



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:06 AM UTC

PDB ID : 4LFZ / pdb_00004lfz
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U in the Absence of Paromomycin
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-27
Resolution : 3.92 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

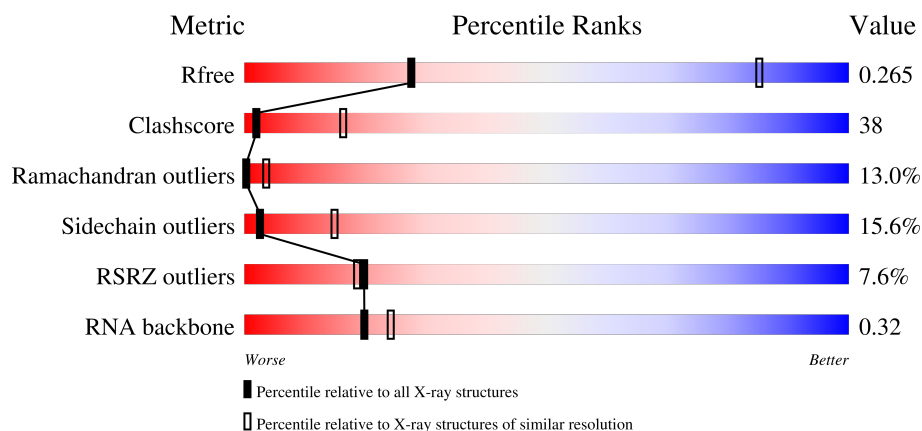
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)
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	4% 29% 51% 18% ..
1	XA	1522	4% 29% 51% 18% ..
2	QB	256	11% 15% 59% 16% • 7%
2	XB	256	5% 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	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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

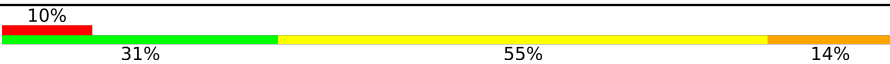
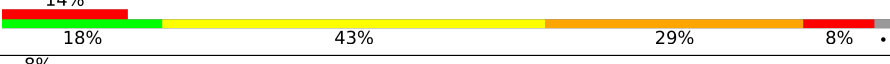
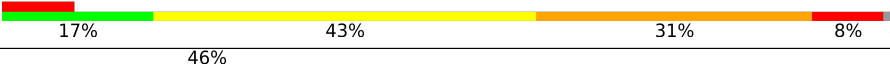
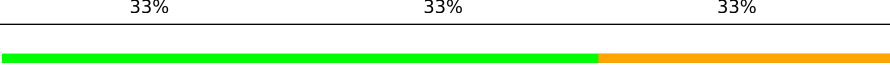
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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4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

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	Z8	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1602	-	-	-	X
57	MG	QA	1603	-	-	-	X
57	MG	QA	1612	-	-	-	X
57	MG	QA	1613	-	-	-	X
57	MG	QA	1614	-	-	-	X
57	MG	QA	1615	-	-	-	X
57	MG	QA	1618	-	-	-	X
57	MG	QA	1642	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3010	-	-	-	X
57	MG	RA	3013	-	-	-	X
57	MG	RA	3015	-	-	-	X
57	MG	RA	3020	-	-	-	X
57	MG	RA	3022	-	-	-	X
57	MG	RA	3026	-	-	-	X
57	MG	RA	3029	-	-	-	X
57	MG	RA	3031	-	-	-	X
57	MG	RA	3032	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3036	-	-	-	X
57	MG	RA	3037	-	-	-	X
57	MG	RA	3039	-	-	-	X
57	MG	RA	3041	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3046	-	-	-	X
57	MG	RA	3049	-	-	-	X
57	MG	RA	3051	-	-	-	X
57	MG	RA	3052	-	-	-	X
57	MG	RA	3058	-	-	-	X
57	MG	RA	3059	-	-	-	X
57	MG	RA	3062	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3069	-	-	-	X
57	MG	RA	3070	-	-	-	X
57	MG	RA	3085	-	-	-	X
57	MG	RA	3087	-	-	-	X
57	MG	RA	3092	-	-	-	X
57	MG	RA	3101	-	-	-	X
57	MG	RA	3121	-	-	-	X
57	MG	RA	3122	-	-	-	X
57	MG	RA	3128	-	-	-	X
57	MG	RA	3131	-	-	-	X
57	MG	RA	3140	-	-	-	X
57	MG	RA	3143	-	-	-	X
57	MG	RA	3153	-	-	-	X
57	MG	RA	3163	-	-	-	X
57	MG	RA	3170	-	-	-	X
57	MG	RA	3187	-	-	-	X
57	MG	RA	3201	-	-	-	X
57	MG	RA	3212	-	-	-	X
57	MG	RA	3229	-	-	-	X
57	MG	XA	1618	-	-	-	X
57	MG	XA	1624	-	-	-	X
57	MG	XA	1632	-	-	-	X
57	MG	YA	3001	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3006	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3014	-	-	-	X
57	MG	YA	3015	-	-	-	X
57	MG	YA	3018	-	-	-	X
57	MG	YA	3029	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3032	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3041	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3043	-	-	-	X
57	MG	YA	3045	-	-	-	X
57	MG	YA	3047	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3052	-	-	-	X
57	MG	YA	3053	-	-	-	X
57	MG	YA	3058	-	-	-	X
57	MG	YA	3060	-	-	-	X
57	MG	YA	3068	-	-	-	X
57	MG	YA	3073	-	-	-	X
57	MG	YA	3076	-	-	-	X
57	MG	YA	3078	-	-	-	X
57	MG	YA	3080	-	-	-	X
57	MG	YA	3087	-	-	-	X
57	MG	YA	3088	-	-	-	X
57	MG	YA	3094	-	-	-	X
57	MG	YA	3096	-	-	-	X
57	MG	YA	3099	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3101	-	-	-	X
57	MG	YA	3106	-	-	-	X
57	MG	YA	3109	-	-	-	X
57	MG	YA	3120	-	-	-	X
57	MG	YA	3121	-	-	-	X
57	MG	YA	3128	-	-	-	X
57	MG	YA	3142	-	-	-	X
57	MG	YA	3167	-	-	-	X
57	MG	YA	3172	-	-	-	X
57	MG	YA	3200	-	-	-	X
57	MG	YA	3201	-	-	-	X
57	MG	YA	3214	-	-	-	X
57	MG	YA	3232	-	-	-	X
57	MG	YA	3237	-	-	-	X
57	MG	YA	3254	-	-	-	X
57	MG	YA	3260	-	-	-	X
57	MG	YB	202	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
23	XX	7	Total	C	N	O	P	0	0	0
			145	65	23	50	7			

- Molecule 24 is a RNA chain called messenger RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	64	Total	Mg	0	0
			64	64		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	1	Total 1	Mg 1	0	0
57	RA	239	Total 239	Mg 239	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	XB	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	2	Total 2	Mg 2	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	269	Total 269	Mg 269	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YE	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0

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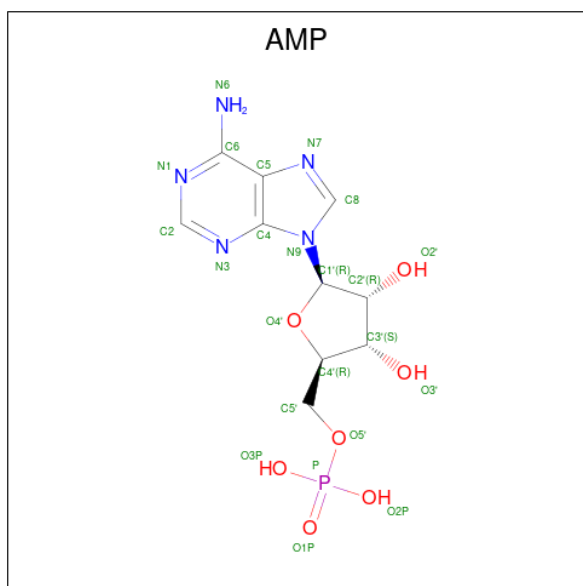
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y5	1	Total	Mg	0	0
			1	1		
57	Y7	1	Total	Mg	0	0
			1	1		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 59 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).

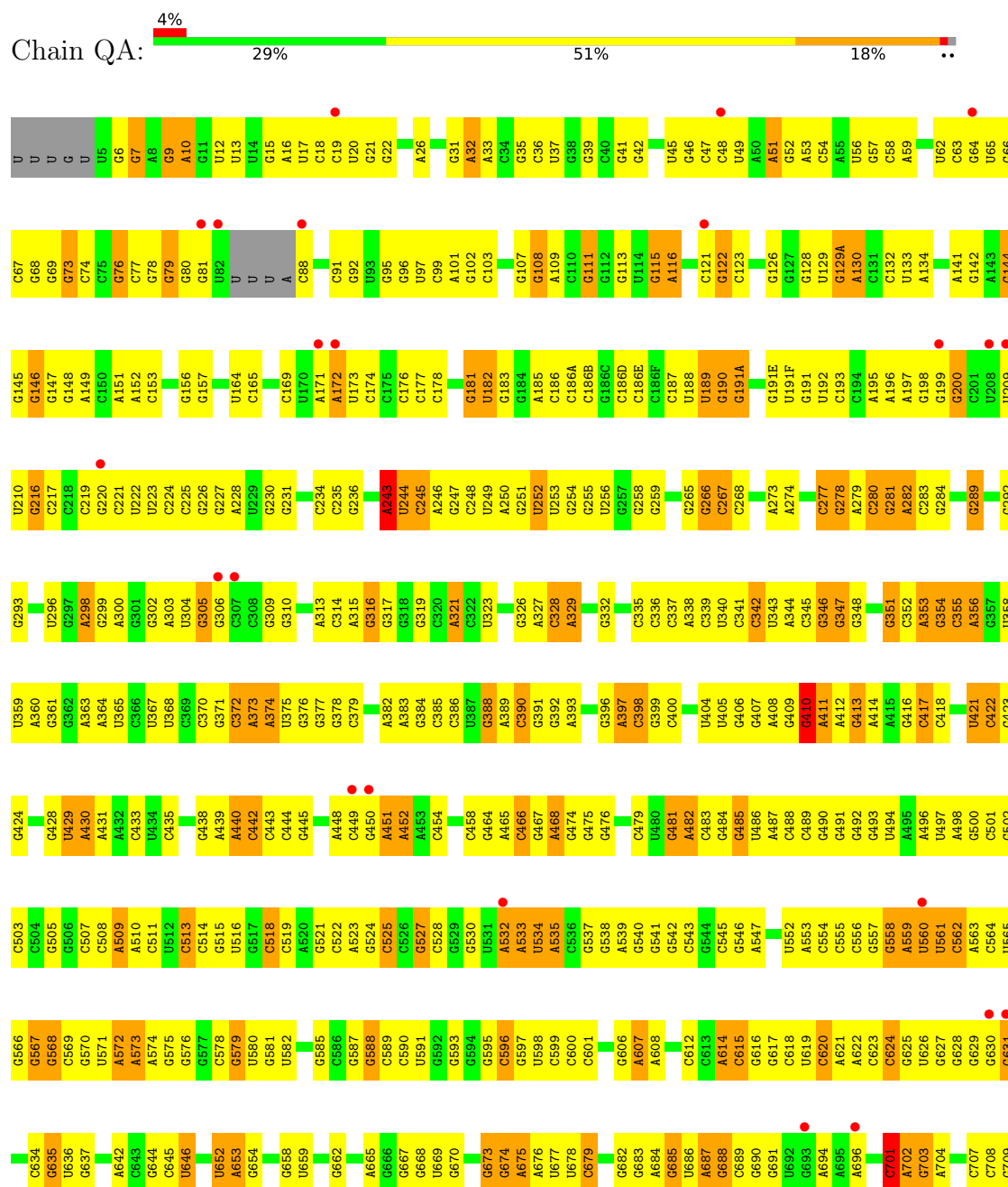


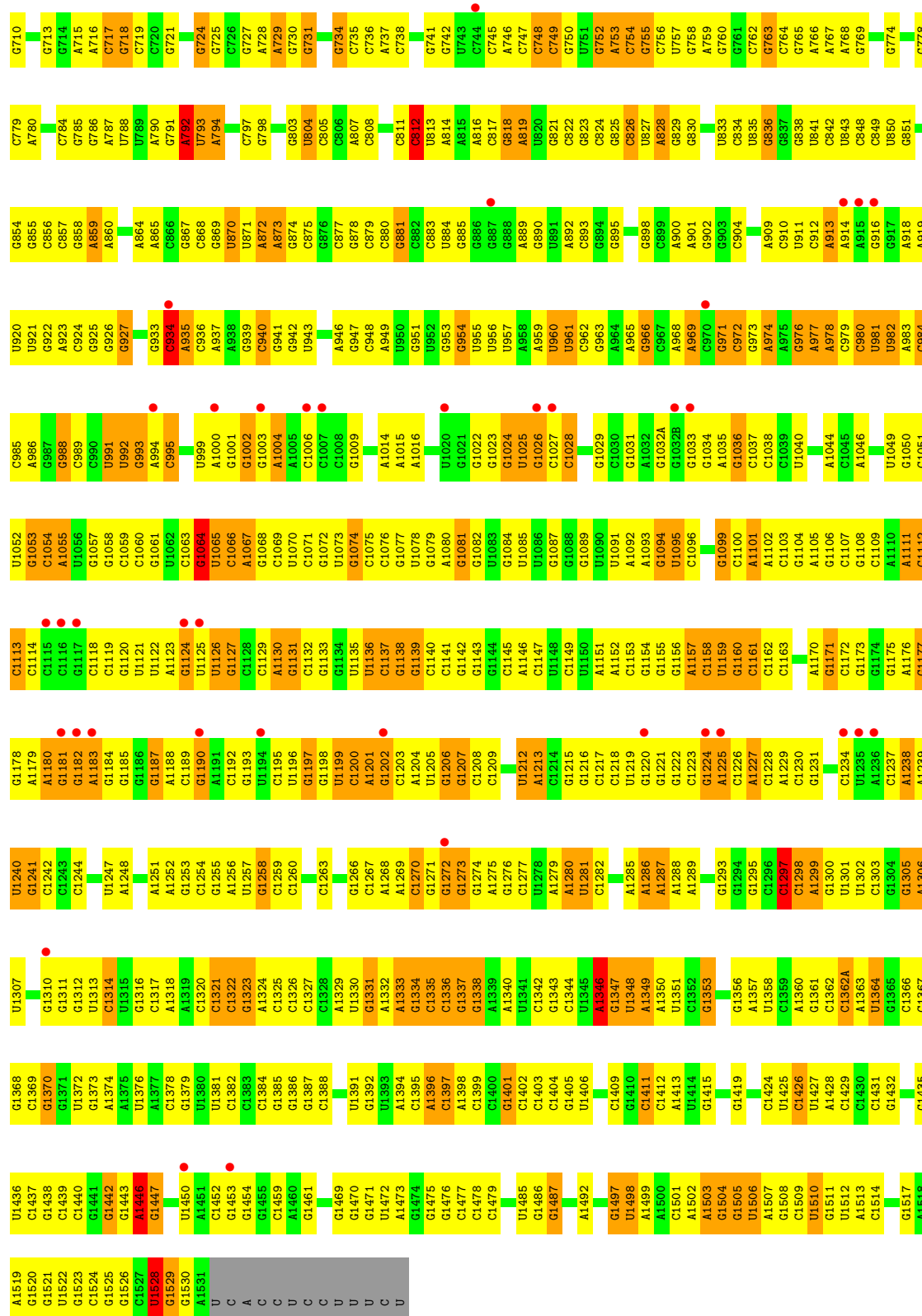
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	XX	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

3 Residue-property plots

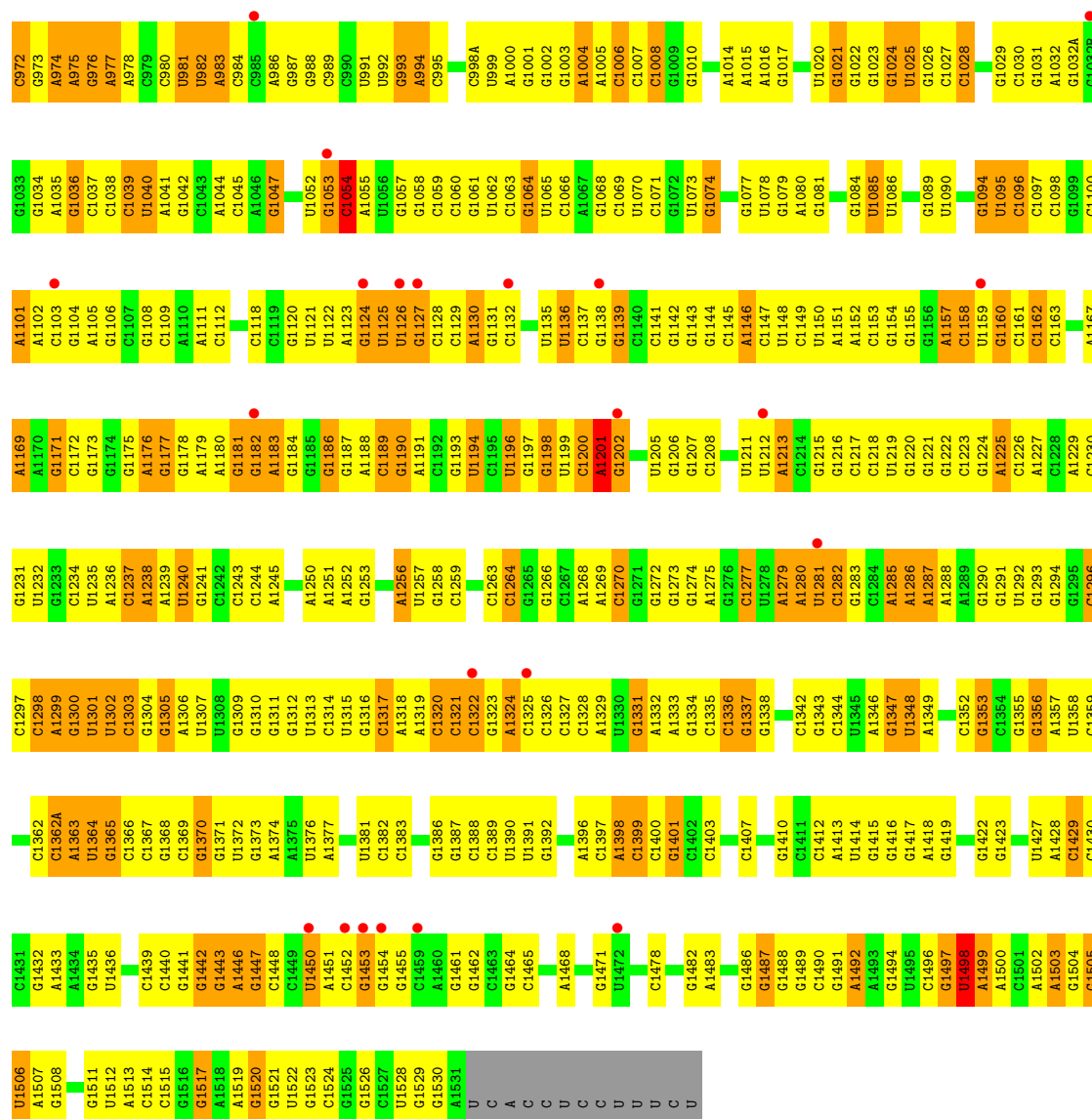
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 rRNA

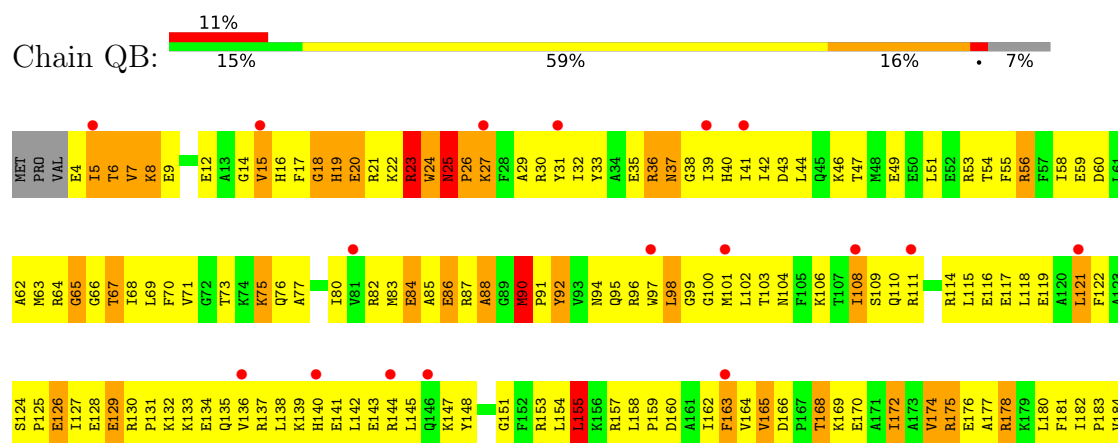


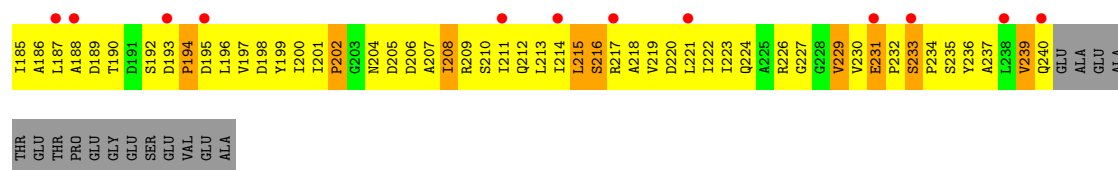




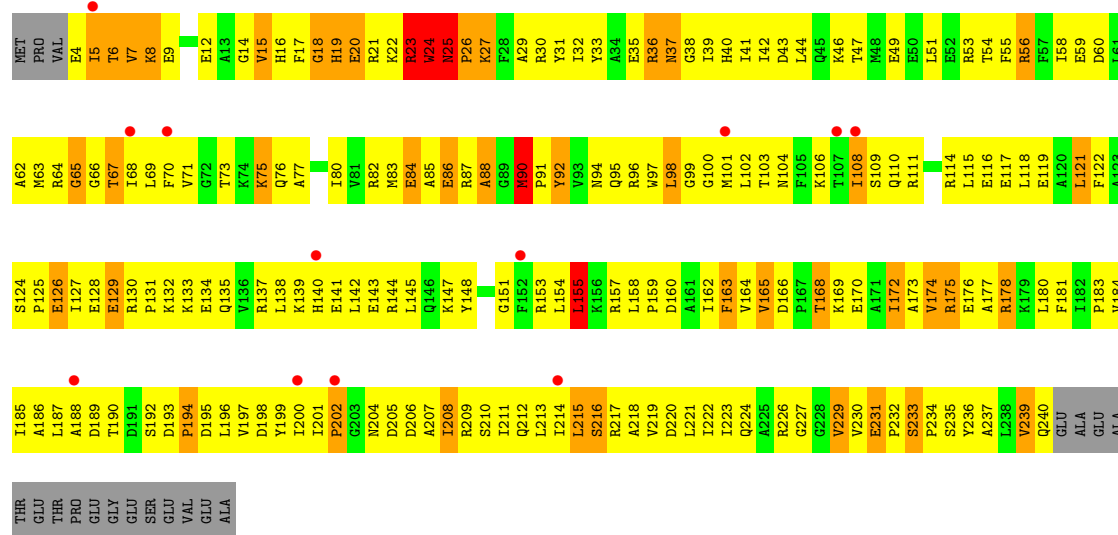
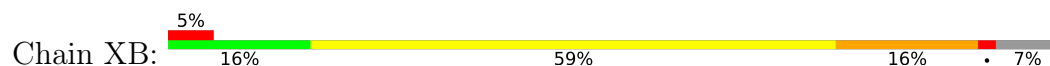


