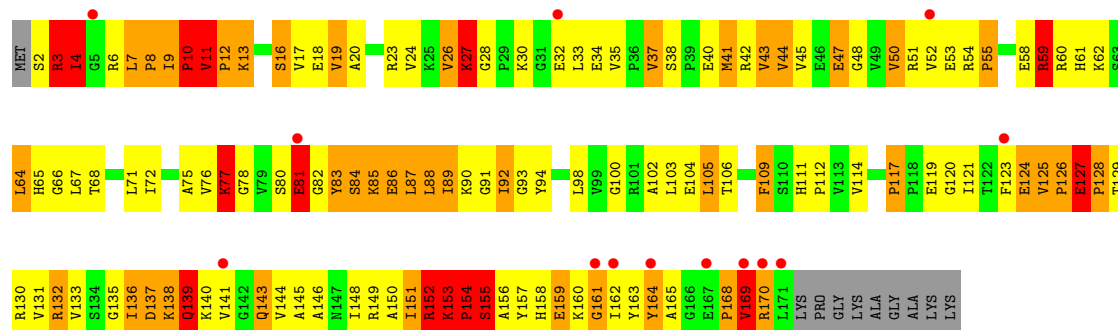


- Molecule 27: 50S ribosomal protein L5

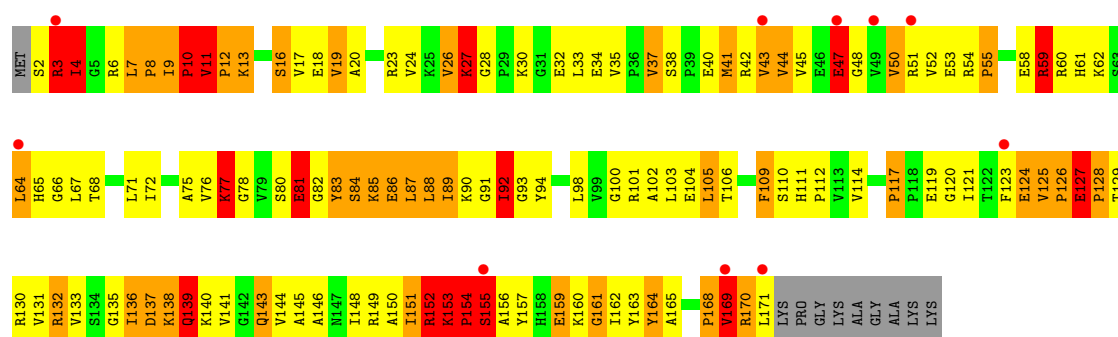
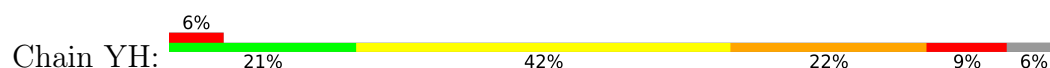


- Molecule 28: 50S ribosomal protein L6

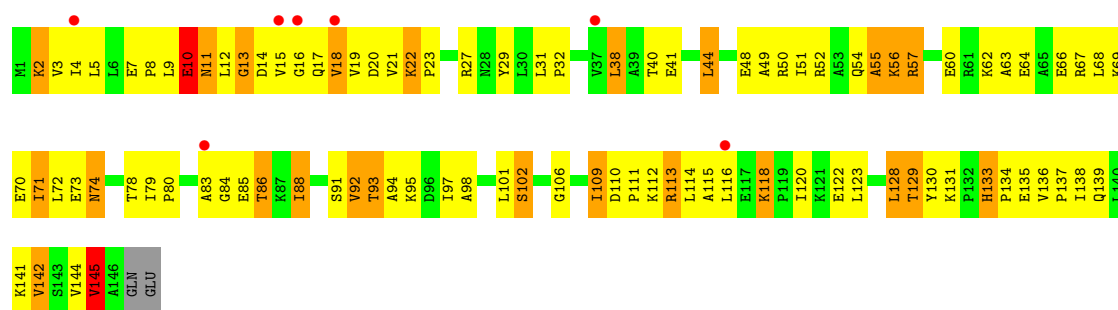




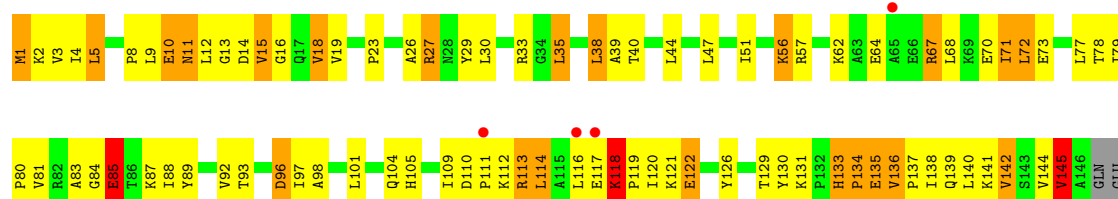
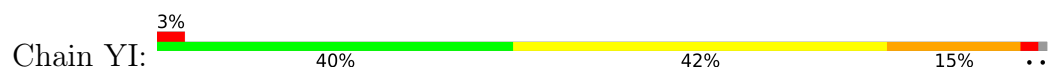
• Molecule 28: 50S ribosomal protein L6



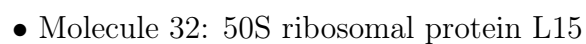
• Molecule 29: 50S ribosomal protein L9



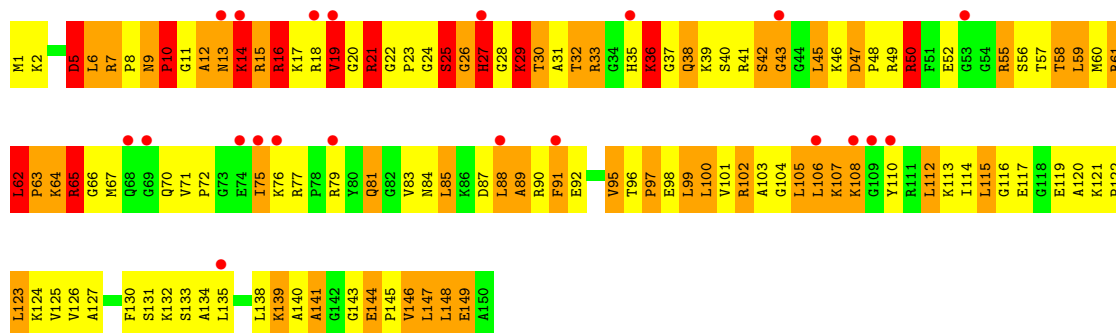
• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein L13

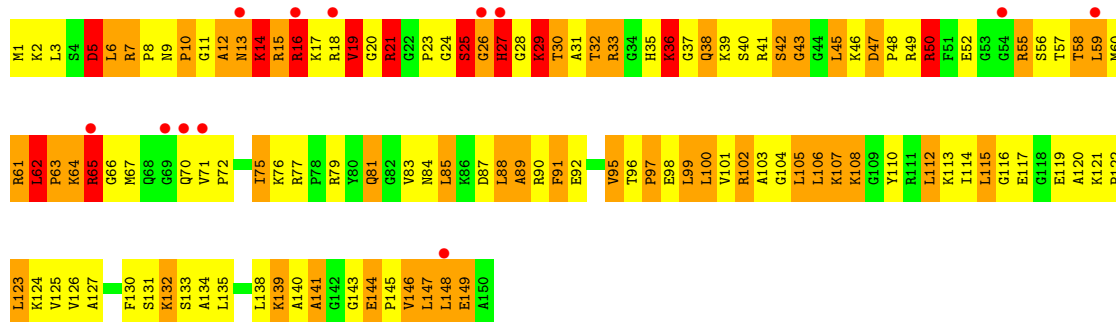


Chain RP: 

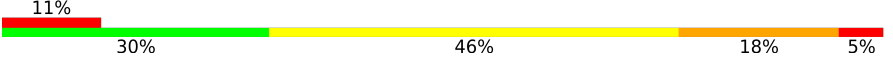


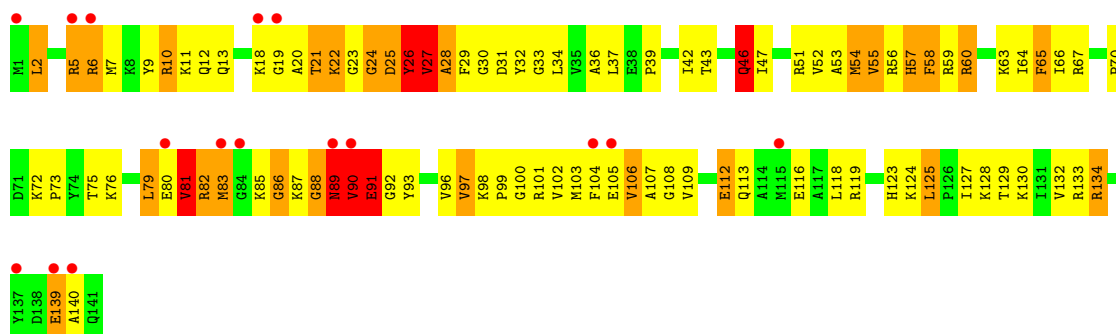
• Molecule 32: 50S ribosomal protein L15

Chain YP: 

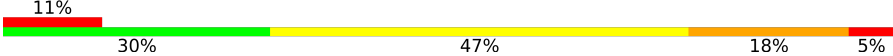


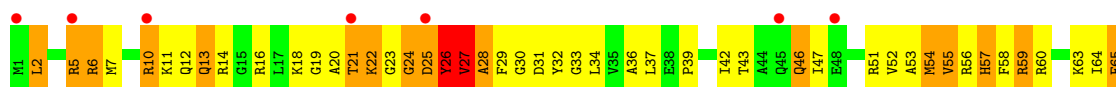
• Molecule 33: 50S ribosomal protein L16

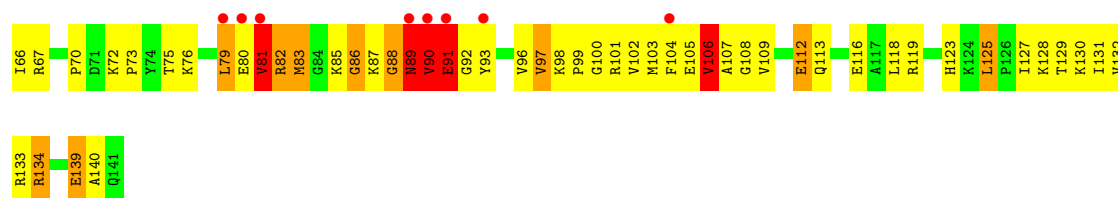
Chain RQ: 



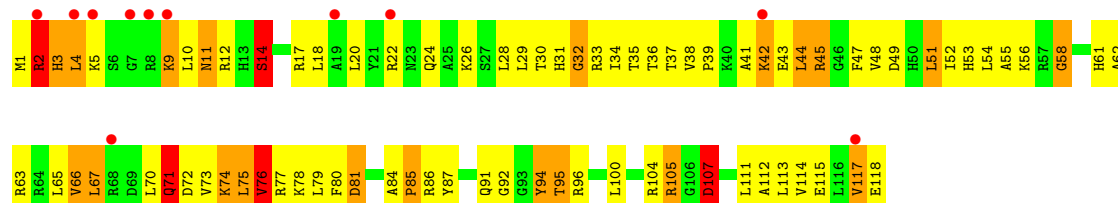
• Molecule 33: 50S ribosomal protein L16

Chain YQ: 

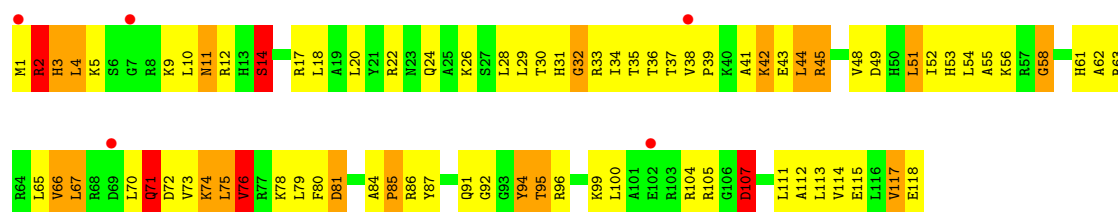




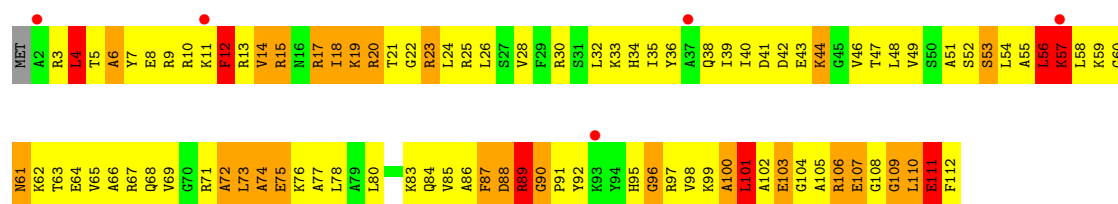
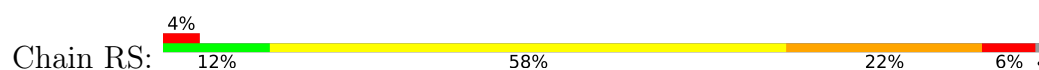
• Molecule 34: 50S ribosomal protein L17



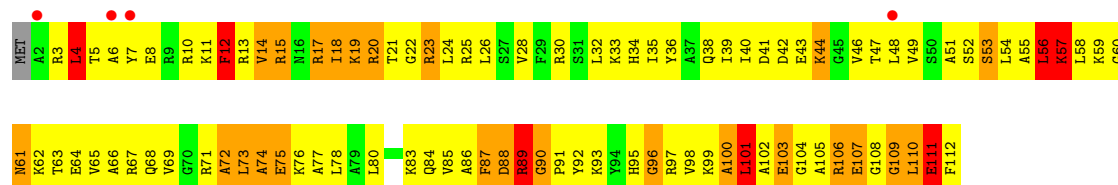
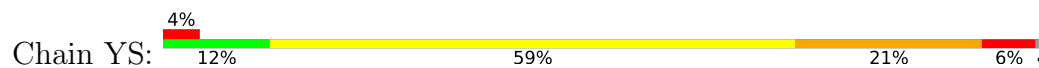
• Molecule 34: 50S ribosomal protein L17



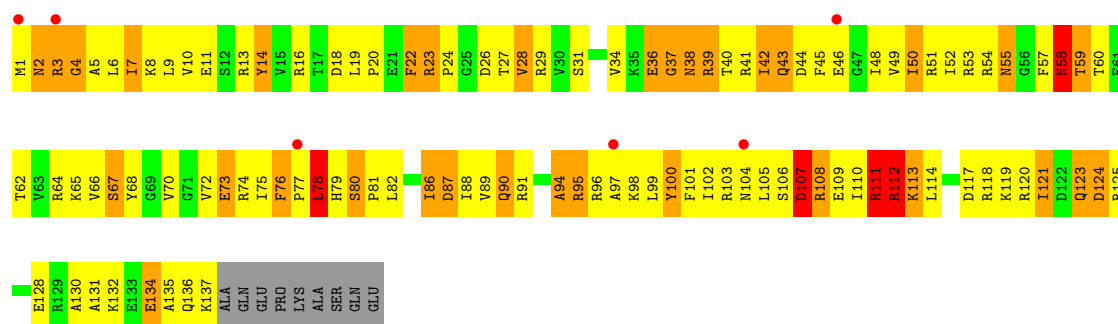
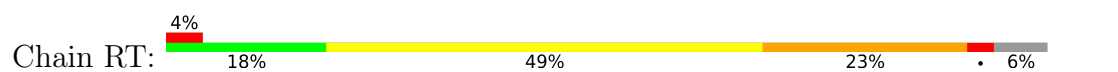
• Molecule 35: 50S ribosomal protein L18



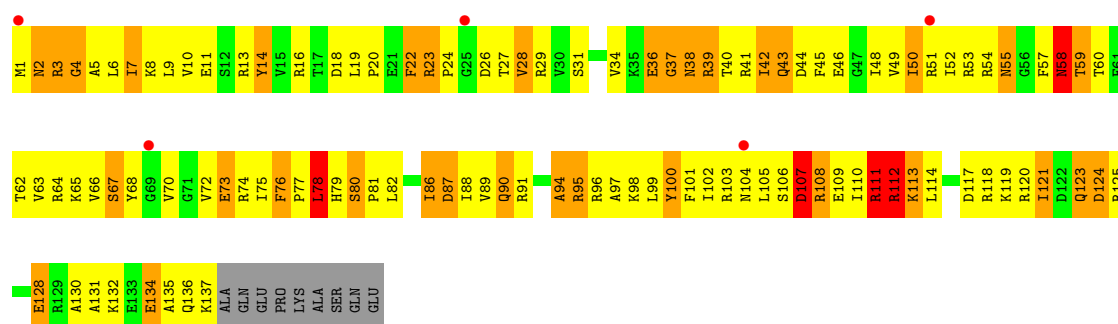
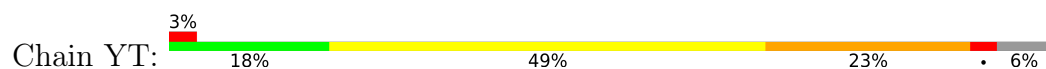
• Molecule 35: 50S ribosomal protein L18



