



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 20, 2024 – 05:34 PM EDT

PDB ID : 4LFZ  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

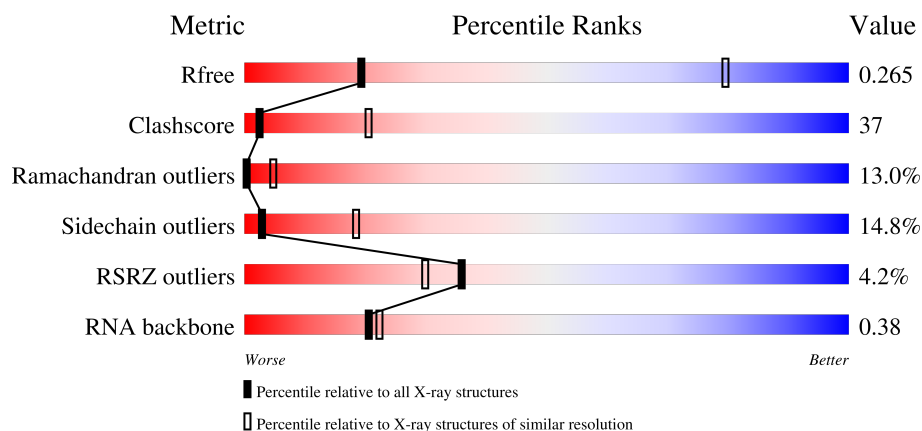
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)
RNA backbone	3102	1041 (4.84-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	

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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	

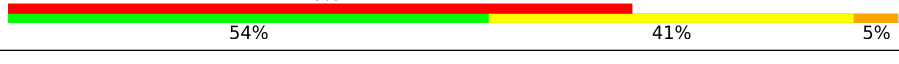
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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	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	1629	-	-	-	X
57	MG	QA	1631	-	-	-	X
57	MG	QF	201	-	-	-	X
57	MG	QX	101	-	-	-	X
57	MG	RA	3003	-	-	-	X
57	MG	RA	3007	-	-	-	X
57	MG	RA	3049	-	-	-	X
57	MG	RA	3062	-	-	-	X
57	MG	RA	3138	-	-	-	X
57	MG	RA	3157	-	-	-	X
57	MG	RA	3173	-	-	-	X
57	MG	RA	3199	-	-	-	X
57	MG	RA	3213	-	-	-	X
57	MG	RA	3219	-	-	-	X
57	MG	RA	3227	-	-	-	X
57	MG	RA	3239	-	-	-	X
57	MG	RP	201	-	-	-	X
57	MG	XA	1642	-	-	-	X
57	MG	YA	3030	-	-	-	X
57	MG	YA	3076	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3121	-	-	-	X
57	MG	YA	3131	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3152	-	-	-	X
57	MG	YA	3172	-	-	-	X
57	MG	YA	3176	-	-	-	X
57	MG	YA	3183	-	-	-	X
57	MG	YA	3196	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3242	-	-	-	X
57	MG	YA	3250	-	-	-	X
57	MG	YA	3254	-	-	-	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 (three-letter code: 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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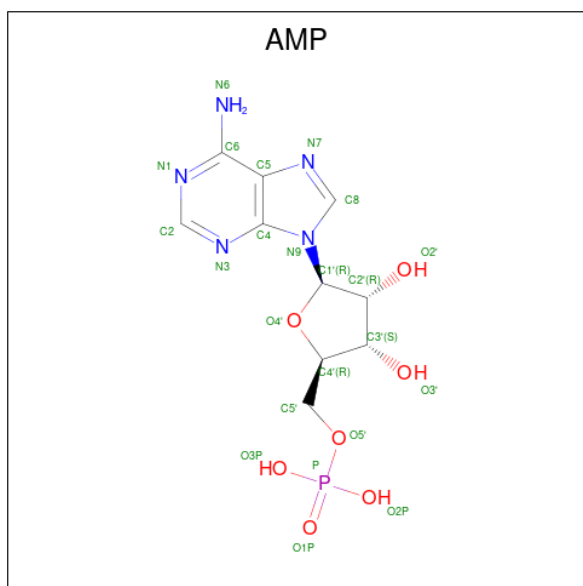
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y5	1	Total	Mg	0	0
			1	1		
57	Y7	1	Total	Mg	0	0
			1	1		

- Molecule 58 is ZINC ION (three-letter code: 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 (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).