• Molecule 2: 30S ribosomal protein S2

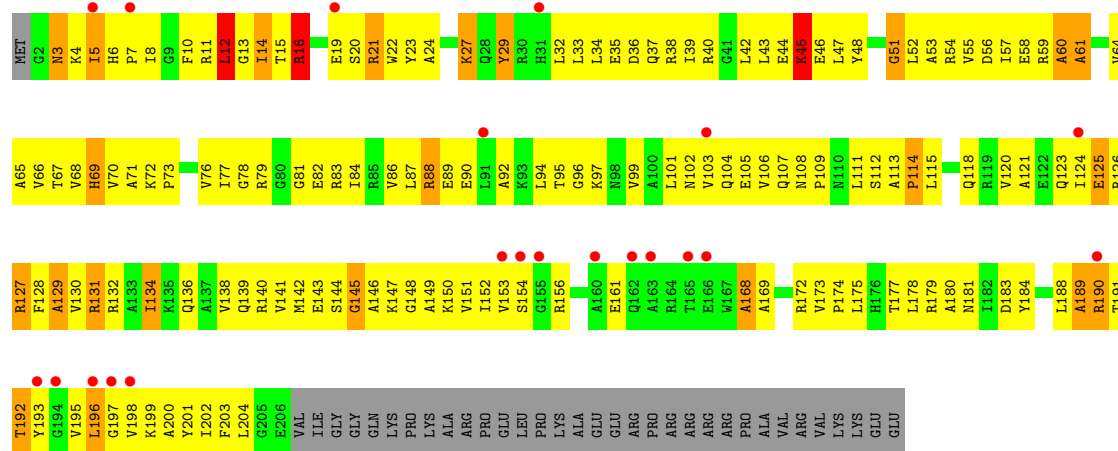




• Molecule 2: 30S ribosomal protein S2

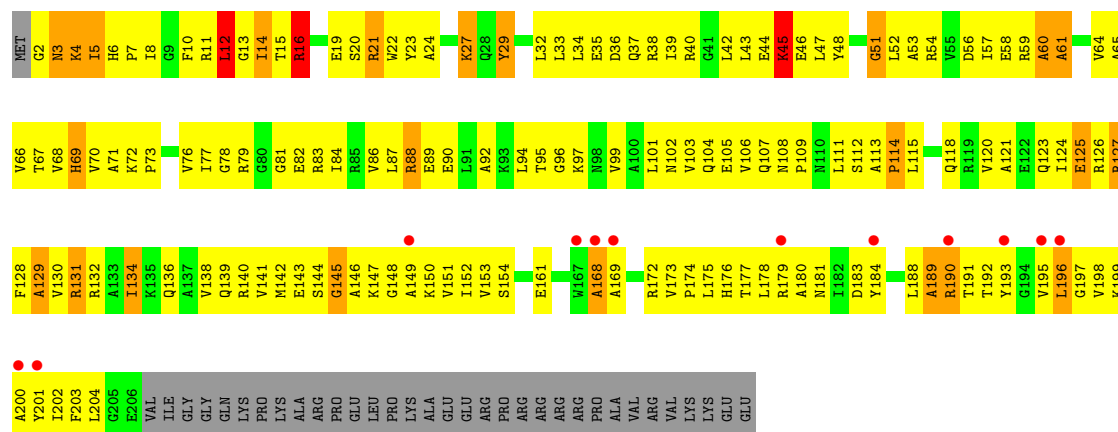


• Molecule 3: 30S ribosomal protein S3

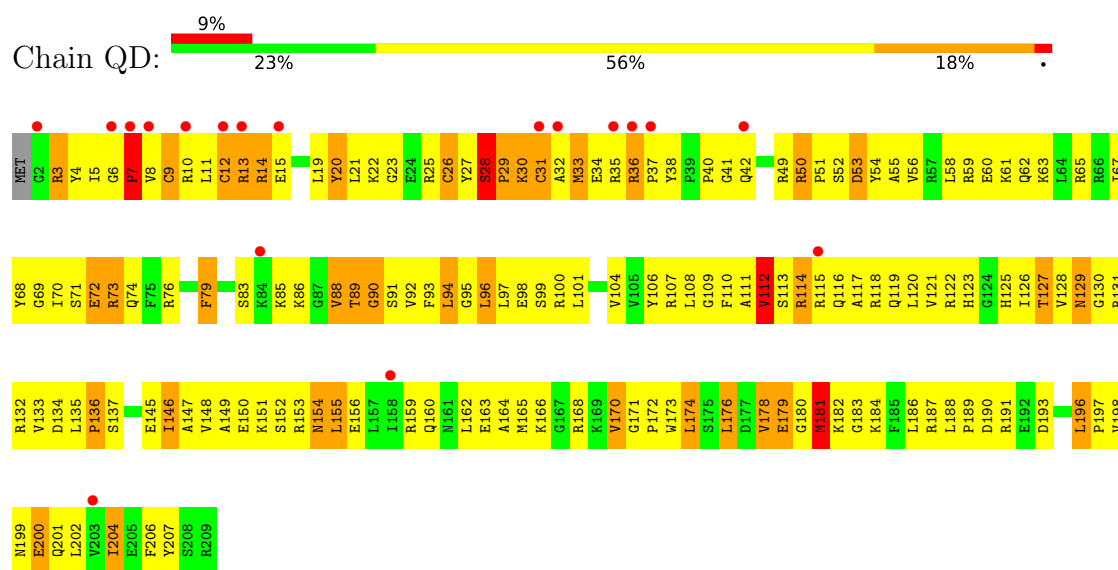


• Molecule 3: 30S ribosomal protein S3

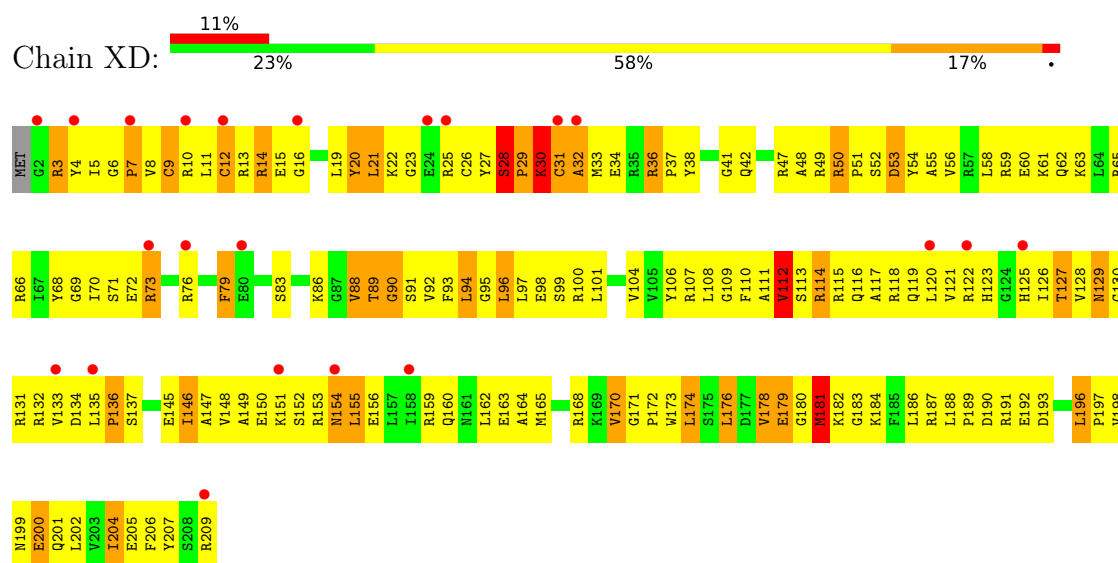




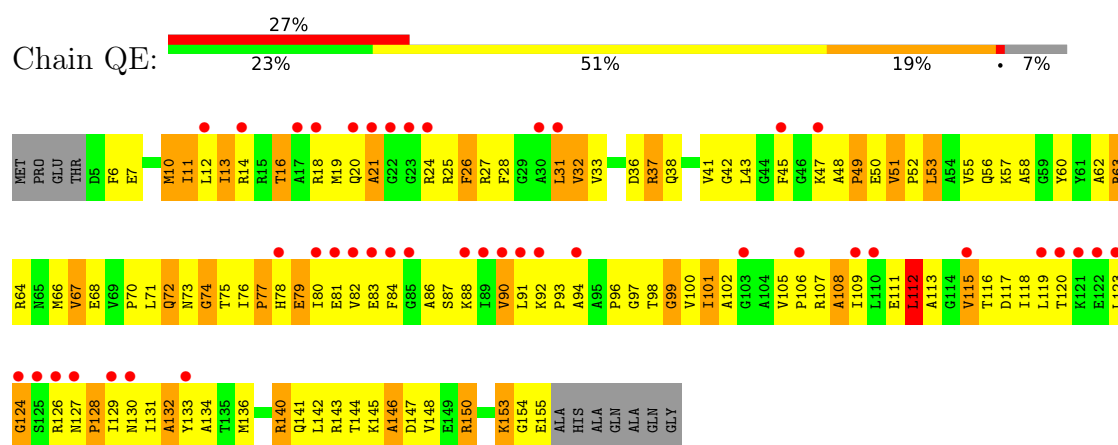
• Molecule 4: 30S ribosomal protein S4



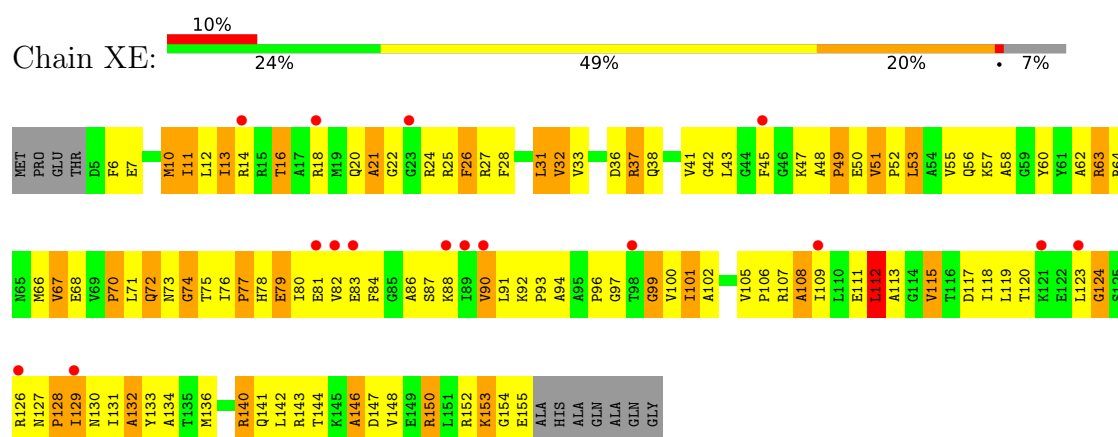
• Molecule 4: 30S ribosomal protein S4



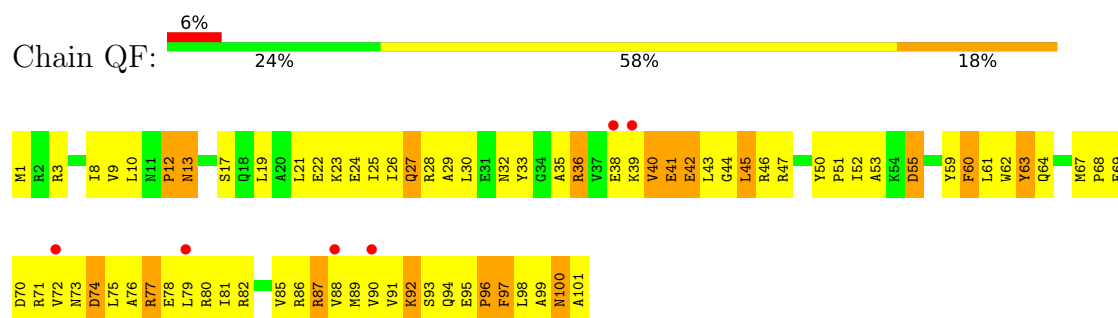
• Molecule 5: 30S ribosomal protein S5



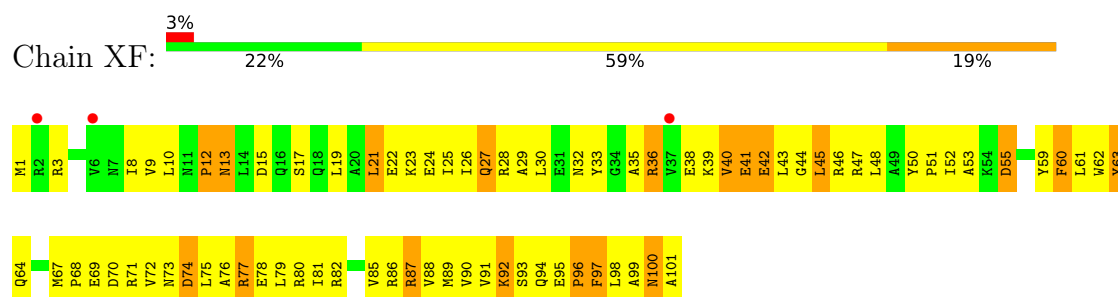
• Molecule 5: 30S ribosomal protein S5



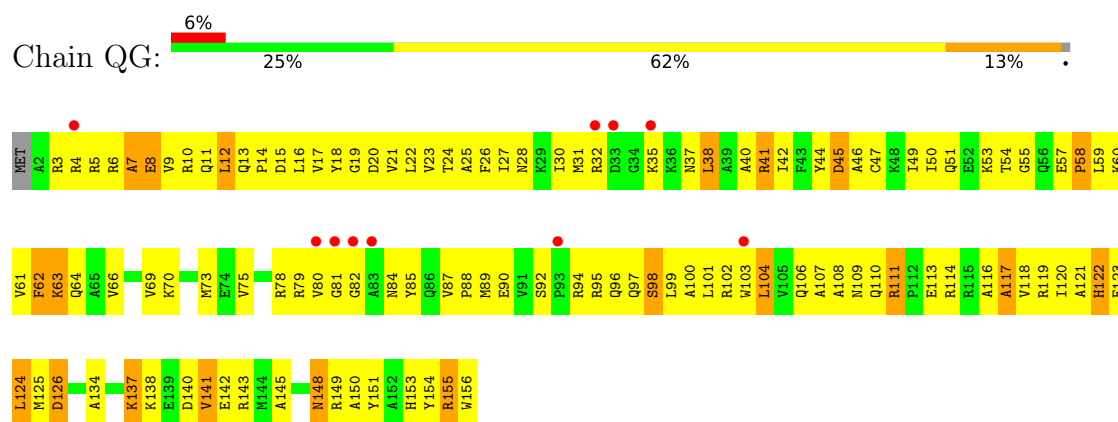
• Molecule 6: 30S ribosomal protein S6



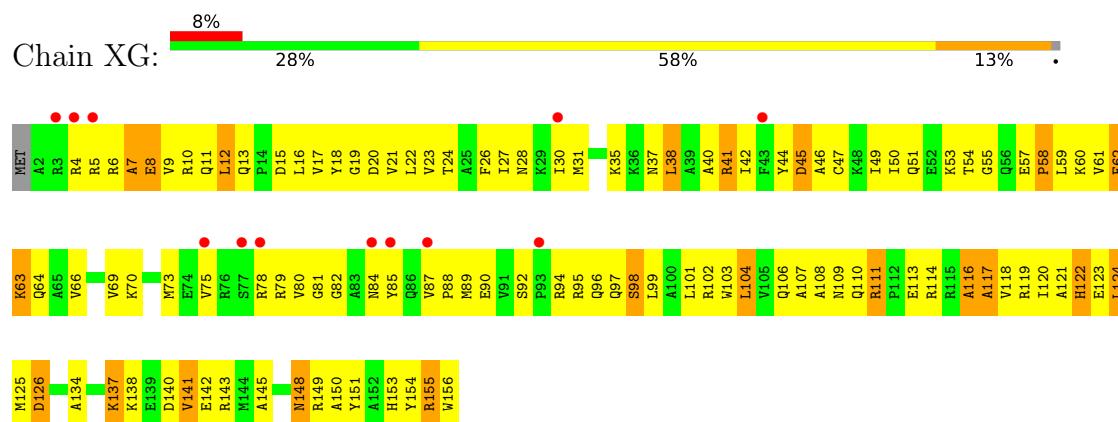
• Molecule 6: 30S ribosomal protein S6



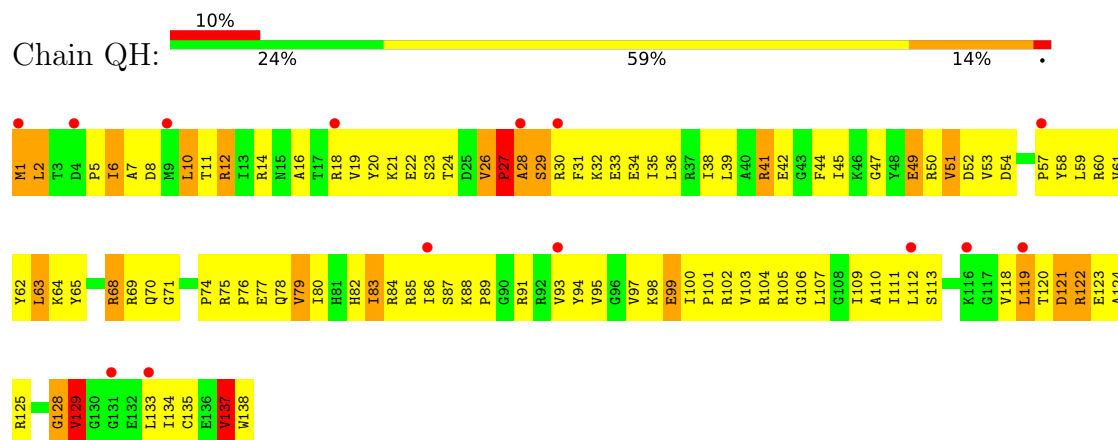
• Molecule 7: 30S ribosomal protein S7



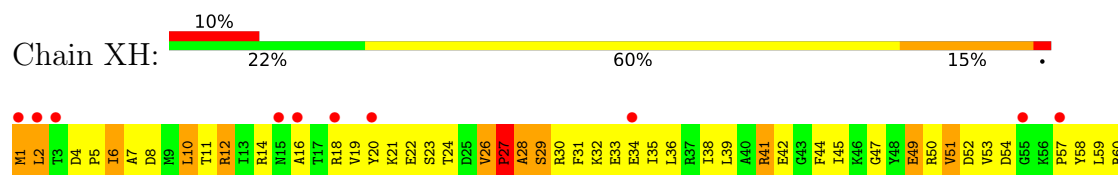
• Molecule 7: 30S ribosomal protein S7

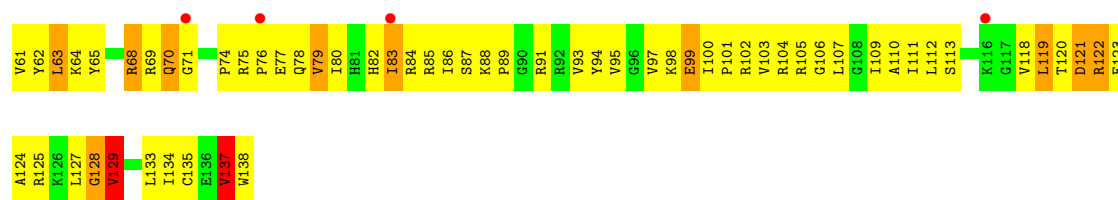


• Molecule 8: 30S ribosomal protein S8

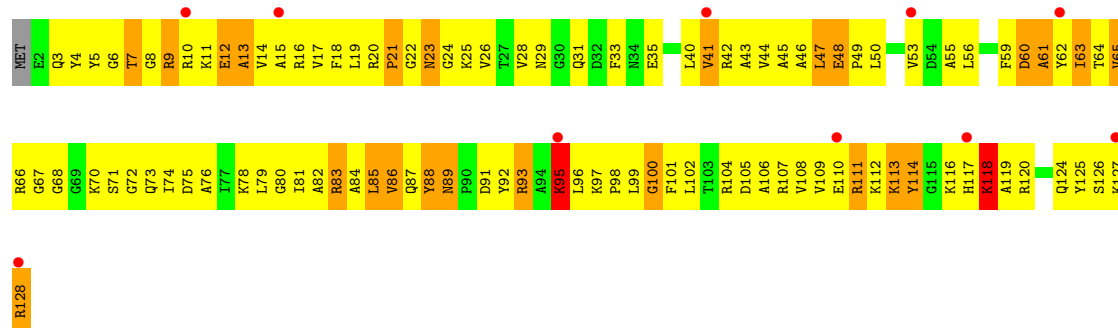


• Molecule 8: 30S ribosomal protein S8

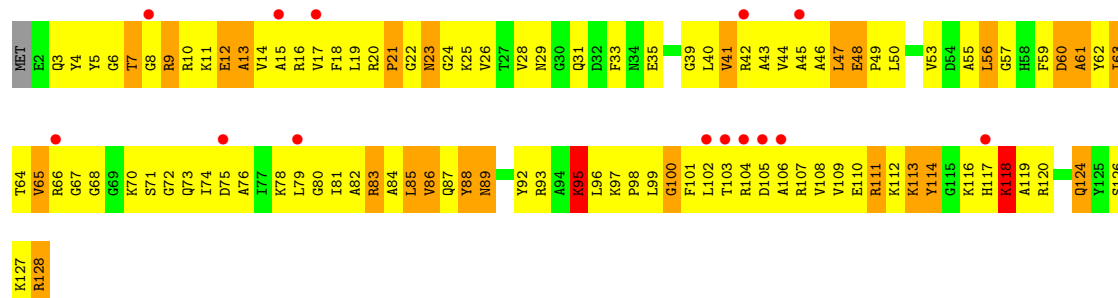




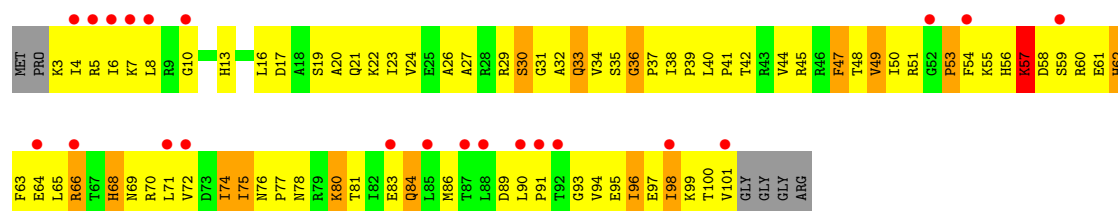
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

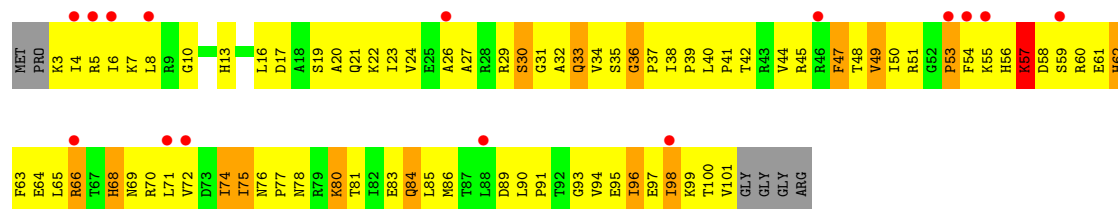


• Molecule 10: 30S ribosomal protein S10

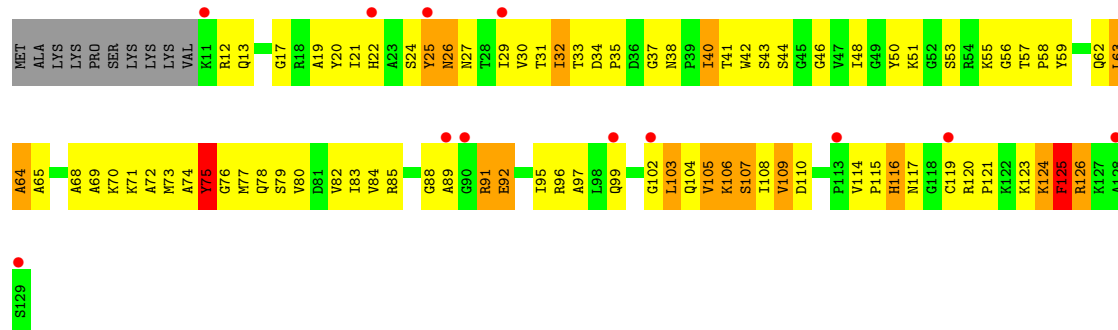


• Molecule 10: 30S ribosomal protein S10

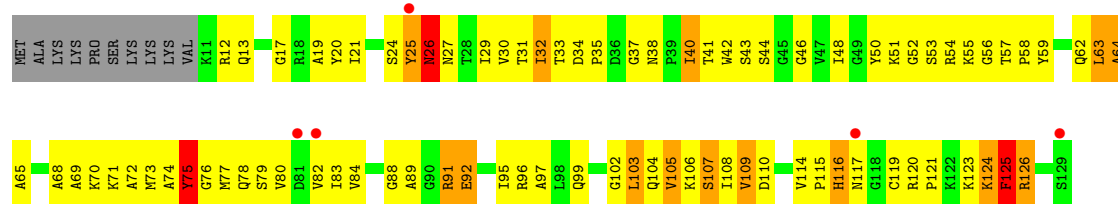




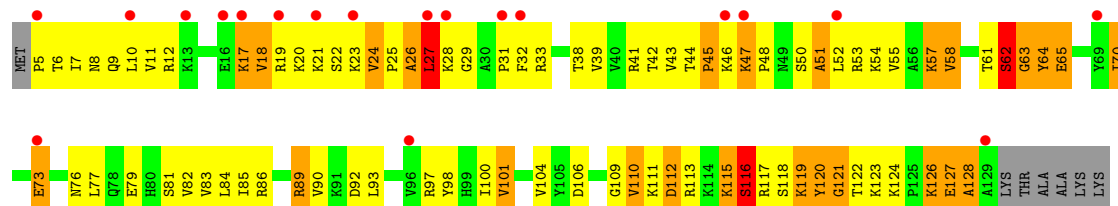
• Molecule 11: 30S ribosomal protein S11



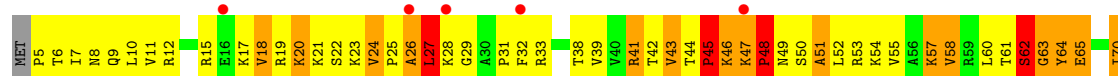
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

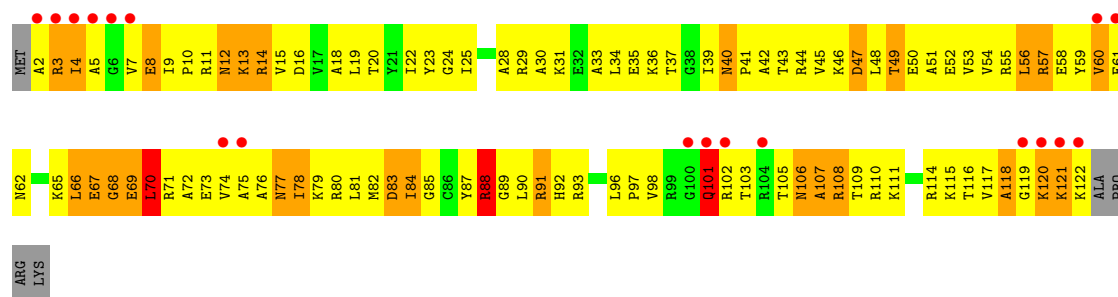
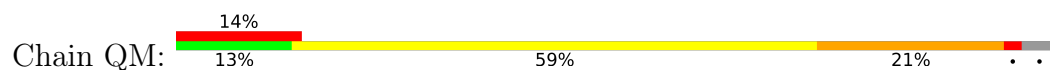


• Molecule 12: 30S ribosomal protein S12

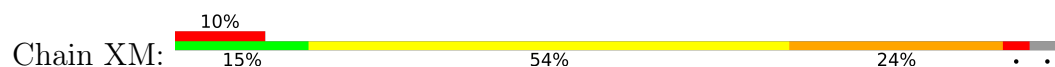




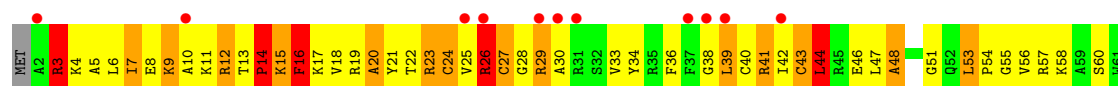
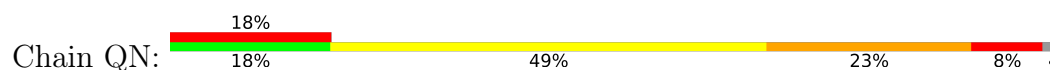
- Molecule 13: 30S ribosomal protein S13



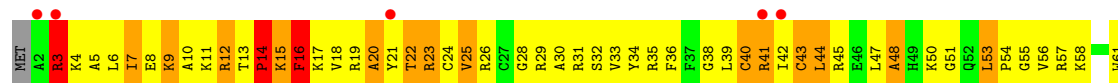
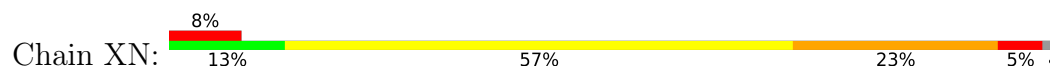
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

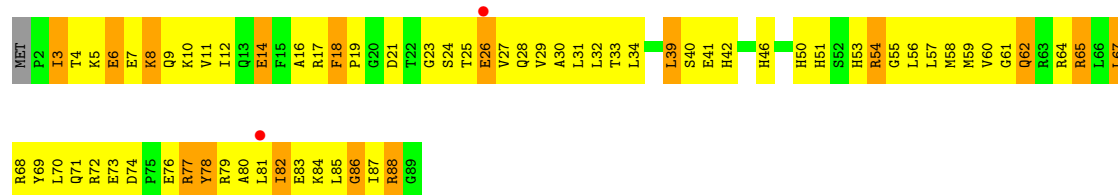


- Molecule 15: 30S ribosomal protein S15

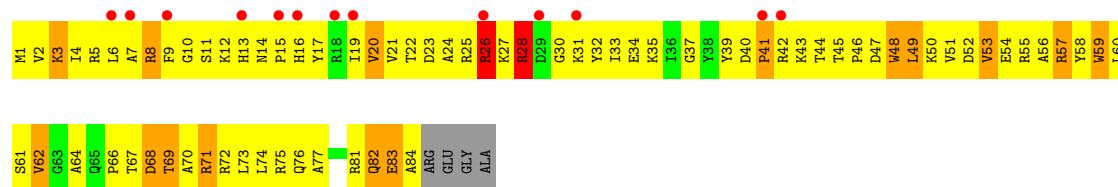
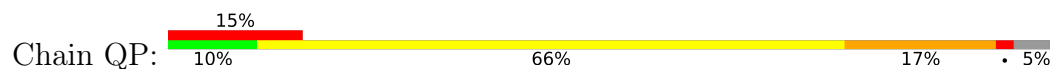




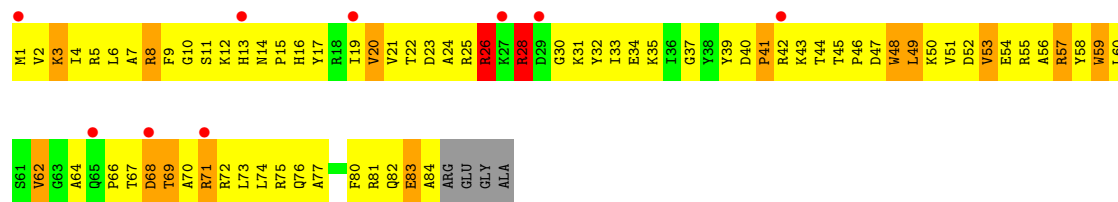
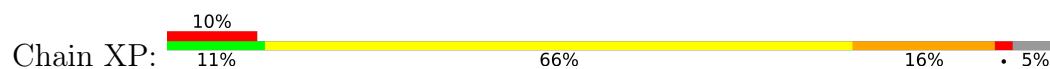
• Molecule 15: 30S ribosomal protein S15