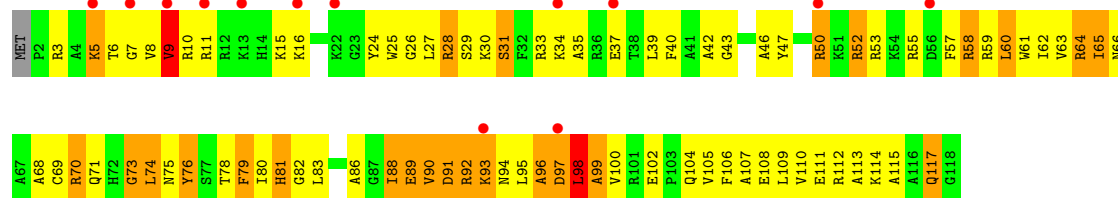
• Molecule 36: 50S ribosomal protein L19



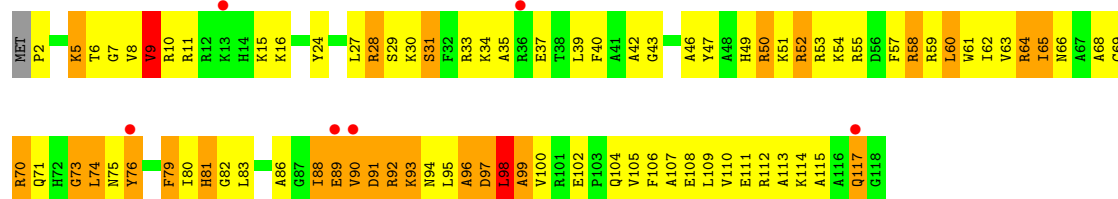
- Molecule 36: 50S ribosomal protein L19



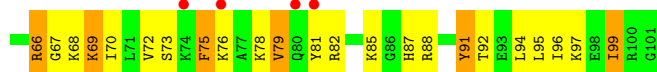
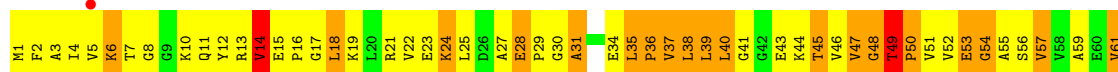
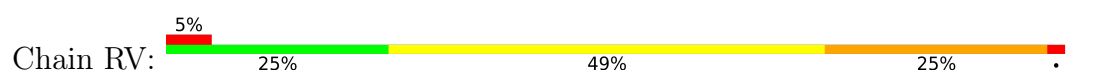
- Molecule 37: 50S ribosomal protein L20



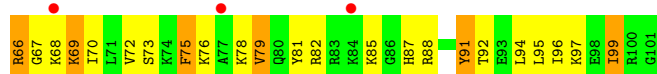
- Molecule 37: 50S ribosomal protein L20



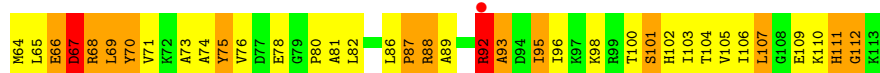
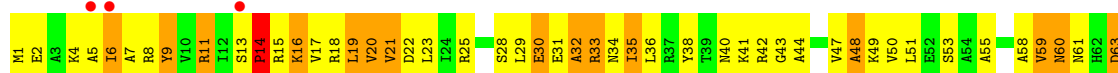
- Molecule 38: 50S ribosomal protein L21



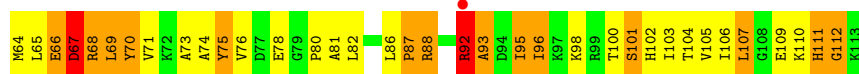
• Molecule 38: 50S ribosomal protein L21



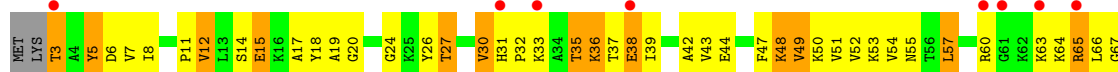
• Molecule 39: 50S ribosomal protein L22

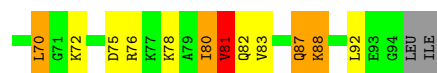


• Molecule 39: 50S ribosomal protein L22

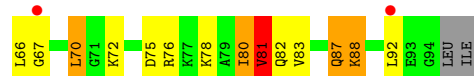
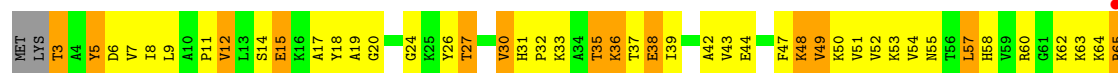


• Molecule 40: 50S ribosomal protein L23

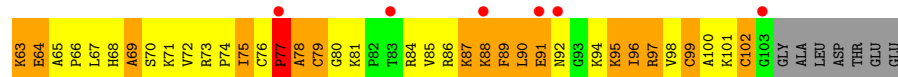
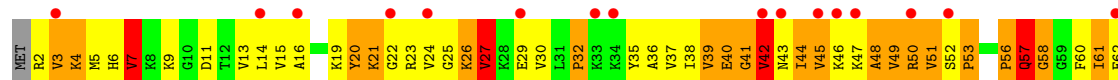
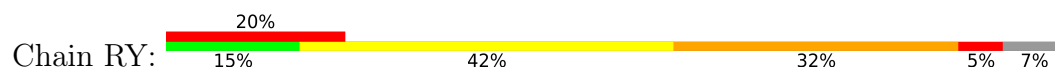




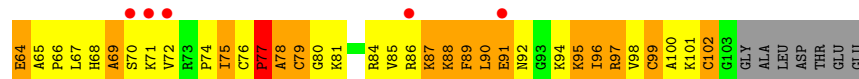
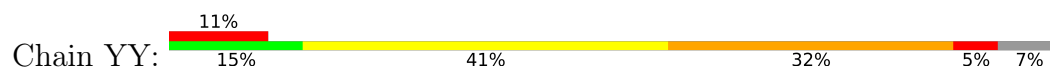
• Molecule 40: 50S ribosomal protein L23



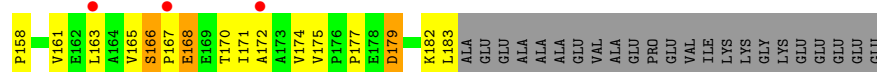
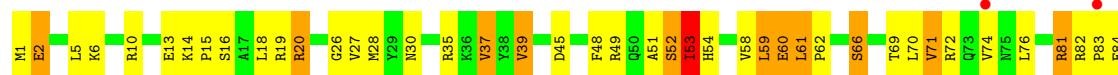
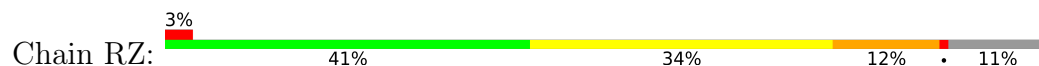
• Molecule 41: 50S ribosomal protein L24



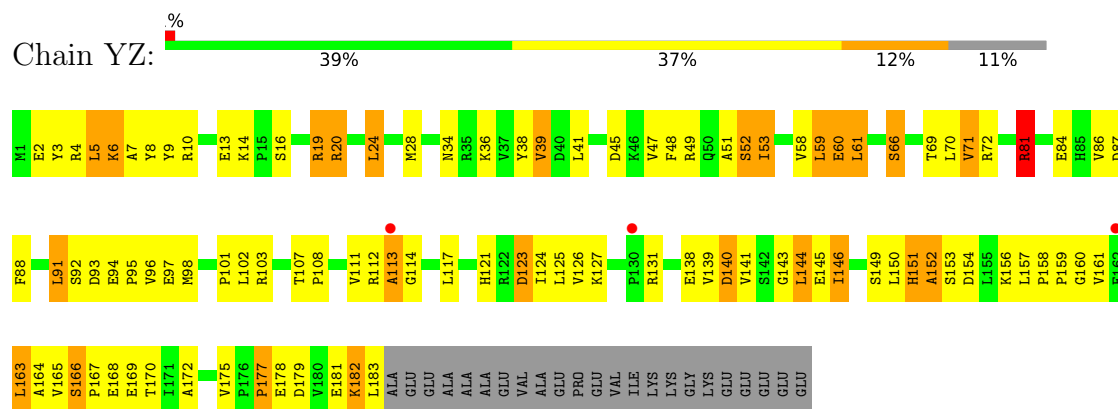
• Molecule 41: 50S ribosomal protein L24



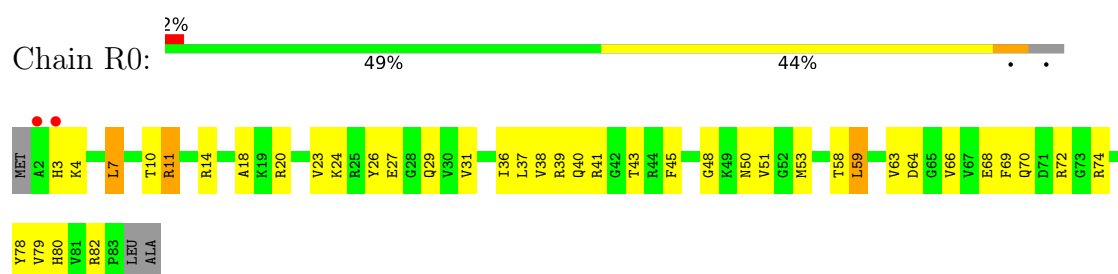
• Molecule 42: 50S ribosomal protein L25



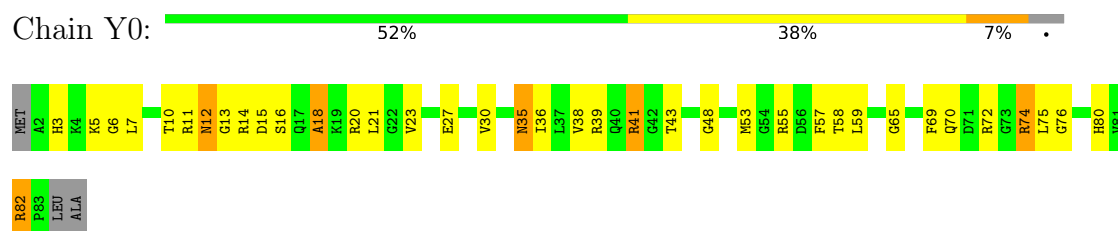
- Molecule 42: 50S ribosomal protein L25



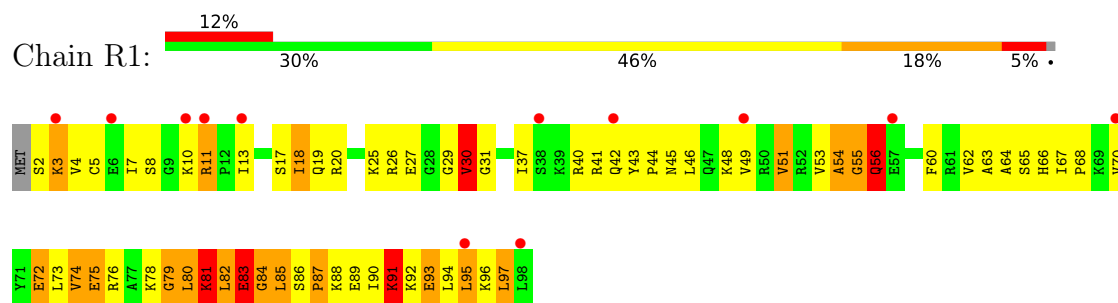
- Molecule 43: 50S ribosomal protein L27



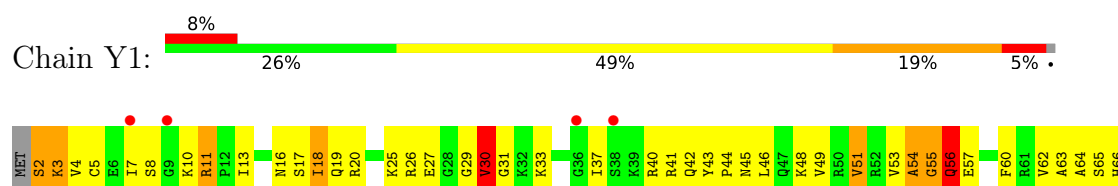
- Molecule 43: 50S ribosomal protein L27



- Molecule 44: 50S ribosomal protein L28

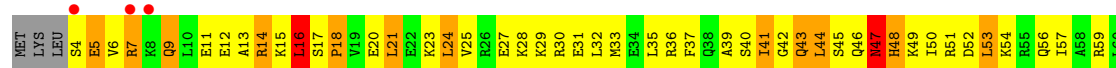
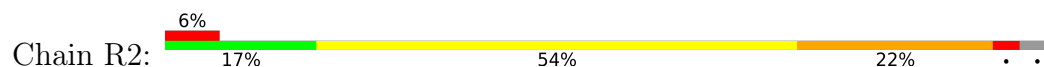


- Molecule 44: 50S ribosomal protein L28

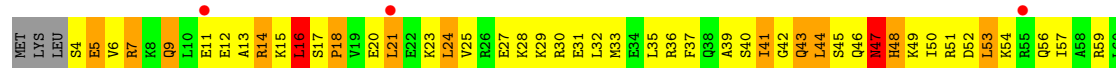
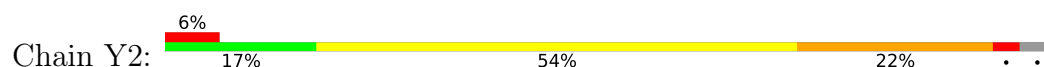




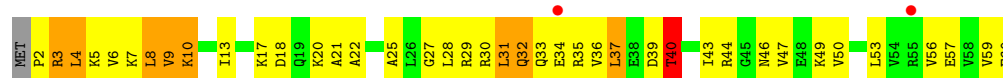
- Molecule 45: 50S ribosomal protein L29



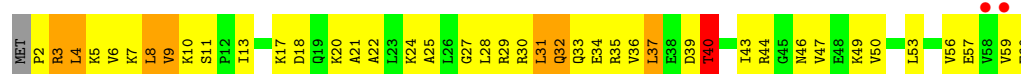
- Molecule 45: 50S ribosomal protein L29



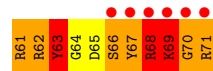
- Molecule 46: 50S ribosomal protein L30



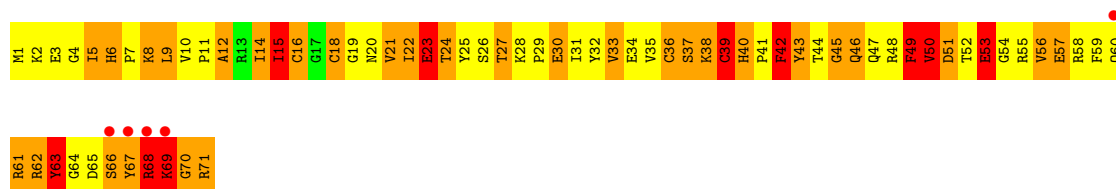
- Molecule 46: 50S ribosomal protein L30



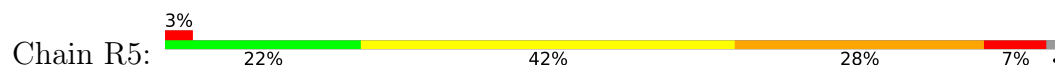
- Molecule 47: 50S ribosomal protein L31



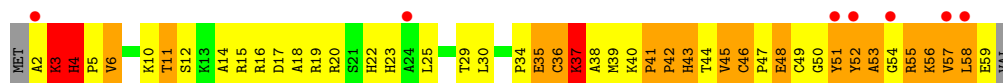
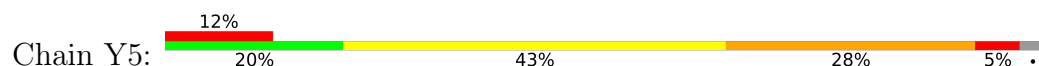
- Molecule 47: 50S ribosomal protein L31



- Molecule 48: 50S ribosomal protein L32



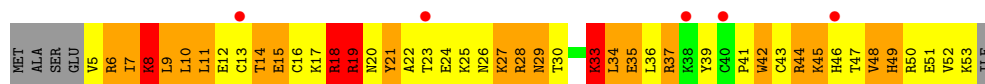
- Molecule 48: 50S ribosomal protein L32



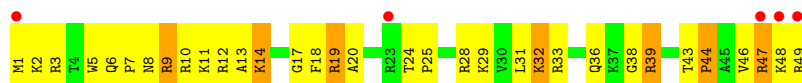
- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34

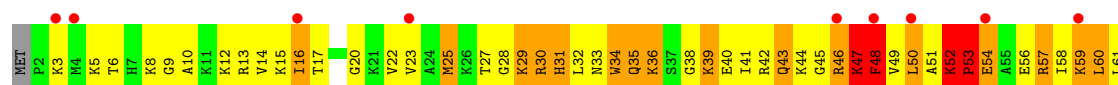
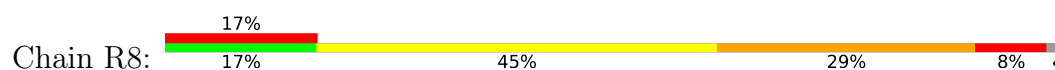


- Molecule 50: 50S ribosomal protein L34

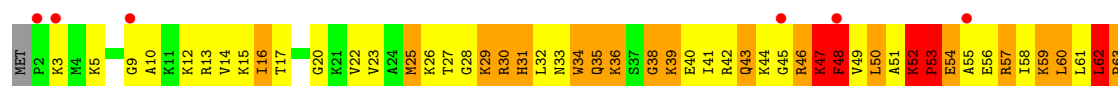
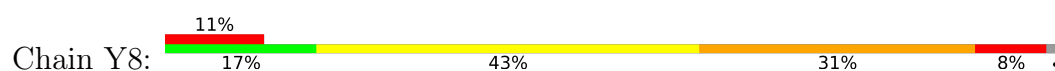