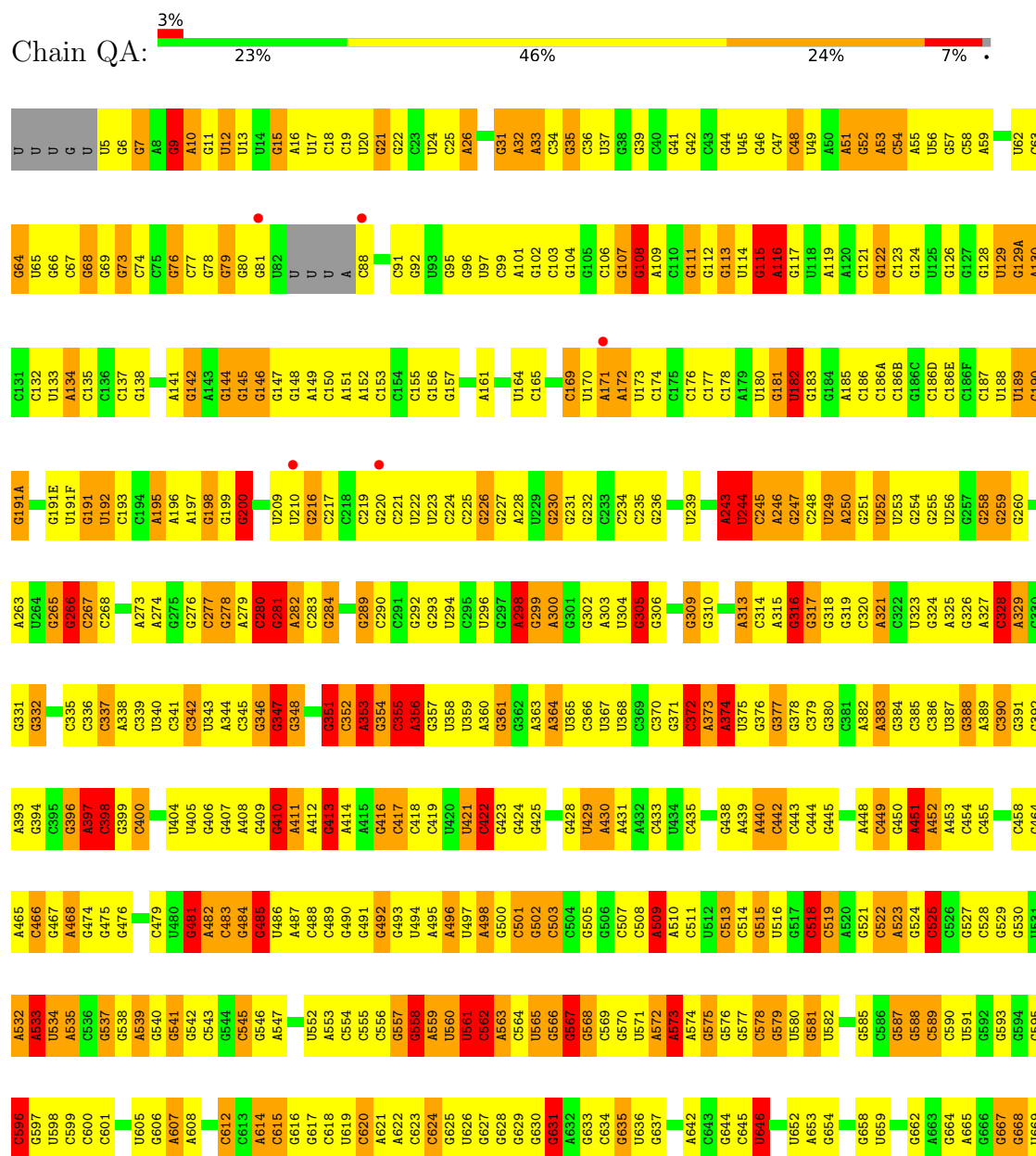


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	XX	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

### 3 Residue-property plots

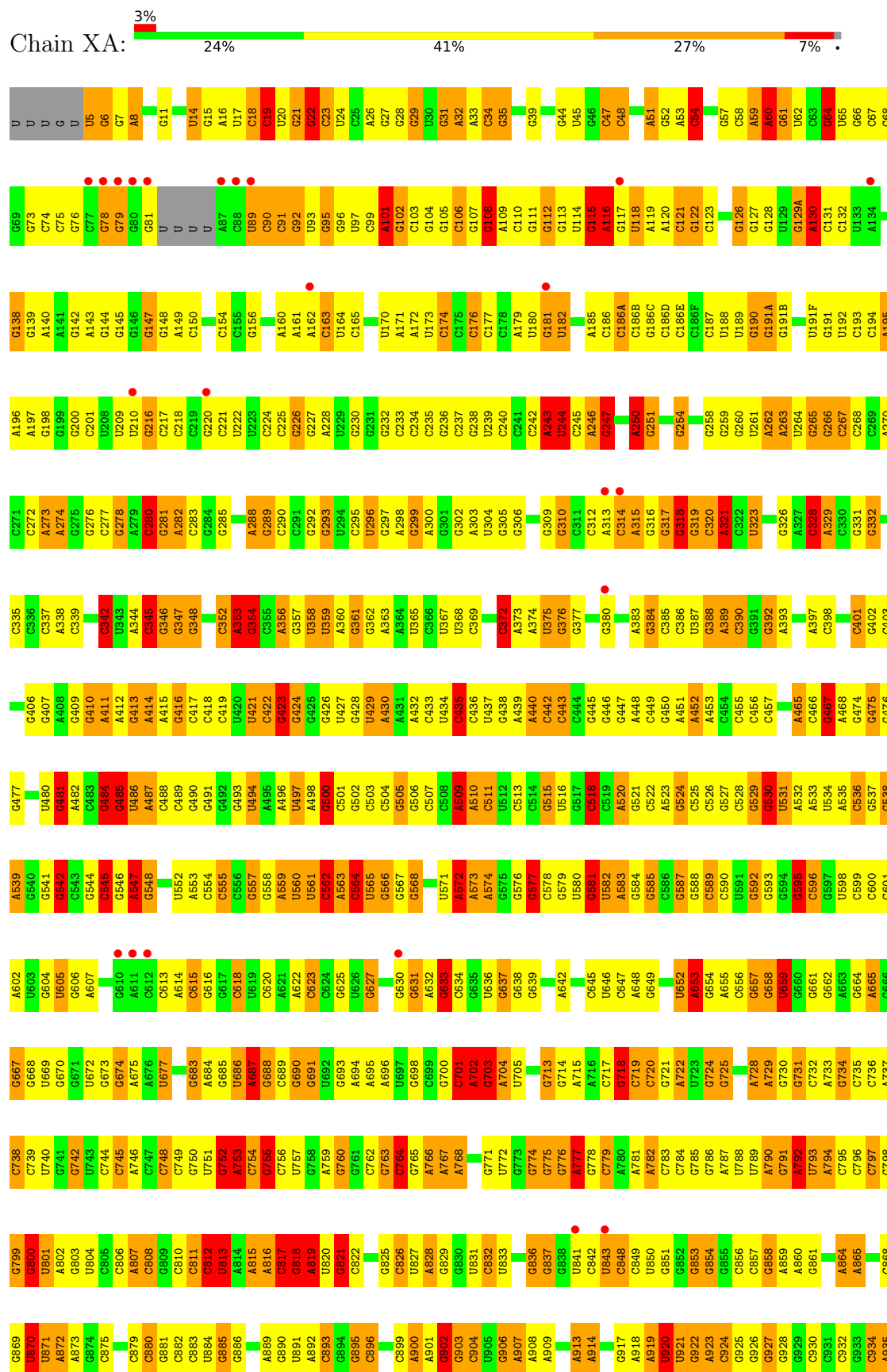
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