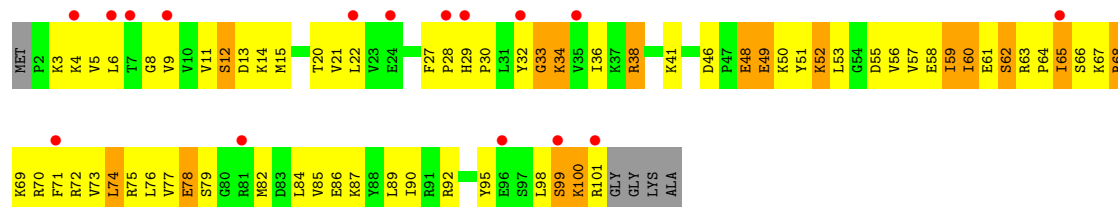
• Molecule 16: 30S ribosomal protein S16



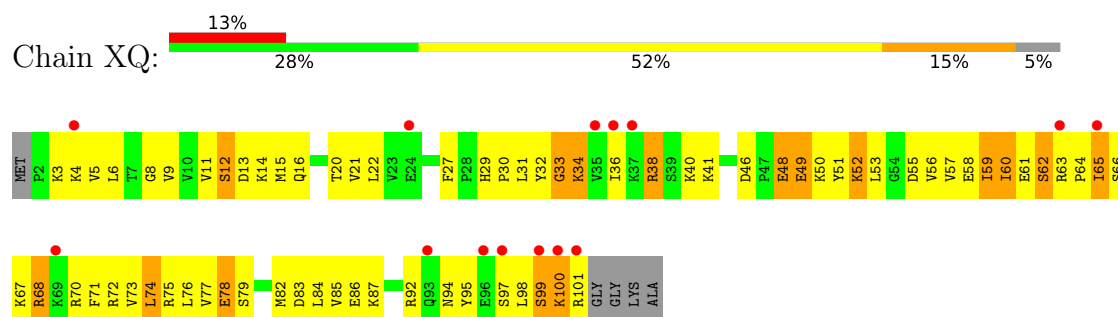
• Molecule 16: 30S ribosomal protein S16



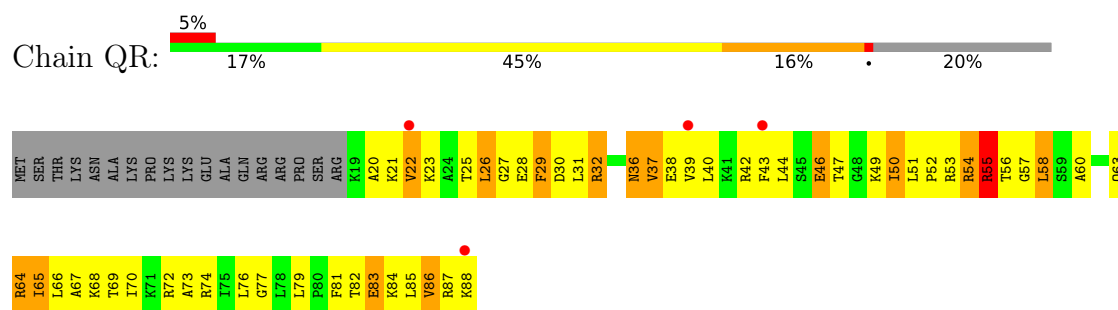
• Molecule 17: 30S ribosomal protein S17



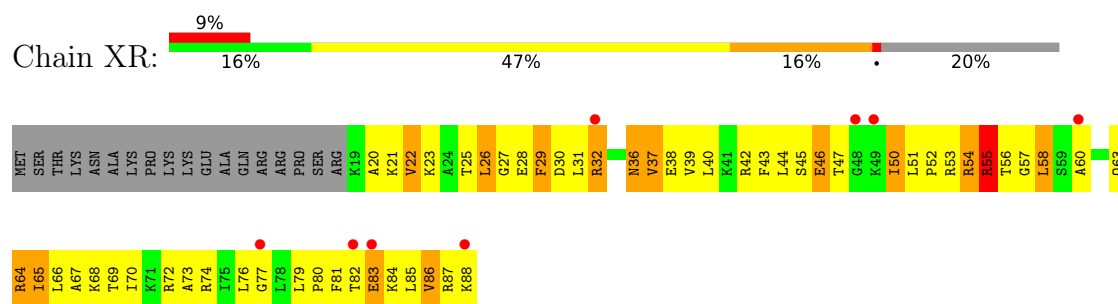
- Molecule 17: 30S ribosomal protein S17



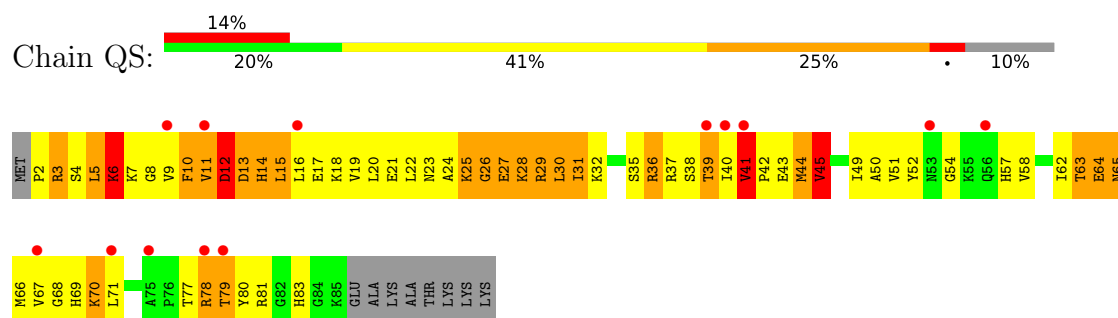
- Molecule 18: 30S ribosomal protein S18



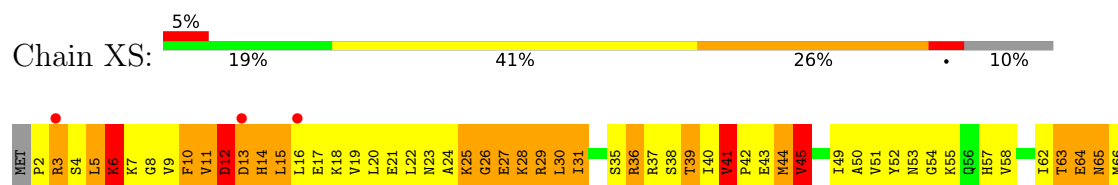
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

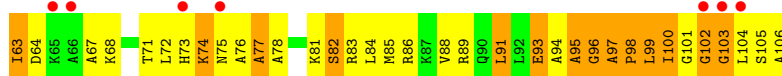
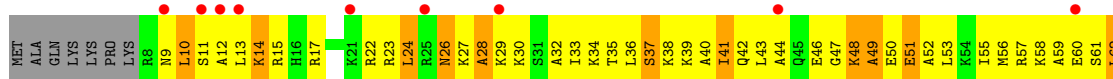
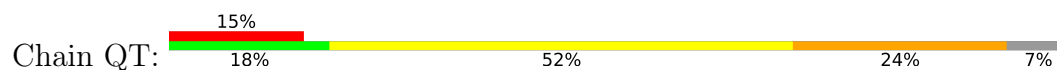


- Molecule 19: 30S ribosomal protein S19

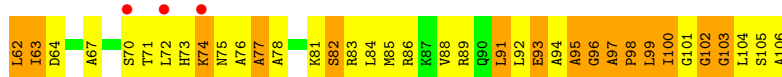
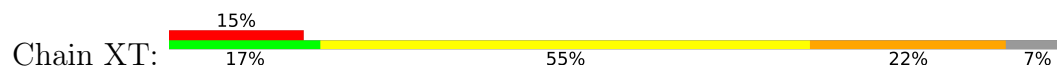




- Molecule 20: 30S ribosomal protein S20



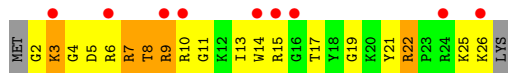
- Molecule 20: 30S ribosomal protein S20



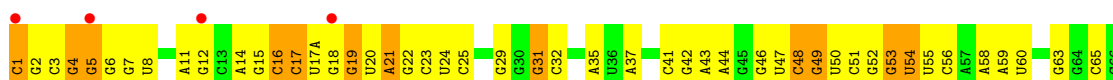
- Molecule 21: 30S ribosomal protein S21



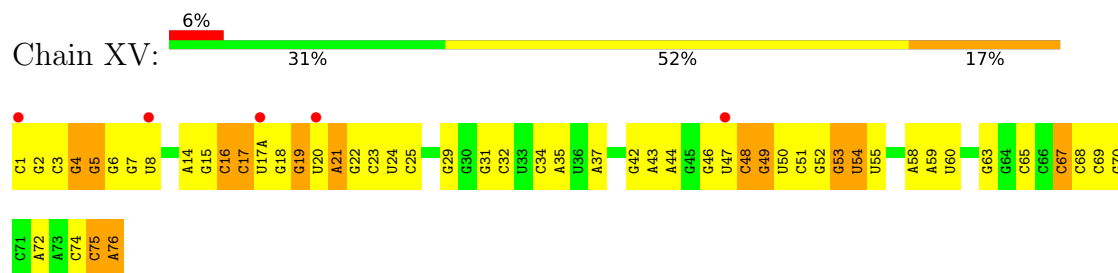
- Molecule 21: 30S ribosomal protein S21



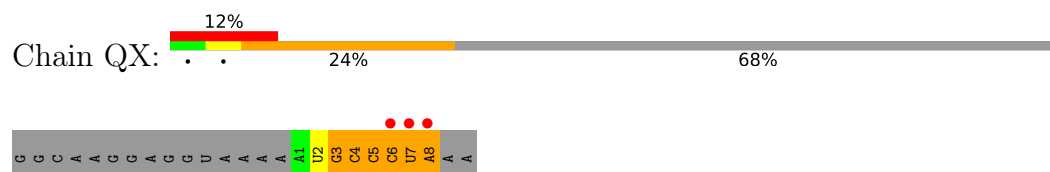
- Molecule 22: P-site tRNA fMet



- Molecule 22: P-site tRNA fMet



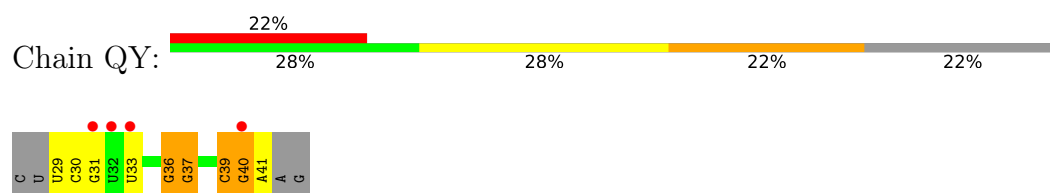
- Molecule 23: A-site ASL SufA6



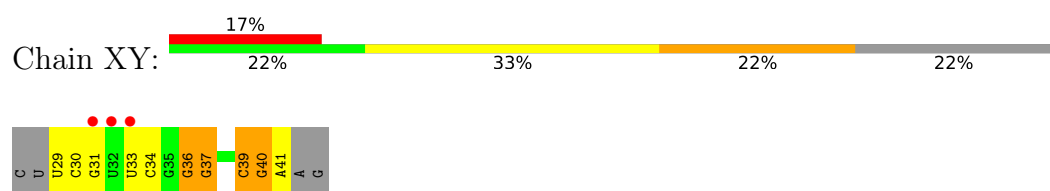
- Molecule 23: A-site ASL SufA6



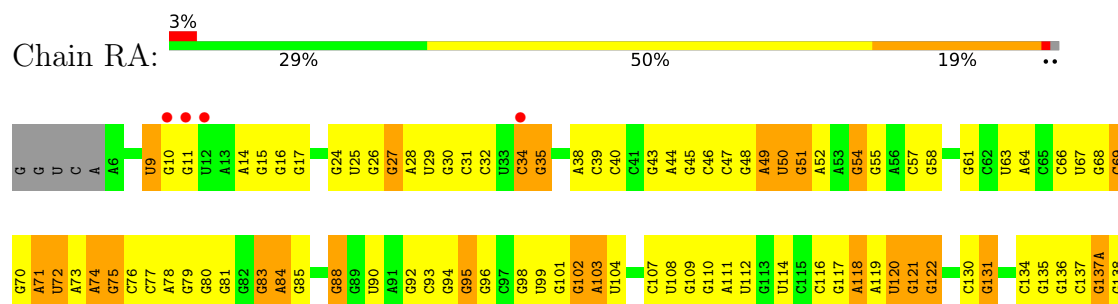
- Molecule 24: messenger RNA



- Molecule 24: messenger RNA



- Molecule 25: 23S rRNA

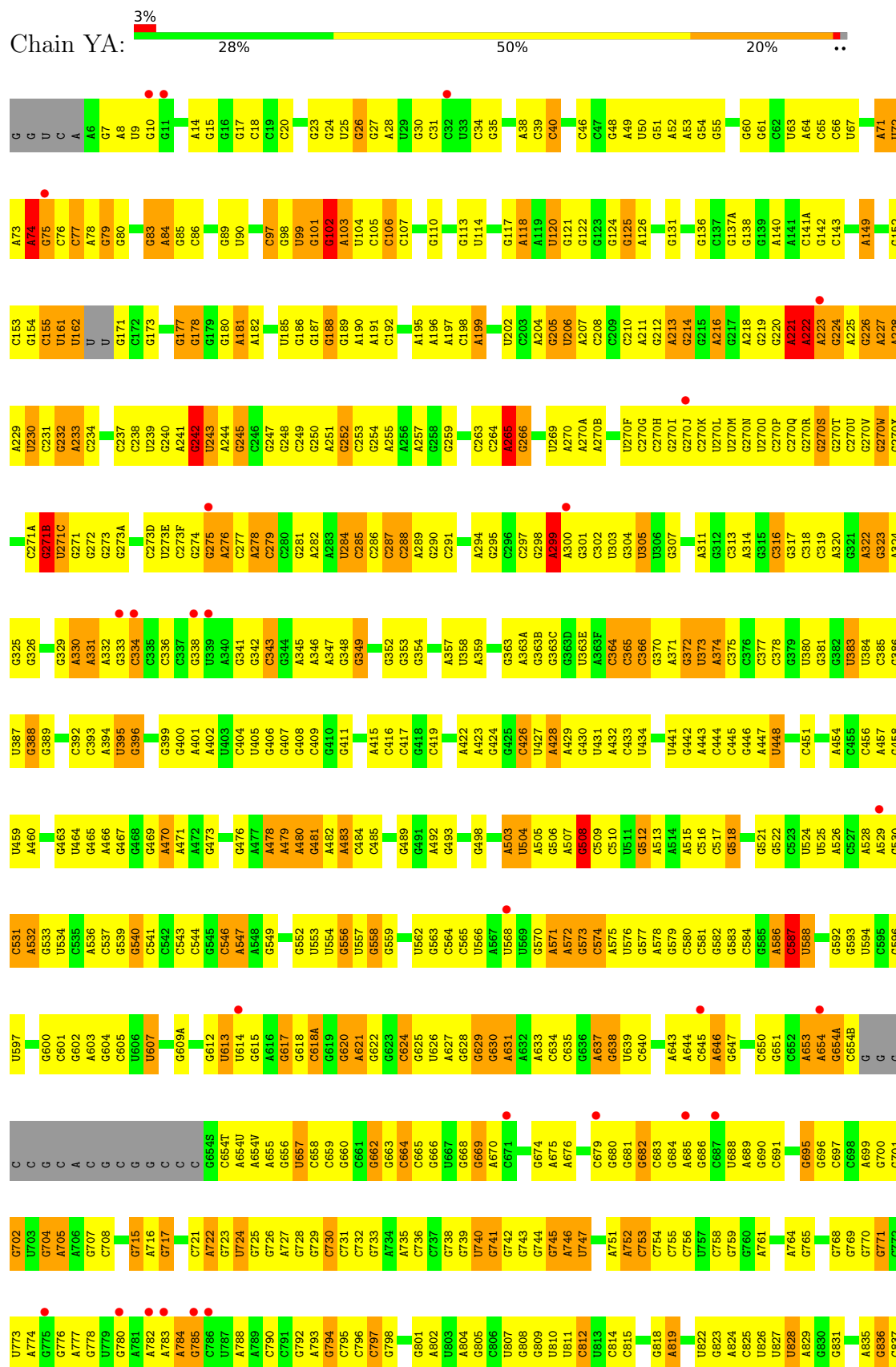


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U1926	G1772	U1840	G1772	U1680	C1604	A1536	A1413	G1348	G1209	G1212	U1142	G1072
A1927	A1773	G1841	A1773	G1681	C1605	C1537	G1414	C1351	A1215	G1216	A1143	A1073
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A2014	U1794	G1869	U1794	U1709	G1628		A1495		C1232			C1092
A2015	C1795	C1870	C1795	G1710	U1629	G1563	A1496		G1233			G1093
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U2017	U1797	G1878	U1797	C1712	G1632	C1565	C1498		G1237			A1095
G2018	U1798		U1798	G1716	G1633	C1566	C1499		A1237			A1096
A2019	G1799	C1880	G1799	U1717	A1632	A1567	G1500		G1238			U1097
A2020	C1801	G1882	C1801	G1718	G1633	A1568	C1501		A1241			A1098
C2021	A1802	G1883	A1802	G1725	C1636	G1569	A1439		A1242			G1099
U2022	U1955	A1884	U1955	G1726	C1636	A1570	G1440		G1243			C1100
G2023	U1956		U1956			A1571	G1441					U1175
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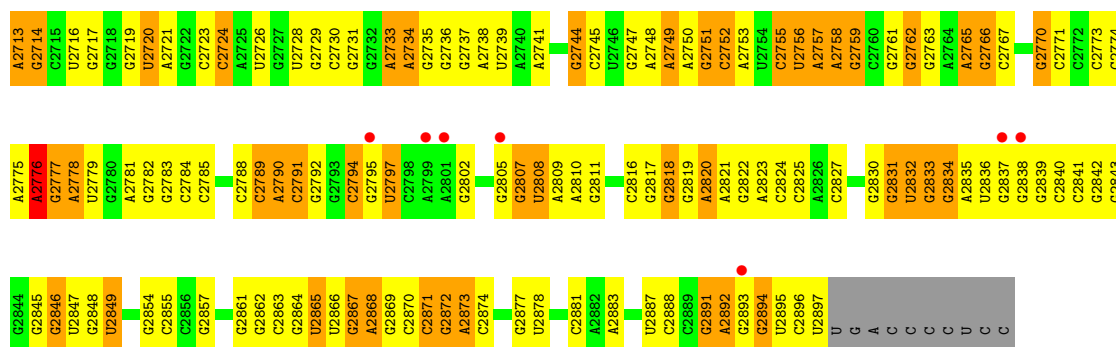


- Molecule 25: 23S rRNA

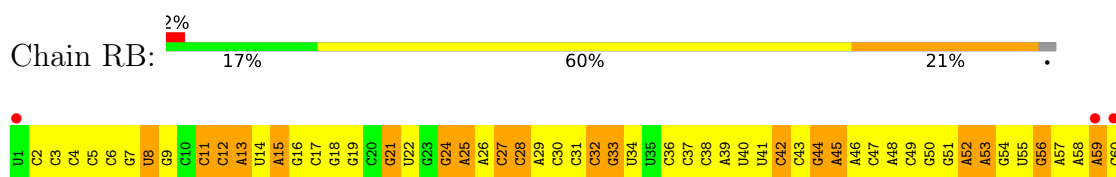




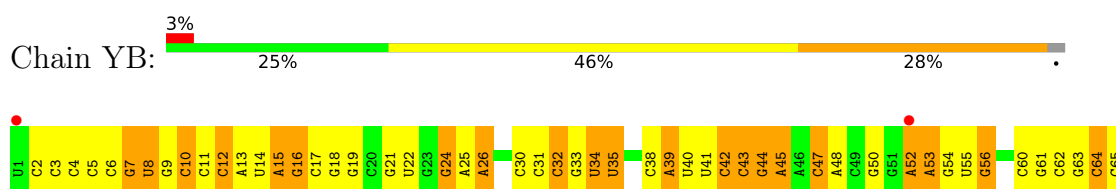
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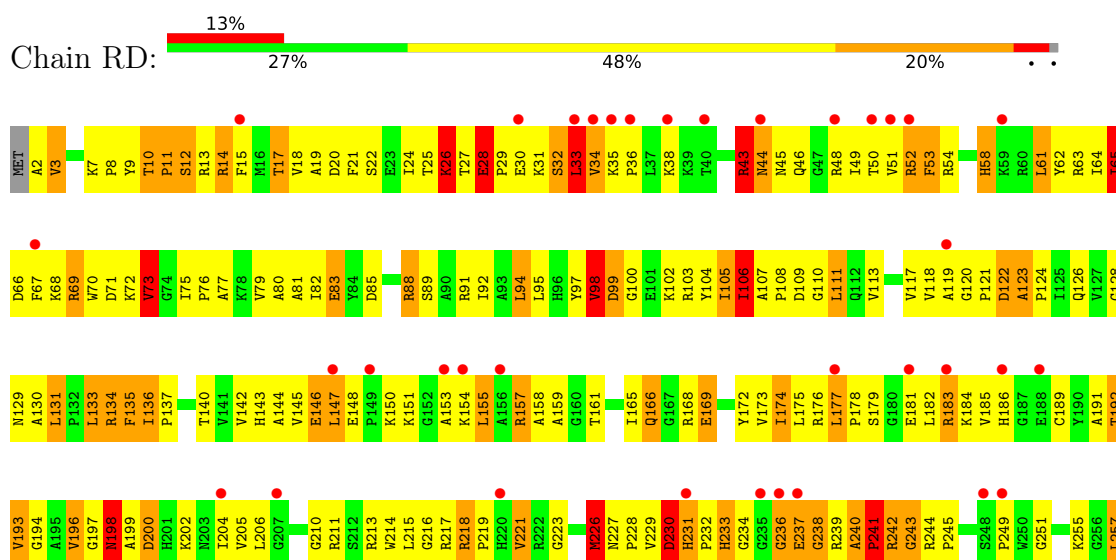
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA

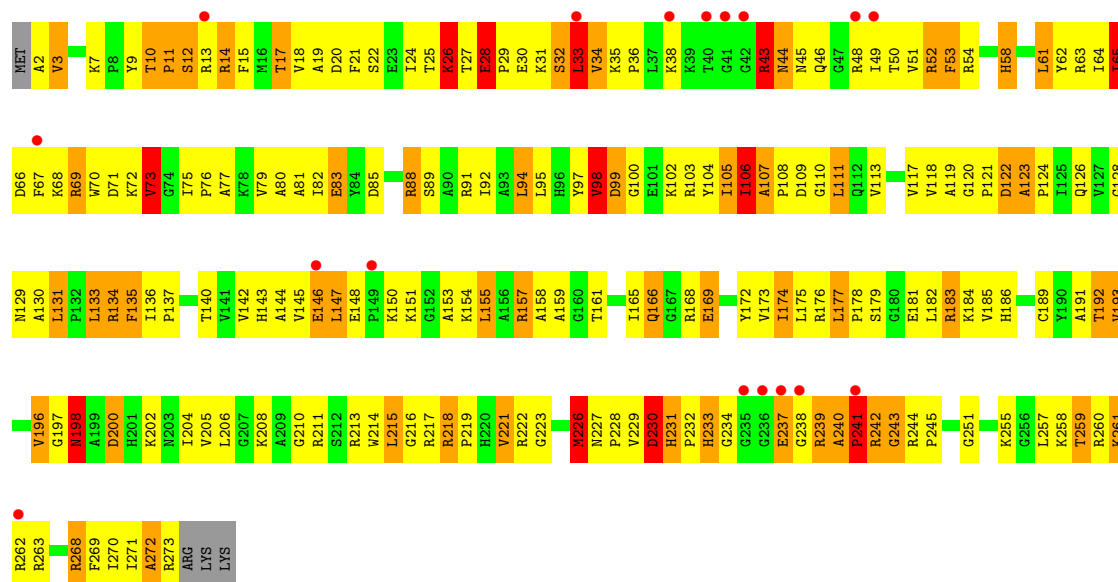


• Molecule 27: 50S ribosomal protein L2

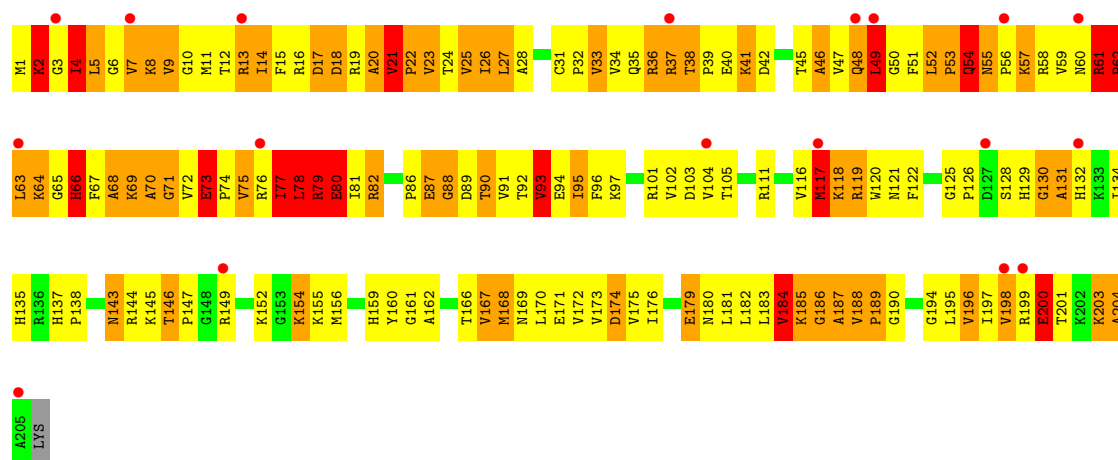
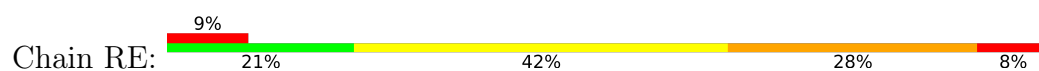




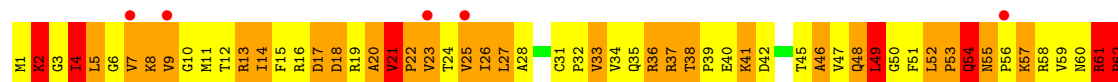
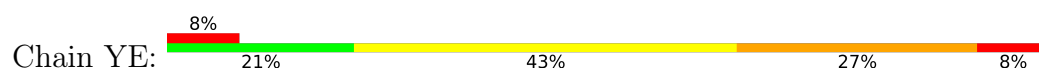
• Molecule 27: 50S ribosomal protein L2