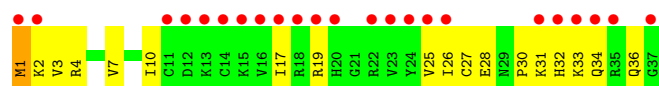
• Molecule 51: 50S ribosomal protein L35



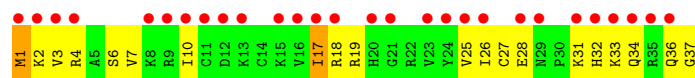
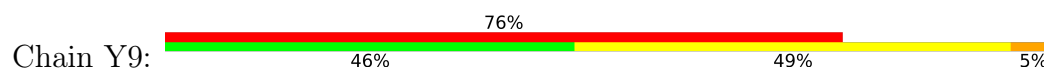
• Molecule 51: 50S ribosomal protein L35



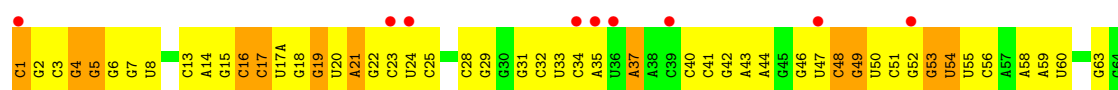
• Molecule 52: 50S ribosomal protein L36



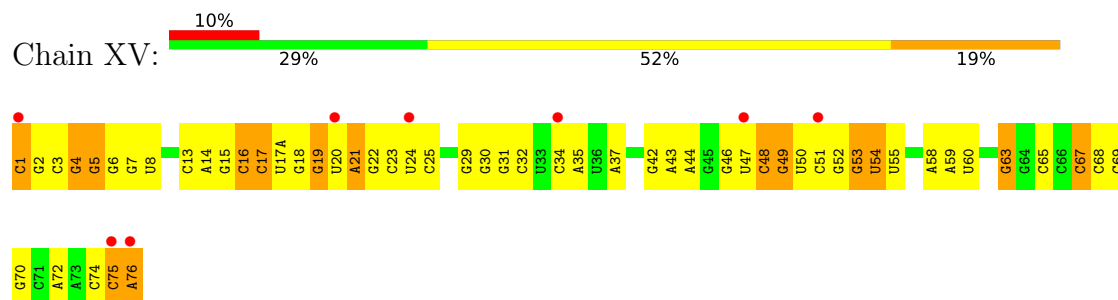
• Molecule 52: 50S ribosomal protein L36



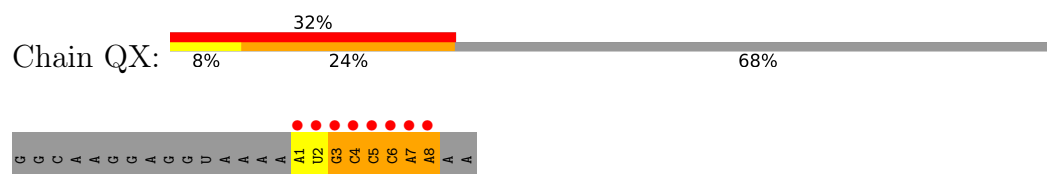
• Molecule 53: P-site tRNA fMet



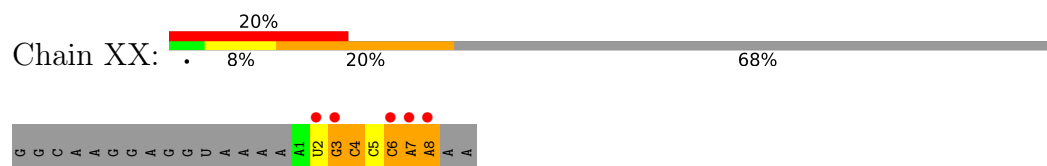
- Molecule 53: P-site tRNA fMet



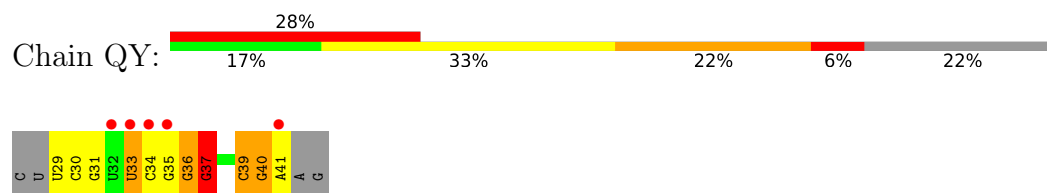
- Molecule 54: A-site ASL SufA6



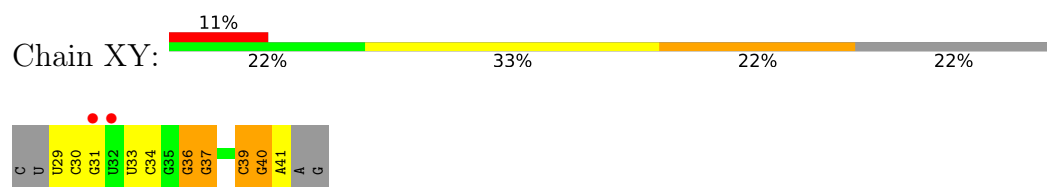
- Molecule 54: A-site ASL SufA6



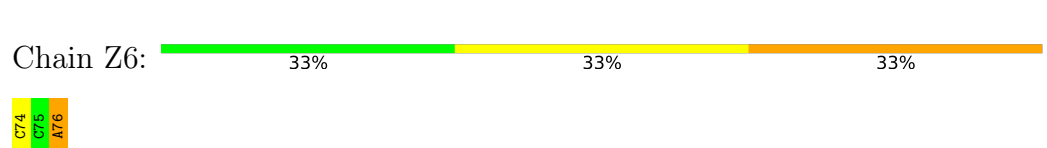
- Molecule 55: messenger RNA



- Molecule 55: messenger RNA



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic



C74
C75
A76

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.24Å 446.10Å 623.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.90 49.68 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.68-3.90) 99.0 (49.68-3.90)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	88.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	291950	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.25	0/36098	0.44	0/56341
1	XA	0.28	0/36101	0.49	3/56346 (0.0%)
2	QB	0.42	0/1959	1.06	15/2642 (0.6%)
2	XB	0.42	0/1959	1.05	10/2642 (0.4%)
3	QC	0.44	0/1629	0.93	1/2195 (0.0%)
3	XC	0.44	0/1629	0.93	1/2195 (0.0%)
4	QD	0.49	0/1733	1.06	12/2318 (0.5%)
4	XD	0.55	0/1733	1.06	14/2318 (0.6%)
5	QE	0.45	0/1171	1.02	9/1576 (0.6%)
5	XE	0.46	0/1171	1.02	9/1576 (0.6%)
6	QF	0.50	0/856	0.97	3/1154 (0.3%)
6	XF	0.50	0/856	0.97	3/1154 (0.3%)
7	QG	0.43	0/1276	0.90	1/1709 (0.1%)
7	XG	0.43	0/1276	0.90	1/1709 (0.1%)
8	QH	0.49	0/1136	1.05	5/1527 (0.3%)
8	XH	0.50	0/1136	1.05	7/1527 (0.5%)
9	QI	0.40	0/1029	1.03	9/1379 (0.7%)
9	XI	0.40	0/1029	1.03	9/1379 (0.7%)
10	QJ	0.46	0/814	0.91	1/1095 (0.1%)
10	XJ	0.46	0/814	0.91	1/1095 (0.1%)
11	QK	0.48	0/900	1.05	6/1213 (0.5%)
11	XK	0.48	0/900	1.04	6/1213 (0.5%)
12	QL	0.58	1/991 (0.1%)	1.20	10/1327 (0.8%)
12	XL	0.57	1/991 (0.1%)	1.21	9/1327 (0.7%)
13	QM	0.43	0/974	1.04	9/1303 (0.7%)
13	XM	0.43	0/974	1.04	9/1303 (0.7%)
14	QN	0.47	0/501	1.08	6/664 (0.9%)
14	XN	0.65	1/501 (0.2%)	1.07	4/664 (0.6%)
15	QO	0.48	0/745	1.00	3/992 (0.3%)
15	XO	0.48	0/745	0.99	3/992 (0.3%)
16	QP	0.45	0/721	1.03	4/970 (0.4%)
16	XP	0.46	0/721	1.04	4/970 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.43	0/847	1.06	6/1131 (0.5%)
17	XQ	0.43	0/847	1.06	6/1131 (0.5%)
18	QR	0.46	0/579	1.04	3/768 (0.4%)
18	XR	0.46	0/579	1.04	3/768 (0.4%)
19	QS	0.46	0/689	1.21	7/926 (0.8%)
19	XS	0.46	0/689	1.21	7/926 (0.8%)
20	QT	0.42	0/765	1.09	5/1007 (0.5%)
20	XT	0.42	0/765	1.09	4/1007 (0.4%)
21	QU	0.42	0/221	1.00	1/288 (0.3%)
21	XU	0.43	0/221	1.01	1/288 (0.3%)
22	RA	0.29	1/69521 (0.0%)	0.50	4/108529 (0.0%)
22	YA	0.33	0/69543	0.53	9/108563 (0.0%)
23	RB	0.24	0/2878	0.42	0/4490
23	YB	0.28	0/2878	0.48	0/4490
24	RD	0.79	2/2165 (0.1%)	1.30	34/2919 (1.2%)
24	YD	0.72	1/2165 (0.0%)	1.30	34/2919 (1.2%)
25	RE	0.62	0/1601	1.35	29/2160 (1.3%)
25	YE	0.62	0/1601	1.35	29/2160 (1.3%)
26	RF	0.62	0/1620	1.20	19/2194 (0.9%)
26	YF	0.62	0/1620	1.20	19/2194 (0.9%)
27	RG	0.47	0/1499	0.99	9/2016 (0.4%)
27	YG	0.47	0/1499	0.99	10/2016 (0.5%)
28	RH	0.58	0/1332	1.22	14/1802 (0.8%)
28	YH	0.58	0/1332	1.22	15/1802 (0.8%)
29	RI	0.74	3/1151 (0.3%)	1.01	3/1558 (0.2%)
29	YI	0.48	0/1151	0.94	2/1558 (0.1%)
30	RN	0.55	0/1131	1.18	10/1525 (0.7%)
30	YN	0.54	0/1131	1.18	10/1525 (0.7%)
31	RO	0.64	0/943	1.03	5/1269 (0.4%)
31	YO	0.65	0/943	1.04	5/1269 (0.4%)
32	RP	0.63	0/1162	1.37	17/1544 (1.1%)
32	YP	0.63	1/1162 (0.1%)	1.37	17/1544 (1.1%)
33	RQ	0.71	0/1143	1.36	19/1527 (1.2%)
33	YQ	0.71	0/1143	1.35	19/1527 (1.2%)
34	RR	0.55	0/982	1.17	10/1312 (0.8%)
34	YR	0.55	0/982	1.17	10/1312 (0.8%)
35	RS	0.53	0/892	1.18	8/1187 (0.7%)
35	YS	0.52	0/892	1.18	8/1187 (0.7%)
36	RT	0.56	0/1155	1.18	16/1542 (1.0%)
36	YT	0.56	0/1155	1.18	17/1542 (1.1%)
37	RU	0.59	0/982	1.21	10/1306 (0.8%)
37	YU	0.60	0/982	1.21	10/1306 (0.8%)
38	RV	0.56	0/790	1.10	6/1057 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YV	0.55	0/790	1.10	6/1057 (0.6%)
39	RW	0.58	0/911	1.18	13/1220 (1.1%)
39	YW	0.57	0/911	1.18	12/1220 (1.0%)
40	RX	0.62	0/739	1.14	5/993 (0.5%)
40	YX	0.62	0/739	1.14	5/993 (0.5%)
41	RY	0.64	0/798	1.17	4/1064 (0.4%)
41	YY	0.64	0/798	1.16	3/1064 (0.3%)
42	RZ	0.50	0/1493	0.95	5/2026 (0.2%)
42	YZ	0.48	0/1493	0.96	2/2026 (0.1%)
43	R0	0.48	0/657	0.92	0/874
43	Y0	0.54	0/657	0.96	0/874
44	R1	0.58	0/770	1.20	9/1022 (0.9%)
44	Y1	0.58	0/770	1.20	9/1022 (0.9%)
45	R2	0.60	0/583	1.32	9/771 (1.2%)
45	Y2	0.60	0/583	1.32	9/771 (1.2%)
46	R3	0.62	1/474 (0.2%)	1.04	0/635
46	Y3	0.54	0/474	1.04	0/635
47	R4	0.47	0/594	1.24	10/795 (1.3%)
47	Y4	0.47	0/594	1.23	10/795 (1.3%)
48	R5	0.65	0/473	1.22	6/639 (0.9%)
48	Y5	0.65	0/465	1.22	7/629 (1.1%)
49	R6	0.53	0/431	1.06	3/575 (0.5%)
49	Y6	0.53	0/431	1.06	3/575 (0.5%)
50	R7	0.73	0/438	1.19	2/575 (0.3%)
50	Y7	0.73	0/438	1.19	2/575 (0.3%)
51	R8	0.79	0/525	1.41	9/691 (1.3%)
51	Y8	0.79	0/525	1.41	9/691 (1.3%)
52	R9	0.42	0/310	0.92	1/407 (0.2%)
52	Y9	0.45	0/310	0.92	1/407 (0.2%)
53	QV	0.34	1/1836 (0.1%)	0.44	0/2859
53	XV	0.34	1/1836 (0.1%)	0.43	0/2859
54	QX	0.67	0/188	0.86	0/290
54	XX	0.40	0/188	0.72	0/290
55	QY	0.47	0/311	0.56	0/483
55	XY	0.37	0/311	0.46	0/483
56	Z6	0.46	0/40	0.62	0/60
56	Z8	0.46	0/40	0.63	0/60
All	All	0.39	14/316321 (0.0%)	0.72	811/472911 (0.2%)

The worst 5 of 14 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	14.27	1.53	1.33
29	RI	54	GLN	C-O	-9.39	1.10	1.23
29	RI	55	ALA	C-O	8.61	1.34	1.24
53	QV	1	C	OP3-P	6.62	1.61	1.48
53	XV	1	C	OP3-P	6.37	1.61	1.48

The worst 5 of 811 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	YP	59	LEU	N-CA-C	-14.62	91.38	111.56
32	RP	59	LEU	N-CA-C	-14.61	91.39	111.56
47	R4	39	CYS	N-CA-C	-13.59	95.96	112.54
47	Y4	39	CYS	N-CA-C	-13.51	96.06	112.54
25	RE	58	ARG	N-CA-C	-11.82	95.21	113.89

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	674	0
1	XA	32249	0	16278	739	1
2	QB	1924	0	1975	303	0
2	XB	1924	0	1975	309	0
3	QC	1605	0	1668	216	0
3	XC	1605	0	1668	213	0
4	QD	1703	0	1764	261	0
4	XD	1703	0	1765	233	1
5	QE	1155	0	1213	174	0
5	XE	1155	0	1213	145	0
6	QF	843	0	857	101	1
6	XF	843	0	857	103	0
7	QG	1257	0	1296	155	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1294	155	0
8	QH	1116	0	1175	160	0
8	XH	1116	0	1177	156	0
9	QI	1010	0	1037	146	0
9	XI	1010	0	1037	159	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	137	0
11	QK	885	0	904	111	0
11	XK	885	0	904	112	0
12	QL	975	0	1062	118	0
12	XL	975	0	1062	118	0
13	QM	964	0	1034	160	0
13	XM	964	0	1034	225	0
14	QN	492	0	529	106	0
14	XN	492	0	529	98	0
15	QO	734	0	771	86	0
15	XO	734	0	771	80	0
16	QP	705	0	725	121	0
16	XP	705	0	725	110	0
17	QQ	834	0	904	79	0
17	XQ	834	0	904	75	0
18	QR	574	0	644	77	0
18	XR	574	0	644	73	0
19	QS	674	0	699	123	0
19	XS	674	0	699	155	0
20	QT	763	0	860	115	0
20	XT	763	0	861	112	0
21	QU	217	0	234	27	0
21	XU	217	0	234	27	0
22	RA	62071	0	31286	1249	0
22	YA	62091	0	31295	1291	0
23	RB	2573	0	1306	70	0
23	YB	2573	0	1306	56	0
24	RD	2115	0	2195	327	0
24	YD	2115	0	2195	329	0
25	RE	1568	0	1634	282	0
25	YE	1568	0	1634	287	0
26	RF	1585	0	1632	192	0
26	YF	1585	0	1632	195	0
27	RG	1474	0	1535	216	0
27	YG	1474	0	1535	217	0
28	RH	1307	0	1382	226	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YH	1307	0	1382	233	3
29	RI	1136	0	1223	62	1
29	YI	1136	0	1223	57	0
30	RN	1104	0	1180	196	0
30	YN	1104	0	1180	194	0
31	RO	933	0	996	132	0
31	YO	933	0	996	139	0
32	RP	1145	0	1227	254	0
32	YP	1145	0	1228	250	0
33	RQ	1122	0	1179	156	0
33	YQ	1122	0	1178	158	0
34	RR	968	0	1033	116	0
34	YR	968	0	1033	118	0
35	RS	882	0	943	163	0
35	YS	882	0	943	163	0
36	RT	1141	0	1202	160	0
36	YT	1141	0	1202	158	0
37	RU	964	0	1022	142	0
37	YU	964	0	1022	144	0
38	RV	779	0	852	138	0
38	YV	779	0	852	133	0
39	RW	900	0	964	105	0
39	YW	900	0	964	106	0
40	RX	725	0	778	69	0
40	YX	725	0	778	68	0
41	RY	785	0	878	172	0
41	YY	785	0	878	163	3
42	RZ	1461	0	1493	65	0
42	YZ	1461	0	1493	73	0
43	R0	648	0	672	28	0
43	Y0	648	0	672	44	0
44	R1	763	0	848	148	0
44	Y1	763	0	848	144	0
45	R2	581	0	629	85	0
45	Y2	581	0	629	83	0
46	R3	469	0	518	44	0
46	Y3	469	0	518	46	0
47	R4	581	0	574	163	0
47	Y4	581	0	574	229	0
48	R5	459	0	480	76	0
48	Y5	451	0	471	69	0
49	R6	424	0	450	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y6	424	0	450	89	0
50	R7	430	0	480	43	0
50	Y7	430	0	480	46	0
51	R8	517	0	582	103	0
51	Y8	517	0	582	106	0
52	R9	307	0	335	20	0
52	Y9	307	0	336	24	0
53	QV	1644	0	836	64	0
53	XV	1644	0	836	56	0
54	QX	169	0	88	56	0
54	XX	169	0	88	18	0
55	QY	303	0	152	21	0
55	XY	303	0	154	31	0
56	Z6	74	0	51	24	0
56	Z8	74	0	51	13	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	16251	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 33.