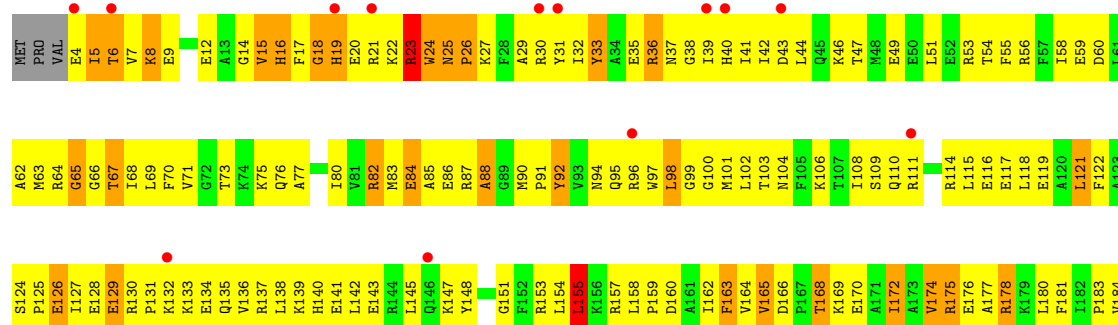


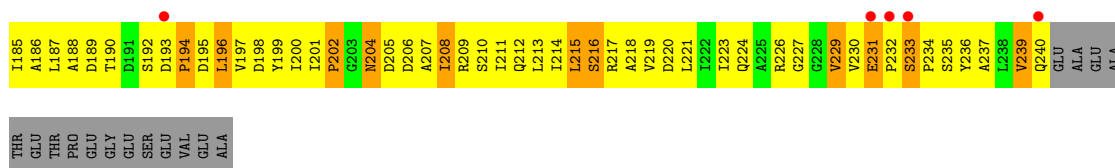
A1513	G1435	G1371	G1312	G1184	G1119	G1058	A994	C934	G869	G799	C736	G670
C1514	U1436	U1372	U1313	G1185	G1120	C1059	C995	A935	U870	G800	A737	G671
G1516	C1437	A1373	C1314	G1186	U1121	C1060	U999	C936	U871	U803	C738	U672
G1517	G1438	A1374	U1315	G1187	U1122	G1061	U999	A937	A872	G803	C739	G673
A1518	G1439	A1375	C1316	A1188	G1123	U1062	A1000	A938	A873	U804	U740	G674
A1519	C1440	U1376	G1317	C1189	G1124	C1063	G1001	G939	G874	G805	A675	A675
G1520	G1441	A1377	A1318	G1190	U1125	U1064	G1002	C940	C875	C806	G742	A676
G1442	G1442	C1378	A1319	A1191	U1126	U1065	A1003	G941	G876	A807	U677	U677
G1443	G1443	G1379	C1320	C1192	G1127	C1066	A1004	G942	C877	C808	U678	U678
U1522	A1446	U1380	C1321	U1194	C1128	U1067	A1005	U943	C878	C811	A746	C679
G1523	G1447	U1381	C1322	U1194	G1129	G1068	C1006	G944	C879	U812	C747	C679
C1524	G1447	C1382	G1323	C1195	A1130	C1069	C1007	G945	C880	C813	G748	G682
G1525	U1450	G1383	A1324	U1196	G1131	U1070	C1008	A946	C881	U813	C749	G683
G1526	A1451	C1384	C1325	G1197	C1132	C1071	G1009	G947	C882	A814	G750	A684
G1452	C1452	G1385	C1326	U1198	G1133	U1072	A1014	C948	C883	A815	G751	G685
G1453	G1453	C1386	C1327	U1199	G1134	U1073	A1015	A949	U884	A816	G752	U686
G1454	G1454	C1387	C1262	U1200	U1135	G1074	A1015	U950	C885	C817	A753	A687
G1455	G1455	C1387	C1328	C1201	U1136	C1075	A1016	U951	C886	G951	C754	A694
G1530	C1459	A1329	U1329	A1201	U1137	U1076	G1017	U952	C886	A819	G755	G689
A1531	U1461	G1330	U1330	G1202	C1137	U1077	C1018	G953	A889	U820	G756	G690
U	A1461	G1331	U1331	G1203	C1138	U1077	C1019	G954	C890	U821	U757	G691
C	A1461	A1332	U1332	A1204	G1139	U1078	C1019	U955	U891	C822	G758	U692
A	G1469	A1333	U1333	U1205	C1140	U1079	U1020	U956	A892	C823	A759	G693
C	G1470	G1334	G1334	G1206	C1141	A1080	G1021	U956	A900	C824	G760	A694
C	C1471	C1335	C1335	G1207	G1142	U1081	G1022	U957	C893	C825	G761	A695
U	G1472	C1336	C1336	C1208	G1143	U1082	G1023	A958	C894	C826	C762	A696
C	U1472	G1337	G1337	C1209	G1144	U1083	G1024	A959	C895	C827	G763	C701
U	A1473	G1338	G1338	G1210	C1145	U1084	U1025	U960	C898	U827	G764	A702
C	G1474	A1339	U1339	C1211	A1146	U1085	U1026	U961	C899	U828	G765	A703
U	G1475	A1340	U1340	U1212	C1147	U1086	C1027	C962	A900	C829	A766	G703
U	G1476	C1341	U1341	C1213	U1148	U1087	C1028	G963	A901	C830	A767	A704