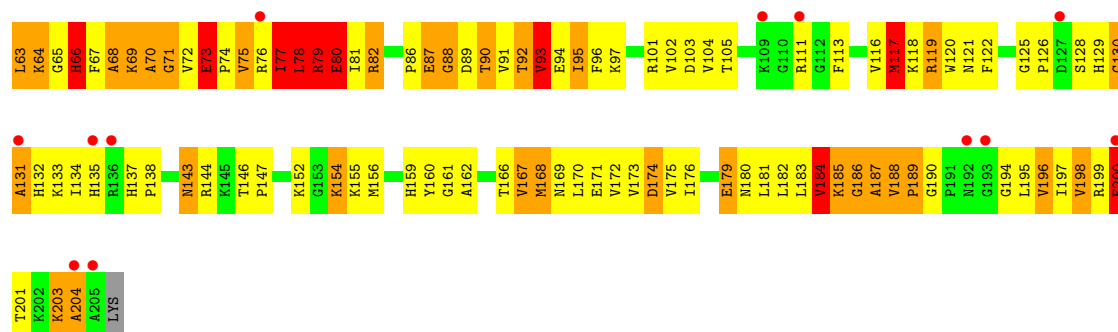


• Molecule 28: 50S ribosomal protein L3

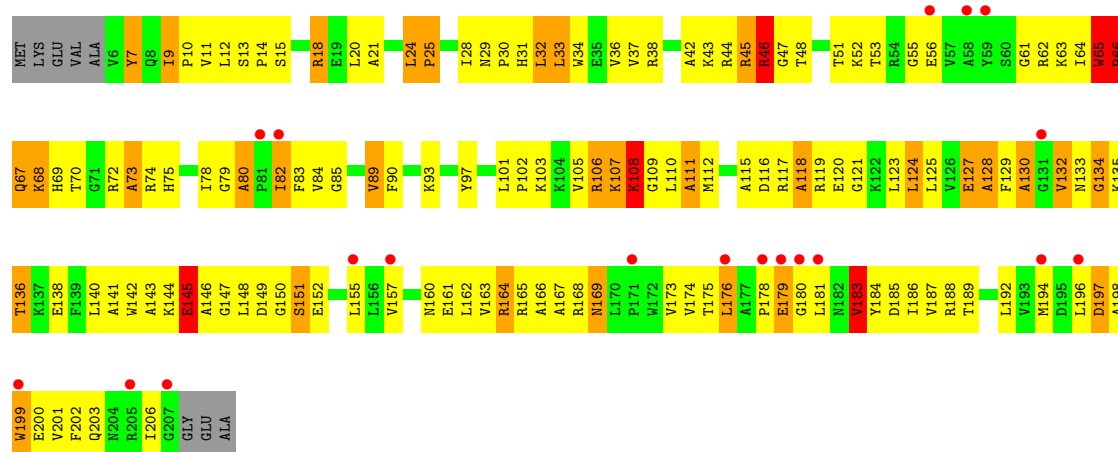


• Molecule 28: 50S ribosomal protein L3

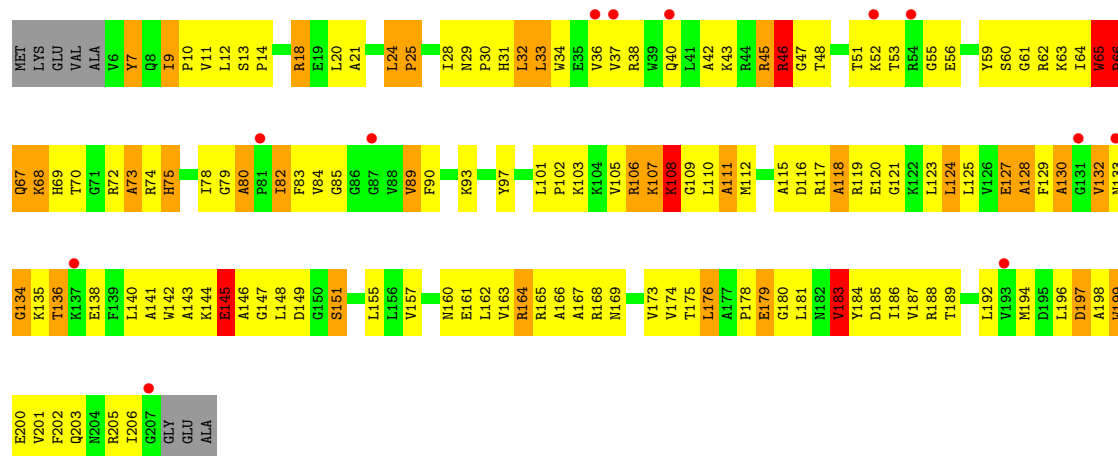




• Molecule 29: 50S ribosomal protein L4

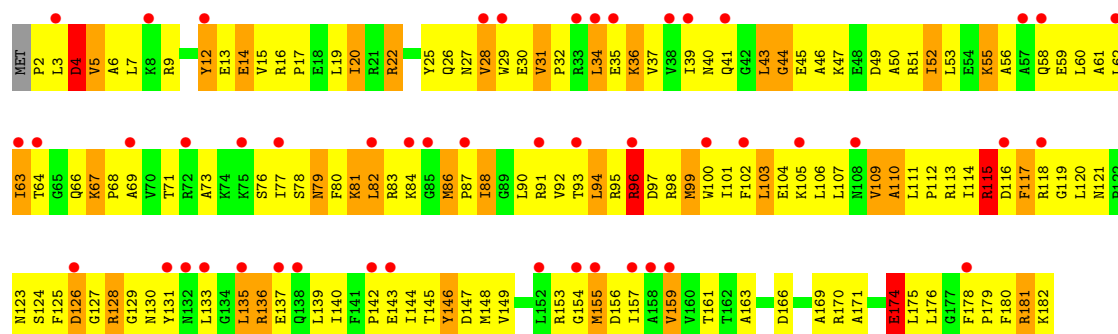


• Molecule 29: 50S ribosomal protein L4

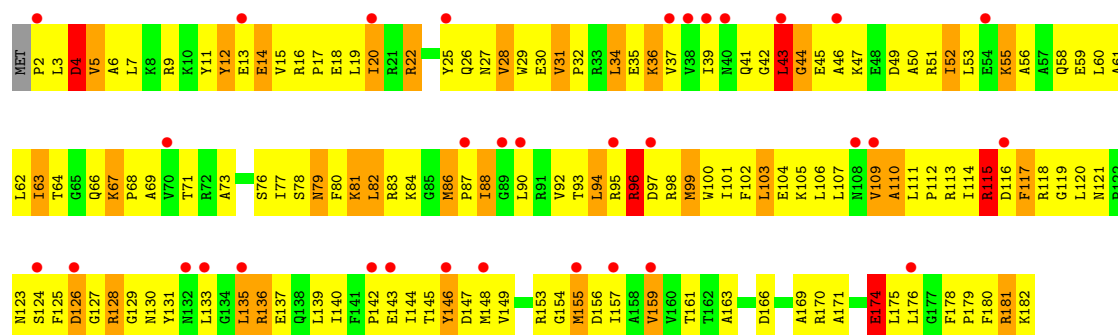


• Molecule 30: 50S ribosomal protein L5

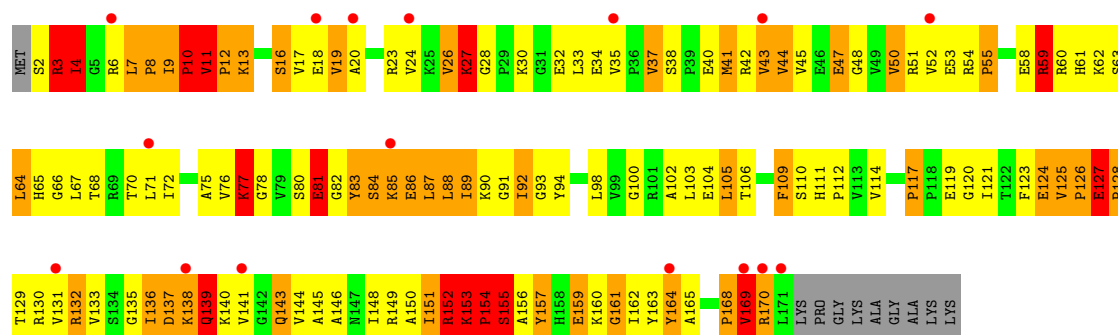
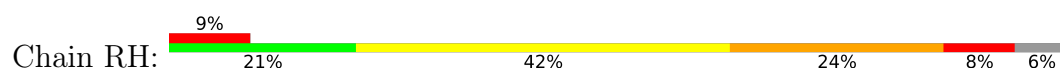




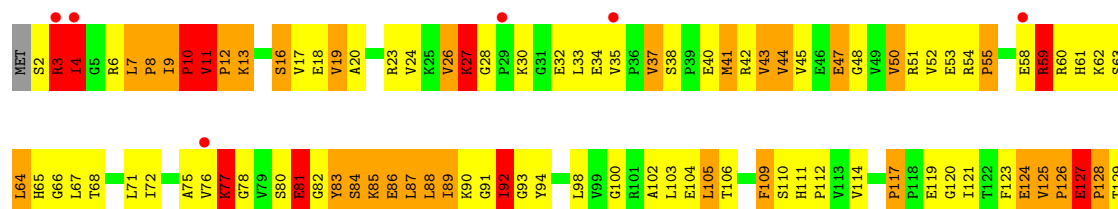
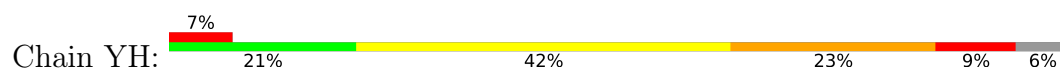
• Molecule 30: 50S ribosomal protein L5

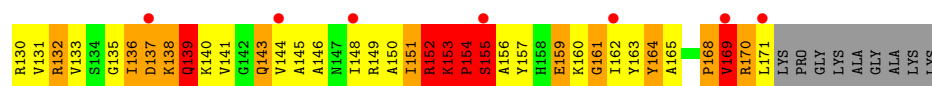


• Molecule 31: 50S ribosomal protein L6

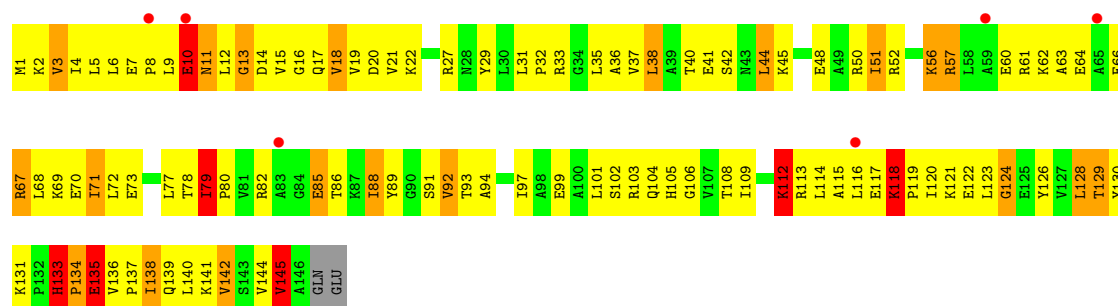


• Molecule 31: 50S ribosomal protein L6

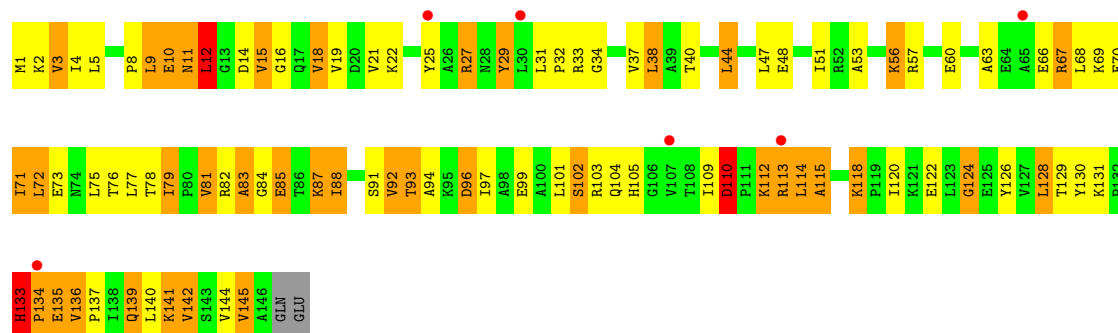




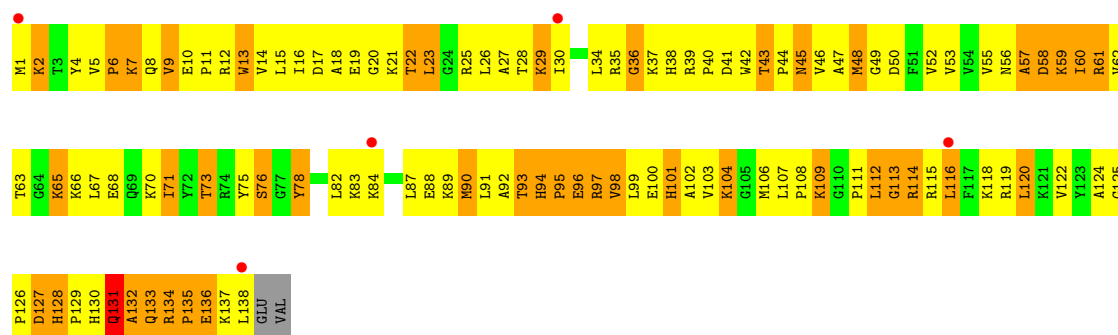
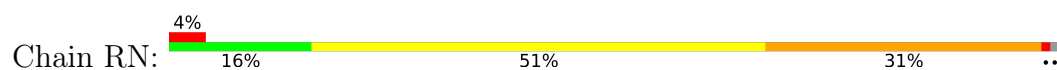
• Molecule 32: 50S ribosomal protein L9



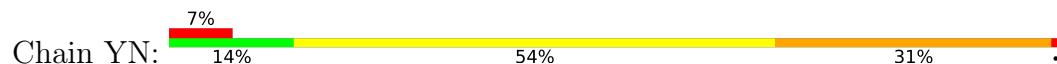
• Molecule 32: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L13

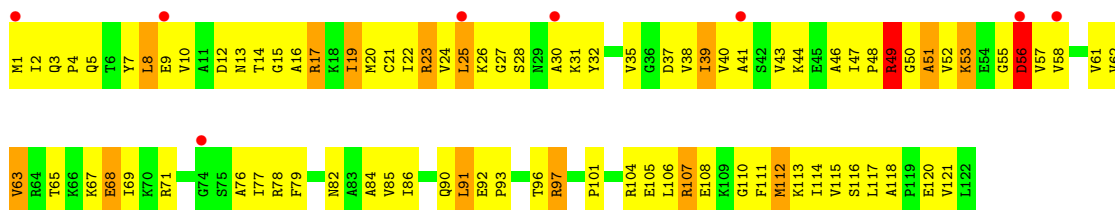


• Molecule 33: 50S ribosomal protein L13

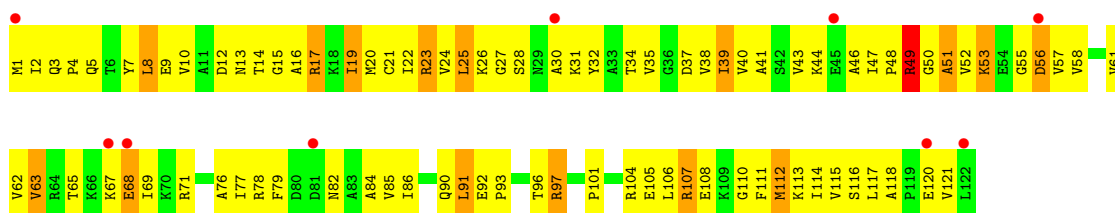




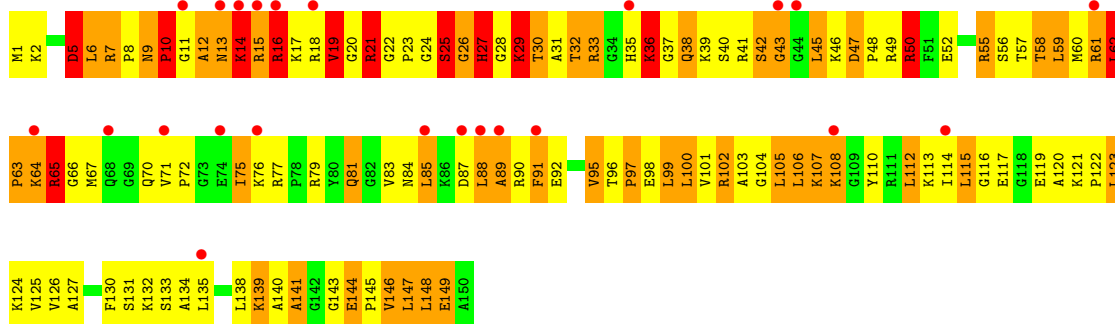
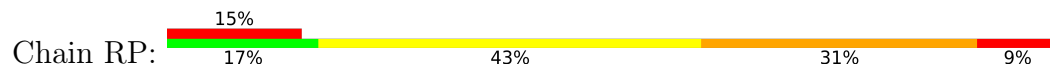
• Molecule 34: 50S ribosomal protein L14



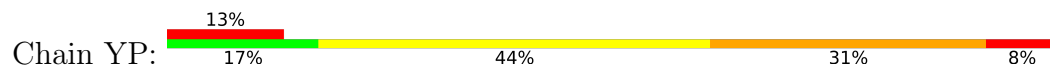
• Molecule 34: 50S ribosomal protein L14

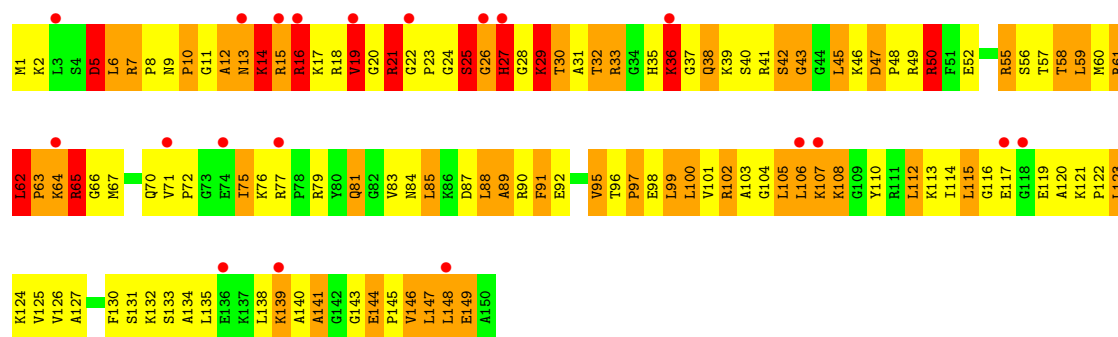


• Molecule 35: 50S ribosomal protein L15

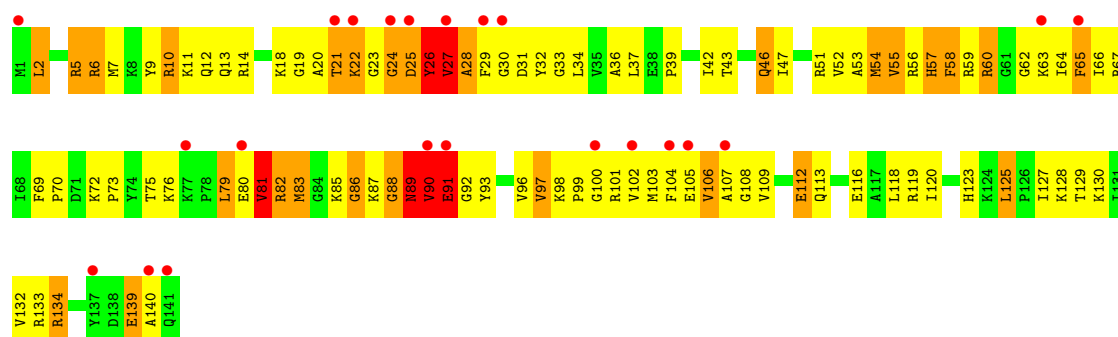


• Molecule 35: 50S ribosomal protein L15

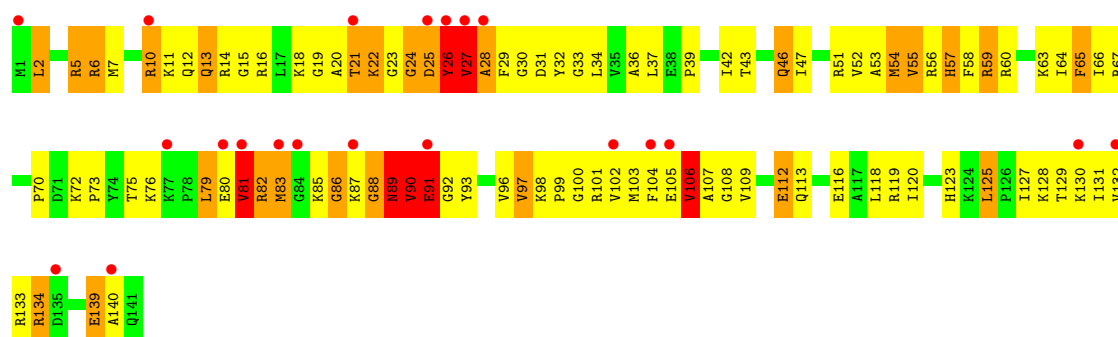




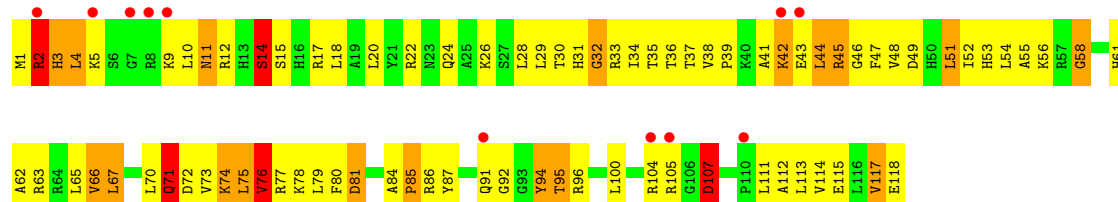
• Molecule 36: 50S ribosomal protein L16



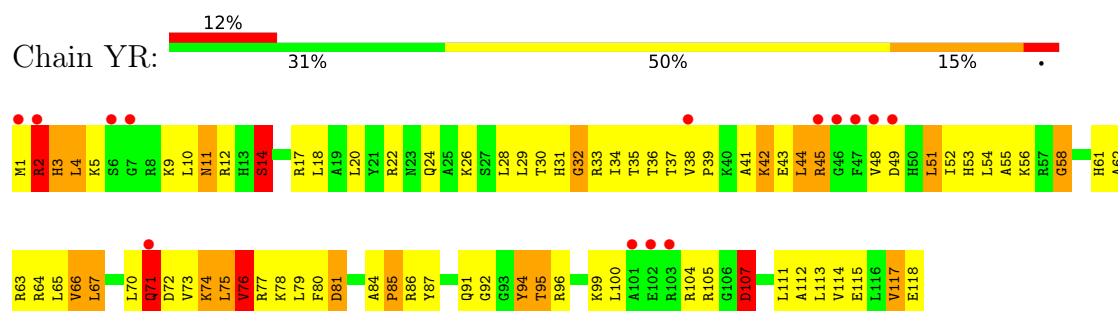
• Molecule 36: 50S ribosomal protein L16



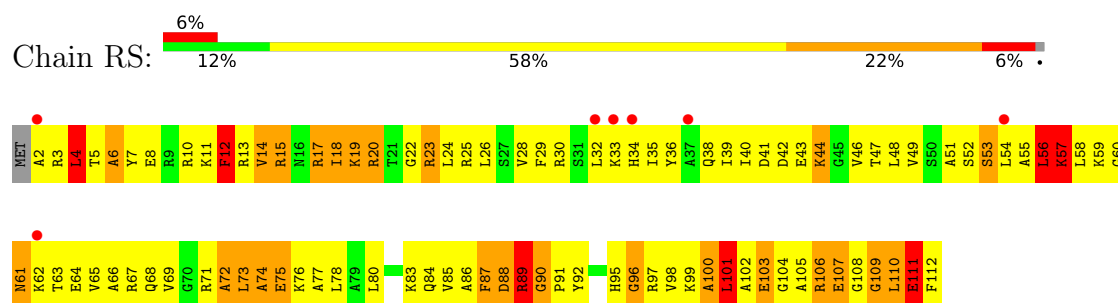
• Molecule 37: 50S ribosomal protein L17



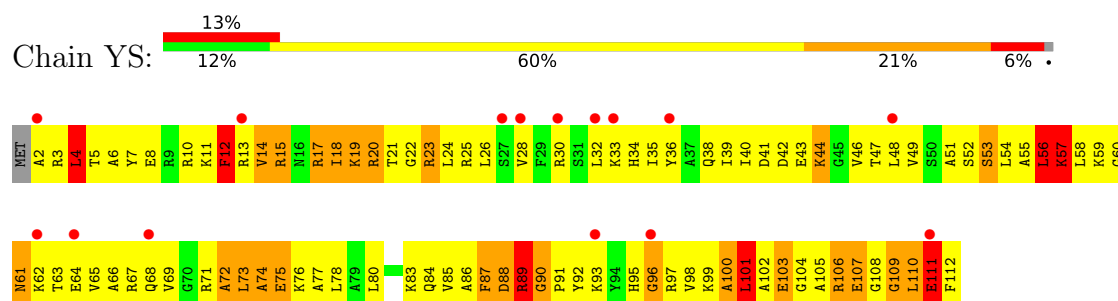
- Molecule 37: 50S ribosomal protein L17



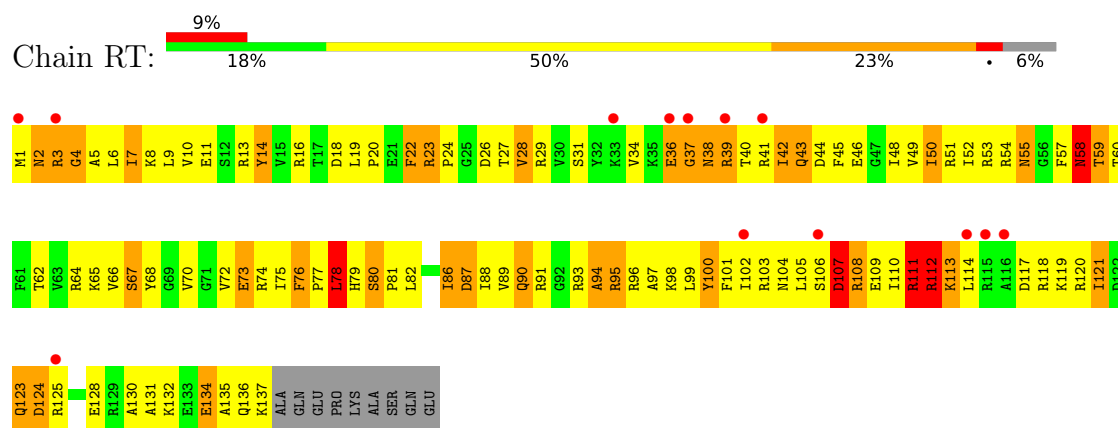
- Molecule 38: 50S ribosomal protein L18



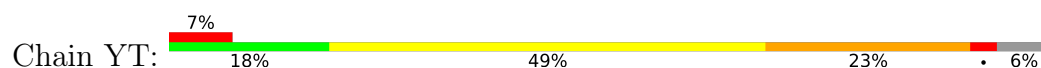
- Molecule 38: 50S ribosomal protein L18