The worst 5 of 16251 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	4
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	4
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	9
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	9
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	8
4	XD	206/209 (99%)	135 (66%)	48 (23%)	23 (11%)	0	6
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	7
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	6
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	0	9
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	0	9
7	QG	153/156 (98%)	101 (66%)	37 (24%)	15 (10%)	0	8
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	0	9
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	6
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	6
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	4
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	4
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	9
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	7
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	14
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	14
12	QL	123/132 (93%)	84 (68%)	23 (19%)	16 (13%)	0	3
12	XL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	0	4
13	QM	119/126 (94%)	71 (60%)	29 (24%)	19 (16%)	0	2
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	2
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	1
14	XN	58/61 (95%)	33 (57%)	13 (22%)	12 (21%)	0	1
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	13
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	13
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	0	11
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	0	11
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	5
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	5
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	1
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
24	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	13
24	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	13
25	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
25	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
26	RF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	7
26	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	7
27	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	5
27	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	5
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	5
29	YI	144/148 (97%)	100 (69%)	27 (19%)	17 (12%)	0	5
30	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
30	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
31	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	12
31	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	12
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	7
33	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	7
34	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
35	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	2
35	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	2
36	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	3
36	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	3
37	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	12
37	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	12
38	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	7
38	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	7
39	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
39	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
40	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1	16
40	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1	16
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	4
42	YZ	181/206 (88%)	128 (71%)	35 (19%)	18 (10%)	0	7
43	R0	80/85 (94%)	67 (84%)	12 (15%)	1 (1%)	9	40
43	Y0	80/85 (94%)	67 (84%)	11 (14%)	2 (2%)	4	29
44	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
44	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
45	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	3
45	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
46	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1	17
46	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1	17
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	15
50	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	15
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	3

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	22
2	XB	205/220 (93%)	182 (89%)	23 (11%)	6	23
3	QC	159/188 (85%)	142 (89%)	17 (11%)	6	24
3	XC	159/188 (85%)	142 (89%)	17 (11%)	6	24
4	QD	180/181 (99%)	156 (87%)	24 (13%)	4	19
4	XD	180/181 (99%)	162 (90%)	18 (10%)	7	27
5	QE	116/123 (94%)	105 (90%)	11 (10%)	8	29
5	XE	116/123 (94%)	105 (90%)	11 (10%)	8	29
6	QF	90/90 (100%)	77 (86%)	13 (14%)	3	17
6	XF	90/90 (100%)	77 (86%)	13 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	QG	126/127 (99%)	112 (89%)	14 (11%)	6	23
7	XG	126/127 (99%)	112 (89%)	14 (11%)	6	23
8	QH	119/119 (100%)	105 (88%)	14 (12%)	5	21
8	XH	119/119 (100%)	105 (88%)	14 (12%)	5	21
9	QI	98/99 (99%)	85 (87%)	13 (13%)	4	19
9	XI	98/99 (99%)	85 (87%)	13 (13%)	4	19
10	QJ	89/92 (97%)	80 (90%)	9 (10%)	7	27
10	XJ	89/92 (97%)	80 (90%)	9 (10%)	7	27
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	27
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	27
12	QL	104/109 (95%)	85 (82%)	19 (18%)	2	11
12	XL	104/109 (95%)	86 (83%)	18 (17%)	2	12
13	QM	97/101 (96%)	83 (86%)	14 (14%)	3	17
13	XM	97/101 (96%)	83 (86%)	14 (14%)	3	17
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	11
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	26
15	QO	79/80 (99%)	70 (89%)	9 (11%)	5	22
15	XO	79/80 (99%)	70 (89%)	9 (11%)	5	22
16	QP	72/74 (97%)	64 (89%)	8 (11%)	6	23
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6	23
17	QQ	95/97 (98%)	86 (90%)	9 (10%)	8	29
17	XQ	95/97 (98%)	86 (90%)	9 (10%)	8	29
18	QR	61/77 (79%)	51 (84%)	10 (16%)	2	13
18	XR	61/77 (79%)	51 (84%)	10 (16%)	2	13
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	16
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	16
20	QT	76/82 (93%)	69 (91%)	7 (9%)	8	30
20	XT	76/82 (93%)	69 (91%)	7 (9%)	8	30
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	RD	214/218 (98%)	174 (81%)	40 (19%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	YD	214/218 (98%)	174 (81%)	40 (19%)	1	10
25	RE	165/166 (99%)	125 (76%)	40 (24%)	1	4
25	YE	165/166 (99%)	125 (76%)	40 (24%)	1	4
26	RF	161/166 (97%)	138 (86%)	23 (14%)	3	17
26	YF	161/166 (97%)	138 (86%)	23 (14%)	3	17
27	RG	155/156 (99%)	133 (86%)	22 (14%)	3	17
27	YG	155/156 (99%)	134 (86%)	21 (14%)	4	18
28	RH	142/148 (96%)	111 (78%)	31 (22%)	1	6
28	YH	142/148 (96%)	111 (78%)	31 (22%)	1	6
29	RI	122/124 (98%)	97 (80%)	25 (20%)	1	8
29	YI	122/124 (98%)	99 (81%)	23 (19%)	1	10
30	RN	117/119 (98%)	97 (83%)	20 (17%)	2	12
30	YN	117/119 (98%)	97 (83%)	20 (17%)	2	12
31	RO	100/100 (100%)	88 (88%)	12 (12%)	5	21
31	YO	100/100 (100%)	89 (89%)	11 (11%)	6	24
32	RP	116/116 (100%)	88 (76%)	28 (24%)	1	4
32	YP	116/116 (100%)	88 (76%)	28 (24%)	1	4
33	RQ	111/111 (100%)	95 (86%)	16 (14%)	3	17
33	YQ	111/111 (100%)	96 (86%)	15 (14%)	4	18
34	RR	101/101 (100%)	85 (84%)	16 (16%)	2	15
34	YR	101/101 (100%)	85 (84%)	16 (16%)	2	15
35	RS	87/88 (99%)	73 (84%)	14 (16%)	2	14
35	YS	87/88 (99%)	73 (84%)	14 (16%)	2	14
36	RT	120/127 (94%)	99 (82%)	21 (18%)	2	12
36	YT	120/127 (94%)	99 (82%)	21 (18%)	2	12
37	RU	93/94 (99%)	81 (87%)	12 (13%)	4	20
37	YU	93/94 (99%)	81 (87%)	12 (13%)	4	20
38	RV	82/82 (100%)	66 (80%)	16 (20%)	1	9
38	YV	82/82 (100%)	67 (82%)	15 (18%)	2	11
39	RW	92/92 (100%)	76 (83%)	16 (17%)	2	12
39	YW	92/92 (100%)	76 (83%)	16 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	RX	74/78 (95%)	61 (82%)	13 (18%)	2	12
40	YX	74/78 (95%)	61 (82%)	13 (18%)	2	12
41	RY	85/91 (93%)	67 (79%)	18 (21%)	1	7
41	YY	85/91 (93%)	66 (78%)	19 (22%)	1	6
42	RZ	162/179 (90%)	140 (86%)	22 (14%)	3	18
42	YZ	162/179 (90%)	136 (84%)	26 (16%)	2	14
43	R0	65/67 (97%)	55 (85%)	10 (15%)	2	15
43	Y0	65/67 (97%)	57 (88%)	8 (12%)	4	20
44	R1	82/83 (99%)	70 (85%)	12 (15%)	3	16
44	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	16
45	R2	64/67 (96%)	56 (88%)	8 (12%)	4	20
45	Y2	64/67 (96%)	56 (88%)	8 (12%)	4	20
46	R3	51/52 (98%)	41 (80%)	10 (20%)	1	9
46	Y3	51/52 (98%)	41 (80%)	10 (20%)	1	9
47	R4	63/63 (100%)	46 (73%)	17 (27%)	0	3
47	Y4	63/63 (100%)	46 (73%)	17 (27%)	0	3
48	R5	51/52 (98%)	40 (78%)	11 (22%)	1	6
48	Y5	50/52 (96%)	39 (78%)	11 (22%)	1	6
49	R6	48/52 (92%)	36 (75%)	12 (25%)	0	4
49	Y6	48/52 (92%)	36 (75%)	12 (25%)	0	4
50	R7	42/42 (100%)	38 (90%)	4 (10%)	8	29
50	Y7	42/42 (100%)	38 (90%)	4 (10%)	8	29
51	R8	54/55 (98%)	40 (74%)	14 (26%)	0	4
51	Y8	54/55 (98%)	40 (74%)	14 (26%)	0	4
52	R9	34/34 (100%)	32 (94%)	2 (6%)	18	44
52	Y9	34/34 (100%)	32 (94%)	2 (6%)	18	44
All	All	9701/10066 (96%)	8218 (85%)	1483 (15%)	3	15

5 of 1483 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	XN	41	ARG
29	YI	81	VAL

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Mol	Chain	Res	Type
18	XR	26	LEU
14	XN	16	PHE
25	YE	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
30	YN	101	HIS
44	Y1	66	HIS
31	YO	29	ASN
37	YU	94	ASN
47	Y4	47	GLN

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%)	659 (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%)	2003 (21%)	240 (2%)

5 of 2003 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
1	XA	60	A
22	YA	2566	A
1	XA	812	C
22	YA	2481	G
55	QY	39	C

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
55	1MG	QY	37	55	23,26,27	1.07	2 (8%)	33,39,42	1.44	3 (9%)
56	PPU	Z6	76	22,56	37,40,41	2.58	8 (21%)	47,57,60	2.57	15 (31%)
55	1MG	XY	37	55	23,26,27	2.63	4 (17%)	33,39,42	2.02	8 (24%)
56	PPU	Z8	76	22,56	37,40,41	2.58	8 (21%)	47,57,60	2.56	15 (31%)

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
55	1MG	QY	37	55	-	0/7/25/26	0/3/3/3
56	PPU	Z6	76	22,56	-	2/25/43/44	0/4/4/4
55	1MG	XY	37	55	-	0/7/25/26	0/3/3/3
56	PPU	Z8	76	22,56	-	2/25/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.63	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.60	1.41	1.23
55	XY	37	1MG	C2-N2	8.10	1.48	1.34
55	XY	37	1MG	C4-N3	6.52	1.49	1.34
56	Z6	76	PPU	C9-N6	-6.28	1.31	1.45

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.55	110.20	123.20
56	Z8	76	PPU	C3'-N3'-C	-8.51	110.25	123.20
55	XY	37	1MG	N2-C2-N1	6.18	123.75	118.79
56	Z6	76	PPU	C2'-C1'-N9	-5.95	98.52	113.30
56	Z8	76	PPU	C2'-C1'-N9	-5.94	98.56	113.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	QY	37	1MG	2	0
56	Z6	76	PPU	14	0
55	XY	37	1MG	8	0
56	Z8	76	PPU	10	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	44,45,45	1.28	6 (13%)	63,67,67	1.33	8 (12%)
58	PAR	XA	1673	-	44,45,45	1.33	6 (13%)	63,67,67	1.30	4 (6%)

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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C52-C42	3.10	1.58	1.52
58	XA	1673	PAR	C52-C42	2.98	1.58	1.52
58	XA	1673	PAR	O54-C14	2.90	1.49	1.41
58	QA	1666	PAR	O54-C14	2.86	1.49	1.41
58	XA	1673	PAR	C11-C21	2.84	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1673	PAR	O33-C14-C24	5.06	116.36	108.08
58	XA	1673	PAR	C14-O54-C54	4.32	122.15	113.72
58	QA	1666	PAR	O33-C14-C24	4.03	114.67	108.08
58	QA	1666	PAR	C14-O54-C54	3.84	121.21	113.72
58	QA	1666	PAR	O11-C42-C52	3.15	115.42	107.42

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

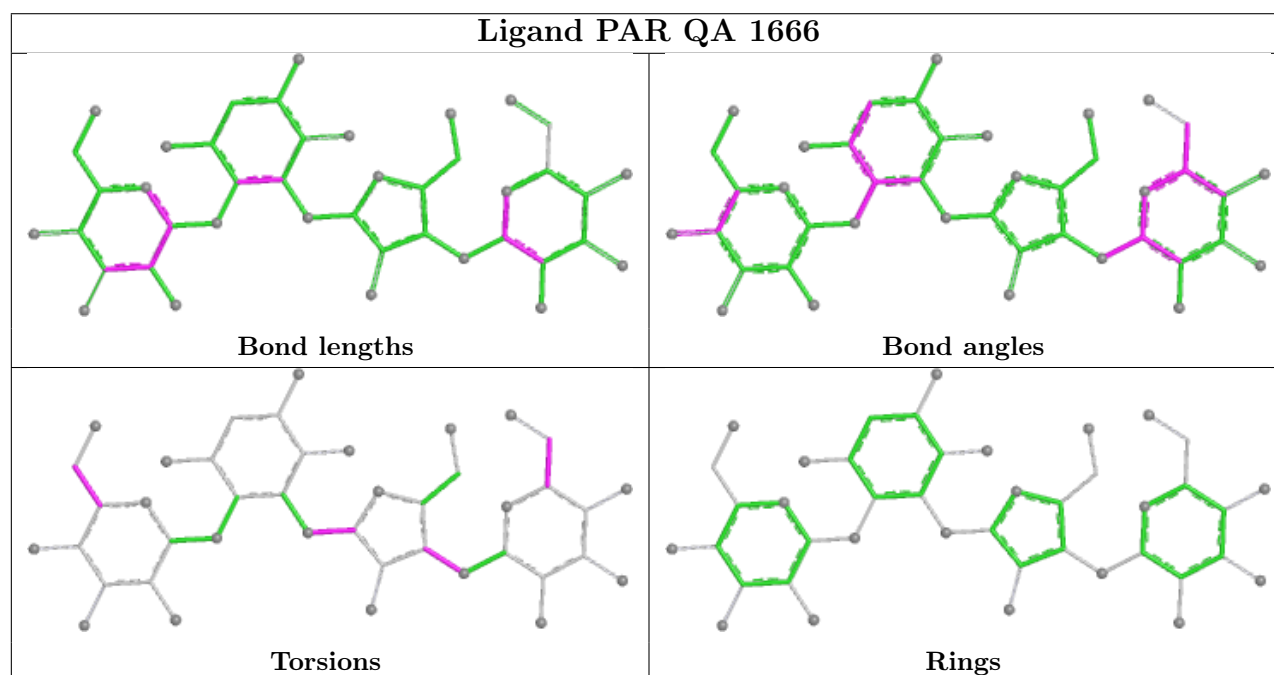
Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	XA	1673	PAR	O51-C51-C61-O61
58	QA	1666	PAR	O51-C51-C61-O61
58	XA	1673	PAR	C41-C51-C61-O61

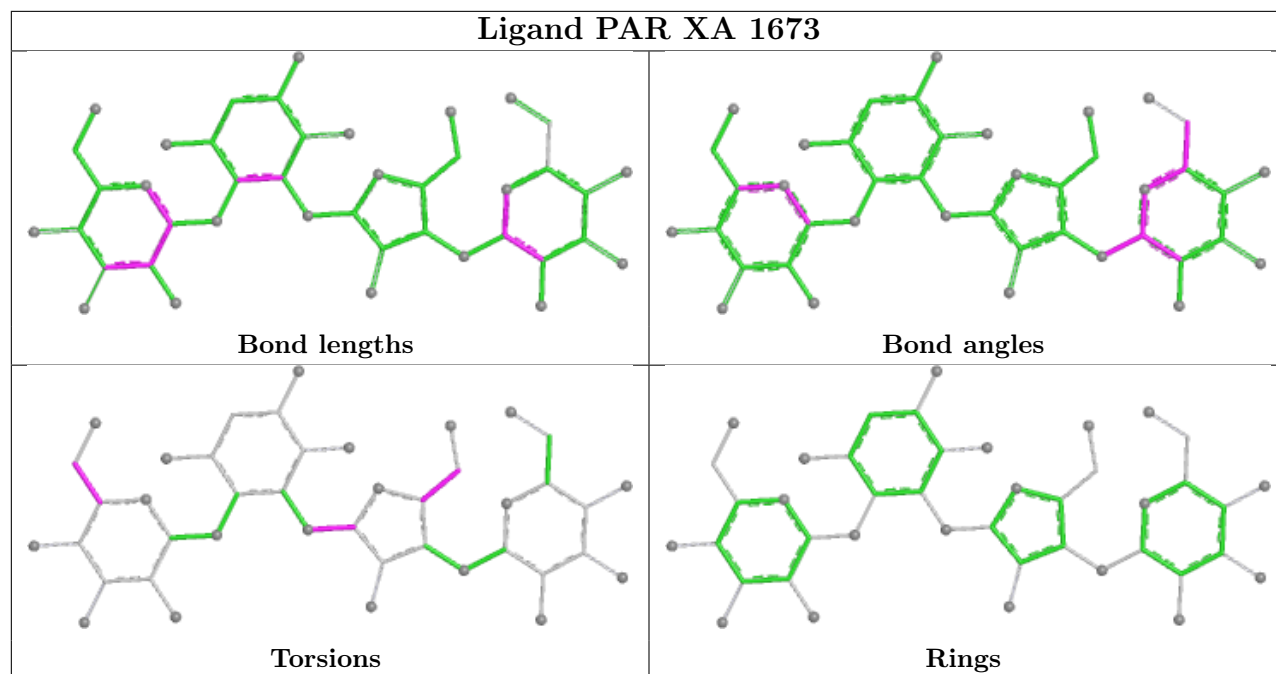
There are no ring outliers.