C	G1477	U1342	U1342	C1214	C1149	U1088	G1029	A964	G902	U833	A768	U705
C	C1478	G1343	G1343	G1215	U1150	U1089	C1030	A965	G903	C834	G769	A706
U	C1479	A1344	U1344	G1216	A1151	U1090	U1031	A966	C904	U835	C770	C707
U	G1480	U1345	U1345	C1217	A1152	U1091	A1032	A968	C904	U836	G771	C708
U	U1481	A1346	U1346	C1218	G1154	A1093	G1032A	A969	C909	U837	U772	G709
U	U1481	G1347	G1347	U1219	G1155	U1094	G1032B	C970	U911	U838	G773	G710
U	U1485	U1348	U1348	G1220	C1156	U1095	G1033	C971	U912	U841	G774	G710
G1486	A1486	A1349	A1349	G1221	A1157	C1096	U1034	C972	C912	U842	A777	G713
G1487	A1487	A1350	U1350	C1222	C1158	U1099	A1035	C973	A913	U843	A777	G714
C1490	C1411	A1288	C1288	C1223	U1159	U1099	G1036	A974	A914	C848	G778	A715
G1491	A1413	A1289	C1352	G1224	C1160	C1100	C1037	A975	A915	C849	C779	A716
A1492	U1414	C1353	G1353	A1225	C1161	A1101	C1038	G976	G916	U850	C779	A716
C1501	G1415	G1354	G1354	C1226	C1162	A1102	C1039	A977	G917	A781	G717	G717
A1502	G1416	G1355	G1355	A1227	C1163	C1103	U1040	A978	A918	A782	C719	G718
A1502	G1497	G1294	G1294	C1228	C1163	C1103	U1040	A978	A918	A782	C719	G718
A1503	U1498	G1295	G1295	C1228	C1163	C1103	U1040	A978	A918	A782	C719	G718
G1504	U1499	C1296	C1296	A1229	G1170	G1104	A1044	C979	A919	C852	G720	C720
G1505	A1500	C1297	C1297	C1230	A1171	A1105	C1045	C980	G920	C853	G721	C721
C1501	A1501	C1298	C1298	G1231	G1172	G1106	U1046	G981	U921	C854	A722	A722
A1502	A1502	A1299	A1299	C1231	C1173	C1107	G1047	U982	G922	C855	U723	U723
A1503	C1361	G1300	G1300	G1234	G1173	C1108	U1047	A983	A923	C856	G724	G724
A1504	C1362	U1301	U1301	U1235	G1174	C1109	G1048	C984	C924	C857	G725	G725
G1505	U1425	U1302	C1362A	A1236	G1175	A1110	U1049	C985	G925	A859	G726	G726
U1506	U1427	C1303	C1363	C1237	A1176	C1111	G1050	A986	A860	U789	G727	G727
A1507	A1428	G1304	G1304	A1238	G1177	C1112	C1051	G987	G927	A790	A728	A728
A1508	C1429	G1305	G1305	A1239	G1178	C1113	U1052	G988	G928	A792	A729	A729
C1509	C1430	A1306	U1240	G1241	A1179	C1114	G1053	C989	G930	U793	G730	G730
C1431	C1367	U1307	U1307	G1241	A1180	C1115	C1054	C990	C931	A794	G731	G731
G1432	G1368	U1307	U1307	C1242	A1181	C1116	A1055	U991	C932	C866	G734	G734
A1433	C1369	G1310	G1310	C1243	G1182	G1117	U1056	U992	C932	C867	C737	C737
U1512	U1512	G1311	G1311	C1244	A1183	C1118	G1057	G993	G933	C868	G798	G798