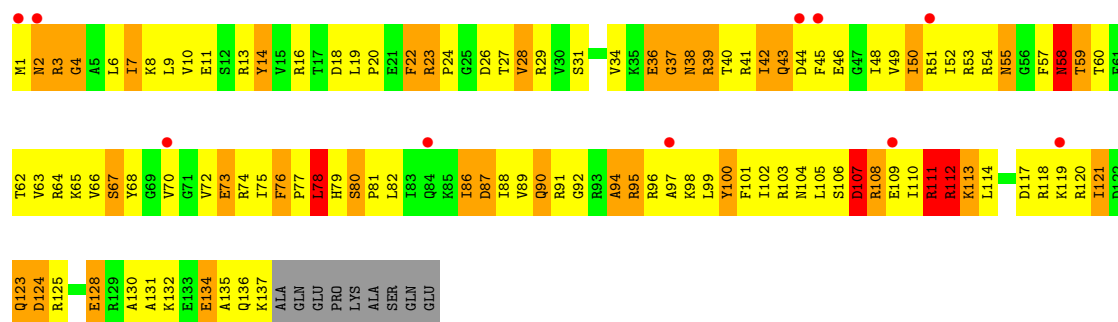


- Molecule 39: 50S ribosomal protein L19

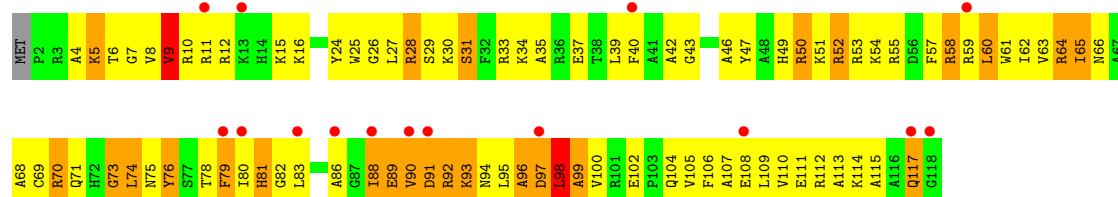


- Molecule 39: 50S ribosomal protein L19

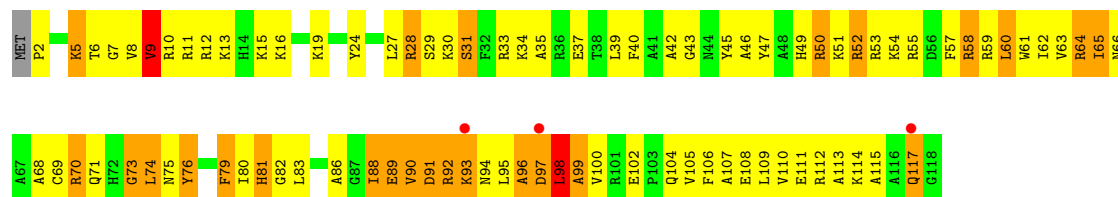




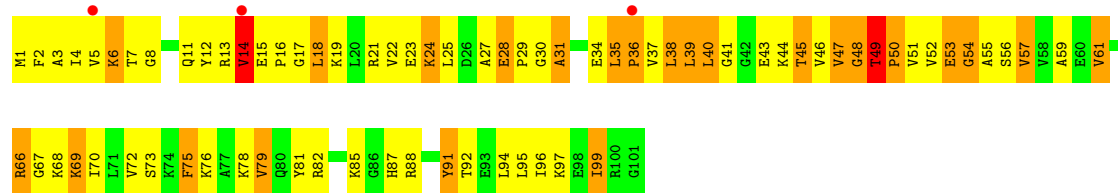
• Molecule 40: 50S ribosomal protein L20



• Molecule 40: 50S ribosomal protein L20

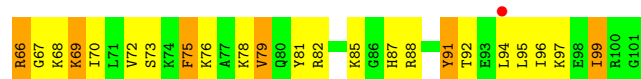


• Molecule 41: 50S ribosomal protein L21

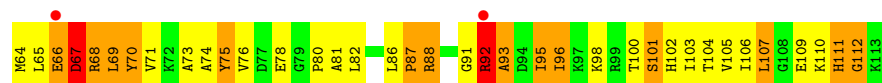
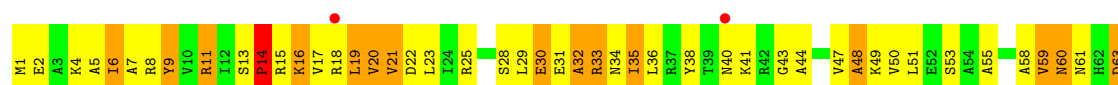


• Molecule 41: 50S ribosomal protein L21

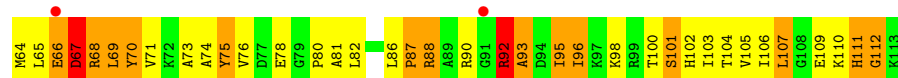




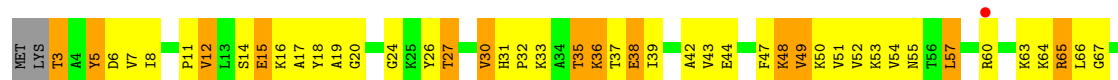
• Molecule 42: 50S ribosomal protein L22



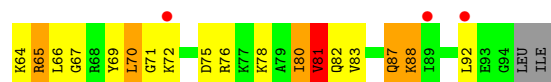
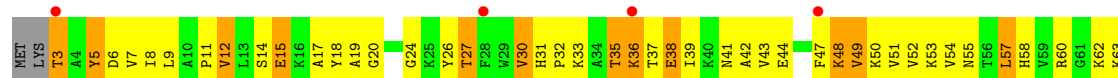
• Molecule 42: 50S ribosomal protein L22



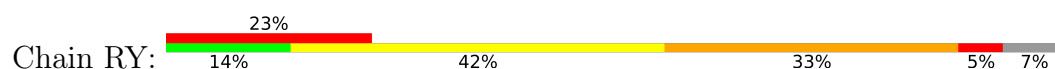
• Molecule 43: 50S ribosomal protein L23

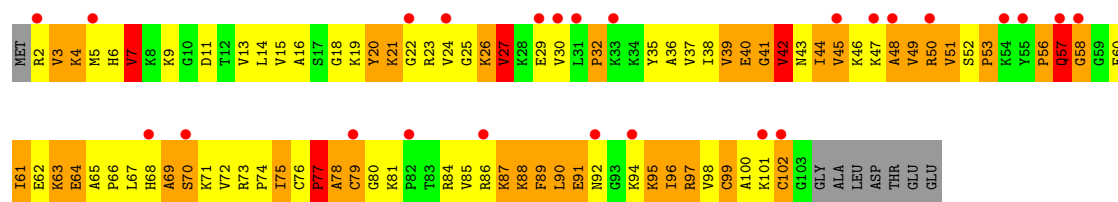


• Molecule 43: 50S ribosomal protein L23

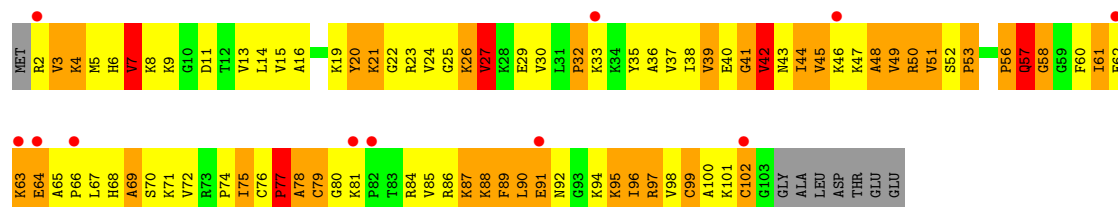
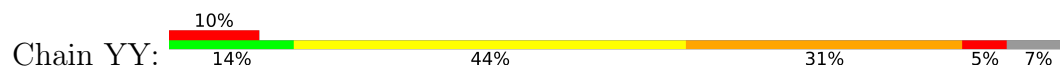


• Molecule 44: 50S ribosomal protein L24

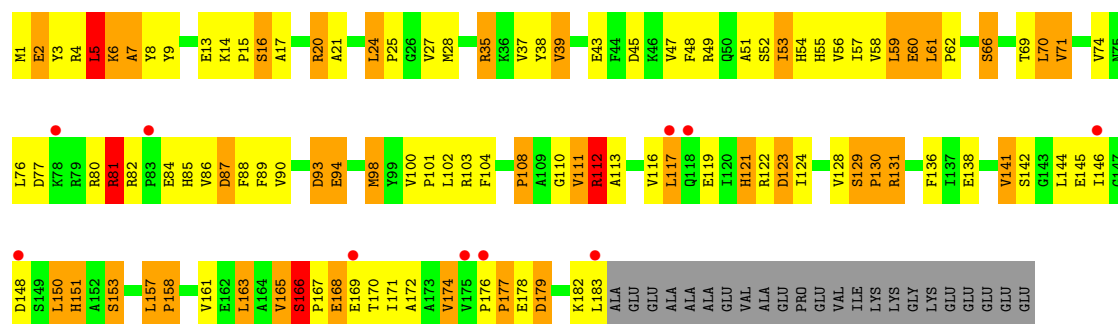




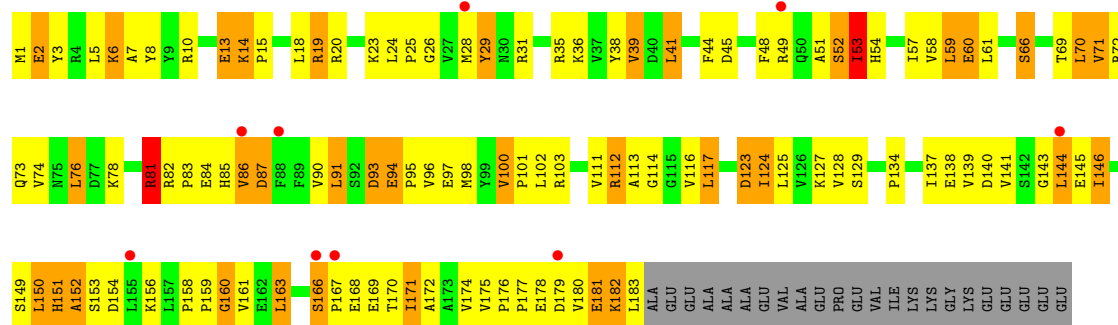
• Molecule 44: 50S ribosomal protein L24



• Molecule 45: 50S ribosomal protein L25

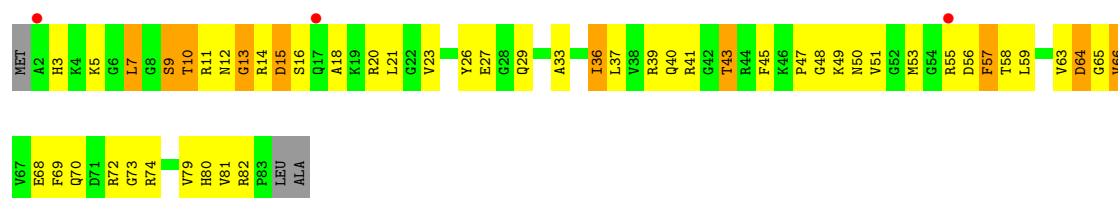


• Molecule 45: 50S ribosomal protein L25

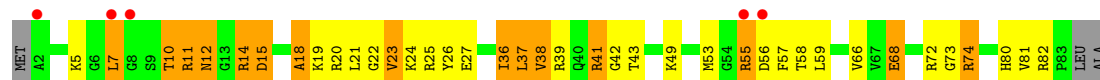


• Molecule 46: 50S ribosomal protein L27

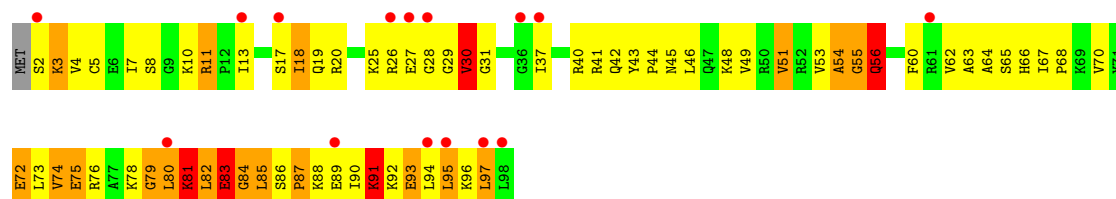




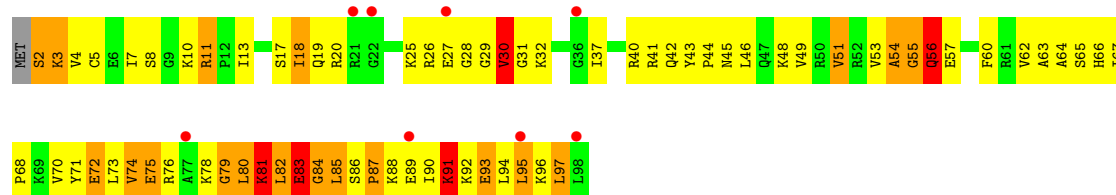
- Molecule 46: 50S ribosomal protein L27



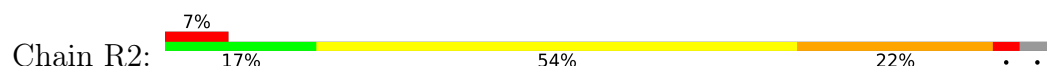
- Molecule 47: 50S ribosomal protein L28



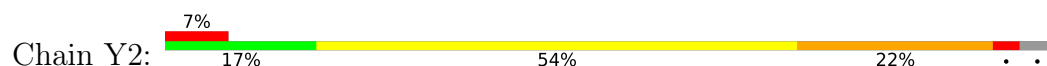
- Molecule 47: 50S ribosomal protein L28

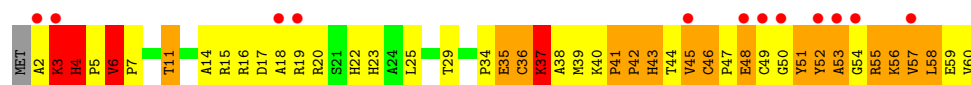


- Molecule 48: 50S ribosomal protein L29

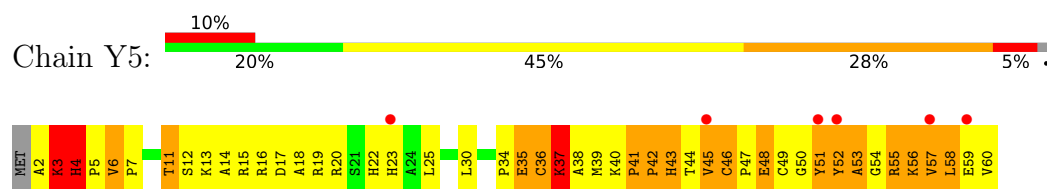


- Molecule 48: 50S ribosomal protein L29

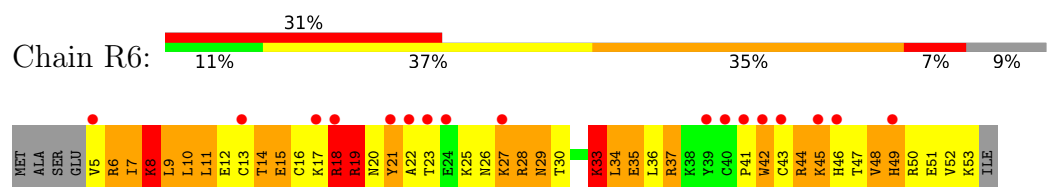




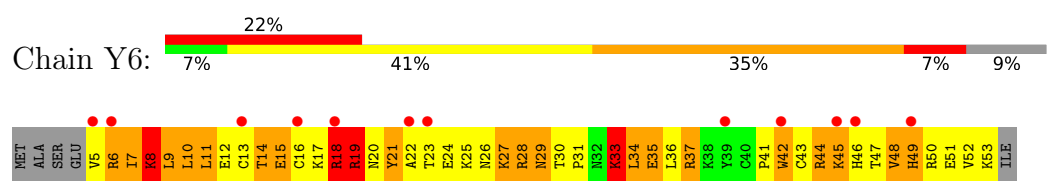
- Molecule 51: 50S ribosomal protein L32



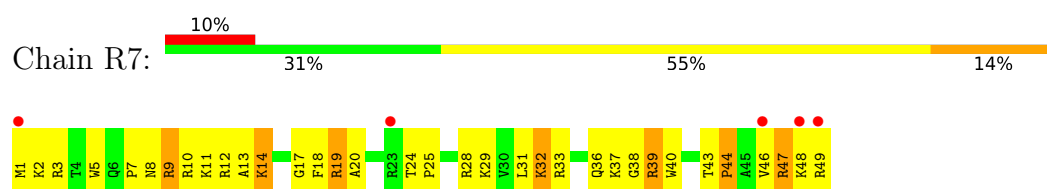
- Molecule 52: 50S ribosomal protein L33



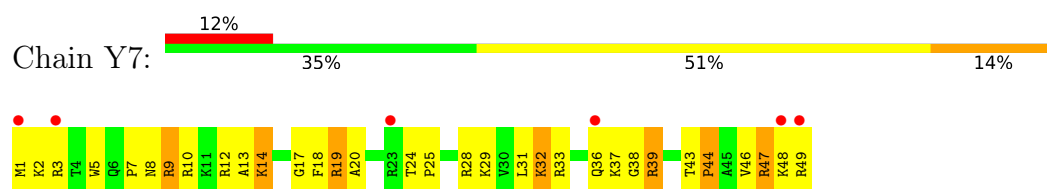
- Molecule 52: 50S ribosomal protein L33



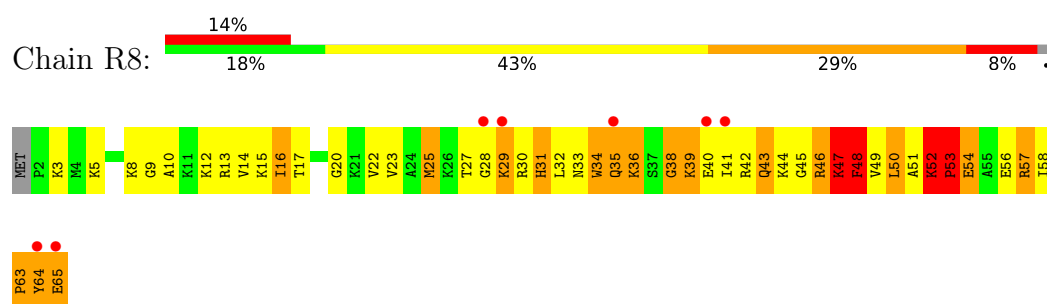
- Molecule 53: 50S ribosomal protein L34



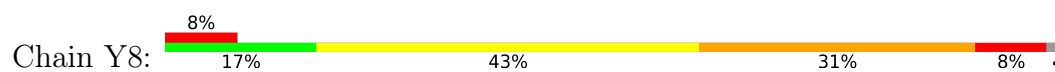
- Molecule 53: 50S ribosomal protein L34



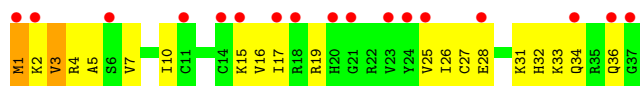
- Molecule 54: 50S ribosomal protein L35



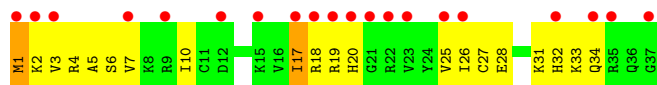
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.38Å 451.02Å 621.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 3.92 34.77 – 3.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.77-3.92) 99.6 (34.77-3.92)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.265 0.208 , 0.265	Depositor DCC
R_{free} test set	25594 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	291868	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, AMP, MG, 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	0.47	0/36098	0.72	18/56341 (0.0%)
1	XA	0.49	5/36101 (0.0%)	0.74	19/56346 (0.0%)
2	QB	0.42	0/1959	1.05	13/2642 (0.5%)
2	XB	0.42	0/1959	1.06	13/2642 (0.5%)
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	0.46	0/1171	1.01	8/1576 (0.5%)
5	XE	0.46	0/1171	1.01	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	0.42	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	1.06	5/1527 (0.3%)
9	QI	0.40	0/1029	1.02	8/1379 (0.6%)
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	0.47	0/900	1.04	6/1213 (0.5%)
12	QL	0.56	0/991	1.18	7/1327 (0.5%)
12	XL	0.62	1/991 (0.1%)	1.20	8/1327 (0.6%)
13	QM	0.43	0/974	1.05	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	0.99	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	0.42	0/847	1.07	7/1131 (0.6%)
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	6/1007 (0.6%)
20	XT	0.41	0/765	1.09	4/1007 (0.4%)
21	QU	0.42	0/221	1.01	1/288 (0.3%)
21	XU	0.42	0/221	1.01	1/288 (0.3%)
22	QV	0.34	1/1836 (0.1%)	0.44	0/2859
22	XV	0.34	1/1836 (0.1%)	0.43	0/2859
23	QX	0.38	0/185	0.64	0/285
23	XX	0.41	0/160	0.69	0/246
24	QY	0.36	0/311	0.46	0/483
24	XY	0.38	0/311	0.49	0/483
25	RA	0.55	1/69521 (0.0%)	0.79	31/108529 (0.0%)
25	YA	0.63	1/69543 (0.0%)	0.85	44/108563 (0.0%)
26	RB	0.45	0/2878	0.69	0/4490
26	YB	0.47	0/2878	0.74	0/4490
27	RD	0.79	2/2165 (0.1%)	1.30	35/2919 (1.2%)
27	YD	0.72	1/2165 (0.0%)	1.30	33/2919 (1.1%)
28	RE	0.62	0/1601	1.35	29/2160 (1.3%)
28	YE	0.62	0/1601	1.35	29/2160 (1.3%)
29	RF	0.62	0/1620	1.19	19/2194 (0.9%)
29	YF	0.62	0/1620	1.19	19/2194 (0.9%)
30	RG	0.47	0/1499	0.99	8/2016 (0.4%)
30	YG	0.47	0/1499	0.99	9/2016 (0.4%)
31	RH	0.58	0/1332	1.22	14/1802 (0.8%)
31	YH	0.57	0/1332	1.22	15/1802 (0.8%)
32	RI	0.64	0/1151	1.15	7/1558 (0.4%)
32	YI	0.62	0/1151	1.13	7/1558 (0.4%)
33	RN	0.55	0/1131	1.18	10/1525 (0.7%)
33	YN	0.54	0/1131	1.18	10/1525 (0.7%)
34	RO	0.65	0/943	1.03	5/1269 (0.4%)
34	YO	0.65	0/943	1.04	5/1269 (0.4%)
35	RP	0.63	0/1162	1.37	17/1544 (1.1%)
35	YP	0.63	1/1162 (0.1%)	1.37	17/1544 (1.1%)
36	RQ	0.71	0/1143	1.36	19/1527 (1.2%)
36	YQ	0.71	0/1143	1.35	19/1527 (1.2%)
37	RR	0.55	0/982	1.17	10/1312 (0.8%)
37	YR	0.55	0/982	1.17	10/1312 (0.8%)
38	RS	0.53	0/892	1.18	8/1187 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.52	0/892	1.18	8/1187 (0.7%)
39	RT	0.56	0/1155	1.18	16/1542 (1.0%)
39	YT	0.56	0/1155	1.18	17/1542 (1.1%)
40	RU	0.59	0/982	1.21	10/1306 (0.8%)
40	YU	0.59	0/982	1.21	10/1306 (0.8%)
41	RV	0.56	0/790	1.10	6/1057 (0.6%)
41	YV	0.55	0/790	1.10	6/1057 (0.6%)
42	RW	0.58	0/911	1.18	13/1220 (1.1%)
42	YW	0.57	0/911	1.18	13/1220 (1.1%)
43	RX	0.62	0/739	1.13	5/993 (0.5%)
43	YX	0.62	0/739	1.14	5/993 (0.5%)
44	RY	0.64	0/798	1.17	4/1064 (0.4%)
44	YY	0.64	0/798	1.16	3/1064 (0.3%)
45	RZ	0.60	1/1493 (0.1%)	1.06	7/2026 (0.3%)
45	YZ	0.60	0/1493	1.06	6/2026 (0.3%)
46	R0	0.67	0/657	1.06	2/874 (0.2%)
46	Y0	0.71	0/657	1.15	3/874 (0.3%)
47	R1	0.58	0/770	1.20	9/1022 (0.9%)
47	Y1	0.58	0/770	1.20	9/1022 (0.9%)
48	R2	0.60	0/583	1.32	9/771 (1.2%)
48	Y2	0.60	0/583	1.32	9/771 (1.2%)
49	R3	0.62	1/474 (0.2%)	1.04	0/635
49	Y3	0.53	0/474	1.04	0/635
50	R4	0.47	0/594	1.24	10/795 (1.3%)
50	Y4	0.47	0/594	1.23	10/795 (1.3%)
51	R5	0.65	0/473	1.22	6/639 (0.9%)
51	Y5	0.65	0/473	1.21	7/639 (1.1%)
52	R6	0.53	0/431	1.06	3/575 (0.5%)
52	Y6	0.53	0/431	1.06	3/575 (0.5%)
53	R7	0.73	0/438	1.19	2/575 (0.3%)
53	Y7	0.73	0/438	1.19	2/575 (0.3%)
54	R8	0.79	0/525	1.41	9/691 (1.3%)
54	Y8	0.79	0/525	1.41	9/691 (1.3%)
55	R9	0.42	0/310	0.92	1/407 (0.2%)
55	Y9	0.44	0/310	0.92	1/407 (0.2%)
56	Z6	0.46	0/40	0.62	0/60
56	Z8	0.46	0/40	0.63	0/60
All	All	0.55	17/316298 (0.0%)	0.89	921/472872 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
45	YZ	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	RD	236	GLY	C-N	14.29	1.53	1.33
1	XA	1201	A	C3'-C2'	8.85	1.66	1.52
1	XA	1054	C	C4'-C3'	8.36	1.65	1.53
1	XA	1054	C	C2'-O2'	7.37	1.52	1.41
22	QV	1	C	OP3-P	6.57	1.61	1.48

The worst 5 of 921 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RP	59	LEU	N-CA-C	-14.61	91.40	111.56
35	YP	59	LEU	N-CA-C	-14.61	91.40	111.56
50	Y4	39	CYS	N-CA-C	-13.55	96.00	112.54
50	R4	39	CYS	N-CA-C	-13.53	96.04	112.54
28	YE	58	ARG	N-CA-C	-11.81	95.23	113.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	YZ	181	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	1130	0
1	XA	32249	0	16279	1069	1
2	QB	1924	0	1975	306	0
2	XB	1924	0	1975	306	0
3	QC	1605	0	1668	211	0
3	XC	1605	0	1668	215	0
4	QD	1703	0	1764	266	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1703	0	1765	232	0
5	QE	1155	0	1213	198	0
5	XE	1155	0	1213	159	0
6	QF	843	0	857	102	0
6	XF	843	0	857	107	0
7	QG	1257	0	1296	159	0
7	XG	1257	0	1294	151	0
8	QH	1116	0	1175	176	0
8	XH	1116	0	1177	158	0
9	QI	1010	0	1037	151	0
9	XI	1010	0	1037	157	0
10	QJ	801	0	849	151	0
10	XJ	801	0	849	134	0
11	QK	885	0	904	110	0
11	XK	885	0	904	109	0
12	QL	975	0	1062	102	0
12	XL	975	0	1062	117	0
13	QM	964	0	1034	176	0
13	XM	964	0	1034	172	0
14	QN	492	0	530	106	0
14	XN	492	0	530	103	0
15	QO	734	0	771	83	0
15	XO	734	0	771	86	0
16	QP	705	0	725	125	0
16	XP	705	0	725	118	0
17	QQ	834	0	904	87	0
17	XQ	834	0	904	83	0
18	QR	574	0	644	74	0
18	XR	574	0	644	72	0
19	QS	674	0	699	115	0
19	XS	674	0	699	137	0
20	QT	763	0	860	115	0
20	XT	763	0	861	119	0
21	QU	217	0	234	31	0
21	XU	217	0	234	27	0
22	QV	1644	0	836	44	0
22	XV	1644	0	836	29	0
23	QX	167	0	87	13	0
23	XX	145	0	75	10	0
24	QY	303	0	154	10	0
24	XY	303	0	154	11	0
25	RA	62071	0	31285	1929	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	YA	62091	0	31293	1983	0
26	RB	2573	0	1306	121	0
26	YB	2573	0	1306	101	0
27	RD	2115	0	2195	331	0
27	YD	2115	0	2195	337	0
28	RE	1568	0	1634	282	0
28	YE	1568	0	1634	277	0
29	RF	1585	0	1632	194	0
29	YF	1585	0	1632	196	0
30	RG	1474	0	1535	214	0
30	YG	1474	0	1535	207	0
31	RH	1307	0	1382	232	0
31	YH	1307	0	1382	234	0
32	RI	1136	0	1223	82	1
32	YI	1136	0	1223	72	0
33	RN	1104	0	1180	208	0
33	YN	1104	0	1180	198	0
34	RO	933	0	996	135	0
34	YO	933	0	996	134	0
35	RP	1145	0	1228	265	0
35	YP	1145	0	1228	254	0
36	RQ	1122	0	1179	164	0
36	YQ	1122	0	1178	173	0
37	RR	968	0	1033	120	0
37	YR	968	0	1033	120	0
38	RS	882	0	943	170	0
38	YS	882	0	943	163	0
39	RT	1141	0	1202	156	0
39	YT	1141	0	1202	161	0
40	RU	964	0	1022	144	0
40	YU	964	0	1022	153	0
41	RV	779	0	852	137	0
41	YV	779	0	852	136	0
42	RW	900	0	964	103	0
42	YW	900	0	964	111	0
43	RX	725	0	778	72	0
43	YX	725	0	778	75	0
44	RY	785	0	878	175	0
44	YY	785	0	878	168	0
45	RZ	1461	0	1493	85	0
45	YZ	1461	0	1493	88	0
46	R0	648	0	671	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Y0	648	0	672	51	0
47	R1	763	0	848	148	0
47	Y1	763	0	848	146	0
48	R2	581	0	629	87	0
48	Y2	581	0	629	81	0
49	R3	469	0	518	44	0
49	Y3	469	0	518	47	0
50	R4	581	0	574	164	0
50	Y4	581	0	574	172	0
51	R5	459	0	480	75	0
51	Y5	459	0	480	78	0
52	R6	424	0	450	91	0
52	Y6	424	0	450	97	0
53	R7	430	0	480	43	0
53	Y7	430	0	480	41	0
54	R8	517	0	582	106	0
54	Y8	517	0	582	108	0
55	R9	307	0	335	28	0
55	Y9	307	0	336	28	0
56	Z6	74	0	51	10	0
56	Z8	74	0	51	10	0
57	QA	64	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	239	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	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	72	0	0	1	0
57	XB	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	269	0	0	1	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	1	0	0	0	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	R9	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y9	1	0	0	0	0
59	XX	22	0	12	1	0
All	All	291868	0	198240	18456	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 18456 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)
14:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.54
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.02	0.18