2 monomers are involved in 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.12	36 (2%) 59 42	22, 75, 152, 231	0
1	XA	1500/1522 (98%)	-0.07	16 (1%) 78 57	7, 55, 142, 232	0
2	QB	237/256 (92%)	0.50	9 (3%) 44 32	47, 109, 145, 182	0
2	XB	237/256 (92%)	0.27	2 (0%) 82 64	38, 88, 133, 159	0
3	QC	205/239 (85%)	0.35	9 (4%) 39 29	39, 98, 133, 150	0
3	XC	205/239 (85%)	0.10	5 (2%) 59 42	20, 67, 110, 138	0
4	QD	208/209 (99%)	0.65	18 (8%) 16 17	29, 79, 128, 167	0
4	XD	208/209 (99%)	0.69	17 (8%) 17 18	10, 72, 110, 139	0
5	QE	151/162 (93%)	0.48	11 (7%) 21 19	25, 85, 122, 159	0
5	XE	151/162 (93%)	0.44	8 (5%) 32 25	1, 62, 104, 134	0
6	QF	101/101 (100%)	0.35	0 100 100	16, 74, 116, 131	0
6	XF	101/101 (100%)	0.16	0 100 100	16, 65, 110, 133	0
7	QG	155/156 (99%)	0.46	11 (7%) 22 20	30, 84, 125, 149	0
7	XG	155/156 (99%)	0.13	4 (2%) 57 40	20, 71, 109, 131	0
8	QH	138/138 (100%)	0.73	12 (8%) 16 17	45, 88, 124, 156	0
8	XH	138/138 (100%)	0.41	4 (2%) 53 37	19, 70, 102, 125	0
9	QI	127/128 (99%)	0.88	14 (11%) 10 13	46, 97, 137, 144	0
9	XI	127/128 (99%)	0.88	16 (12%) 8 11	16, 79, 119, 129	0
10	QJ	99/105 (94%)	1.15	17 (17%) 4 7	44, 108, 142, 161	0
10	XJ	99/105 (94%)	0.81	7 (7%) 22 20	9, 83, 129, 147	0
11	QK	119/129 (92%)	0.56	7 (5%) 28 24	18, 71, 123, 149	0
11	XK	119/129 (92%)	0.34	5 (4%) 40 30	15, 63, 110, 147	0
12	QL	125/132 (94%)	0.87	14 (11%) 10 13	20, 72, 108, 139	0
12	XL	125/132 (94%)	0.56	15 (12%) 9 12	0, 48, 91, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.88	17 (14%) 6 9	39, 96, 131, 170	0
13	XM	121/126 (96%)	0.53	9 (7%) 20 19	4, 68, 125, 149	0
14	QN	60/61 (98%)	1.42	17 (28%) 1 3	52, 98, 137, 146	0
14	XN	60/61 (98%)	0.85	6 (10%) 12 15	4, 60, 100, 120	0
15	QO	88/89 (98%)	0.51	4 (4%) 38 28	30, 79, 120, 136	0
15	XO	88/89 (98%)	0.27	3 (3%) 48 34	10, 64, 93, 107	0
16	QP	84/88 (95%)	0.94	10 (11%) 9 12	12, 68, 103, 138	0
16	XP	84/88 (95%)	0.67	4 (4%) 35 27	30, 70, 106, 135	0
17	QQ	100/105 (95%)	0.99	16 (16%) 5 8	33, 82, 115, 141	0
17	XQ	100/105 (95%)	0.61	6 (6%) 27 23	14, 64, 102, 124	0
18	QR	70/88 (79%)	0.33	2 (2%) 53 37	18, 78, 119, 147	0
18	XR	70/88 (79%)	0.27	3 (4%) 40 30	22, 67, 109, 135	0
19	QS	84/93 (90%)	1.05	14 (16%) 4 7	60, 102, 132, 147	0
19	XS	84/93 (90%)	0.40	4 (4%) 35 27	15, 73, 112, 164	0
20	QT	99/106 (93%)	0.86	12 (12%) 8 12	3, 77, 111, 131	0
20	XT	99/106 (93%)	0.90	15 (15%) 5 8	19, 77, 117, 126	0
21	QU	25/27 (92%)	1.24	7 (28%) 1 3	37, 85, 131, 145	0
21	XU	25/27 (92%)	1.53	8 (32%) 1 2	30, 75, 103, 134	0
22	RA	2882/2916 (98%)	-0.13	57 (1%) 65 45	2, 45, 174, 236	0
22	YA	2883/2916 (98%)	-0.18	44 (1%) 72 50	1, 35, 165, 227	0
23	RB	120/122 (98%)	0.19	1 (0%) 82 64	46, 89, 131, 152	0
23	YB	120/122 (98%)	-0.13	2 (1%) 69 48	18, 58, 93, 139	0
24	RD	272/276 (98%)	0.48	20 (7%) 20 19	4, 41, 81, 123	0
24	YD	272/276 (98%)	0.61	20 (7%) 20 19	1, 33, 74, 140	0
25	RE	205/206 (99%)	0.83	24 (11%) 9 12	7, 62, 112, 141	0
25	YE	205/206 (99%)	0.41	6 (2%) 53 37	6, 56, 103, 125	0
26	RF	202/210 (96%)	0.39	6 (2%) 52 36	1, 64, 110, 129	0
26	YF	202/210 (96%)	0.48	6 (2%) 52 36	1, 47, 95, 112	0
27	RG	181/182 (99%)	0.95	19 (10%) 11 14	34, 99, 142, 166	0
27	YG	181/182 (99%)	0.37	6 (3%) 49 34	9, 66, 115, 163	0
28	RH	170/180 (94%)	0.65	13 (7%) 20 19	32, 108, 152, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YH	170/180 (94%)	0.61	10 (5%) 28 24	14, 68, 110, 133	0
29	RI	146/148 (98%)	0.30	7 (4%) 35 27	16, 78, 122, 154	0
29	YI	146/148 (98%)	0.16	4 (2%) 56 39	8, 72, 119, 159	0
30	RN	138/140 (98%)	0.61	7 (5%) 33 26	14, 70, 110, 124	0
30	YN	138/140 (98%)	0.68	10 (7%) 21 20	8, 55, 103, 128	0
31	RO	122/122 (100%)	0.73	13 (10%) 11 14	5, 56, 97, 126	0
31	YO	122/122 (100%)	0.24	3 (2%) 58 41	0, 42, 79, 94	0
32	RP	150/150 (100%)	0.94	21 (14%) 6 9	6, 65, 126, 159	0
32	YP	150/150 (100%)	0.70	12 (8%) 18 18	5, 53, 105, 154	0
33	RQ	141/141 (100%)	0.76	16 (11%) 10 13	2, 62, 106, 142	0
33	YQ	141/141 (100%)	0.59	15 (10%) 11 14	3, 42, 94, 132	0
34	RR	118/118 (100%)	0.65	11 (9%) 14 16	8, 50, 92, 118	0
34	YR	118/118 (100%)	0.40	5 (4%) 40 30	6, 43, 89, 109	0
35	RS	111/112 (99%)	0.56	5 (4%) 38 28	35, 78, 114, 141	0
35	YS	111/112 (99%)	0.24	4 (3%) 46 33	7, 61, 94, 111	0
36	RT	137/146 (93%)	0.59	6 (4%) 39 29	13, 64, 125, 165	0
36	YT	137/146 (93%)	0.43	5 (3%) 46 33	10, 58, 111, 158	0
37	RU	117/118 (99%)	0.76	13 (11%) 10 13	10, 61, 104, 147	0
37	YU	117/118 (99%)	0.68	6 (5%) 33 26	0, 44, 108, 129	0
38	RV	101/101 (100%)	0.44	5 (4%) 34 26	20, 75, 116, 144	0
38	YV	101/101 (100%)	0.56	8 (7%) 18 18	11, 65, 104, 156	0
39	RW	113/113 (100%)	0.39	4 (3%) 47 33	3, 43, 93, 149	0
39	YW	113/113 (100%)	0.12	1 (0%) 81 62	2, 42, 91, 144	0
40	RX	92/96 (95%)	0.66	8 (8%) 16 17	15, 52, 96, 125	0
40	YX	92/96 (95%)	0.38	3 (3%) 49 34	3, 37, 76, 96	0
41	RY	102/110 (92%)	1.35	22 (21%) 2 4	26, 88, 132, 159	0
41	YY	102/110 (92%)	0.76	12 (11%) 9 12	9, 63, 120, 140	0
42	RZ	183/206 (88%)	0.41	7 (3%) 44 32	21, 88, 132, 152	0
42	YZ	183/206 (88%)	0.22	3 (1%) 70 49	20, 70, 123, 155	0
43	R0	82/85 (96%)	0.36	2 (2%) 59 42	14, 48, 79, 112	0
43	Y0	82/85 (96%)	0.02	0 100 100	3, 36, 66, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	R1	97/98 (98%)	0.96	12 (12%) 8 11	5, 53, 126, 159	0
44	Y1	97/98 (98%)	0.56	8 (8%) 17 18	5, 43, 104, 139	0
45	R2	69/72 (95%)	0.64	4 (5%) 29 24	13, 72, 111, 129	0
45	Y2	69/72 (95%)	0.41	4 (5%) 29 24	5, 50, 104, 121	0
46	R3	59/60 (98%)	0.52	2 (3%) 48 34	12, 63, 111, 138	0
46	Y3	59/60 (98%)	0.52	2 (3%) 48 34	2, 44, 101, 174	0
47	R4	71/71 (100%)	0.80	6 (8%) 16 17	75, 131, 170, 189	0
47	Y4	71/71 (100%)	0.71	5 (7%) 22 20	46, 102, 154, 161	0
48	R5	59/60 (98%)	0.42	2 (3%) 48 34	6, 55, 133, 141	0
48	Y5	58/60 (96%)	0.62	7 (12%) 8 12	10, 59, 143, 162	0
49	R6	49/54 (90%)	1.18	12 (24%) 2 4	83, 118, 150, 157	0
49	Y6	49/54 (90%)	0.94	5 (10%) 12 15	51, 109, 141, 149	0
50	R7	49/49 (100%)	0.67	5 (10%) 12 15	8, 35, 87, 146	0
50	Y7	49/49 (100%)	0.51	4 (8%) 17 18	1, 29, 71, 121	0
51	R8	64/65 (98%)	1.02	11 (17%) 4 7	1, 52, 96, 158	0
51	Y8	64/65 (98%)	0.97	7 (10%) 10 13	5, 40, 81, 149	0
52	R9	37/37 (100%)	2.60	23 (62%) 0 0	66, 110, 156, 168	0
52	Y9	37/37 (100%)	2.59	28 (75%) 0 0	78, 107, 132, 166	0
53	QV	77/77 (100%)	0.93	11 (14%) 6 9	46, 99, 145, 169	0
53	XV	77/77 (100%)	0.68	8 (10%) 11 14	28, 72, 119, 180	0
54	QX	8/25 (32%)	3.85	8 (100%) 0 0	103, 130, 144, 183	0
54	XX	8/25 (32%)	3.19	5 (62%) 0 0	56, 75, 115, 190	0
55	QY	13/18 (72%)	1.90	5 (38%) 1 1	112, 161, 199, 206	0
55	XY	13/18 (72%)	1.21	2 (15%) 5 8	72, 116, 180, 193	0
56	Z6	2/3 (66%)	0.90	0 100 100	52, 52, 52, 57	0
56	Z8	2/3 (66%)	0.70	0 100 100	46, 46, 46, 46	0
All	All	20870/21494 (97%)	0.30	1072 (5%) 33 26	0, 61, 135, 236	0

The worst 5 of 1072 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	XX	8	A	9.5
11	XK	129	SER	7.7