● Molecule 1: 16S rRNA

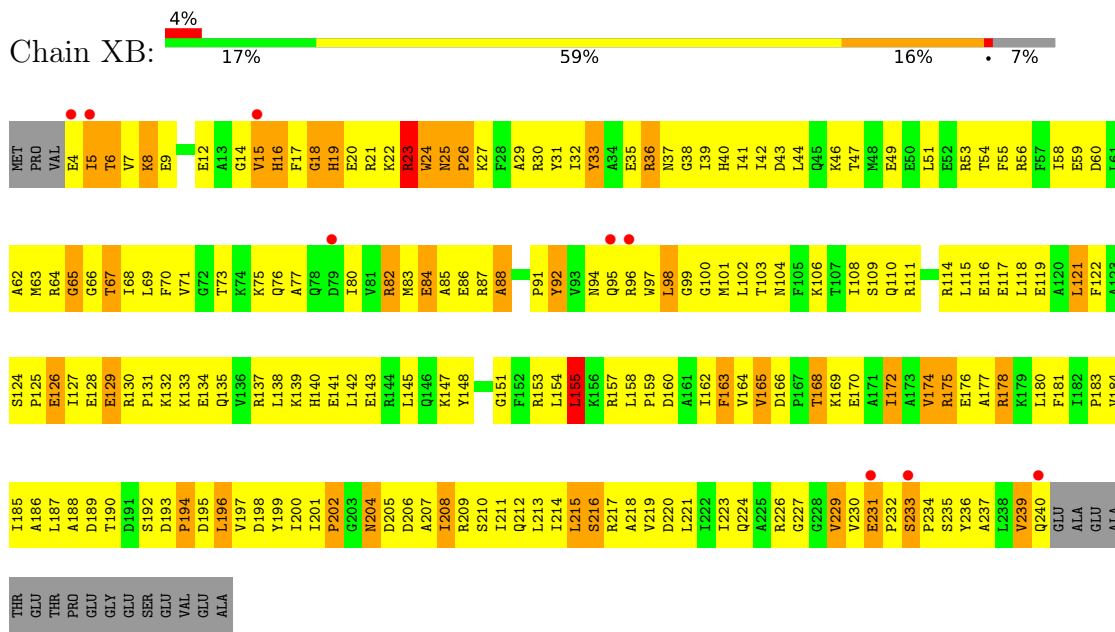




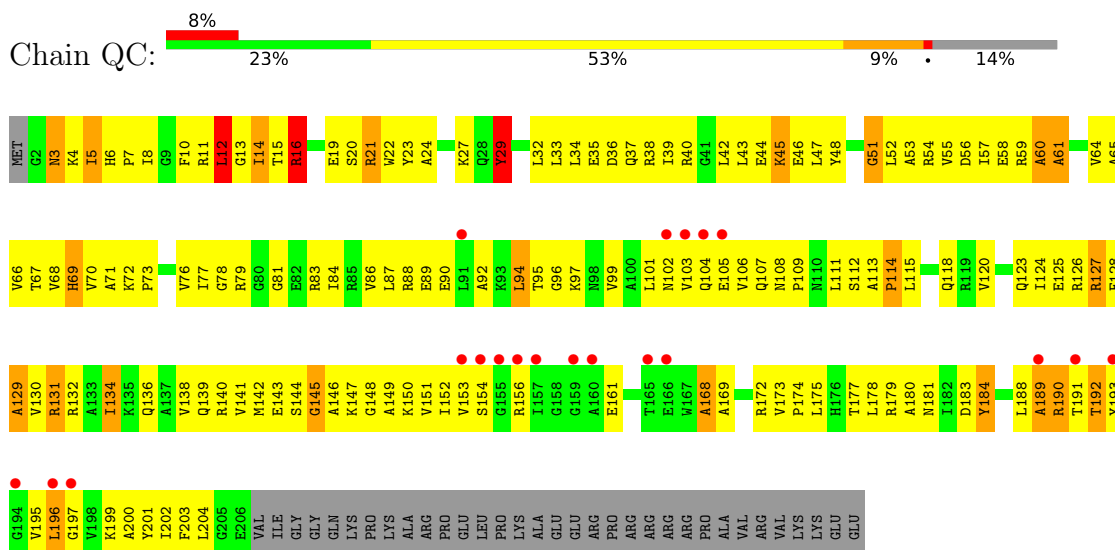




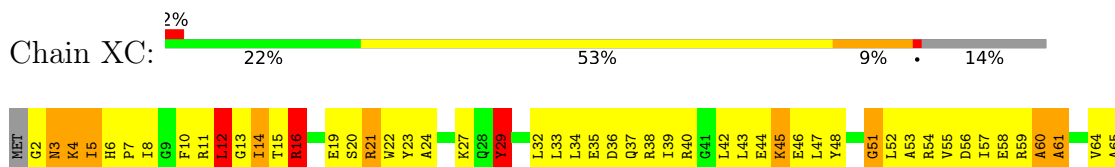
• Molecule 2: 30S ribosomal protein S2

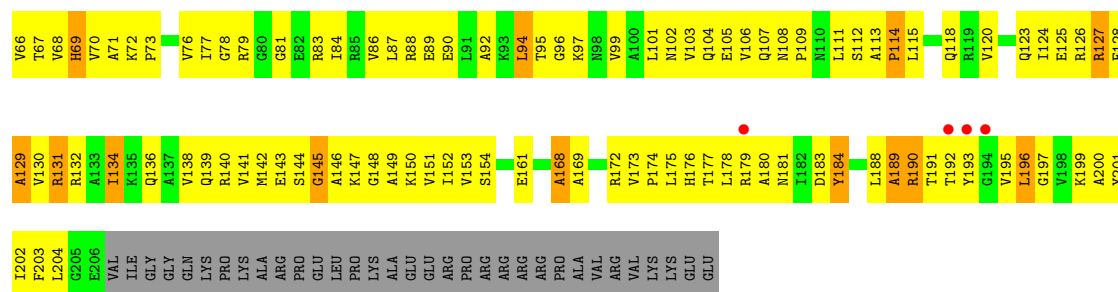


• Molecule 3: 30S ribosomal protein S3

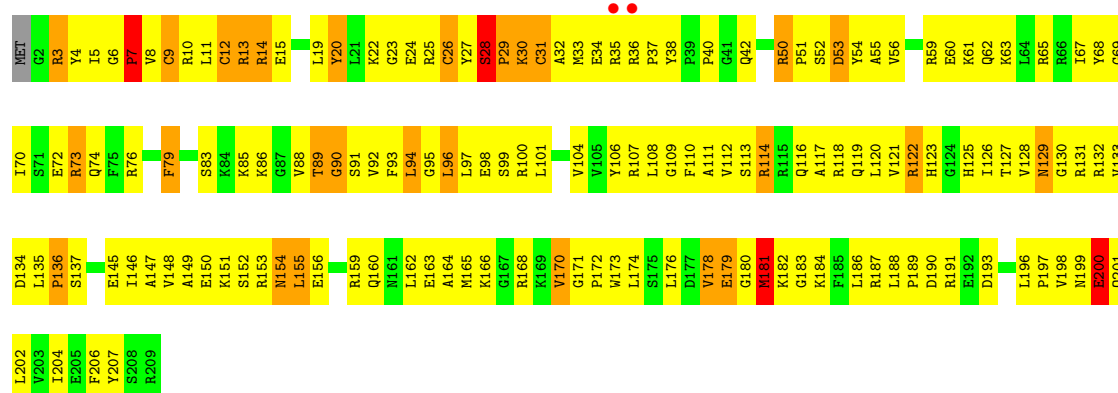


• Molecule 3: 30S ribosomal protein S3