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%)	49 (24%)	22 (11%)	0	6
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	8
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	10
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	0	10
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	8
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	0	10
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	10
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	7
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	12
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	14
12	QL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	0	4
12	XL	123/132 (93%)	83 (68%)	24 (20%)	16 (13%)	0	3
13	QM	119/126 (94%)	71 (60%)	29 (24%)	19 (16%)	0	3
13	XM	119/126 (94%)	72 (60%)	25 (21%)	22 (18%)	0	2
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	1
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	14
15	XO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	14
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
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%)	46 (68%)	14 (21%)	8 (12%)	0	5
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	5
19	QS	82/93 (88%)	46 (56%)	18 (22%)	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%)	16 (70%)	3 (13%)	4 (17%)	0	2
21	XU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	2
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	14
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	14
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	8
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	8
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	5
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	5
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	99 (69%)	32 (22%)	13 (9%)	0	10
32	YI	144/148 (97%)	93 (65%)	30 (21%)	21 (15%)	0	3
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	13
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	8
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	8
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	2
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	2
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	3
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	3
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	12
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	12
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	8
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	8
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1	17
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1	17
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	1
44	YY	100/110 (91%)	57 (57%)	16 (16%)	27 (27%)	0	1
45	RZ	181/206 (88%)	113 (62%)	46 (25%)	22 (12%)	0	4
45	YZ	181/206 (88%)	128 (71%)	36 (20%)	17 (9%)	0	9
46	R0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	1	18
46	Y0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	1	18
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
48	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	3
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	3
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1	18
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1	18
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	15
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	15
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7621 (66%)	2356 (20%)	1493 (13%)	0	3

5 of 1493 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%)	182 (89%)	23 (11%)	6	23
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	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	180/181 (99%)	162 (90%)	18 (10%)	7	27
5	QE	116/123 (94%)	105 (90%)	11 (10%)	8	28
5	XE	116/123 (94%)	105 (90%)	11 (10%)	8	28
6	QF	90/90 (100%)	77 (86%)	13 (14%)	3	17
6	XF	90/90 (100%)	77 (86%)	13 (14%)	3	17
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%)	104 (87%)	15 (13%)	4	20
9	QI	98/99 (99%)	85 (87%)	13 (13%)	4	18
9	XI	98/99 (99%)	85 (87%)	13 (13%)	4	18
10	QJ	89/92 (97%)	80 (90%)	9 (10%)	7	26
10	XJ	89/92 (97%)	80 (90%)	9 (10%)	7	26
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%)	87 (84%)	17 (16%)	2	14
12	XL	104/109 (95%)	84 (81%)	20 (19%)	1	10
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	25
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	28
17	XQ	95/97 (98%)	86 (90%)	9 (10%)	8	28
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
27	RD	214/218 (98%)	174 (81%)	40 (19%)	1	10
27	YD	214/218 (98%)	174 (81%)	40 (19%)	1	10
28	RE	165/166 (99%)	125 (76%)	40 (24%)	1	5
28	YE	165/166 (99%)	125 (76%)	40 (24%)	1	5
29	RF	161/166 (97%)	138 (86%)	23 (14%)	3	17
29	YF	161/166 (97%)	138 (86%)	23 (14%)	3	17
30	RG	155/156 (99%)	133 (86%)	22 (14%)	3	17
30	YG	155/156 (99%)	134 (86%)	21 (14%)	4	18
31	RH	142/148 (96%)	111 (78%)	31 (22%)	1	6
31	YH	142/148 (96%)	111 (78%)	31 (22%)	1	6
32	RI	122/124 (98%)	88 (72%)	34 (28%)	0	3
32	YI	122/124 (98%)	93 (76%)	29 (24%)	1	5
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	13
33	YN	117/119 (98%)	97 (83%)	20 (17%)	2	13
34	RO	100/100 (100%)	88 (88%)	12 (12%)	5	21
34	YO	100/100 (100%)	89 (89%)	11 (11%)	6	23
35	RP	116/116 (100%)	88 (76%)	28 (24%)	1	5
35	YP	116/116 (100%)	88 (76%)	28 (24%)	1	5
36	RQ	111/111 (100%)	96 (86%)	15 (14%)	4	18
36	YQ	111/111 (100%)	96 (86%)	15 (14%)	4	18
37	RR	101/101 (100%)	85 (84%)	16 (16%)	2	15
37	YR	101/101 (100%)	85 (84%)	16 (16%)	2	15
38	RS	87/88 (99%)	73 (84%)	14 (16%)	2	14
38	YS	87/88 (99%)	73 (84%)	14 (16%)	2	14
39	RT	120/127 (94%)	99 (82%)	21 (18%)	2	12
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	12
40	RU	93/94 (99%)	81 (87%)	12 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YU	93/94 (99%)	81 (87%)	12 (13%)	4	19
41	RV	82/82 (100%)	67 (82%)	15 (18%)	2	11
41	YV	82/82 (100%)	67 (82%)	15 (18%)	2	11
42	RW	92/92 (100%)	76 (83%)	16 (17%)	2	12
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	12
43	RX	74/78 (95%)	61 (82%)	13 (18%)	2	12
43	YX	74/78 (95%)	61 (82%)	13 (18%)	2	12
44	RY	85/91 (93%)	67 (79%)	18 (21%)	1	7
44	YY	85/91 (93%)	66 (78%)	19 (22%)	1	6
45	RZ	162/179 (90%)	126 (78%)	36 (22%)	1	6
45	YZ	162/179 (90%)	127 (78%)	35 (22%)	1	6
46	R0	65/67 (97%)	58 (89%)	7 (11%)	6	24
46	Y0	65/67 (97%)	57 (88%)	8 (12%)	4	20
47	R1	82/83 (99%)	70 (85%)	12 (15%)	3	16
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	16
48	R2	64/67 (96%)	56 (88%)	8 (12%)	4	20
48	Y2	64/67 (96%)	56 (88%)	8 (12%)	4	20
49	R3	51/52 (98%)	41 (80%)	10 (20%)	1	9
49	Y3	51/52 (98%)	41 (80%)	10 (20%)	1	9
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0	3
50	Y4	63/63 (100%)	46 (73%)	17 (27%)	0	3
51	R5	51/52 (98%)	40 (78%)	11 (22%)	1	6
51	Y5	51/52 (98%)	40 (78%)	11 (22%)	1	6
52	R6	48/52 (92%)	36 (75%)	12 (25%)	0	4
52	Y6	48/52 (92%)	36 (75%)	12 (25%)	0	4
53	R7	42/42 (100%)	38 (90%)	4 (10%)	8	28
53	Y7	42/42 (100%)	38 (90%)	4 (10%)	8	28
54	R8	54/55 (98%)	41 (76%)	13 (24%)	1	5
54	Y8	54/55 (98%)	40 (74%)	14 (26%)	0	4
55	R9	34/34 (100%)	32 (94%)	2 (6%)	18	43
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9702/10066 (96%)	8187 (84%)	1515 (16%)	2 15

5 of 1515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	XM	8	GLU
31	YH	143	GLN
16	XP	11	SER
13	XM	3	ARG
28	YE	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
32	YI	43	ASN
48	Y2	46	GLN
33	YN	131	GLN
41	YV	11	GLN
52	Y6	32	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	387 (25%)	49 (3%)
1	XA	1498/1522 (98%)	379 (25%)	60 (4%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	5 (71%)	1 (14%)
23	XX	6/25 (24%)	3 (50%)	0
24	QY	13/18 (72%)	5 (38%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2879/2916 (98%)	838 (29%)	82 (2%)
25	YA	2880/2916 (98%)	873 (30%)	93 (3%)
26	RB	119/122 (97%)	32 (26%)	3 (2%)
26	YB	119/122 (97%)	42 (35%)	2 (1%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9186/9366 (98%)	2629 (28%)	294 (3%)

5 of 2629 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	7	G
1	QA	9	G
1	QA	10	A
1	QA	22	G
1	QA	32	A

5 of 294 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	961	C
25	YA	2751	G
25	YA	1045	A
25	YA	1899	G
25	RA	1265	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	PPU	Z8	76	56,25	37,40,41	2.57	8 (21%)	47,57,60	2.56	15 (31%)
56	PPU	Z6	76	56,25	37,40,41	2.58	8 (21%)	47,57,60	2.57	15 (31%)
24	1MG	QY	37	24	23,26,27	2.64	4 (17%)	33,39,42	2.01	8 (24%)
24	1MG	XY	37	24	23,26,27	2.64	4 (17%)	33,39,42	2.03	9 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z8	76	56,25	-	2/25/43/44	0/4/4/4
56	PPU	Z6	76	56,25	-	2/25/43/44	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	QY	37	24	-	0/7/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/7/25/26	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.58	1.41	1.23
56	Z8	76	PPU	O-C	9.54	1.41	1.23
24	XY	37	1MG	C2-N2	8.11	1.48	1.34
24	QY	37	1MG	C2-N2	8.06	1.48	1.34
24	XY	37	1MG	C4-N3	6.58	1.49	1.34

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.57	110.17	123.20
56	Z8	76	PPU	C3'-N3'-C	-8.55	110.20	123.20
24	QY	37	1MG	N2-C2-N1	6.16	123.73	118.79
24	XY	37	1MG	N2-C2-N1	6.16	123.73	118.79
56	Z8	76	PPU	C2'-C1'-N9	-6.00	98.40	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 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	10	0
56	Z6	76	PPU	7	0
24	QY	37	1MG	1	0
24	XY	37	1MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 681 ligands modelled in this entry, 680 are monoatomic - leaving 1 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	$\# Z > 2$
59	AMP	XX	101	-	21,24,25	1.11	3 (14%)	30,35,38	0.78	1 (3%)

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
59	AMP	XX	101	-	-	1/7/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	XX	101	AMP	C1'-N9	3.52	1.56	1.46
59	XX	101	AMP	C5-C6	2.15	1.47	1.41
59	XX	101	AMP	C6-N6	2.11	1.39	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	XX	101	AMP	C4-N9-C1'	2.42	132.29	126.63

There are no chirality outliers.

All (1) torsion outliers are listed below:

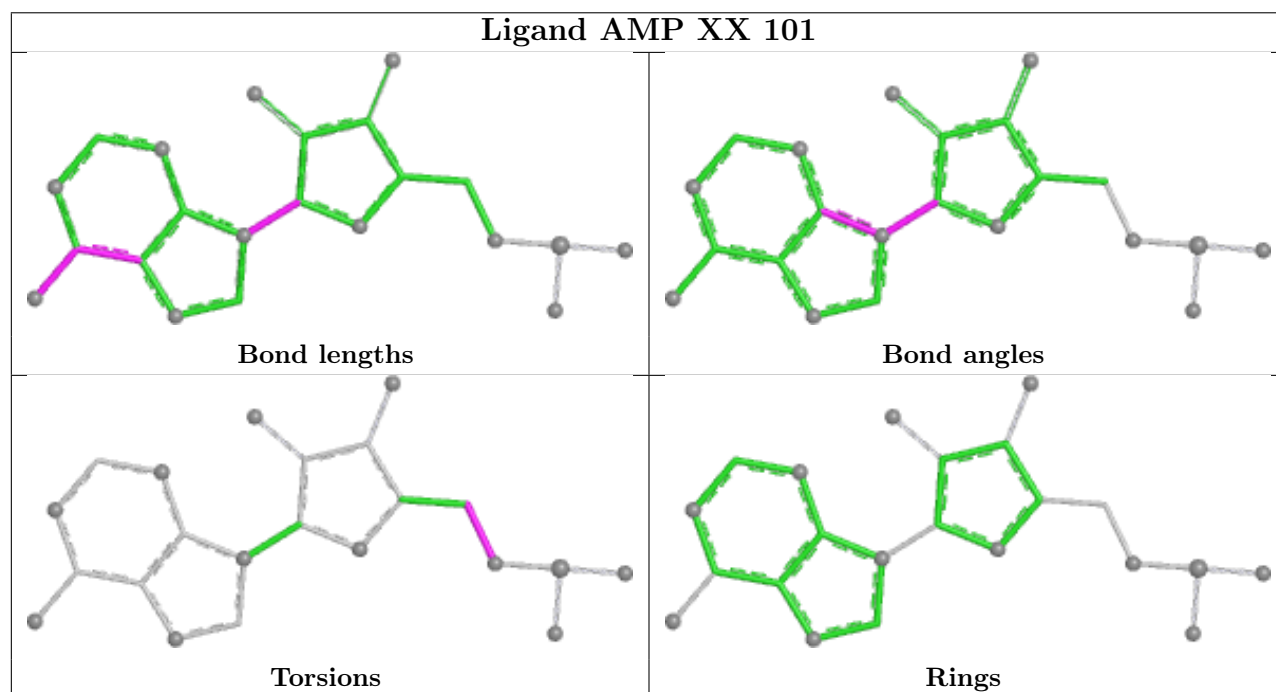
Mol	Chain	Res	Type	Atoms
59	XX	101	AMP	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	XX	101	AMP	1	0

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.20	61 (4%)	41	31	3, 59, 153, 236	0
1	XA	1500/1522 (98%)	0.19	68 (4%)	38	29	1, 53, 148, 240	0
2	QB	237/256 (92%)	0.85	29 (12%)	8	11	41, 113, 151, 177	0
2	XB	237/256 (92%)	0.46	12 (5%)	33	26	21, 96, 142, 157	0
3	QC	205/239 (85%)	0.74	21 (10%)	12	14	22, 104, 139, 161	0
3	XC	205/239 (85%)	0.29	12 (5%)	28	24	22, 79, 122, 161	0
4	QD	208/209 (99%)	0.68	18 (8%)	16	16	8, 69, 116, 153	0
4	XD	208/209 (99%)	0.64	22 (10%)	11	13	16, 74, 114, 158	0
5	QE	151/162 (93%)	1.36	43 (28%)	1	3	32, 95, 133, 161	0
5	XE	151/162 (93%)	0.57	16 (10%)	11	13	20, 63, 108, 140	0
6	QF	101/101 (100%)	0.50	6 (5%)	28	24	15, 68, 105, 139	0
6	XF	101/101 (100%)	0.49	3 (2%)	52	37	4, 66, 107, 134	0
7	QG	155/156 (99%)	0.58	10 (6%)	25	21	26, 89, 133, 154	0
7	XG	155/156 (99%)	0.47	12 (7%)	19	18	28, 83, 124, 148	0
8	QH	138/138 (100%)	0.77	14 (10%)	12	14	21, 79, 122, 132	0
8	XH	138/138 (100%)	0.69	14 (10%)	12	14	14, 68, 108, 133	0
9	QI	127/128 (99%)	0.79	10 (7%)	18	18	49, 102, 138, 161	0
9	XI	127/128 (99%)	0.79	14 (11%)	10	13	13, 91, 134, 162	0
10	QJ	99/105 (94%)	1.29	22 (22%)	2	4	57, 108, 148, 192	0
10	XJ	99/105 (94%)	0.96	15 (15%)	5	8	40, 94, 140, 165	0
11	QK	119/129 (92%)	0.70	12 (10%)	12	14	25, 72, 127, 150	0
11	XK	119/129 (92%)	0.43	5 (4%)	40	30	4, 59, 109, 129	0
12	QL	125/132 (94%)	0.99	19 (15%)	5	8	15, 64, 124, 159	0
12	XL	125/132 (94%)	0.57	8 (6%)	25	22	6, 48, 102, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.84	18 (14%) 5 8	48, 101, 151, 159	0
13	XM	121/126 (96%)	0.66	12 (9%) 13 14	38, 85, 119, 158	0
14	QN	60/61 (98%)	1.05	11 (18%) 3 6	52, 108, 148, 159	0
14	XN	60/61 (98%)	0.65	5 (8%) 17 17	33, 72, 116, 130	0
15	QO	88/89 (98%)	0.45	5 (5%) 29 24	17, 71, 119, 151	0
15	XO	88/89 (98%)	0.31	2 (2%) 61 43	7, 59, 102, 127	0
16	QP	84/88 (95%)	0.91	13 (15%) 5 8	14, 59, 114, 134	0
16	XP	84/88 (95%)	0.75	9 (10%) 11 13	28, 68, 122, 176	0
17	QQ	100/105 (95%)	1.07	16 (16%) 5 8	30, 70, 116, 148	0
17	XQ	100/105 (95%)	0.93	14 (14%) 6 9	19, 71, 106, 144	0
18	QR	70/88 (79%)	0.47	4 (5%) 29 24	22, 70, 125, 150	0
18	XR	70/88 (79%)	0.59	8 (11%) 10 12	9, 65, 106, 140	0
19	QS	84/93 (90%)	0.87	13 (15%) 5 8	69, 116, 148, 161	0
19	XS	84/93 (90%)	0.58	5 (5%) 27 23	48, 87, 132, 145	0
20	QT	99/106 (93%)	0.93	16 (16%) 4 7	16, 73, 113, 135	0
20	XT	99/106 (93%)	1.04	16 (16%) 4 7	23, 77, 124, 157	0
21	QU	25/27 (92%)	1.86	12 (48%) 0 1	31, 92, 141, 158	0
21	XU	25/27 (92%)	1.44	9 (36%) 1 2	32, 83, 121, 143	0
22	QV	77/77 (100%)	0.78	4 (5%) 33 26	21, 85, 147, 180	0
22	XV	77/77 (100%)	0.52	5 (6%) 25 21	6, 64, 119, 169	0
23	QX	8/25 (32%)	1.28	3 (37%) 1 2	50, 74, 138, 138	0
23	XX	7/25 (28%)	0.96	0 100 100	18, 51, 81, 90	0
24	QY	13/18 (72%)	1.60	4 (30%) 1 3	106, 175, 223, 238	0
24	XY	13/18 (72%)	1.39	3 (23%) 2 4	55, 149, 189, 217	0
25	RA	2882/2916 (98%)	-0.03	100 (3%) 47 33	0, 30, 174, 252	0
25	YA	2883/2916 (98%)	-0.05	101 (3%) 47 33	0, 20, 159, 242	0
26	RB	120/122 (98%)	0.30	3 (2%) 58 41	39, 82, 133, 170	0
26	YB	120/122 (98%)	0.18	4 (3%) 49 34	16, 68, 104, 146	0
27	RD	272/276 (98%)	0.67	37 (13%) 7 10	0, 34, 82, 147	0
27	YD	272/276 (98%)	0.45	17 (6%) 26 22	0, 18, 64, 125	0
28	RE	205/206 (99%)	0.68	18 (8%) 15 16	1, 49, 112, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.61	17 (8%) 17 17	0, 47, 104, 155	0
29	RF	202/210 (96%)	0.69	19 (9%) 14 16	0, 55, 108, 143	0
29	YF	202/210 (96%)	0.44	12 (5%) 28 24	0, 32, 96, 124	0
30	RG	181/182 (99%)	1.43	49 (27%) 1 3	39, 113, 160, 177	0
30	YG	181/182 (99%)	1.15	33 (18%) 3 6	18, 92, 131, 177	0
31	RH	170/180 (94%)	0.87	16 (9%) 14 16	45, 112, 156, 177	0
31	YH	170/180 (94%)	0.53	13 (7%) 20 18	11, 66, 116, 131	0
32	RI	146/148 (98%)	0.20	6 (4%) 41 31	3, 77, 124, 177	0
32	YI	146/148 (98%)	0.13	6 (4%) 41 31	3, 64, 125, 140	0
33	RN	138/140 (98%)	0.41	5 (3%) 46 33	6, 61, 118, 144	0
33	YN	138/140 (98%)	0.51	10 (7%) 21 19	4, 45, 98, 131	0
34	RO	122/122 (100%)	0.51	8 (6%) 24 21	2, 42, 80, 107	0
34	YO	122/122 (100%)	0.56	9 (7%) 20 19	2, 41, 82, 126	0
35	RP	150/150 (100%)	0.85	23 (15%) 5 8	1, 58, 130, 158	0
35	YP	150/150 (100%)	0.79	20 (13%) 7 10	1, 46, 101, 160	0
36	RQ	141/141 (100%)	0.93	22 (15%) 5 8	3, 58, 103, 133	0
36	YQ	141/141 (100%)	0.79	21 (14%) 5 8	0, 47, 97, 115	0
37	RR	118/118 (100%)	0.73	11 (9%) 14 16	1, 34, 87, 136	0
37	YR	118/118 (100%)	0.61	14 (11%) 9 11	2, 38, 98, 136	0
38	RS	111/112 (99%)	0.53	7 (6%) 26 22	23, 83, 117, 138	0
38	YS	111/112 (99%)	0.67	15 (13%) 7 10	13, 73, 115, 168	0
39	RT	137/146 (93%)	0.78	13 (9%) 14 15	8, 58, 130, 152	0
39	YT	137/146 (93%)	0.69	10 (7%) 21 19	9, 56, 122, 170	0
40	RU	117/118 (99%)	0.81	15 (12%) 7 10	1, 49, 113, 166	0
40	YU	117/118 (99%)	0.35	3 (2%) 57 40	1, 31, 97, 145	0
41	RV	101/101 (100%)	0.44	3 (2%) 52 37	1, 68, 120, 193	0
41	YV	101/101 (100%)	0.22	4 (3%) 42 31	1, 45, 97, 171	0
42	RW	113/113 (100%)	0.40	4 (3%) 47 33	2, 34, 95, 131	0
42	YW	113/113 (100%)	0.12	4 (3%) 47 33	1, 24, 84, 155	0
43	RX	92/96 (95%)	0.32	2 (2%) 62 44	4, 44, 91, 131	0
43	YX	92/96 (95%)	0.53	7 (7%) 20 18	1, 25, 64, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.37	25 (24%) 2 4	10, 84, 138, 174	0
44	YY	102/110 (92%)	0.73	11 (10%) 11 13	2, 50, 106, 160	0
45	RZ	183/206 (88%)	0.44	10 (5%) 30 25	20, 88, 136, 160	0
45	YZ	183/206 (88%)	0.39	9 (4%) 35 27	20, 78, 137, 167	0
46	R0	82/85 (96%)	0.21	3 (3%) 45 32	6, 44, 83, 137	0
46	Y0	82/85 (96%)	0.29	5 (6%) 27 23	2, 32, 70, 88	0
47	R1	97/98 (98%)	0.90	15 (15%) 5 8	2, 47, 126, 202	0
47	Y1	97/98 (98%)	0.50	8 (8%) 17 18	0, 32, 114, 142	0
48	R2	69/72 (95%)	0.71	5 (7%) 21 19	8, 72, 116, 128	0
48	Y2	69/72 (95%)	0.59	5 (7%) 21 19	0, 39, 97, 137	0
49	R3	59/60 (98%)	0.47	2 (3%) 48 34	7, 60, 126, 152	0
49	Y3	59/60 (98%)	0.32	3 (5%) 33 26	3, 40, 87, 128	0
50	R4	71/71 (100%)	1.36	12 (16%) 4 7	78, 145, 193, 235	0
50	Y4	71/71 (100%)	0.82	7 (9%) 13 14	69, 122, 166, 194	0
51	R5	59/60 (98%)	1.22	12 (20%) 3 5	4, 39, 139, 166	0
51	Y5	59/60 (98%)	0.74	6 (10%) 12 14	1, 40, 132, 156	0
52	R6	49/54 (90%)	1.85	17 (34%) 1 2	48, 122, 152, 191	0
52	Y6	49/54 (90%)	1.26	12 (24%) 2 4	47, 108, 148, 175	0
53	R7	49/49 (100%)	0.65	5 (10%) 12 14	1, 27, 75, 161	0
53	Y7	49/49 (100%)	0.88	6 (12%) 8 11	1, 15, 84, 140	0
54	R8	64/65 (98%)	1.08	9 (14%) 6 9	4, 41, 94, 153	0
54	Y8	64/65 (98%)	0.71	5 (7%) 19 18	2, 34, 85, 138	0
55	R9	37/37 (100%)	2.18	17 (45%) 0 1	53, 103, 154, 162	0
55	Y9	37/37 (100%)	2.37	20 (54%) 0 1	60, 98, 136, 154	0
56	Z6	2/3 (66%)	0.16	0 100 100	17, 17, 17, 30	0
56	Z8	2/3 (66%)	1.07	0 100 100	19, 19, 19, 22	0
All	All	20870/21494 (97%)	0.41	1583 (7%) 20 18	0, 55, 139, 252	0

The worst 5 of 1583 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
47	R1	98	LEU	10.7
37	RR	7	GLY	9.8