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Mol	Chain	Res	Type	RSRZ
50	Y7	48	LYS	7.2
52	R9	11	CYS	6.9
11	QK	129	SER	6.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	1MG	QY	37	24/25	0.88	0.14	125,125,125,125	0
55	1MG	XY	37	24/25	0.90	0.10	64,64,64,64	0
56	PPU	Z6	76	37/38	0.91	0.18	51,51,51,51	0
56	PPU	Z8	76	37/38	0.92	0.13	48,48,48,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	YA	3041	1/1	0.34	0.66	50,50,50,50	0
57	MG	QA	1655	1/1	0.35	0.15	66,66,66,66	0
57	MG	YA	3043	1/1	0.35	0.65	50,50,50,50	0
57	MG	YA	3098	1/1	0.35	0.53	50,50,50,50	0
57	MG	RA	3157	1/1	0.36	0.20	39,39,39,39	0
57	MG	RA	3140	1/1	0.36	0.21	61,61,61,61	0
57	MG	RA	3064	1/1	0.39	1.03	50,50,50,50	0
57	MG	YA	3014	1/1	0.40	0.49	1,1,1,1	0
57	MG	RA	3032	1/1	0.41	0.38	50,50,50,50	0
57	MG	XA	1658	1/1	0.45	0.20	17,17,17,17	0
57	MG	RA	3027	1/1	0.46	1.05	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	3067	1/1	0.48	0.45	7,7,7,7	0
57	MG	RA	3123	1/1	0.48	0.50	50,50,50,50	0
57	MG	RA	3230	1/1	0.49	0.18	45,45,45,45	0
57	MG	RA	3039	1/1	0.52	0.40	50,50,50,50	0
57	MG	QA	1605	1/1	0.52	0.25	4,4,4,4	0
57	MG	RA	3002	1/1	0.54	0.17	8,8,8,8	0
57	MG	QA	1617	1/1	0.54	0.30	2,2,2,2	0
57	MG	RA	3219	1/1	0.54	0.16	40,40,40,40	0
57	MG	YA	3033	1/1	0.54	0.68	50,50,50,50	0
57	MG	XA	1635	1/1	0.55	0.75	50,50,50,50	0
57	MG	RA	3071	1/1	0.55	0.58	50,50,50,50	0
57	MG	YA	3053	1/1	0.55	0.60	50,50,50,50	0
57	MG	RA	3229	1/1	0.55	0.17	50,50,50,50	0
57	MG	RA	3051	1/1	0.55	0.67	50,50,50,50	0
57	MG	YA	3250	1/1	0.55	0.54	50,50,50,50	0
57	MG	QA	1628	1/1	0.57	0.12	21,21,21,21	0
57	MG	XA	1621	1/1	0.57	0.46	6,6,6,6	0
57	MG	YA	3082	1/1	0.57	0.42	50,50,50,50	0
57	MG	RA	3222	1/1	0.57	0.29	4,4,4,4	0
57	MG	YA	3148	1/1	0.57	0.15	38,38,38,38	0
57	MG	RA	3031	1/1	0.57	0.62	50,50,50,50	0
57	MG	QA	1608	1/1	0.58	0.15	63,63,63,63	0
57	MG	RA	3139	1/1	0.58	0.27	18,18,18,18	0
57	MG	QH	201	1/1	0.58	0.12	27,27,27,27	0
57	MG	RA	3043	1/1	0.59	0.48	50,50,50,50	0
57	MG	YA	3012	1/1	0.59	0.62	50,50,50,50	0
57	MG	XA	1624	1/1	0.59	0.32	8,8,8,8	0
57	MG	YA	3224	1/1	0.59	0.57	50,50,50,50	0
57	MG	RA	3093	1/1	0.59	0.40	50,50,50,50	0
57	MG	RA	3041	1/1	0.60	0.55	50,50,50,50	0
57	MG	YA	3220	1/1	0.60	0.15	26,26,26,26	0
57	MG	YA	3099	1/1	0.60	0.43	50,50,50,50	0
57	MG	YA	3117	1/1	0.60	0.65	50,50,50,50	0
59	ZN	R9	101	1/1	0.60	0.36	177,177,177,177	0
57	MG	YA	3080	1/1	0.61	0.45	50,50,50,50	0
57	MG	RE	302	1/1	0.61	0.29	15,15,15,15	0
57	MG	YA	3113	1/1	0.62	0.49	50,50,50,50	0
57	MG	YA	3009	1/1	0.62	0.54	50,50,50,50	0
57	MG	YA	3081	1/1	0.62	0.29	7,7,7,7	0
57	MG	RA	3096	1/1	0.62	0.49	11,11,11,11	0
57	MG	YA	3085	1/1	0.62	0.78	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	RP	202	1/1	0.62	0.15	75,75,75,75	0
57	MG	RA	3217	1/1	0.62	0.28	16,16,16,16	0
57	MG	RA	3023	1/1	0.63	0.55	50,50,50,50	0
57	MG	QA	1610	1/1	0.63	0.54	50,50,50,50	0
57	MG	RA	3013	1/1	0.63	0.30	0,0,0,0	0
57	MG	RA	3194	1/1	0.64	0.09	82,82,82,82	0
57	MG	RA	3127	1/1	0.64	0.34	15,15,15,15	0
57	MG	RA	3007	1/1	0.64	0.67	50,50,50,50	0
57	MG	YA	3156	1/1	0.64	0.23	8,8,8,8	0
57	MG	YA	3191	1/1	0.64	0.24	14,14,14,14	0
57	MG	YA	3045	1/1	0.64	0.26	0,0,0,0	0
57	MG	RA	3065	1/1	0.64	0.74	50,50,50,50	0
57	MG	RA	3030	1/1	0.64	0.41	50,50,50,50	0
57	MG	YA	3107	1/1	0.64	0.45	2,2,2,2	0
57	MG	YA	3021	1/1	0.65	0.47	50,50,50,50	0
57	MG	YA	3119	1/1	0.65	0.20	66,66,66,66	0
57	MG	YA	3049	1/1	0.65	0.69	50,50,50,50	0
57	MG	XA	1616	1/1	0.66	0.57	50,50,50,50	0
57	MG	RA	3035	1/1	0.67	0.69	50,50,50,50	0
57	MG	RA	3042	1/1	0.67	0.41	50,50,50,50	0
57	MG	XA	1662	1/1	0.67	0.59	50,50,50,50	0
57	MG	YA	3001	1/1	0.67	0.54	50,50,50,50	0
57	MG	RA	3016	1/1	0.67	0.44	50,50,50,50	0
57	MG	RA	3111	1/1	0.67	0.39	4,4,4,4	0
57	MG	YA	3083	1/1	0.67	0.12	16,16,16,16	0
59	ZN	Y9	101	1/1	0.67	0.37	158,158,158,158	0
57	MG	QA	1612	1/1	0.68	0.38	4,4,4,4	0
57	MG	YA	3059	1/1	0.68	0.38	3,3,3,3	0
57	MG	YA	3134	1/1	0.68	0.49	50,50,50,50	0
57	MG	RA	3239	1/1	0.68	0.34	10,10,10,10	0
57	MG	XA	1643	1/1	0.68	0.54	50,50,50,50	0
57	MG	YA	3164	1/1	0.68	0.43	97,97,97,97	0
57	MG	YA	3137	1/1	0.69	0.18	22,22,22,22	0
57	MG	YA	3094	1/1	0.69	0.36	8,8,8,8	0
57	MG	YA	3197	1/1	0.69	0.72	50,50,50,50	0
57	MG	XA	1614	1/1	0.69	0.30	25,25,25,25	0
57	MG	RA	3231	1/1	0.70	0.22	3,3,3,3	0
57	MG	YA	3061	1/1	0.70	0.34	9,9,9,9	0
57	MG	RA	3233	1/1	0.70	0.51	50,50,50,50	0
57	MG	RA	3052	1/1	0.70	0.27	50,50,50,50	0
57	MG	RA	3005	1/1	0.70	0.63	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	3132	1/1	0.70	0.24	26,26,26,26	0
57	MG	XA	1656	1/1	0.71	0.22	12,12,12,12	0
57	MG	RA	3003	1/1	0.71	0.68	50,50,50,50	0
57	MG	YA	3201	1/1	0.71	0.25	10,10,10,10	0
57	MG	YA	3202	1/1	0.71	0.36	13,13,13,13	0
57	MG	YA	3079	1/1	0.71	0.80	50,50,50,50	0
57	MG	RA	3021	1/1	0.71	0.65	50,50,50,50	0
57	MG	YA	3018	1/1	0.71	0.59	50,50,50,50	0
57	MG	RA	3006	1/1	0.71	0.49	50,50,50,50	0
57	MG	YA	3006	1/1	0.71	0.77	50,50,50,50	0
57	MG	RA	3081	1/1	0.72	0.44	10,10,10,10	0
57	MG	RA	3180	1/1	0.72	0.11	1,1,1,1	0
57	MG	YA	3022	1/1	0.72	0.68	50,50,50,50	0
57	MG	YA	3253	1/1	0.72	0.67	50,50,50,50	0
57	MG	YA	3261	1/1	0.72	0.81	50,50,50,50	0
57	MG	XA	1615	1/1	0.72	0.61	50,50,50,50	0
57	MG	RA	3145	1/1	0.72	0.39	3,3,3,3	0
57	MG	QA	1664	1/1	0.73	0.15	10,10,10,10	0
57	MG	RA	3033	1/1	0.73	0.33	16,16,16,16	0
57	MG	YA	3057	1/1	0.73	0.34	8,8,8,8	0
57	MG	RA	3186	1/1	0.73	0.23	51,51,51,51	0
57	MG	YA	3026	1/1	0.73	1.55	50,50,50,50	0
57	MG	QA	1621	1/1	0.73	0.18	35,35,35,35	0
57	MG	XA	1602	1/1	0.73	0.54	50,50,50,50	0
57	MG	XX	101	1/1	0.73	0.13	88,88,88,88	0
57	MG	XA	1612	1/1	0.73	0.32	23,23,23,23	0
57	MG	RA	3060	1/1	0.73	0.67	13,13,13,13	0
57	MG	RA	3212	1/1	0.74	0.16	33,33,33,33	0
57	MG	YA	3125	1/1	0.74	0.24	15,15,15,15	0
57	MG	YA	3211	1/1	0.74	0.16	3,3,3,3	0
57	MG	YA	3213	1/1	0.74	0.11	15,15,15,15	0
57	MG	RA	3232	1/1	0.74	0.24	5,5,5,5	0
57	MG	RA	3182	1/1	0.74	0.28	10,10,10,10	0
57	MG	RA	3142	1/1	0.74	0.26	8,8,8,8	0
57	MG	QA	1603	1/1	0.74	0.14	10,10,10,10	0
57	MG	YA	3040	1/1	0.74	0.79	50,50,50,50	0
57	MG	RA	3201	1/1	0.74	0.09	41,41,41,41	0
57	MG	RR	201	1/1	0.74	0.32	9,9,9,9	0
57	MG	RA	3206	1/1	0.74	0.21	11,11,11,11	0
57	MG	YA	3050	1/1	0.75	0.57	50,50,50,50	0
57	MG	QA	1622	1/1	0.75	0.30	52,52,52,52	0
57	MG	YA	3255	1/1	0.75	0.80	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	3025	1/1	0.75	0.39	3,3,3,3	0
57	MG	YA	3002	1/1	0.75	0.66	50,50,50,50	0
57	MG	YA	3151	1/1	0.75	0.51	50,50,50,50	0
57	MG	YA	3235	1/1	0.75	0.10	34,34,34,34	0
57	MG	RA	3099	1/1	0.76	0.49	20,20,20,20	0
57	MG	YA	3172	1/1	0.76	0.21	19,19,19,19	0
57	MG	YA	3176	1/1	0.76	0.16	11,11,11,11	0
57	MG	RA	3014	1/1	0.76	0.66	50,50,50,50	0
57	MG	YA	3054	1/1	0.76	0.49	50,50,50,50	0
57	MG	XA	1605	1/1	0.76	0.34	16,16,16,16	0
57	MG	RA	3077	1/1	0.76	0.37	50,50,50,50	0
57	MG	RA	3170	1/1	0.76	0.28	2,2,2,2	0
57	MG	YA	3030	1/1	0.76	0.45	50,50,50,50	0
57	MG	YA	3074	1/1	0.76	0.30	4,4,4,4	0
57	MG	RA	3048	1/1	0.76	0.63	50,50,50,50	0
57	MG	RA	3057	1/1	0.76	0.73	50,50,50,50	0
57	MG	XA	1618	1/1	0.76	0.26	4,4,4,4	0
57	MG	YA	3144	1/1	0.76	0.39	6,6,6,6	0
57	MG	RA	3220	1/1	0.76	0.19	25,25,25,25	0
57	MG	YA	3150	1/1	0.76	0.22	16,16,16,16	0
57	MG	RA	3067	1/1	0.76	0.32	6,6,6,6	0
57	MG	XA	1633	1/1	0.76	0.16	13,13,13,13	0
57	MG	YA	3159	1/1	0.76	0.27	22,22,22,22	0
57	MG	YA	3019	1/1	0.77	0.55	50,50,50,50	0
57	MG	QA	1618	1/1	0.77	0.21	8,8,8,8	0
57	MG	YA	3138	1/1	0.77	0.41	4,4,4,4	0
57	MG	RA	3020	1/1	0.77	0.46	50,50,50,50	0
57	MG	YA	3024	1/1	0.77	0.61	50,50,50,50	0
57	MG	YA	3198	1/1	0.77	0.27	2,2,2,2	0
57	MG	RA	3038	1/1	0.77	0.60	50,50,50,50	0
57	MG	RA	3100	1/1	0.77	0.60	50,50,50,50	0
57	MG	YA	3093	1/1	0.77	0.24	4,4,4,4	0
57	MG	RA	3092	1/1	0.77	0.21	59,59,59,59	0
57	MG	XA	1654	1/1	0.78	0.19	17,17,17,17	0
57	MG	YA	3124	1/1	0.78	0.28	13,13,13,13	0
57	MG	YA	3149	1/1	0.78	0.34	7,7,7,7	0
57	MG	YA	3252	1/1	0.78	0.21	4,4,4,4	0
57	MG	RA	3078	1/1	0.78	0.37	50,50,50,50	0
57	MG	RA	3146	1/1	0.78	0.28	7,7,7,7	0
57	MG	YA	3072	1/1	0.78	0.64	50,50,50,50	0
57	MG	RU	201	1/1	0.78	0.13	86,86,86,86	0
57	MG	YA	3010	1/1	0.78	0.42	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	3139	1/1	0.78	0.19	13,13,13,13	0
57	MG	RA	3008	1/1	0.79	0.08	0,0,0,0	0
57	MG	RA	3124	1/1	0.79	0.27	19,19,19,19	0
57	MG	YA	3076	1/1	0.79	0.32	1,1,1,1	0
57	MG	RA	3181	1/1	0.79	0.09	9,9,9,9	0
57	MG	YA	3187	1/1	0.79	0.12	47,47,47,47	0
57	MG	YA	3188	1/1	0.79	0.20	36,36,36,36	0
57	MG	YA	3029	1/1	0.79	0.34	6,6,6,6	0
57	MG	RA	3019	1/1	0.79	0.46	50,50,50,50	0
57	MG	XA	1622	1/1	0.79	0.20	6,6,6,6	0
57	MG	Y7	101	1/1	0.79	0.32	14,14,14,14	0
57	MG	XA	1606	1/1	0.79	0.41	13,13,13,13	0
58	PAR	QA	1666	42/42	0.79	0.31	104,104,104,104	0
57	MG	RA	3207	1/1	0.79	0.31	5,5,5,5	0
57	MG	RA	3184	1/1	0.79	0.30	40,40,40,40	0
57	MG	RA	3084	1/1	0.80	0.26	6,6,6,6	0
57	MG	YA	3232	1/1	0.80	0.16	15,15,15,15	0
57	MG	YA	3182	1/1	0.80	0.34	14,14,14,14	0
57	MG	YA	3103	1/1	0.80	0.17	31,31,31,31	0
57	MG	YA	3031	1/1	0.80	0.74	50,50,50,50	0
57	MG	RA	3095	1/1	0.80	0.30	24,24,24,24	0
57	MG	RA	3234	1/1	0.80	0.83	50,50,50,50	0
57	MG	YA	3260	1/1	0.80	0.77	50,50,50,50	0
57	MG	QA	1604	1/1	0.80	0.21	7,7,7,7	0
57	MG	YA	3084	1/1	0.80	0.18	2,2,2,2	0
57	MG	XA	1625	1/1	0.80	0.21	50,50,50,50	0
57	MG	RA	3193	1/1	0.80	0.19	17,17,17,17	0
57	MG	XA	1670	1/1	0.80	0.16	44,44,44,44	0
57	MG	YA	3015	1/1	0.80	0.70	50,50,50,50	0
57	MG	RA	3068	1/1	0.81	0.28	4,4,4,4	0
57	MG	XA	1626	1/1	0.81	0.24	1,1,1,1	0
57	MG	YA	3032	1/1	0.81	0.65	50,50,50,50	0
57	MG	YA	3126	1/1	0.81	0.34	50,50,50,50	0
57	MG	YA	3127	1/1	0.81	0.27	12,12,12,12	0
57	MG	RA	3034	1/1	0.81	0.85	50,50,50,50	0
57	MG	YA	3092	1/1	0.81	0.38	2,2,2,2	0
57	MG	RA	3025	1/1	0.81	0.24	7,7,7,7	0
57	MG	XA	1641	1/1	0.81	0.25	14,14,14,14	0
57	MG	RA	3141	1/1	0.81	0.30	5,5,5,5	0
57	MG	YA	3044	1/1	0.81	0.53	16,16,16,16	0
57	MG	RA	3066	1/1	0.81	0.36	23,23,23,23	0
57	MG	YA	3047	1/1	0.81	0.54	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	3202	1/1	0.81	0.23	2,2,2,2	0
57	MG	RA	3001	1/1	0.81	0.24	1,1,1,1	0
57	MG	RA	3010	1/1	0.82	0.27	56,56,56,56	0
57	MG	RA	3235	1/1	0.82	0.15	2,2,2,2	0
57	MG	QA	1648	1/1	0.82	0.17	16,16,16,16	0
57	MG	QA	1625	1/1	0.82	0.08	74,74,74,74	0
57	MG	XA	1632	1/1	0.82	0.31	2,2,2,2	0
57	MG	RA	3059	1/1	0.82	0.60	50,50,50,50	0
57	MG	RA	3208	1/1	0.82	0.20	50,50,50,50	0
57	MG	XA	1636	1/1	0.82	0.24	9,9,9,9	0
57	MG	RA	3168	1/1	0.82	0.24	10,10,10,10	0
57	MG	RA	3073	1/1	0.82	0.24	36,36,36,36	0
57	MG	XA	1603	1/1	0.82	0.64	50,50,50,50	0
57	MG	RA	3171	1/1	0.82	0.27	15,15,15,15	0
57	MG	RA	3024	1/1	0.82	0.26	15,15,15,15	0
57	MG	XA	1607	1/1	0.82	0.24	17,17,17,17	0
57	MG	XA	1663	1/1	0.82	0.07	3,3,3,3	0
57	MG	XA	1666	1/1	0.82	0.13	34,34,34,34	0
57	MG	RA	3061	1/1	0.82	0.42	50,50,50,50	0
57	MG	RA	3063	1/1	0.82	0.13	19,19,19,19	0
57	MG	QA	1613	1/1	0.82	0.30	1,1,1,1	0
57	MG	RA	3086	1/1	0.82	0.34	50,50,50,50	0
57	MG	RA	3089	1/1	0.82	0.35	0,0,0,0	0
57	MG	XA	1619	1/1	0.82	0.25	8,8,8,8	0
57	MG	QF	201	1/1	0.82	0.12	40,40,40,40	0
57	MG	YA	3052	1/1	0.83	0.23	5,5,5,5	0
57	MG	RA	3225	1/1	0.83	0.12	47,47,47,47	0
57	MG	RA	3172	1/1	0.83	0.13	17,17,17,17	0
57	MG	RA	3173	1/1	0.83	0.20	3,3,3,3	0
57	MG	YA	3243	1/1	0.83	0.77	50,50,50,50	0
57	MG	YA	3245	1/1	0.83	0.19	3,3,3,3	0
57	MG	YA	3179	1/1	0.83	0.37	20,20,20,20	0
57	MG	YA	3035	1/1	0.83	0.56	50,50,50,50	0
57	MG	RA	3044	1/1	0.83	0.25	8,8,8,8	0
57	MG	QA	1637	1/1	0.83	0.14	3,3,3,3	0
57	MG	YA	3042	1/1	0.83	0.49	50,50,50,50	0
57	MG	YA	3023	1/1	0.83	0.26	5,5,5,5	0
57	MG	RA	3062	1/1	0.83	0.37	2,2,2,2	0
57	MG	RA	3205	1/1	0.83	0.09	33,33,33,33	0
57	MG	RA	3221	1/1	0.83	0.30	79,79,79,79	0
57	MG	RA	3070	1/1	0.83	0.16	21,21,21,21	0
57	MG	RA	3241	1/1	0.83	0.29	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1626	1/1	0.84	0.09	17,17,17,17	0
57	MG	RA	3240	1/1	0.84	0.27	12,12,12,12	0
57	MG	YA	3003	1/1	0.84	0.35	50,50,50,50	0
57	MG	RA	3153	1/1	0.84	0.29	36,36,36,36	0
57	MG	RA	3244	1/1	0.84	0.15	9,9,9,9	0
57	MG	YA	3249	1/1	0.84	0.29	5,5,5,5	0
57	MG	XA	1655	1/1	0.84	0.14	7,7,7,7	0
57	MG	YA	3011	1/1	0.84	0.24	3,3,3,3	0
57	MG	RD	301	1/1	0.84	0.17	15,15,15,15	0
57	MG	YA	3013	1/1	0.84	0.31	1,1,1,1	0
57	MG	YA	3257	1/1	0.84	0.57	50,50,50,50	0
57	MG	YA	3096	1/1	0.84	0.19	17,17,17,17	0
57	MG	XA	1608	1/1	0.84	0.08	50,50,50,50	0
57	MG	XA	1659	1/1	0.84	0.16	15,15,15,15	0
57	MG	RA	3087	1/1	0.84	0.34	0,0,0,0	0
57	MG	RA	3125	1/1	0.84	0.19	14,14,14,14	0
57	MG	RA	3213	1/1	0.84	0.20	10,10,10,10	0
57	MG	RA	3174	1/1	0.84	0.09	40,40,40,40	0
57	MG	RA	3121	1/1	0.85	0.21	0,0,0,0	0
57	MG	RA	3026	1/1	0.85	0.13	13,13,13,13	0
57	MG	RA	3158	1/1	0.85	0.29	15,15,15,15	0
57	MG	YA	3204	1/1	0.85	0.14	11,11,11,11	0
57	MG	RA	3166	1/1	0.85	0.41	9,9,9,9	0
57	MG	RA	3167	1/1	0.85	0.10	26,26,26,26	0
57	MG	RA	3185	1/1	0.85	0.21	3,3,3,3	0
57	MG	RA	3074	1/1	0.85	0.18	20,20,20,20	0
57	MG	RA	3218	1/1	0.85	0.27	10,10,10,10	0
57	MG	QA	1611	1/1	0.85	0.22	4,4,4,4	0
57	MG	YA	3153	1/1	0.85	0.23	16,16,16,16	0
57	MG	RA	3143	1/1	0.85	0.16	12,12,12,12	0
57	MG	YA	3157	1/1	0.85	0.14	8,8,8,8	0
57	MG	YA	3071	1/1	0.85	0.18	6,6,6,6	0
57	MG	XA	1649	1/1	0.85	0.17	16,16,16,16	0
57	MG	RA	3243	1/1	0.85	0.32	18,18,18,18	0
57	MG	YA	3174	1/1	0.85	0.29	3,3,3,3	0
57	MG	YA	3075	1/1	0.85	0.61	50,50,50,50	0
57	MG	YA	3122	1/1	0.85	0.54	50,50,50,50	0
57	MG	RA	3196	1/1	0.85	0.14	22,22,22,22	0
57	MG	YA	3183	1/1	0.85	0.11	17,17,17,17	0
57	MG	XA	1617	1/1	0.85	0.25	2,2,2,2	0
57	MG	QA	1639	1/1	0.85	0.09	27,27,27,27	0
57	MG	RA	3223	1/1	0.85	0.07	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3138	1/1	0.85	0.34	8,8,8,8	0
57	MG	YA	3007	1/1	0.86	0.25	1,1,1,1	0
57	MG	QA	1656	1/1	0.86	0.14	63,63,63,63	0
57	MG	XA	1650	1/1	0.86	0.18	22,22,22,22	0
57	MG	XA	1651	1/1	0.86	0.10	84,84,84,84	0
57	MG	YA	3208	1/1	0.86	0.22	0,0,0,0	0
57	MG	XA	1620	1/1	0.86	0.19	0,0,0,0	0
57	MG	YA	3100	1/1	0.86	0.23	0,0,0,0	0
57	MG	RA	3116	1/1	0.86	0.18	0,0,0,0	0
57	MG	RA	3160	1/1	0.86	0.29	2,2,2,2	0
57	MG	RA	3162	1/1	0.86	0.24	18,18,18,18	0
57	MG	YA	3234	1/1	0.86	0.14	2,2,2,2	0
57	MG	YA	3116	1/1	0.86	0.26	11,11,11,11	0
57	MG	QA	1614	1/1	0.86	0.25	21,21,21,21	0
57	MG	YA	3118	1/1	0.86	0.33	12,12,12,12	0
57	MG	YA	3247	1/1	0.86	0.27	16,16,16,16	0
57	MG	YA	3168	1/1	0.86	0.16	13,13,13,13	0
57	MG	RA	3053	1/1	0.86	0.60	50,50,50,50	0
57	MG	YA	3121	1/1	0.86	0.25	8,8,8,8	0
57	MG	XA	1629	1/1	0.86	0.16	32,32,32,32	0
57	MG	RA	3083	1/1	0.86	0.16	3,3,3,3	0
57	MG	YA	3180	1/1	0.86	0.28	5,5,5,5	0
57	MG	YA	3181	1/1	0.86	0.39	5,5,5,5	0
57	MG	RA	3009	1/1	0.86	0.20	7,7,7,7	0
57	MG	RA	3046	1/1	0.86	0.21	0,0,0,0	0
57	MG	RA	3215	1/1	0.86	0.17	14,14,14,14	0
57	MG	RA	3216	1/1	0.86	0.22	1,1,1,1	0
57	MG	YA	3086	1/1	0.86	0.50	19,19,19,19	0
57	MG	QA	1643	1/1	0.86	0.09	20,20,20,20	0
57	MG	RA	3190	1/1	0.87	0.20	4,4,4,4	0
57	MG	RA	3094	1/1	0.87	0.39	3,3,3,3	0
57	MG	RA	3004	1/1	0.87	0.21	9,9,9,9	0
57	MG	YA	3089	1/1	0.87	0.17	13,13,13,13	0
57	MG	YA	3048	1/1	0.87	0.48	50,50,50,50	0
57	MG	XA	1611	1/1	0.87	0.22	1,1,1,1	0
57	MG	YA	3185	1/1	0.87	0.09	74,74,74,74	0
57	MG	YA	3248	1/1	0.87	0.26	15,15,15,15	0
57	MG	QA	1631	1/1	0.87	0.04	63,63,63,63	0
57	MG	XA	1601	1/1	0.87	0.69	50,50,50,50	0
57	MG	YA	3154	1/1	0.87	0.23	5,5,5,5	0
57	MG	YA	3193	1/1	0.87	0.23	7,7,7,7	0
57	MG	RA	3119	1/1	0.87	0.17	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3256	1/1	0.87	0.18	9,9,9,9	0
57	MG	QA	1650	1/1	0.87	0.21	8,8,8,8	0
57	MG	YA	3056	1/1	0.87	0.54	50,50,50,50	0
57	MG	YA	3163	1/1	0.87	0.18	9,9,9,9	0
57	MG	YB	201	1/1	0.87	0.15	14,14,14,14	0
57	MG	RA	3178	1/1	0.87	0.16	5,5,5,5	0
57	MG	YA	3106	1/1	0.87	0.41	50,50,50,50	0
57	MG	YA	3171	1/1	0.87	0.15	7,7,7,7	0
57	MG	YA	3135	1/1	0.87	0.24	9,9,9,9	0
57	MG	XM	201	1/1	0.87	0.07	78,78,78,78	0
57	MG	YA	3111	1/1	0.88	0.25	7,7,7,7	0
57	MG	YA	3140	1/1	0.88	0.21	19,19,19,19	0
57	MG	YA	3112	1/1	0.88	0.18	19,19,19,19	0
57	MG	QA	1602	1/1	0.88	0.38	11,11,11,11	0
57	MG	YA	3114	1/1	0.88	0.17	16,16,16,16	0
57	MG	QA	1601	1/1	0.88	0.12	21,21,21,21	0
57	MG	XA	1660	1/1	0.88	0.17	19,19,19,19	0
57	MG	YA	3189	1/1	0.88	0.25	7,7,7,7	0
57	MG	RA	3227	1/1	0.88	0.22	39,39,39,39	0
57	MG	RA	3133	1/1	0.88	0.25	4,4,4,4	0
57	MG	RA	3137	1/1	0.88	0.09	3,3,3,3	0
57	MG	YA	3062	1/1	0.88	0.24	0,0,0,0	0
57	MG	RA	3147	1/1	0.88	0.12	6,6,6,6	0
57	MG	YA	3259	1/1	0.88	0.37	2,2,2,2	0
57	MG	XA	1647	1/1	0.88	0.24	11,11,11,11	0
57	MG	QA	1635	1/1	0.88	0.08	11,11,11,11	0
57	MG	QA	1644	1/1	0.88	0.18	24,24,24,24	0
57	MG	YP	202	1/1	0.88	0.22	5,5,5,5	0
57	MG	YQ	201	1/1	0.88	0.20	79,79,79,79	0
57	MG	RA	3090	1/1	0.88	0.27	4,4,4,4	0
57	MG	QA	1659	1/1	0.88	0.22	4,4,4,4	0
57	MG	XA	1628	1/1	0.88	0.14	2,2,2,2	0
57	MG	R5	101	1/1	0.88	0.21	14,14,14,14	0
57	MG	XA	1657	1/1	0.88	0.16	4,4,4,4	0
57	MG	YA	3039	1/1	0.89	0.22	0,0,0,0	0
57	MG	YA	3231	1/1	0.89	0.27	11,11,11,11	0
57	MG	YA	3131	1/1	0.89	0.26	17,17,17,17	0
57	MG	YA	3233	1/1	0.89	0.08	3,3,3,3	0
57	MG	RA	3228	1/1	0.89	0.10	7,7,7,7	0
57	MG	YA	3068	1/1	0.89	0.26	1,1,1,1	0
57	MG	YA	3070	1/1	0.89	0.11	33,33,33,33	0
57	MG	RA	3037	1/1	0.89	0.26	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3101	1/1	0.89	0.15	11,11,11,11	0
57	MG	RA	3197	1/1	0.89	0.08	9,9,9,9	0
57	MG	YA	3184	1/1	0.89	0.36	50,50,50,50	0
57	MG	RA	3183	1/1	0.89	0.18	11,11,11,11	0
57	MG	RA	3011	1/1	0.89	0.25	7,7,7,7	0
57	MG	RA	3203	1/1	0.89	0.12	34,34,34,34	0
57	MG	YA	3077	1/1	0.89	0.31	0,0,0,0	0
57	MG	RA	3204	1/1	0.89	0.23	15,15,15,15	0
57	MG	QA	1629	1/1	0.89	0.14	38,38,38,38	0
57	MG	RA	3238	1/1	0.89	0.29	3,3,3,3	0
57	MG	RA	3122	1/1	0.89	0.24	19,19,19,19	0
57	MG	RA	3045	1/1	0.89	0.20	0,0,0,0	0
57	MG	YA	3265	1/1	0.89	0.36	11,11,11,11	0
57	MG	QA	1658	1/1	0.89	0.14	46,46,46,46	0
57	MG	YE	301	1/1	0.89	0.18	1,1,1,1	0
57	MG	RA	3211	1/1	0.89	0.14	11,11,11,11	0
57	MG	YA	3205	1/1	0.89	0.29	40,40,40,40	0
57	MG	XA	1627	1/1	0.89	0.27	9,9,9,9	0
57	MG	XA	1609	1/1	0.89	0.27	8,8,8,8	0
57	MG	RA	3047	1/1	0.89	0.21	2,2,2,2	0
58	PAR	XA	1673	42/42	0.89	0.34	132,132,132,132	0
57	MG	YA	3036	1/1	0.89	0.22	3,3,3,3	0
57	MG	YA	3223	1/1	0.89	0.32	11,11,11,11	0
57	MG	YA	3240	1/1	0.90	0.30	15,15,15,15	0
57	MG	YA	3190	1/1	0.90	0.19	17,17,17,17	0
57	MG	YA	3244	1/1	0.90	0.34	6,6,6,6	0
57	MG	RA	3036	1/1	0.90	0.25	0,0,0,0	0
57	MG	YA	3102	1/1	0.90	0.21	6,6,6,6	0
57	MG	RA	3117	1/1	0.90	0.19	4,4,4,4	0
57	MG	YA	3060	1/1	0.90	0.18	9,9,9,9	0
57	MG	YA	3170	1/1	0.90	0.09	8,8,8,8	0
57	MG	XA	1638	1/1	0.90	0.11	27,27,27,27	0
57	MG	YA	3203	1/1	0.90	0.37	29,29,29,29	0
57	MG	RA	3161	1/1	0.90	0.20	8,8,8,8	0
57	MG	YA	3008	1/1	0.90	0.20	1,1,1,1	0
57	MG	RA	3134	1/1	0.90	0.07	23,23,23,23	0
57	MG	YA	3087	1/1	0.90	0.28	6,6,6,6	0
57	MG	RA	3164	1/1	0.90	0.15	15,15,15,15	0
57	MG	YA	3214	1/1	0.90	0.19	23,23,23,23	0
57	MG	YA	3218	1/1	0.90	0.23	5,5,5,5	0
57	MG	YA	3091	1/1	0.90	0.18	12,12,12,12	0
57	MG	RA	3226	1/1	0.90	0.16	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1664	1/1	0.90	0.21	27,27,27,27	0
57	MG	YA	3225	1/1	0.90	0.27	23,23,23,23	0
57	MG	YA	3226	1/1	0.90	0.09	10,10,10,10	0
57	MG	XV	101	1/1	0.90	0.24	1,1,1,1	0
57	MG	RE	301	1/1	0.90	0.15	2,2,2,2	0
57	MG	XA	1668	1/1	0.90	0.09	6,6,6,6	0
57	MG	RA	3103	1/1	0.90	0.16	8,8,8,8	0
57	MG	RF	301	1/1	0.90	0.17	10,10,10,10	0
57	MG	RA	3085	1/1	0.90	0.21	27,27,27,27	0
57	MG	YA	3128	1/1	0.91	0.11	0,0,0,0	0
57	MG	YA	3169	1/1	0.91	0.35	7,7,7,7	0
57	MG	RA	3072	1/1	0.91	0.26	0,0,0,0	0
57	MG	RA	3040	1/1	0.91	0.19	11,11,11,11	0
57	MG	XA	1648	1/1	0.91	0.14	10,10,10,10	0
57	MG	RA	3242	1/1	0.91	0.32	8,8,8,8	0
57	MG	XA	1604	1/1	0.91	0.71	50,50,50,50	0
57	MG	RA	3015	1/1	0.91	0.18	15,15,15,15	0
57	MG	RA	3075	1/1	0.91	0.21	37,37,37,37	0
57	MG	RB	202	1/1	0.91	0.15	15,15,15,15	0
57	MG	YA	3221	1/1	0.91	0.09	7,7,7,7	0
57	MG	RA	3155	1/1	0.91	0.20	9,9,9,9	0
57	MG	RA	3156	1/1	0.91	0.18	7,7,7,7	0
57	MG	RA	3076	1/1	0.91	0.10	3,3,3,3	0
57	MG	XA	1630	1/1	0.91	0.21	1,1,1,1	0
57	MG	QA	1651	1/1	0.91	0.12	16,16,16,16	0
57	MG	RP	201	1/1	0.91	0.66	85,85,85,85	0
57	MG	QA	1619	1/1	0.91	0.10	29,29,29,29	0
57	MG	YA	3123	1/1	0.91	0.24	0,0,0,0	0
57	MG	RA	3236	1/1	0.91	0.32	2,2,2,2	0
57	MG	XA	1637	1/1	0.91	0.19	13,13,13,13	0
57	MG	QA	1640	1/1	0.91	0.14	6,6,6,6	0
57	MG	RA	3113	1/1	0.91	0.17	1,1,1,1	0
57	MG	YA	3165	1/1	0.91	0.15	42,42,42,42	0
57	MG	RA	3108	1/1	0.92	0.19	5,5,5,5	0
57	MG	XA	1672	1/1	0.92	0.13	5,5,5,5	0
57	MG	RA	3120	1/1	0.92	0.11	31,31,31,31	0
57	MG	RA	3098	1/1	0.92	0.29	4,4,4,4	0
57	MG	YA	3173	1/1	0.92	0.12	14,14,14,14	0
57	MG	YA	3142	1/1	0.92	0.17	9,9,9,9	0
57	MG	RA	3159	1/1	0.92	0.18	18,18,18,18	0
57	MG	YA	3178	1/1	0.92	0.27	32,32,32,32	0
57	MG	YA	3147	1/1	0.92	0.10	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3217	1/1	0.92	0.10	52,52,52,52	0
57	MG	RA	3136	1/1	0.92	0.18	14,14,14,14	0
57	MG	YA	3219	1/1	0.92	0.10	22,22,22,22	0
57	MG	YA	3095	1/1	0.92	0.16	8,8,8,8	0
57	MG	QA	1630	1/1	0.92	0.09	14,14,14,14	0
57	MG	RA	3114	1/1	0.92	0.14	3,3,3,3	0
57	MG	XA	1634	1/1	0.92	0.14	11,11,11,11	0
57	MG	YB	202	1/1	0.92	0.18	5,5,5,5	0
57	MG	RA	3175	1/1	0.92	0.12	12,12,12,12	0
57	MG	RA	3176	1/1	0.92	0.10	30,30,30,30	0
57	MG	RA	3195	1/1	0.92	0.11	23,23,23,23	0
57	MG	RA	3177	1/1	0.92	0.11	30,30,30,30	0
57	MG	RA	3029	1/1	0.92	0.23	5,5,5,5	0
57	MG	XA	1642	1/1	0.92	0.24	11,11,11,11	0
57	MG	RA	3200	1/1	0.92	0.05	31,31,31,31	0
57	MG	YA	3239	1/1	0.92	0.09	13,13,13,13	0
57	MG	YA	3167	1/1	0.92	0.29	39,39,39,39	0
57	MG	QA	1646	1/1	0.92	0.20	11,11,11,11	0
57	MG	QA	1645	1/1	0.93	0.11	37,37,37,37	0
57	MG	QA	1636	1/1	0.93	0.17	11,11,11,11	0
57	MG	YA	3038	1/1	0.93	0.20	5,5,5,5	0
57	MG	YA	3160	1/1	0.93	0.07	4,4,4,4	0
57	MG	YA	3194	1/1	0.93	0.11	15,15,15,15	0
57	MG	YA	3195	1/1	0.93	0.15	21,21,21,21	0
57	MG	YA	3162	1/1	0.93	0.25	30,30,30,30	0
57	MG	YA	3065	1/1	0.93	0.31	8,8,8,8	0
57	MG	YA	3200	1/1	0.93	0.09	35,35,35,35	0
57	MG	XA	1665	1/1	0.93	0.10	18,18,18,18	0
57	MG	RA	3209	1/1	0.93	0.10	44,44,44,44	0
57	MG	YA	3251	1/1	0.93	0.65	50,50,50,50	0
57	MG	RA	3028	1/1	0.93	0.15	23,23,23,23	0
57	MG	YA	3097	1/1	0.93	0.61	50,50,50,50	0
57	MG	RA	3097	1/1	0.93	0.22	11,11,11,11	0
57	MG	YA	3020	1/1	0.93	0.36	6,6,6,6	0
57	MG	YA	3073	1/1	0.93	0.17	4,4,4,4	0
57	MG	RA	3022	1/1	0.93	0.19	5,5,5,5	0
57	MG	RA	3163	1/1	0.93	0.26	38,38,38,38	0
57	MG	YA	3046	1/1	0.93	0.30	12,12,12,12	0
57	MG	YA	3105	1/1	0.93	0.16	8,8,8,8	0
57	MG	RA	3199	1/1	0.93	0.12	1,1,1,1	0
57	MG	RA	3128	1/1	0.93	0.18	10,10,10,10	0
57	MG	RA	3131	1/1	0.93	0.07	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	QA	1647	1/1	0.93	0.07	55,55,55,55	0
57	MG	YA	3028	1/1	0.93	0.19	8,8,8,8	0
57	MG	RA	3118	1/1	0.93	0.15	1,1,1,1	0
57	MG	RA	3237	1/1	0.93	0.24	4,4,4,4	0
57	MG	XV	102	1/1	0.93	0.10	16,16,16,16	0
57	MG	YA	3229	1/1	0.93	0.16	5,5,5,5	0
57	MG	YA	3230	1/1	0.93	0.28	19,19,19,19	0
57	MG	QA	1627	1/1	0.93	0.09	1,1,1,1	0
57	MG	RA	3012	1/1	0.93	0.18	1,1,1,1	0
57	MG	RA	3105	1/1	0.93	0.13	1,1,1,1	0
57	MG	QA	1623	1/1	0.94	0.15	13,13,13,13	0
57	MG	RA	3191	1/1	0.94	0.13	38,38,38,38	0
57	MG	YA	3246	1/1	0.94	0.31	2,2,2,2	0
57	MG	XA	1613	1/1	0.94	0.08	16,16,16,16	0
57	MG	RA	3154	1/1	0.94	0.20	6,6,6,6	0
57	MG	RA	3088	1/1	0.94	0.16	10,10,10,10	0
57	MG	RA	3058	1/1	0.94	0.14	0,0,0,0	0
57	MG	YA	3104	1/1	0.94	0.21	11,11,11,11	0
57	MG	RA	3101	1/1	0.94	0.07	9,9,9,9	0
57	MG	RA	3079	1/1	0.94	0.20	0,0,0,0	0
57	MG	RA	3104	1/1	0.94	0.13	5,5,5,5	0
57	MG	YA	3109	1/1	0.94	0.12	9,9,9,9	0
57	MG	QA	1632	1/1	0.94	0.07	71,71,71,71	0
57	MG	XA	1644	1/1	0.94	0.16	11,11,11,11	0
57	MG	RA	3082	1/1	0.94	0.13	5,5,5,5	0
57	MG	QA	1634	1/1	0.94	0.05	44,44,44,44	0
57	MG	RA	3054	1/1	0.94	0.28	4,4,4,4	0
57	MG	RA	3055	1/1	0.94	0.15	12,12,12,12	0
57	MG	YA	3004	1/1	0.94	0.26	5,5,5,5	0
57	MG	YA	3227	1/1	0.94	0.09	15,15,15,15	0
57	MG	RA	3165	1/1	0.94	0.19	3,3,3,3	0
57	MG	XA	1652	1/1	0.94	0.14	50,50,50,50	0
57	MG	YA	3158	1/1	0.94	0.10	6,6,6,6	0
57	MG	XA	1653	1/1	0.94	0.07	29,29,29,29	0
57	MG	YA	3063	1/1	0.94	0.15	15,15,15,15	0
57	MG	YA	3161	1/1	0.94	0.19	14,14,14,14	0
57	MG	RA	3130	1/1	0.94	0.16	19,19,19,19	0
57	MG	RA	3069	1/1	0.94	0.20	9,9,9,9	0
57	MG	RB	201	1/1	0.94	0.06	38,38,38,38	0
57	MG	RA	3148	1/1	0.94	0.14	0,0,0,0	0
57	MG	YA	3145	1/1	0.95	0.27	25,25,25,25	0
57	MG	YA	3146	1/1	0.95	0.16	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3210	1/1	0.95	0.07	30,30,30,30	0
57	MG	RA	3049	1/1	0.95	0.16	1,1,1,1	0
57	MG	RA	3112	1/1	0.95	0.15	2,2,2,2	0
57	MG	RA	3129	1/1	0.95	0.16	19,19,19,19	0
57	MG	YA	3215	1/1	0.95	0.15	2,2,2,2	0
57	MG	RA	3050	1/1	0.95	0.10	8,8,8,8	0
57	MG	XA	1667	1/1	0.95	0.24	4,4,4,4	0
57	MG	YA	3254	1/1	0.95	0.28	0,0,0,0	0
57	MG	YA	3051	1/1	0.95	0.19	5,5,5,5	0
57	MG	QA	1642	1/1	0.95	0.16	9,9,9,9	0
57	MG	YA	3155	1/1	0.95	0.20	8,8,8,8	0
57	MG	QA	1662	1/1	0.95	0.07	39,39,39,39	0
57	MG	YA	3078	1/1	0.95	0.18	10,10,10,10	0
57	MG	YA	3034	1/1	0.95	0.33	7,7,7,7	0
57	MG	YA	3055	1/1	0.95	0.10	24,24,24,24	0
57	MG	YA	3129	1/1	0.95	0.16	1,1,1,1	0
57	MG	XA	1671	1/1	0.95	0.07	28,28,28,28	0
57	MG	YA	3016	1/1	0.95	0.10	8,8,8,8	0
57	MG	YA	3133	1/1	0.95	0.16	12,12,12,12	0
57	MG	RA	3189	1/1	0.95	0.15	16,16,16,16	0
57	MG	Y5	101	1/1	0.95	0.14	2,2,2,2	0
57	MG	QA	1606	1/1	0.95	0.09	23,23,23,23	0
57	MG	RA	3214	1/1	0.95	0.07	43,43,43,43	0
57	MG	QA	1665	1/1	0.95	0.07	37,37,37,37	0
57	MG	RA	3126	1/1	0.95	0.21	14,14,14,14	0
57	MG	XA	1645	1/1	0.95	0.19	8,8,8,8	0
57	MG	YA	3242	1/1	0.95	0.14	5,5,5,5	0
57	MG	XA	1646	1/1	0.95	0.21	8,8,8,8	0
57	MG	XA	1631	1/1	0.95	0.12	10,10,10,10	0
57	MG	YA	3212	1/1	0.96	0.07	8,8,8,8	0
57	MG	RA	3192	1/1	0.96	0.19	27,27,27,27	0
57	MG	XA	1610	1/1	0.96	0.16	1,1,1,1	0
57	MG	XA	1640	1/1	0.96	0.08	119,119,119,119	0
57	MG	RA	3150	1/1	0.96	0.23	4,4,4,4	0
57	MG	RA	3132	1/1	0.96	0.30	7,7,7,7	0
57	MG	RA	3210	1/1	0.96	0.09	11,11,11,11	0
57	MG	YB	203	1/1	0.96	0.10	17,17,17,17	0
57	MG	YA	3199	1/1	0.96	0.07	11,11,11,11	0
57	MG	RA	3091	1/1	0.96	0.15	2,2,2,2	0
57	MG	QA	1649	1/1	0.96	0.08	19,19,19,19	0
57	MG	YA	3088	1/1	0.96	0.14	3,3,3,3	0
57	MG	YA	3027	1/1	0.96	0.09	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3186	1/1	0.96	0.12	10,10,10,10	0
57	MG	YA	3090	1/1	0.96	0.14	17,17,17,17	0
57	MG	YA	3206	1/1	0.96	0.27	20,20,20,20	0
57	MG	YA	3207	1/1	0.96	0.09	0,0,0,0	0
57	MG	RA	3107	1/1	0.96	0.15	9,9,9,9	0
59	ZN	QN	101	1/1	0.96	0.04	56,56,56,56	0
57	MG	YA	3064	1/1	0.96	0.16	4,4,4,4	0
57	MG	QA	1615	1/1	0.96	0.10	54,54,54,54	0
57	MG	RA	3110	1/1	0.97	0.07	15,15,15,15	0
57	MG	YA	3209	1/1	0.97	0.10	9,9,9,9	0
57	MG	RA	3018	1/1	0.97	0.20	3,3,3,3	0
57	MG	YA	3115	1/1	0.97	0.24	15,15,15,15	0
57	MG	XA	1669	1/1	0.97	0.06	15,15,15,15	0
57	MG	RA	3135	1/1	0.97	0.14	28,28,28,28	0
57	MG	RA	3080	1/1	0.97	0.11	5,5,5,5	0
57	MG	RA	3179	1/1	0.97	0.11	10,10,10,10	0
57	MG	YA	3216	1/1	0.97	0.14	30,30,30,30	0
57	MG	YA	3152	1/1	0.97	0.09	7,7,7,7	0
57	MG	YA	3120	1/1	0.97	0.09	16,16,16,16	0
57	MG	YA	3069	1/1	0.97	0.06	8,8,8,8	0
57	MG	RA	3151	1/1	0.97	0.27	37,37,37,37	0
57	MG	RA	3198	1/1	0.97	0.04	35,35,35,35	0
57	MG	RA	3102	1/1	0.97	0.06	10,10,10,10	0
57	MG	YA	3262	1/1	0.97	0.17	9,9,9,9	0
57	MG	YA	3264	1/1	0.97	0.20	14,14,14,14	0
57	MG	QA	1633	1/1	0.97	0.27	1,1,1,1	0
57	MG	QA	1652	1/1	0.97	0.12	24,24,24,24	0
57	MG	RA	3169	1/1	0.97	0.03	19,19,19,19	0
57	MG	QA	1654	1/1	0.97	0.07	17,17,17,17	0
57	MG	RA	3106	1/1	0.97	0.18	3,3,3,3	0
57	MG	YA	3196	1/1	0.97	0.12	76,76,76,76	0
57	MG	RA	3187	1/1	0.97	0.08	10,10,10,10	0
57	MG	YX	101	1/1	0.97	0.06	50,50,50,50	0
57	MG	XA	1661	1/1	0.97	0.05	14,14,14,14	0
57	MG	QA	1620	1/1	0.97	0.04	21,21,21,21	0
57	MG	XA	1623	1/1	0.97	0.11	23,23,23,23	0
57	MG	RA	3224	1/1	0.97	0.07	16,16,16,16	0
57	MG	YA	3058	1/1	0.97	0.09	13,13,13,13	0
57	MG	YA	3108	1/1	0.97	0.04	10,10,10,10	0
57	MG	QA	1663	1/1	0.97	0.04	19,19,19,19	0
57	MG	YA	3110	1/1	0.97	0.08	5,5,5,5	0
57	MG	YA	3037	1/1	0.97	0.22	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3109	1/1	0.97	0.13	11,11,11,11	0
57	MG	YA	3237	1/1	0.98	0.23	38,38,38,38	0
57	MG	YA	3238	1/1	0.98	0.07	33,33,33,33	0
57	MG	YA	3136	1/1	0.98	0.15	1,1,1,1	0
57	MG	YA	3017	1/1	0.98	0.18	7,7,7,7	0
57	MG	QA	1607	1/1	0.98	0.04	30,30,30,30	0
57	MG	RA	3144	1/1	0.98	0.13	29,29,29,29	0
57	MG	YA	3222	1/1	0.98	0.04	2,2,2,2	0
57	MG	QA	1641	1/1	0.98	0.06	3,3,3,3	0
57	MG	RA	3188	1/1	0.98	0.09	16,16,16,16	0
57	MG	YP	201	1/1	0.98	0.05	83,83,83,83	0
57	MG	YA	3192	1/1	0.98	0.04	15,15,15,15	0
57	MG	QA	1609	1/1	0.98	0.08	10,10,10,10	0
57	MG	QA	1661	1/1	0.98	0.05	44,44,44,44	0
57	MG	YA	3228	1/1	0.98	0.12	67,67,67,67	0
57	MG	QM	201	1/1	0.98	0.03	34,34,34,34	0
57	MG	QX	101	1/1	0.98	0.06	6,6,6,6	0
57	MG	YA	3130	1/1	0.98	0.05	3,3,3,3	0
57	MG	QA	1638	1/1	0.98	0.14	8,8,8,8	0
57	MG	QA	1616	1/1	0.98	0.11	10,10,10,10	0
57	MG	RA	3017	1/1	0.98	0.18	0,0,0,0	0
57	MG	XA	1639	1/1	0.98	0.06	11,11,11,11	0
57	MG	RA	3115	1/1	0.98	0.14	8,8,8,8	0
57	MG	YA	3258	1/1	0.98	0.33	4,4,4,4	0
59	ZN	XD	301	1/1	0.98	0.30	50,50,50,50	0
59	ZN	XN	101	1/1	0.98	0.06	59,59,59,59	0
57	MG	YA	3236	1/1	0.98	0.20	12,12,12,12	0
57	MG	QA	1660	1/1	0.99	0.03	16,16,16,16	0
57	MG	YA	3241	1/1	0.99	0.15	13,13,13,13	0
57	MG	QA	1657	1/1	0.99	0.04	19,19,19,19	0
57	MG	YA	3066	1/1	0.99	0.11	9,9,9,9	0
57	MG	RA	3152	1/1	0.99	0.04	26,26,26,26	0
57	MG	QA	1653	1/1	0.99	0.04	6,6,6,6	0
57	MG	YA	3175	1/1	0.99	0.04	2,2,2,2	0
57	MG	YA	3141	1/1	0.99	0.04	18,18,18,18	0
57	MG	YA	3263	1/1	0.99	0.29	2,2,2,2	0
57	MG	YA	3177	1/1	0.99	0.04	92,92,92,92	0
57	MG	R8	101	1/1	0.99	0.21	6,6,6,6	0
57	MG	YA	3143	1/1	0.99	0.14	11,11,11,11	0
57	MG	YA	3166	1/1	0.99	0.06	14,14,14,14	0
57	MG	YA	3005	1/1	0.99	0.09	2,2,2,2	0
57	MG	QA	1624	1/1	0.99	0.07	16,16,16,16	0