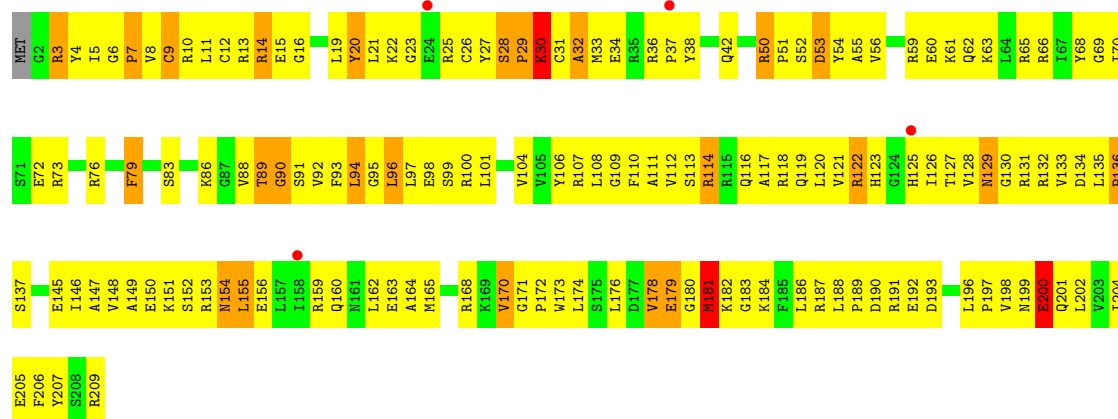




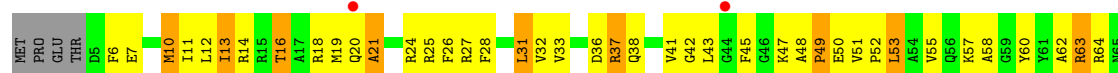
• Molecule 4: 30S ribosomal protein S4

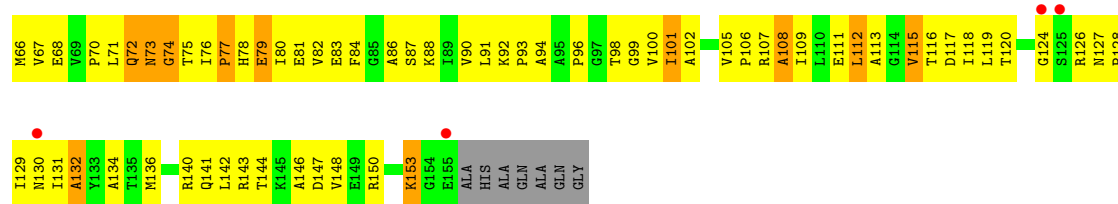


• Molecule 4: 30S ribosomal protein S4



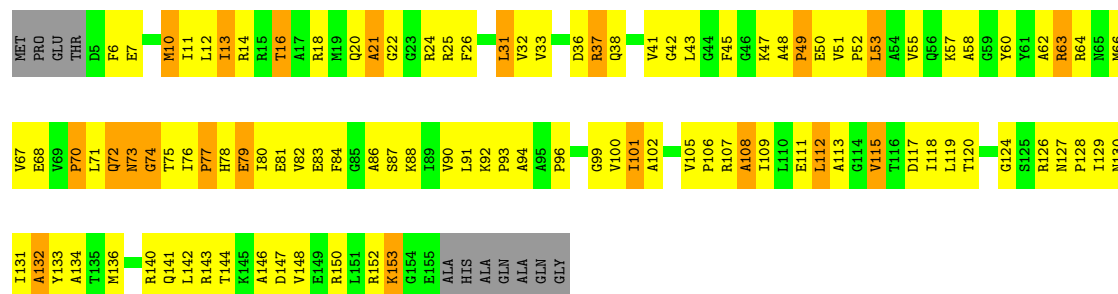
• Molecule 5: 30S ribosomal protein S5





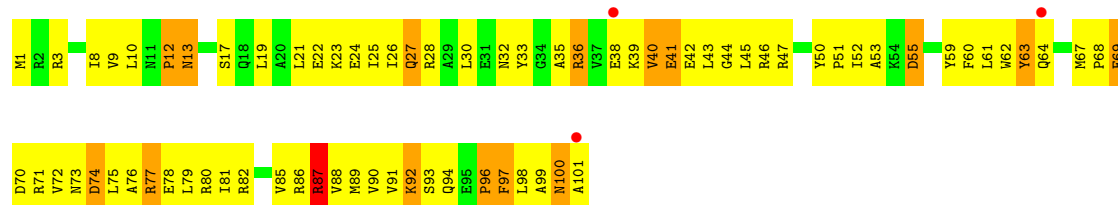
• Molecule 5: 30S ribosomal protein S5