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Mol	Chain	Res	Type	RSRZ
50	R4	69	LYS	9.5
36	RQ	25	ASP	9.1
52	R6	42	TRP	9.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	1MG	QY	37	24/25	0.76	0.11	130,130,130,130	0
24	1MG	XY	37	24/25	0.88	0.10	56,56,56,56	0
56	PPU	Z8	76	37/38	0.89	0.19	10,10,10,10	0
56	PPU	Z6	76	37/38	0.94	0.14	14,14,14,14	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	3100	1/1	-0.77	0.49	6,6,6,6	0
57	MG	RA	3166	1/1	-0.13	0.40	34,34,34,34	0
57	MG	RA	3122	1/1	0.13	0.42	5,5,5,5	0
57	MG	RA	3070	1/1	0.17	0.52	0,0,0,0	0
57	MG	RA	3049	1/1	0.17	0.64	13,13,13,13	0
57	MG	QA	1618	1/1	0.20	0.40	3,3,3,3	0
57	MG	QA	1629	1/1	0.29	0.35	0,0,0,0	0
57	MG	YA	3167	1/1	0.30	0.47	2,2,2,2	0
57	MG	RA	3121	1/1	0.31	0.50	5,5,5,5	0
57	MG	YA	3041	1/1	0.32	0.56	0,0,0,0	0
57	MG	XA	1624	1/1	0.41	0.45	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	XA	1618	1/1	0.41	0.52	3,3,3,3	0
57	MG	YA	3068	1/1	0.43	0.48	2,2,2,2	0
57	MG	YA	3214	1/1	0.44	0.47	2,2,2,2	0
57	MG	YA	3006	1/1	0.45	0.59	3,3,3,3	0
57	MG	RA	3022	1/1	0.45	0.41	4,4,4,4	0
57	MG	QA	1612	1/1	0.45	0.44	7,7,7,7	0
57	MG	YA	3001	1/1	0.46	0.86	50,50,50,50	0
57	MG	YA	3121	1/1	0.47	0.45	62,62,62,62	0
57	MG	XA	1631	1/1	0.48	0.17	31,31,31,31	0
57	MG	YA	3078	1/1	0.50	0.43	2,2,2,2	0
57	MG	YB	202	1/1	0.50	0.52	24,24,24,24	0
57	MG	RA	3138	1/1	0.51	0.33	29,29,29,29	0
57	MG	RA	3020	1/1	0.53	0.68	50,50,50,50	0
57	MG	YA	3060	1/1	0.54	0.43	10,10,10,10	0
57	MG	RA	3085	1/1	0.54	0.53	5,5,5,5	0
57	MG	QA	1614	1/1	0.56	0.55	9,9,9,9	0
57	MG	YA	3014	1/1	0.57	1.08	50,50,50,50	0
57	MG	YA	3032	1/1	0.57	0.43	1,1,1,1	0
57	MG	QA	1626	1/1	0.57	0.17	57,57,57,57	0
57	MG	YA	3043	1/1	0.57	0.67	2,2,2,2	0
57	MG	RA	3065	1/1	0.58	0.55	7,7,7,7	0
57	MG	RA	3170	1/1	0.58	0.44	5,5,5,5	0
57	MG	QH	201	1/1	0.58	0.18	47,47,47,47	0
57	MG	YA	3120	1/1	0.58	0.60	8,8,8,8	0
57	MG	RA	3173	1/1	0.59	0.24	48,48,48,48	0
57	MG	YA	3128	1/1	0.60	0.47	12,12,12,12	0
57	MG	YA	3237	1/1	0.60	0.45	7,7,7,7	0
57	MG	RA	3137	1/1	0.60	0.38	10,10,10,10	0
57	MG	RA	3179	1/1	0.61	0.34	4,4,4,4	0
57	MG	YA	3031	1/1	0.61	0.51	0,0,0,0	0
57	MG	QA	1619	1/1	0.61	0.34	4,4,4,4	0
57	MG	RA	3083	1/1	0.61	0.31	6,6,6,6	0
59	AMP	XX	101	22/23	0.61	0.18	91,91,91,91	0
57	MG	RA	3032	1/1	0.62	0.99	50,50,50,50	0
57	MG	YA	3015	1/1	0.62	1.04	50,50,50,50	0
57	MG	YA	3076	1/1	0.62	0.81	50,50,50,50	0
57	MG	YA	3194	1/1	0.62	0.23	0,0,0,0	0
57	MG	RA	3037	1/1	0.63	0.40	5,5,5,5	0
57	MG	RA	3041	1/1	0.63	0.43	4,4,4,4	0
57	MG	QA	1613	1/1	0.63	0.63	15,15,15,15	0
57	MG	RA	3050	1/1	0.63	0.32	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3216	1/1	0.63	0.37	7,7,7,7	0
57	MG	RA	3031	1/1	0.64	0.46	5,5,5,5	0
57	MG	XA	1632	1/1	0.64	0.48	14,14,14,14	0
57	MG	XA	1638	1/1	0.64	0.26	20,20,20,20	0
57	MG	YA	3094	1/1	0.64	0.45	11,11,11,11	0
57	MG	YA	3096	1/1	0.64	0.47	3,3,3,3	0
57	MG	YA	3087	1/1	0.65	0.44	11,11,11,11	0
57	MG	YA	3200	1/1	0.65	0.57	4,4,4,4	0
57	MG	YA	3029	1/1	0.66	0.58	10,10,10,10	0
57	MG	YA	3203	1/1	0.66	0.12	53,53,53,53	0
57	MG	YA	3053	1/1	0.66	0.50	4,4,4,4	0
57	MG	QA	1655	1/1	0.66	0.34	20,20,20,20	0
57	MG	RA	3039	1/1	0.66	0.45	10,10,10,10	0
57	MG	RA	3010	1/1	0.66	0.49	14,14,14,14	0
57	MG	RA	3221	1/1	0.67	0.26	22,22,22,22	0
57	MG	RA	3224	1/1	0.67	0.31	5,5,5,5	0
57	MG	YA	3198	1/1	0.67	0.30	51,51,51,51	0
57	MG	RA	3108	1/1	0.67	0.13	0,0,0,0	0
57	MG	RA	3034	1/1	0.67	0.50	9,9,9,9	0
57	MG	RA	3079	1/1	0.67	0.39	5,5,5,5	0
57	MG	RA	3029	1/1	0.67	0.41	1,1,1,1	0
57	MG	RA	3046	1/1	0.67	0.62	50,50,50,50	0
57	MG	YA	3162	1/1	0.67	0.25	0,0,0,0	0
57	MG	YA	3201	1/1	0.68	0.43	9,9,9,9	0
57	MG	YA	3141	1/1	0.68	0.40	0,0,0,0	0
57	MG	RA	3213	1/1	0.68	0.33	8,8,8,8	0
57	MG	YA	3002	1/1	0.69	0.72	50,50,50,50	0
57	MG	YA	3172	1/1	0.69	0.54	1,1,1,1	0
57	MG	QA	1603	1/1	0.69	0.46	14,14,14,14	0
57	MG	YA	3045	1/1	0.69	0.44	13,13,13,13	0
57	MG	RA	3219	1/1	0.69	0.32	40,40,40,40	0
57	MG	YA	3106	1/1	0.69	0.54	8,8,8,8	0
57	MG	RA	3212	1/1	0.69	0.41	1,1,1,1	0
57	MG	RA	3007	1/1	0.69	0.22	16,16,16,16	0
57	MG	RA	3228	1/1	0.69	0.39	11,11,11,11	0
57	MG	XA	1611	1/1	0.69	0.35	7,7,7,7	0
57	MG	YA	3084	1/1	0.69	0.20	17,17,17,17	0
57	MG	QA	1615	1/1	0.70	0.45	4,4,4,4	0
57	MG	RA	3153	1/1	0.70	0.46	15,15,15,15	0
57	MG	YA	3140	1/1	0.70	0.22	12,12,12,12	0
57	MG	YA	3099	1/1	0.70	0.45	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3150	1/1	0.70	0.35	4,4,4,4	0
57	MG	YA	3157	1/1	0.70	0.39	0,0,0,0	0
57	MG	YA	3049	1/1	0.70	0.69	50,50,50,50	0
57	MG	RA	3087	1/1	0.70	0.56	11,11,11,11	0
57	MG	RA	3013	1/1	0.70	0.43	4,4,4,4	0
57	MG	RA	3059	1/1	0.71	0.42	11,11,11,11	0
57	MG	YA	3010	1/1	0.71	0.36	5,5,5,5	0
57	MG	XA	1672	1/1	0.71	0.29	0,0,0,0	0
57	MG	RA	3101	1/1	0.71	0.40	11,11,11,11	0
57	MG	YA	3186	1/1	0.71	0.31	11,11,11,11	0
57	MG	YA	3021	1/1	0.71	0.29	12,12,12,12	0
57	MG	RA	3226	1/1	0.71	0.15	9,9,9,9	0
57	MG	RA	3135	1/1	0.72	0.20	7,7,7,7	0
57	MG	XV	101	1/1	0.72	0.36	14,14,14,14	0
57	MG	RA	3069	1/1	0.72	0.47	4,4,4,4	0
57	MG	XA	1657	1/1	0.72	0.22	8,8,8,8	0
57	MG	YA	3018	1/1	0.72	0.60	3,3,3,3	0
57	MG	RA	3199	1/1	0.73	0.31	6,6,6,6	0
57	MG	RA	3203	1/1	0.73	0.16	24,24,24,24	0
57	MG	QA	1664	1/1	0.73	0.17	54,54,54,54	0
57	MG	QA	1642	1/1	0.73	0.57	16,16,16,16	0
57	MG	YA	3011	1/1	0.73	0.36	0,0,0,0	0
57	MG	YA	3052	1/1	0.73	0.42	14,14,14,14	0
57	MG	YA	3116	1/1	0.73	0.27	3,3,3,3	0
57	MG	RA	3214	1/1	0.73	0.35	5,5,5,5	0
57	MG	QA	1640	1/1	0.73	0.36	9,9,9,9	0
57	MG	QA	1661	1/1	0.73	0.13	64,64,64,64	0
57	MG	RA	3140	1/1	0.73	0.41	9,9,9,9	0
57	MG	YA	3222	1/1	0.73	0.20	8,8,8,8	0
57	MG	RA	3182	1/1	0.73	0.26	4,4,4,4	0
57	MG	RA	3191	1/1	0.73	0.18	67,67,67,67	0
57	MG	YA	3156	1/1	0.73	0.29	2,2,2,2	0
57	MG	RA	3077	1/1	0.74	0.37	0,0,0,0	0
57	MG	XA	1628	1/1	0.74	0.33	10,10,10,10	0
57	MG	QF	201	1/1	0.74	0.27	36,36,36,36	0
57	MG	YA	3071	1/1	0.74	0.17	28,28,28,28	0
57	MG	YA	3254	1/1	0.74	0.44	2,2,2,2	0
57	MG	RA	3015	1/1	0.74	0.61	5,5,5,5	0
57	MG	YA	3036	1/1	0.74	0.26	2,2,2,2	0
57	MG	RA	3006	1/1	0.75	0.71	50,50,50,50	0
57	MG	YA	3101	1/1	0.75	0.40	2,2,2,2	0
57	MG	RA	3131	1/1	0.75	0.52	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3115	1/1	0.75	0.33	4,4,4,4	0
57	MG	RA	3081	1/1	0.75	0.37	1,1,1,1	0
57	MG	YA	3166	1/1	0.75	0.22	4,4,4,4	0
57	MG	RA	3062	1/1	0.75	1.02	50,50,50,50	0
57	MG	YA	3062	1/1	0.75	0.37	6,6,6,6	0
57	MG	YA	3260	1/1	0.75	0.96	50,50,50,50	0
57	MG	RA	3058	1/1	0.75	0.70	3,3,3,3	0
57	MG	YA	3047	1/1	0.75	0.53	3,3,3,3	0
57	MG	RA	3151	1/1	0.76	0.29	9,9,9,9	0
57	MG	RA	3111	1/1	0.76	0.31	11,11,11,11	0
57	MG	RA	3160	1/1	0.76	0.36	4,4,4,4	0
57	MG	QA	1623	1/1	0.76	0.29	14,14,14,14	0
57	MG	YA	3050	1/1	0.76	0.63	50,50,50,50	0
57	MG	YA	3033	1/1	0.76	0.44	4,4,4,4	0
57	MG	RA	3143	1/1	0.76	0.84	7,7,7,7	0
57	MG	RA	3229	1/1	0.76	0.94	50,50,50,50	0
57	MG	RA	3043	1/1	0.77	0.30	10,10,10,10	0
57	MG	RA	3051	1/1	0.77	0.57	7,7,7,7	0
57	MG	YA	3009	1/1	0.77	0.49	8,8,8,8	0
57	MG	RA	3236	1/1	0.77	0.31	0,0,0,0	0
57	MG	YA	3142	1/1	0.77	0.46	19,19,19,19	0
57	MG	XA	1648	1/1	0.77	0.39	3,3,3,3	0
57	MG	RA	3128	1/1	0.77	0.41	7,7,7,7	0
57	MG	YA	3221	1/1	0.77	0.32	18,18,18,18	0
57	MG	RA	3208	1/1	0.77	0.38	15,15,15,15	0
57	MG	YA	3109	1/1	0.77	0.45	2,2,2,2	0
57	MG	YA	3164	1/1	0.77	0.31	8,8,8,8	0
57	MG	RA	3052	1/1	0.77	0.69	50,50,50,50	0
57	MG	YA	3019	1/1	0.77	0.31	5,5,5,5	0
58	ZN	Y9	101	1/1	0.77	0.24	138,138,138,138	0
57	MG	RA	3163	1/1	0.77	0.60	12,12,12,12	0
57	MG	YA	3192	1/1	0.78	0.36	11,11,11,11	0
57	MG	YA	3055	1/1	0.78	0.28	0,0,0,0	0
57	MG	YA	3058	1/1	0.78	0.43	15,15,15,15	0
57	MG	RA	3125	1/1	0.78	0.36	1,1,1,1	0
57	MG	YA	3147	1/1	0.78	0.37	4,4,4,4	0
57	MG	RA	3188	1/1	0.78	0.29	5,5,5,5	0
57	MG	YA	3207	1/1	0.78	0.34	7,7,7,7	0
57	MG	YA	3063	1/1	0.78	0.34	11,11,11,11	0
57	MG	YA	3025	1/1	0.78	0.24	4,4,4,4	0
57	MG	XA	1658	1/1	0.78	0.28	9,9,9,9	0
57	MG	YA	3227	1/1	0.78	0.30	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	RA	3096	1/1	0.78	0.32	4,4,4,4	0
57	MG	QA	1649	1/1	0.78	0.32	6,6,6,6	0
57	MG	YA	3082	1/1	0.78	0.36	3,3,3,3	0
57	MG	RA	3092	1/1	0.78	0.40	7,7,7,7	0
57	MG	YA	3176	1/1	0.78	0.26	6,6,6,6	0
57	MG	RA	3181	1/1	0.78	0.31	3,3,3,3	0
57	MG	YA	3098	1/1	0.79	0.30	1,1,1,1	0
57	MG	RA	3018	1/1	0.79	0.40	6,6,6,6	0
57	MG	QA	1646	1/1	0.79	0.25	10,10,10,10	0
57	MG	RA	3124	1/1	0.79	0.28	10,10,10,10	0
57	MG	RA	3187	1/1	0.79	0.40	3,3,3,3	0
57	MG	RA	3036	1/1	0.79	0.44	6,6,6,6	0
57	MG	YA	3114	1/1	0.79	0.24	13,13,13,13	0
57	MG	QA	1638	1/1	0.79	0.29	34,34,34,34	0
57	MG	XA	1659	1/1	0.79	0.28	0,0,0,0	0
57	MG	RA	3026	1/1	0.79	0.89	50,50,50,50	0
57	MG	RA	3201	1/1	0.79	0.52	10,10,10,10	0
57	MG	YA	3204	1/1	0.79	0.34	11,11,11,11	0
57	MG	YA	3073	1/1	0.79	0.42	1,1,1,1	0
57	MG	RA	3232	1/1	0.79	0.33	13,13,13,13	0
57	MG	QA	1604	1/1	0.79	0.30	0,0,0,0	0
57	MG	RA	3207	1/1	0.79	0.15	11,11,11,11	0
57	MG	RA	3169	1/1	0.79	0.23	16,16,16,16	0
57	MG	YA	3232	1/1	0.79	0.47	2,2,2,2	0
57	MG	XA	1621	1/1	0.79	0.33	3,3,3,3	0
57	MG	YA	3088	1/1	0.79	0.64	50,50,50,50	0
57	MG	QA	1602	1/1	0.79	0.52	12,12,12,12	0
57	MG	YA	3159	1/1	0.79	0.18	6,6,6,6	0
57	MG	YA	3095	1/1	0.79	0.35	2,2,2,2	0
57	MG	RA	3082	1/1	0.79	0.28	0,0,0,0	0
57	MG	XA	1617	1/1	0.80	0.28	15,15,15,15	0
57	MG	YA	3080	1/1	0.80	1.03	50,50,50,50	0
57	MG	XA	1630	1/1	0.80	0.31	10,10,10,10	0
57	MG	YA	3179	1/1	0.80	0.18	0,0,0,0	0
57	MG	YA	3004	1/1	0.80	0.32	12,12,12,12	0
57	MG	YA	3086	1/1	0.80	0.34	6,6,6,6	0
57	MG	YA	3067	1/1	0.80	0.34	5,5,5,5	0
57	MG	YA	3243	1/1	0.80	0.21	32,32,32,32	0
57	MG	RA	3068	1/1	0.80	0.27	6,6,6,6	0
57	MG	RA	3159	1/1	0.80	0.31	6,6,6,6	0
57	MG	XA	1616	1/1	0.80	0.24	1,1,1,1	0
57	MG	YA	3075	1/1	0.80	0.37	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	XA	1647	1/1	0.80	0.26	1,1,1,1	0
57	MG	RP	201	1/1	0.81	0.82	21,21,21,21	0
57	MG	YA	3118	1/1	0.81	0.40	14,14,14,14	0
57	MG	YA	3236	1/1	0.81	0.19	5,5,5,5	0
57	MG	RA	3076	1/1	0.81	0.41	7,7,7,7	0
57	MG	YA	3013	1/1	0.81	0.39	5,5,5,5	0
57	MG	YA	3097	1/1	0.81	0.35	5,5,5,5	0
57	MG	YA	3184	1/1	0.81	0.31	7,7,7,7	0
57	MG	YA	3129	1/1	0.81	0.39	15,15,15,15	0
57	MG	RA	3227	1/1	0.81	0.48	22,22,22,22	0
57	MG	RA	3112	1/1	0.81	0.19	6,6,6,6	0
57	MG	RA	3218	1/1	0.82	0.46	23,23,23,23	0
57	MG	QA	1663	1/1	0.82	0.19	47,47,47,47	0
57	MG	YA	3034	1/1	0.82	0.37	2,2,2,2	0
57	MG	XA	1615	1/1	0.82	0.33	6,6,6,6	0
57	MG	YA	3091	1/1	0.82	0.38	13,13,13,13	0
57	MG	QA	1660	1/1	0.82	0.29	2,2,2,2	0
57	MG	YA	3223	1/1	0.82	0.27	34,34,34,34	0
57	MG	RA	3073	1/1	0.82	0.25	2,2,2,2	0
57	MG	RA	3110	1/1	0.82	0.34	3,3,3,3	0
57	MG	RA	3019	1/1	0.82	0.38	8,8,8,8	0
57	MG	YA	3135	1/1	0.82	0.28	6,6,6,6	0
57	MG	QA	1641	1/1	0.82	0.27	7,7,7,7	0
57	MG	RA	3089	1/1	0.82	0.32	11,11,11,11	0
57	MG	YA	3259	1/1	0.82	0.54	8,8,8,8	0
57	MG	QA	1662	1/1	0.82	0.11	37,37,37,37	0
57	MG	RA	3234	1/1	0.82	0.32	9,9,9,9	0
57	MG	RA	3197	1/1	0.82	0.26	3,3,3,3	0
57	MG	YA	3107	1/1	0.82	0.30	15,15,15,15	0
57	MG	RA	3238	1/1	0.83	0.39	16,16,16,16	0
57	MG	QA	1644	1/1	0.83	0.26	4,4,4,4	0
57	MG	YA	3035	1/1	0.83	0.33	9,9,9,9	0
57	MG	YA	3012	1/1	0.83	0.86	50,50,50,50	0
57	MG	QA	1622	1/1	0.83	0.24	14,14,14,14	0
57	MG	XA	1670	1/1	0.83	0.15	43,43,43,43	0
57	MG	RA	3093	1/1	0.83	0.54	10,10,10,10	0
57	MG	RA	3205	1/1	0.83	0.32	12,12,12,12	0
57	MG	XA	1636	1/1	0.83	0.32	3,3,3,3	0
57	MG	YA	3242	1/1	0.83	0.48	4,4,4,4	0
57	MG	RA	3094	1/1	0.83	0.41	0,0,0,0	0
57	MG	QA	1620	1/1	0.83	0.16	6,6,6,6	0
57	MG	YA	3104	1/1	0.83	0.35	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3161	1/1	0.83	0.25	1,1,1,1	0
57	MG	YA	3083	1/1	0.83	0.29	9,9,9,9	0
57	MG	YA	3008	1/1	0.83	0.38	10,10,10,10	0
57	MG	XA	1653	1/1	0.83	0.20	8,8,8,8	0
57	MG	RA	3028	1/1	0.84	0.37	14,14,14,14	0
57	MG	RA	3114	1/1	0.84	0.24	1,1,1,1	0
57	MG	RA	3192	1/1	0.84	0.11	21,21,21,21	0
57	MG	RA	3088	1/1	0.84	0.56	15,15,15,15	0
57	MG	QA	1643	1/1	0.84	0.18	33,33,33,33	0
57	MG	RA	3055	1/1	0.84	0.53	5,5,5,5	0
57	MG	YA	3217	1/1	0.84	0.35	35,35,35,35	0
57	MG	QA	1632	1/1	0.84	0.14	42,42,42,42	0
57	MG	RA	3231	1/1	0.84	0.16	14,14,14,14	0
57	MG	RA	3126	1/1	0.84	0.30	2,2,2,2	0
57	MG	QA	1645	1/1	0.84	0.14	38,38,38,38	0
57	MG	RA	3033	1/1	0.84	0.72	50,50,50,50	0
57	MG	YA	3234	1/1	0.84	0.57	17,17,17,17	0
57	MG	RA	3209	1/1	0.84	0.27	17,17,17,17	0
57	MG	YA	3171	1/1	0.84	0.22	13,13,13,13	0
57	MG	RA	3063	1/1	0.84	0.78	3,3,3,3	0
57	MG	RA	3105	1/1	0.84	0.32	11,11,11,11	0
57	MG	YA	3245	1/1	0.84	0.10	2,2,2,2	0
57	MG	YA	3250	1/1	0.84	0.58	11,11,11,11	0
57	MG	QA	1659	1/1	0.84	0.28	4,4,4,4	0
57	MG	YA	3256	1/1	0.84	0.24	7,7,7,7	0
57	MG	YA	3054	1/1	0.84	0.22	1,1,1,1	0
57	MG	YA	3126	1/1	0.84	0.23	7,7,7,7	0
57	MG	RA	3067	1/1	0.84	0.28	2,2,2,2	0
57	MG	YA	3024	1/1	0.84	0.78	50,50,50,50	0
57	MG	RA	3016	1/1	0.84	0.24	8,8,8,8	0
57	MG	RA	3145	1/1	0.85	0.29	3,3,3,3	0
57	MG	YA	3122	1/1	0.85	0.28	3,3,3,3	0
57	MG	YA	3125	1/1	0.85	0.59	12,12,12,12	0
57	MG	QA	1625	1/1	0.85	0.29	0,0,0,0	0
57	MG	YA	3127	1/1	0.85	0.24	2,2,2,2	0
57	MG	YA	3077	1/1	0.85	0.34	2,2,2,2	0
57	MG	RA	3123	1/1	0.85	0.24	7,7,7,7	0
57	MG	XA	1663	1/1	0.85	0.25	15,15,15,15	0
57	MG	YA	3190	1/1	0.85	0.12	21,21,21,21	0
57	MG	XA	1664	1/1	0.85	0.29	8,8,8,8	0
57	MG	RA	3014	1/1	0.85	0.24	13,13,13,13	0
57	MG	RA	3194	1/1	0.85	0.30	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	3085	1/1	0.85	0.37	13,13,13,13	0
57	MG	RA	3211	1/1	0.85	0.24	2,2,2,2	0
57	MG	YA	3257	1/1	0.85	0.17	3,3,3,3	0
57	MG	RA	3195	1/1	0.85	0.08	24,24,24,24	0
57	MG	RA	3091	1/1	0.85	0.27	9,9,9,9	0
57	MG	QA	1636	1/1	0.85	0.13	16,16,16,16	0
57	MG	Y5	101	1/1	0.85	0.34	6,6,6,6	0
57	MG	YA	3022	1/1	0.85	0.30	1,1,1,1	0
57	MG	QA	1637	1/1	0.85	0.18	0,0,0,0	0
57	MG	YA	3188	1/1	0.86	0.36	1,1,1,1	0
57	MG	RA	3047	1/1	0.86	0.40	5,5,5,5	0
57	MG	RE	301	1/1	0.86	0.26	12,12,12,12	0
57	MG	QX	101	1/1	0.86	0.28	4,4,4,4	0
57	MG	YA	3195	1/1	0.86	0.19	9,9,9,9	0
57	MG	XA	1656	1/1	0.86	0.31	10,10,10,10	0
57	MG	RA	3045	1/1	0.86	0.21	1,1,1,1	0
57	MG	RA	3098	1/1	0.86	0.41	14,14,14,14	0
57	MG	RA	3005	1/1	0.86	0.40	12,12,12,12	0
57	MG	YA	3090	1/1	0.86	0.27	1,1,1,1	0
57	MG	RA	3190	1/1	0.86	0.18	16,16,16,16	0
57	MG	YA	3092	1/1	0.86	0.19	12,12,12,12	0
57	MG	YA	3174	1/1	0.86	0.13	40,40,40,40	0
57	MG	YA	3261	1/1	0.86	0.22	4,4,4,4	0
57	MG	RA	3103	1/1	0.86	0.30	9,9,9,9	0
57	MG	YP	201	1/1	0.86	0.16	94,94,94,94	0
57	MG	YA	3059	1/1	0.86	0.34	5,5,5,5	0
57	MG	Y7	101	1/1	0.86	0.48	15,15,15,15	0
57	MG	XA	1665	1/1	0.86	0.26	7,7,7,7	0
57	MG	YA	3149	1/1	0.86	0.18	15,15,15,15	0
57	MG	RE	302	1/1	0.87	0.22	1,1,1,1	0
57	MG	RA	3165	1/1	0.87	0.42	13,13,13,13	0
57	MG	YA	3175	1/1	0.87	0.16	9,9,9,9	0
57	MG	RR	201	1/1	0.87	0.27	13,13,13,13	0
57	MG	RA	3225	1/1	0.87	0.13	10,10,10,10	0
57	MG	YA	3180	1/1	0.87	0.27	38,38,38,38	0
57	MG	XA	1655	1/1	0.87	0.19	9,9,9,9	0
57	MG	RA	3129	1/1	0.87	0.12	31,31,31,31	0
57	MG	RA	3167	1/1	0.87	0.22	3,3,3,3	0
57	MG	YA	3042	1/1	0.87	0.34	2,2,2,2	0
57	MG	RA	3023	1/1	0.87	0.27	16,16,16,16	0
57	MG	RA	3044	1/1	0.87	0.52	10,10,10,10	0
57	MG	RA	3158	1/1	0.87	0.26	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3174	1/1	0.87	0.24	4,4,4,4	0
57	MG	XA	1627	1/1	0.87	0.32	14,14,14,14	0
57	MG	QV	101	1/1	0.87	0.25	1,1,1,1	0
57	MG	RA	3017	1/1	0.87	0.31	11,11,11,11	0
57	MG	RA	3115	1/1	0.87	0.33	6,6,6,6	0
57	MG	YA	3205	1/1	0.87	0.12	10,10,10,10	0
57	MG	RA	3239	1/1	0.87	0.31	14,14,14,14	0
57	MG	YA	3027	1/1	0.87	0.19	1,1,1,1	0
57	MG	YA	3028	1/1	0.87	0.41	6,6,6,6	0
57	MG	RA	3008	1/1	0.87	0.26	0,0,0,0	0
57	MG	YA	3051	1/1	0.88	0.27	3,3,3,3	0
57	MG	RA	3171	1/1	0.88	0.13	12,12,12,12	0
57	MG	YA	3218	1/1	0.88	0.19	5,5,5,5	0
57	MG	RA	3196	1/1	0.88	0.19	0,0,0,0	0
57	MG	RA	3109	1/1	0.88	0.28	8,8,8,8	0
57	MG	RA	3080	1/1	0.88	0.23	21,21,21,21	0
57	MG	QA	1633	1/1	0.88	0.47	4,4,4,4	0
57	MG	RA	3027	1/1	0.88	0.39	13,13,13,13	0
57	MG	QA	1648	1/1	0.88	0.22	12,12,12,12	0
57	MG	R5	101	1/1	0.88	0.34	5,5,5,5	0
57	MG	RA	3206	1/1	0.88	0.09	3,3,3,3	0
57	MG	XA	1650	1/1	0.88	0.16	18,18,18,18	0
57	MG	XA	1612	1/1	0.88	0.24	19,19,19,19	0
57	MG	YA	3139	1/1	0.88	0.35	7,7,7,7	0
57	MG	YA	3189	1/1	0.88	0.33	6,6,6,6	0
57	MG	XA	1654	1/1	0.88	0.13	26,26,26,26	0
57	MG	RA	3003	1/1	0.88	0.36	5,5,5,5	0
57	MG	RA	3147	1/1	0.88	0.25	9,9,9,9	0
57	MG	RA	3150	1/1	0.88	0.55	37,37,37,37	0
57	MG	YA	3102	1/1	0.88	0.40	14,14,14,14	0
57	MG	RA	3168	1/1	0.88	0.19	1,1,1,1	0
57	MG	YA	3264	1/1	0.88	0.27	9,9,9,9	0
57	MG	RA	3119	1/1	0.88	0.29	3,3,3,3	0
57	MG	XA	1662	1/1	0.88	0.50	11,11,11,11	0
57	MG	RA	3025	1/1	0.88	0.15	3,3,3,3	0
57	MG	YA	3160	1/1	0.88	0.25	1,1,1,1	0
57	MG	YA	3020	1/1	0.88	0.50	0,0,0,0	0
57	MG	YA	3209	1/1	0.88	0.30	15,15,15,15	0
57	MG	RA	3142	1/1	0.89	0.43	36,36,36,36	0
57	MG	YA	3170	1/1	0.89	0.18	8,8,8,8	0
57	MG	XA	1671	1/1	0.89	0.15	3,3,3,3	0
57	MG	QA	1650	1/1	0.89	0.38	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	R0	101	1/1	0.89	0.17	0,0,0,0	0
57	MG	RA	3061	1/1	0.89	0.13	53,53,53,53	0
57	MG	XA	1646	1/1	0.89	0.23	7,7,7,7	0
57	MG	XA	1603	1/1	0.89	0.63	8,8,8,8	0
57	MG	XA	1607	1/1	0.89	0.17	16,16,16,16	0
57	MG	YA	3181	1/1	0.89	0.33	3,3,3,3	0
57	MG	YA	3182	1/1	0.89	0.26	8,8,8,8	0
57	MG	YA	3130	1/1	0.89	0.35	20,20,20,20	0
57	MG	RA	3120	1/1	0.89	0.24	1,1,1,1	0
57	MG	RA	3086	1/1	0.89	0.14	0,0,0,0	0
57	MG	RA	3048	1/1	0.89	0.17	3,3,3,3	0
57	MG	YA	3069	1/1	0.89	0.36	2,2,2,2	0
57	MG	YA	3255	1/1	0.89	0.62	0,0,0,0	0
57	MG	RA	3202	1/1	0.89	0.17	16,16,16,16	0
57	MG	YA	3040	1/1	0.89	0.41	10,10,10,10	0
57	MG	RA	3233	1/1	0.89	0.47	2,2,2,2	0
57	MG	RA	3217	1/1	0.89	0.21	74,74,74,74	0
57	MG	XA	1619	1/1	0.89	0.22	5,5,5,5	0
57	MG	RA	3042	1/1	0.89	0.13	2,2,2,2	0
57	MG	YA	3265	1/1	0.89	0.65	4,4,4,4	0
57	MG	YA	3268	1/1	0.89	0.18	6,6,6,6	0
57	MG	YA	3046	1/1	0.89	0.40	3,3,3,3	0
57	MG	RA	3155	1/1	0.89	0.40	10,10,10,10	0
57	MG	RA	3072	1/1	0.89	0.25	3,3,3,3	0
57	MG	RA	3222	1/1	0.89	0.38	14,14,14,14	0
57	MG	QA	1624	1/1	0.89	0.21	0,0,0,0	0
57	MG	YA	3212	1/1	0.89	0.15	8,8,8,8	0
57	MG	QA	1611	1/1	0.90	0.28	6,6,6,6	0
57	MG	QA	1631	1/1	0.90	0.14	26,26,26,26	0
57	MG	XA	1652	1/1	0.90	0.10	66,66,66,66	0
57	MG	YA	3030	1/1	0.90	0.44	5,5,5,5	0
57	MG	RA	3040	1/1	0.90	0.26	14,14,14,14	0
57	MG	YA	3089	1/1	0.90	0.32	5,5,5,5	0
57	MG	YA	3124	1/1	0.90	0.30	9,9,9,9	0
57	MG	RA	3078	1/1	0.90	0.25	3,3,3,3	0
57	MG	RA	3148	1/1	0.90	0.30	5,5,5,5	0
57	MG	QA	1628	1/1	0.90	0.15	8,8,8,8	0
57	MG	YA	3093	1/1	0.90	0.22	7,7,7,7	0
57	MG	RA	3056	1/1	0.90	0.19	5,5,5,5	0
57	MG	RA	3133	1/1	0.90	0.21	0,0,0,0	0
57	MG	YA	3131	1/1	0.90	0.15	3,3,3,3	0
57	MG	YA	3247	1/1	0.90	0.46	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1602	1/1	0.90	0.22	7,7,7,7	0
57	MG	YA	3252	1/1	0.90	0.36	8,8,8,8	0
57	MG	YA	3138	1/1	0.90	0.16	0,0,0,0	0
57	MG	RA	3090	1/1	0.90	0.24	75,75,75,75	0
57	MG	YA	3070	1/1	0.90	0.26	15,15,15,15	0
57	MG	XA	1605	1/1	0.90	0.40	3,3,3,3	0
57	MG	XA	1635	1/1	0.90	0.29	4,4,4,4	0
57	MG	YA	3146	1/1	0.90	0.28	0,0,0,0	0
57	MG	YA	3196	1/1	0.90	0.42	1,1,1,1	0
57	MG	YA	3044	1/1	0.90	0.48	6,6,6,6	0
57	MG	RA	3136	1/1	0.90	0.28	0,0,0,0	0
57	MG	RA	3106	1/1	0.90	0.35	13,13,13,13	0
57	MG	YB	201	1/1	0.90	0.17	7,7,7,7	0
57	MG	XA	1641	1/1	0.90	0.72	21,21,21,21	0
57	MG	RA	3071	1/1	0.90	0.17	1,1,1,1	0
57	MG	XB	301	1/1	0.90	0.05	2,2,2,2	0
57	MG	YA	3113	1/1	0.90	0.18	1,1,1,1	0
57	MG	YA	3161	1/1	0.90	0.09	1,1,1,1	0
57	MG	RA	3064	1/1	0.90	0.27	5,5,5,5	0
57	MG	YA	3153	1/1	0.91	0.27	20,20,20,20	0
57	MG	YA	3155	1/1	0.91	0.18	7,7,7,7	0
57	MG	RA	3223	1/1	0.91	0.13	47,47,47,47	0
57	MG	YA	3208	1/1	0.91	0.41	15,15,15,15	0
57	MG	YA	3048	1/1	0.91	0.30	4,4,4,4	0
57	MG	YA	3117	1/1	0.91	0.47	6,6,6,6	0
57	MG	YA	3039	1/1	0.91	0.20	6,6,6,6	0
57	MG	QA	1635	1/1	0.91	0.28	13,13,13,13	0
57	MG	YA	3079	1/1	0.91	0.19	4,4,4,4	0
57	MG	RA	3215	1/1	0.91	0.19	27,27,27,27	0
57	MG	YA	3123	1/1	0.91	0.16	18,18,18,18	0
57	MG	YA	3263	1/1	0.91	0.48	4,4,4,4	0
57	MG	YA	3193	1/1	0.91	0.11	3,3,3,3	0
57	MG	XA	1637	1/1	0.91	0.17	25,25,25,25	0
57	MG	YA	3266	1/1	0.91	0.37	2,2,2,2	0
57	MG	YA	3229	1/1	0.91	0.19	3,3,3,3	0
57	MG	RA	3193	1/1	0.91	0.21	22,22,22,22	0
57	MG	XA	1608	1/1	0.91	0.12	37,37,37,37	0
57	MG	YA	3148	1/1	0.91	0.17	7,7,7,7	0
57	MG	XA	1642	1/1	0.91	0.28	5,5,5,5	0
57	MG	YA	3239	1/1	0.91	0.29	5,5,5,5	0
58	ZN	R9	101	1/1	0.91	0.21	145,145,145,145	0
57	MG	RA	3004	1/1	0.91	0.70	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3152	1/1	0.91	0.28	5,5,5,5	0
57	MG	RA	3001	1/1	0.92	0.25	3,3,3,3	0
57	MG	YA	3158	1/1	0.92	0.26	6,6,6,6	0
57	MG	QA	1606	1/1	0.92	0.16	16,16,16,16	0
57	MG	RA	3177	1/1	0.92	0.47	7,7,7,7	0
57	MG	RA	3038	1/1	0.92	0.24	8,8,8,8	0
57	MG	YA	3249	1/1	0.92	0.24	10,10,10,10	0
57	MG	YA	3007	1/1	0.92	0.19	7,7,7,7	0
57	MG	RA	3127	1/1	0.92	0.24	0,0,0,0	0
57	MG	YA	3103	1/1	0.92	0.17	5,5,5,5	0
57	MG	YA	3133	1/1	0.92	0.18	1,1,1,1	0
57	MG	RA	3024	1/1	0.92	0.22	16,16,16,16	0
57	MG	XA	1633	1/1	0.92	0.15	3,3,3,3	0
57	MG	XA	1610	1/1	0.92	0.21	3,3,3,3	0
57	MG	RA	3183	1/1	0.92	0.14	57,57,57,57	0
57	MG	RA	3117	1/1	0.92	0.21	25,25,25,25	0
57	MG	YA	3038	1/1	0.92	0.15	7,7,7,7	0
57	MG	YA	3177	1/1	0.92	0.21	3,3,3,3	0
57	MG	QA	1657	1/1	0.92	0.11	7,7,7,7	0
57	MG	YA	3219	1/1	0.92	0.18	7,7,7,7	0
57	MG	RA	3060	1/1	0.92	0.30	6,6,6,6	0
57	MG	YA	3064	1/1	0.92	0.16	8,8,8,8	0
57	MG	XA	1668	1/1	0.92	0.17	18,18,18,18	0
57	MG	QA	1654	1/1	0.92	0.16	17,17,17,17	0
57	MG	YA	3151	1/1	0.92	0.19	5,5,5,5	0
57	MG	RA	3021	1/1	0.92	0.22	2,2,2,2	0
58	ZN	QN	101	1/1	0.92	0.05	104,104,104,104	0
57	MG	RA	3154	1/1	0.92	0.10	11,11,11,11	0
57	MG	XA	1620	1/1	0.92	0.14	2,2,2,2	0
57	MG	RA	3035	1/1	0.92	0.33	11,11,11,11	0
57	MG	RA	3235	1/1	0.93	0.45	1,1,1,1	0
57	MG	R8	101	1/1	0.93	0.18	0,0,0,0	0
57	MG	XA	1666	1/1	0.93	0.07	50,50,50,50	0
57	MG	YA	3136	1/1	0.93	0.20	21,21,21,21	0
57	MG	YA	3119	1/1	0.93	0.52	8,8,8,8	0
57	MG	RA	3116	1/1	0.93	0.26	9,9,9,9	0
57	MG	RA	3184	1/1	0.93	0.23	8,8,8,8	0
57	MG	YA	3238	1/1	0.93	0.09	11,11,11,11	0
57	MG	YA	3183	1/1	0.93	0.12	16,16,16,16	0
57	MG	YA	3240	1/1	0.93	0.49	72,72,72,72	0
57	MG	RA	3220	1/1	0.93	0.17	26,26,26,26	0
57	MG	QA	1610	1/1	0.93	0.23	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YB	203	1/1	0.93	0.09	37,37,37,37	0
57	MG	QA	1601	1/1	0.93	0.23	9,9,9,9	0
57	MG	YQ	201	1/1	0.93	0.09	99,99,99,99	0
57	MG	QA	1616	1/1	0.93	0.11	29,29,29,29	0
57	MG	RA	3053	1/1	0.93	0.18	2,2,2,2	0
57	MG	YA	3111	1/1	0.93	0.20	15,15,15,15	0
57	MG	XA	1660	1/1	0.93	0.11	24,24,24,24	0
57	MG	RR	202	1/1	0.93	0.19	0,0,0,0	0
57	MG	RA	3157	1/1	0.93	0.51	0,0,0,0	0
57	MG	YA	3137	1/1	0.94	0.23	10,10,10,10	0
57	MG	RA	3204	1/1	0.94	0.31	18,18,18,18	0
57	MG	YA	3081	1/1	0.94	0.25	9,9,9,9	0
57	MG	RA	3104	1/1	0.94	0.21	3,3,3,3	0
57	MG	YA	3191	1/1	0.94	0.15	7,7,7,7	0
57	MG	YA	3165	1/1	0.94	0.21	11,11,11,11	0
57	MG	XA	1667	1/1	0.94	0.18	17,17,17,17	0
57	MG	RA	3100	1/1	0.94	0.07	2,2,2,2	0
57	MG	QA	1647	1/1	0.94	0.11	33,33,33,33	0
57	MG	RA	3152	1/1	0.94	0.11	4,4,4,4	0
57	MG	RA	3200	1/1	0.94	0.08	1,1,1,1	0
57	MG	XA	1604	1/1	0.94	0.49	10,10,10,10	0
57	MG	XM	201	1/1	0.94	0.05	85,85,85,85	0
57	MG	YA	3072	1/1	0.94	0.16	2,2,2,2	0
57	MG	XA	1640	1/1	0.94	0.07	75,75,75,75	0
57	MG	YE	301	1/1	0.94	0.21	0,0,0,0	0
57	MG	RD	301	1/1	0.94	0.08	1,1,1,1	0
57	MG	RA	3144	1/1	0.94	0.18	0,0,0,0	0
57	MG	YA	3244	1/1	0.94	0.33	9,9,9,9	0
57	MG	RA	3230	1/1	0.94	0.54	5,5,5,5	0
57	MG	YA	3134	1/1	0.94	0.32	11,11,11,11	0
57	MG	RA	3130	1/1	0.94	0.44	2,2,2,2	0
57	MG	QA	1605	1/1	0.94	0.63	7,7,7,7	0
57	MG	YA	3215	1/1	0.94	0.14	14,14,14,14	0
57	MG	QA	1621	1/1	0.95	0.10	5,5,5,5	0
57	MG	RA	3132	1/1	0.95	0.10	3,3,3,3	0
57	MG	RA	3057	1/1	0.95	0.26	2,2,2,2	0
57	MG	YA	3112	1/1	0.95	0.08	21,21,21,21	0
57	MG	YA	3185	1/1	0.95	0.18	2,2,2,2	0
57	MG	RA	3134	1/1	0.95	0.21	25,25,25,25	0
57	MG	QA	1607	1/1	0.95	0.14	13,13,13,13	0
57	MG	XA	1661	1/1	0.95	0.06	2,2,2,2	0
57	MG	RA	3084	1/1	0.95	0.23	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3016	1/1	0.95	0.14	6,6,6,6	0
57	MG	XA	1601	1/1	0.95	0.47	1,1,1,1	0
57	MG	YA	3154	1/1	0.95	0.14	1,1,1,1	0
57	MG	RA	3102	1/1	0.95	0.09	4,4,4,4	0
57	MG	XA	1634	1/1	0.95	0.28	0,0,0,0	0
57	MG	YA	3251	1/1	0.95	0.07	9,9,9,9	0
57	MG	RA	3186	1/1	0.95	0.25	8,8,8,8	0
57	MG	QA	1658	1/1	0.95	0.15	16,16,16,16	0
57	MG	RA	3139	1/1	0.95	0.16	2,2,2,2	0
57	MG	XA	1669	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3026	1/1	0.95	0.73	1,1,1,1	0
57	MG	XA	1606	1/1	0.95	0.36	10,10,10,10	0
57	MG	RA	3210	1/1	0.95	0.12	45,45,45,45	0
57	MG	YA	3206	1/1	0.95	0.40	26,26,26,26	0
57	MG	YA	3262	1/1	0.95	0.48	8,8,8,8	0
57	MG	YA	3061	1/1	0.95	0.18	17,17,17,17	0
57	MG	QA	1630	1/1	0.95	0.14	7,7,7,7	0
57	MG	QA	1609	1/1	0.95	0.38	4,4,4,4	0
57	MG	RA	3074	1/1	0.95	0.08	8,8,8,8	0
57	MG	YA	3267	1/1	0.95	0.45	4,4,4,4	0
57	MG	RA	3075	1/1	0.95	0.26	3,3,3,3	0
57	MG	YA	3269	1/1	0.95	0.49	1,1,1,1	0
57	MG	QA	1627	1/1	0.95	0.09	10,10,10,10	0
57	MG	YA	3173	1/1	0.95	0.06	35,35,35,35	0
57	MG	QA	1639	1/1	0.95	0.10	3,3,3,3	0
57	MG	RA	3011	1/1	0.95	0.18	6,6,6,6	0
57	MG	YA	3220	1/1	0.95	0.52	33,33,33,33	0
57	MG	YA	3005	1/1	0.95	0.21	3,3,3,3	0
57	MG	RA	3012	1/1	0.95	0.39	4,4,4,4	0
57	MG	YA	3178	1/1	0.95	0.14	2,2,2,2	0
57	MG	RA	3198	1/1	0.95	0.15	12,12,12,12	0
57	MG	YA	3228	1/1	0.95	0.34	17,17,17,17	0
57	MG	RA	3002	1/1	0.95	0.55	6,6,6,6	0
57	MG	YA	3230	1/1	0.95	0.06	8,8,8,8	0
57	MG	YA	3216	1/1	0.96	0.46	19,19,19,19	0
57	MG	RA	3141	1/1	0.96	0.11	2,2,2,2	0
57	MG	YA	3253	1/1	0.96	0.42	6,6,6,6	0
57	MG	RA	3189	1/1	0.96	0.20	4,4,4,4	0
57	MG	RA	3009	1/1	0.96	0.30	10,10,10,10	0
57	MG	XA	1613	1/1	0.96	0.07	0,0,0,0	0
57	MG	RA	3180	1/1	0.96	0.11	6,6,6,6	0
57	MG	RA	3066	1/1	0.96	0.42	6,6,6,6	0