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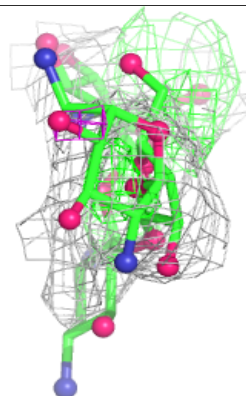
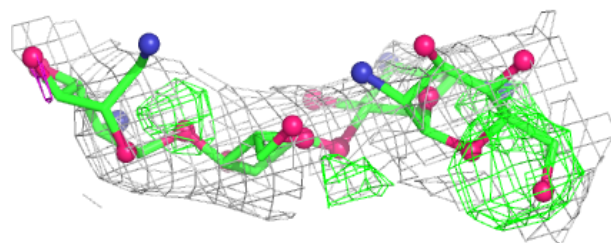
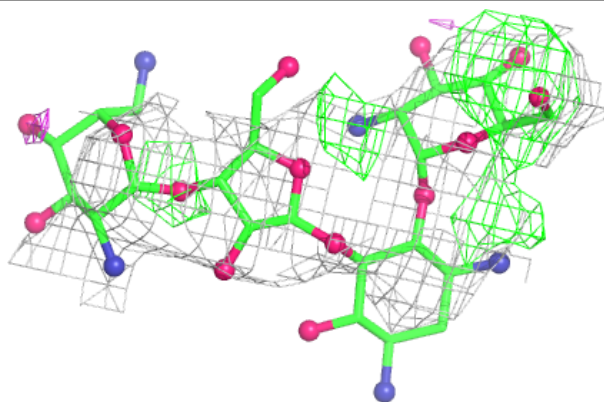
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3149	1/1	0.99	0.57	17,17,17,17	0
59	ZN	QD	301	1/1	1.00	0.08	12,12,12,12	0
57	MG	RA	3056	1/1	1.00	0.13	0,0,0,0	0