Chain XE: 28% 52% 13% 7%



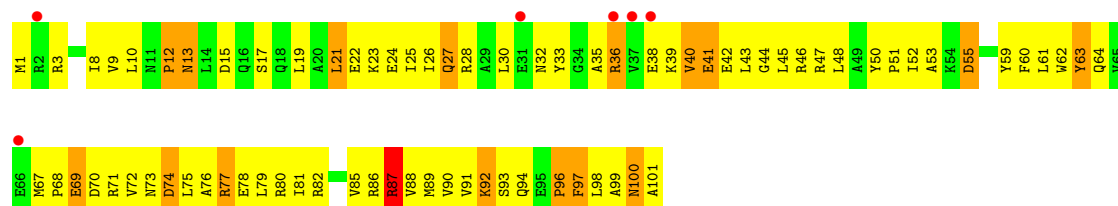
• Molecule 6: 30S ribosomal protein S6

Chain QF: 3% 26% 58% 15%



• Molecule 6: 30S ribosomal protein S6

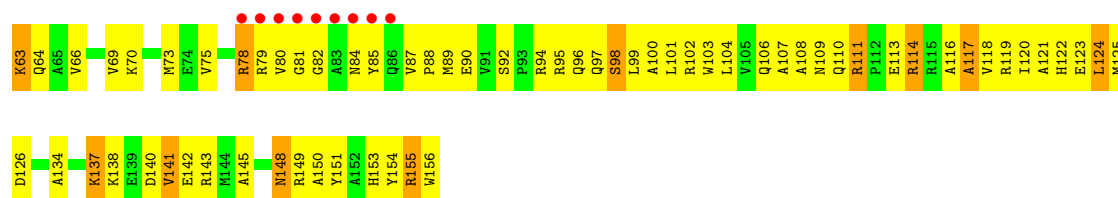
Chain XF: 6% 24% 59% 16%



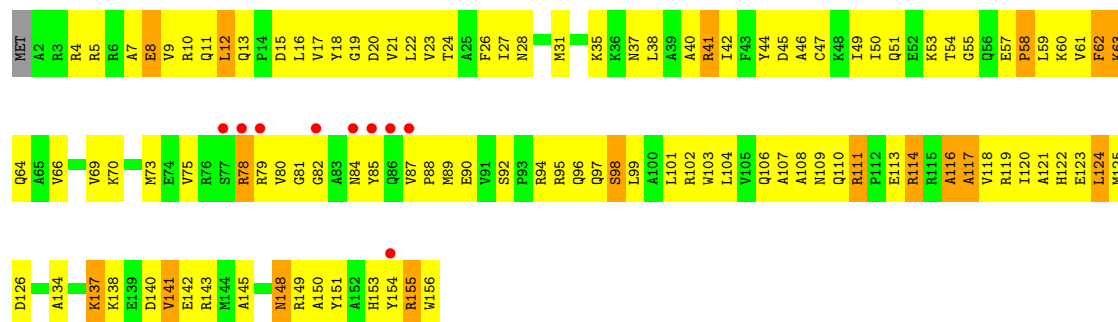
• Molecule 7: 30S ribosomal protein S7

Chain QG: 6% 26% 63% 10%