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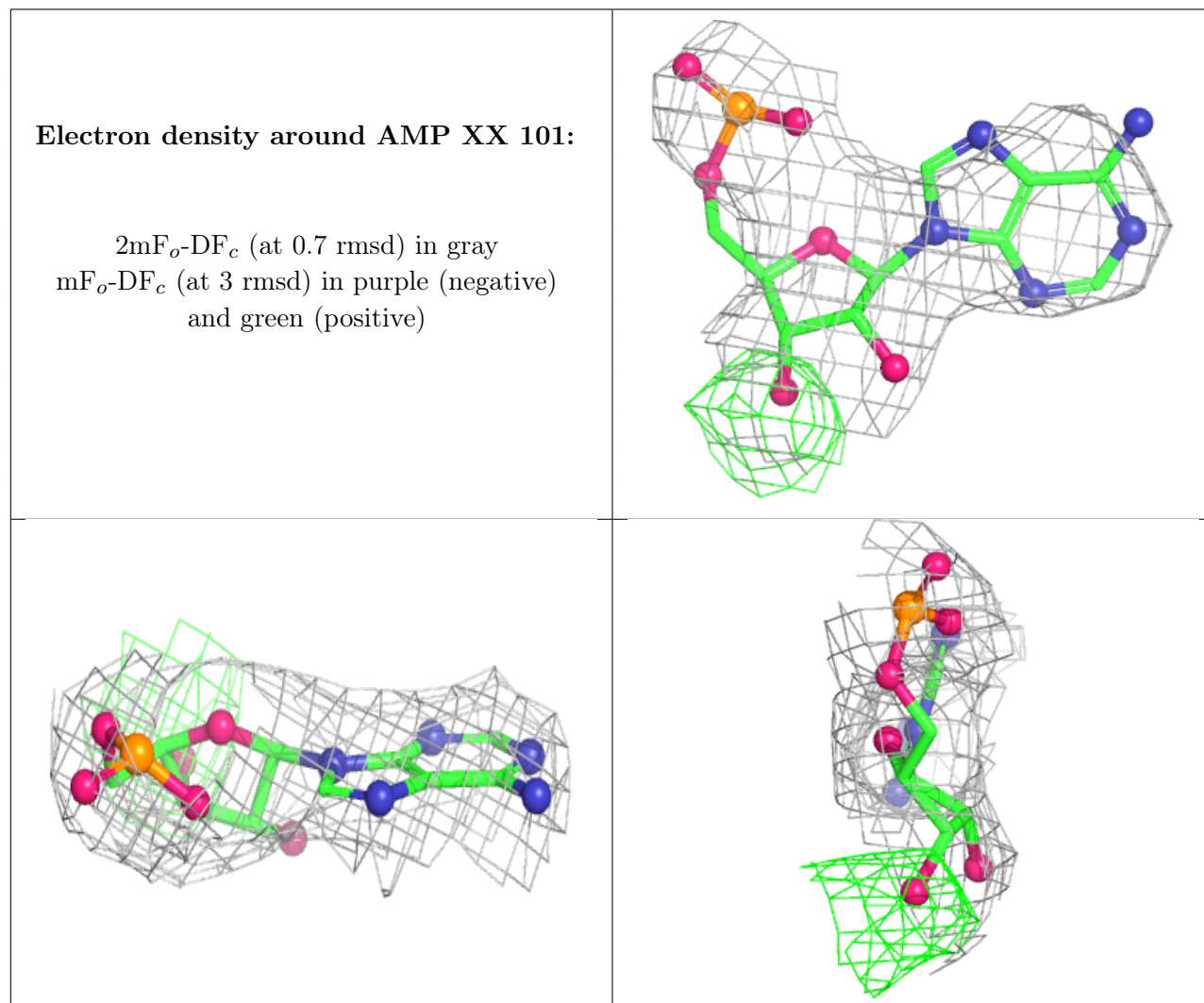
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XX	102	1/1	0.96	0.04	50,50,50,50	0
57	MG	YA	3226	1/1	0.96	0.24	1,1,1,1	0
57	MG	RA	3237	1/1	0.96	0.48	1,1,1,1	0
57	MG	YA	3023	1/1	0.96	0.17	2,2,2,2	0
57	MG	RA	3054	1/1	0.96	0.18	3,3,3,3	0
57	MG	RA	3030	1/1	0.96	0.21	5,5,5,5	0
57	MG	YA	3143	1/1	0.96	0.13	8,8,8,8	0
57	MG	YA	3233	1/1	0.96	0.33	7,7,7,7	0
57	MG	RA	3146	1/1	0.96	0.11	5,5,5,5	0
57	MG	RA	3185	1/1	0.96	0.08	9,9,9,9	0
57	MG	RA	3164	1/1	0.96	0.15	4,4,4,4	0
57	MG	XA	1643	1/1	0.96	0.11	5,5,5,5	0
57	MG	XA	1626	1/1	0.96	0.12	6,6,6,6	0
57	MG	RF	301	1/1	0.96	0.17	2,2,2,2	0
57	MG	YA	3241	1/1	0.96	0.12	5,5,5,5	0
57	MG	QA	1652	1/1	0.96	0.17	12,12,12,12	0
57	MG	XA	1629	1/1	0.96	0.23	8,8,8,8	0
57	MG	XA	1651	1/1	0.96	0.12	25,25,25,25	0
57	MG	YA	3211	1/1	0.96	0.45	7,7,7,7	0
57	MG	YA	3056	1/1	0.96	0.14	5,5,5,5	0
57	MG	YA	3057	1/1	0.96	0.61	4,4,4,4	0
57	MG	YA	3105	1/1	0.96	0.12	4,4,4,4	0
57	MG	YA	3108	1/1	0.97	0.35	1,1,1,1	0
57	MG	XA	1609	1/1	0.97	0.52	10,10,10,10	0
57	MG	YA	3145	1/1	0.97	0.11	9,9,9,9	0
57	MG	YA	3037	1/1	0.97	0.17	13,13,13,13	0
57	MG	XV	102	1/1	0.97	0.36	9,9,9,9	0
57	MG	YA	3066	1/1	0.97	0.48	7,7,7,7	0
57	MG	YA	3168	1/1	0.97	0.20	41,41,41,41	0
57	MG	YA	3213	1/1	0.97	0.10	19,19,19,19	0
57	MG	RA	3162	1/1	0.97	0.08	2,2,2,2	0
57	MG	RA	3149	1/1	0.97	0.06	20,20,20,20	0
57	MG	YA	3132	1/1	0.97	0.15	5,5,5,5	0
57	MG	RA	3175	1/1	0.97	0.15	1,1,1,1	0
57	MG	XA	1644	1/1	0.97	0.12	5,5,5,5	0
57	MG	XA	1622	1/1	0.97	0.07	7,7,7,7	0
57	MG	YA	3246	1/1	0.97	0.12	7,7,7,7	0
57	MG	XA	1623	1/1	0.97	0.11	14,14,14,14	0
57	MG	YA	3197	1/1	0.97	0.06	1,1,1,1	0
57	MG	QA	1608	1/1	0.97	0.05	10,10,10,10	0
57	MG	YA	3074	1/1	0.97	0.15	11,11,11,11	0
57	MG	YA	3224	1/1	0.97	0.24	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	RA	3178	1/1	0.97	0.05	1,1,1,1	0
57	MG	YA	3202	1/1	0.97	0.06	1,1,1,1	0
57	MG	QA	1656	1/1	0.97	0.08	30,30,30,30	0
57	MG	QA	1651	1/1	0.97	0.07	9,9,9,9	0
57	MG	XA	1645	1/1	0.98	0.11	1,1,1,1	0
57	MG	YA	3163	1/1	0.98	0.06	4,4,4,4	0
57	MG	YA	3003	1/1	0.98	0.15	2,2,2,2	0
57	MG	RA	3097	1/1	0.98	0.38	2,2,2,2	0
57	MG	YA	3225	1/1	0.98	0.05	10,10,10,10	0
57	MG	QA	1617	1/1	0.98	0.17	4,4,4,4	0
57	MG	YA	3210	1/1	0.98	0.21	3,3,3,3	0
57	MG	RA	3099	1/1	0.98	0.05	10,10,10,10	0
57	MG	YA	3248	1/1	0.98	0.47	0,0,0,0	0
57	MG	RA	3172	1/1	0.98	0.08	4,4,4,4	0
57	MG	RA	3113	1/1	0.98	0.10	0,0,0,0	0
57	MG	YA	3231	1/1	0.98	0.19	45,45,45,45	0
57	MG	QA	1634	1/1	0.98	0.06	7,7,7,7	0
57	MG	YA	3199	1/1	0.98	0.08	55,55,55,55	0
57	MG	RA	3156	1/1	0.98	0.05	9,9,9,9	0
57	MG	YA	3235	1/1	0.98	0.08	3,3,3,3	0
57	MG	RB	201	1/1	0.98	0.10	8,8,8,8	0
57	MG	YA	3187	1/1	0.98	0.09	2,2,2,2	0
57	MG	YA	3258	1/1	0.98	0.38	1,1,1,1	0
57	MG	RB	202	1/1	0.98	0.08	4,4,4,4	0
57	MG	RA	3176	1/1	0.98	0.14	3,3,3,3	0
57	MG	XA	1625	1/1	0.99	0.05	5,5,5,5	0
57	MG	RA	3095	1/1	0.99	0.34	1,1,1,1	0
57	MG	RA	3118	1/1	0.99	0.05	2,2,2,2	0
57	MG	QA	1653	1/1	0.99	0.07	67,67,67,67	0
57	MG	YA	3169	1/1	0.99	0.04	6,6,6,6	0
58	ZN	QD	301	1/1	0.99	0.27	50,50,50,50	0
57	MG	QM	201	1/1	0.99	0.03	44,44,44,44	0
57	MG	XA	1649	1/1	0.99	0.17	0,0,0,0	0
58	ZN	XD	301	1/1	0.99	0.30	50,50,50,50	0
58	ZN	XN	101	1/1	0.99	0.09	84,84,84,84	0
57	MG	YA	3065	1/1	0.99	0.04	5,5,5,5	0
57	MG	XA	1614	1/1	0.99	0.05	26,26,26,26	0
57	MG	RA	3107	1/1	1.00	0.09	10,10,10,10	0
57	MG	XA	1639	1/1	1.00	0.07	5,5,5,5	0
57	MG	YA	3110	1/1	1.00	0.03	2,2,2,2	0
57	MG	YA	3017	1/1	1.00	0.12	1,1,1,1	0
57	MG	YA	3144	1/1	1.00	0.06	4,4,4,4	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.