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.

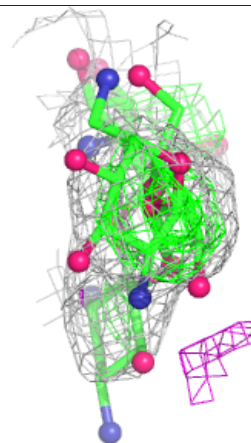
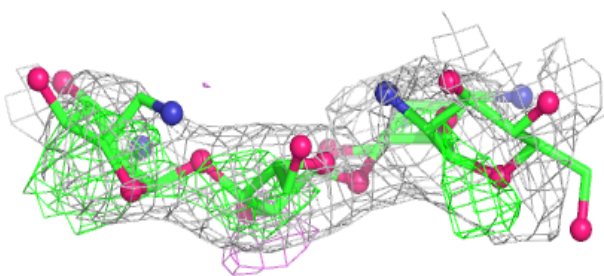
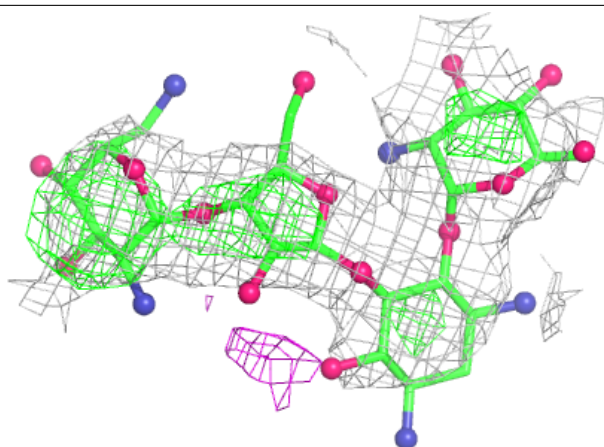
Electron density around PAR QA 1666:

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



Electron density around PAR XA 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.