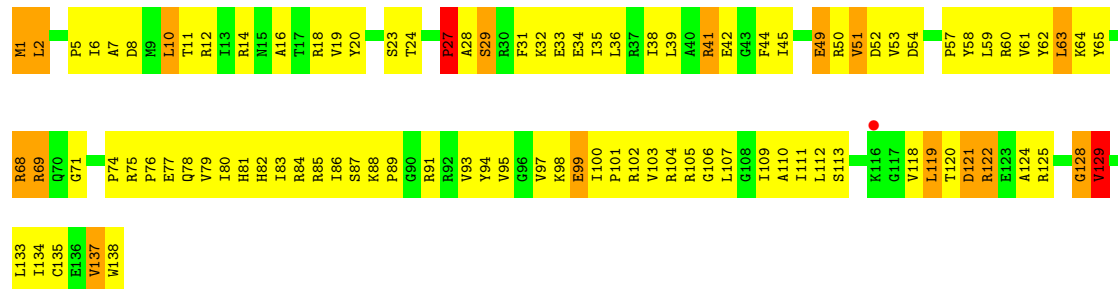




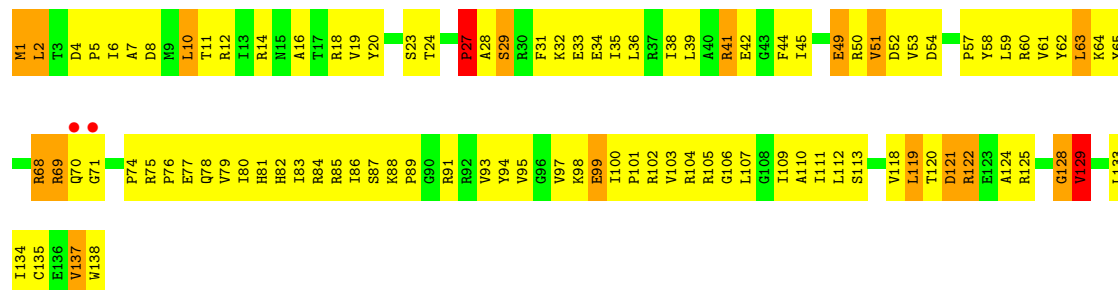
• Molecule 7: 30S ribosomal protein S7



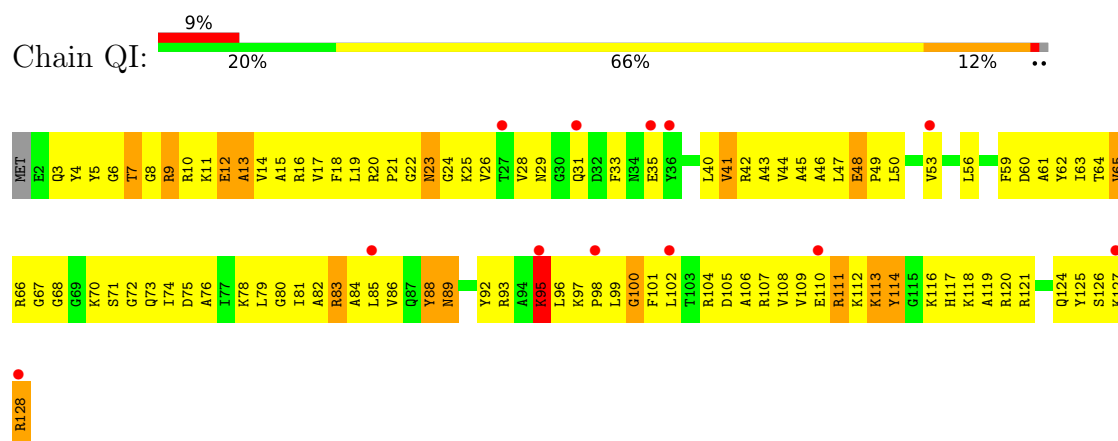
• Molecule 8: 30S ribosomal protein S8



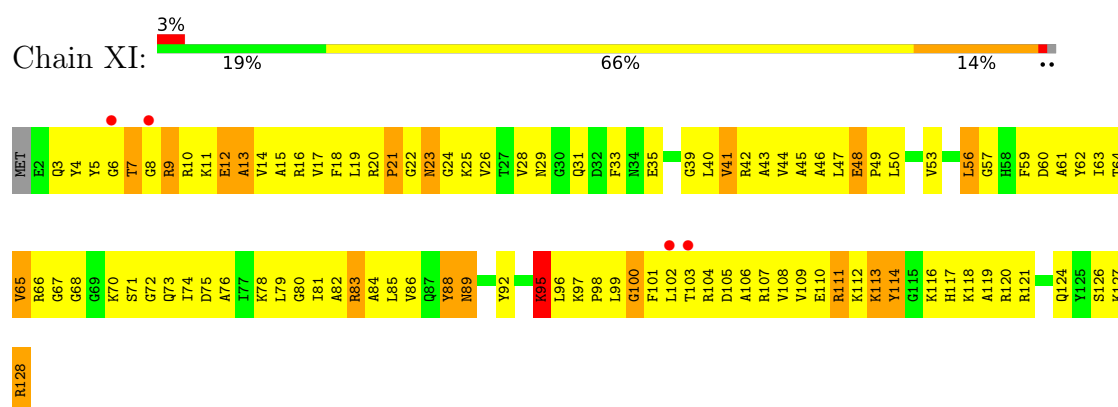
• Molecule 8: 30S ribosomal protein S8



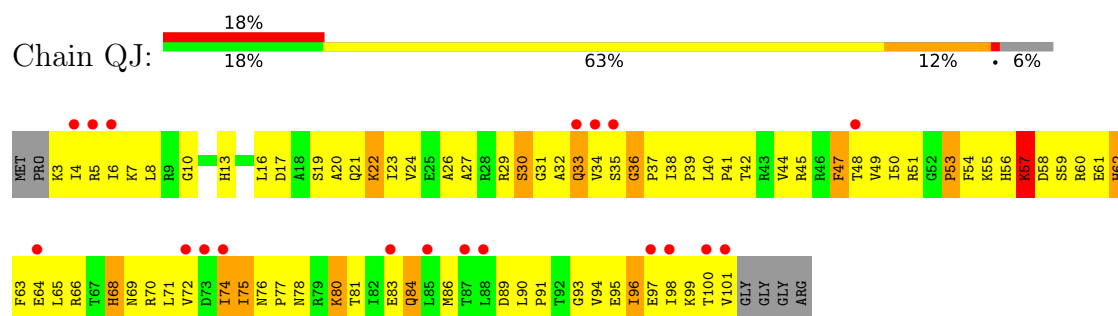
• Molecule 9: 30S ribosomal protein S9



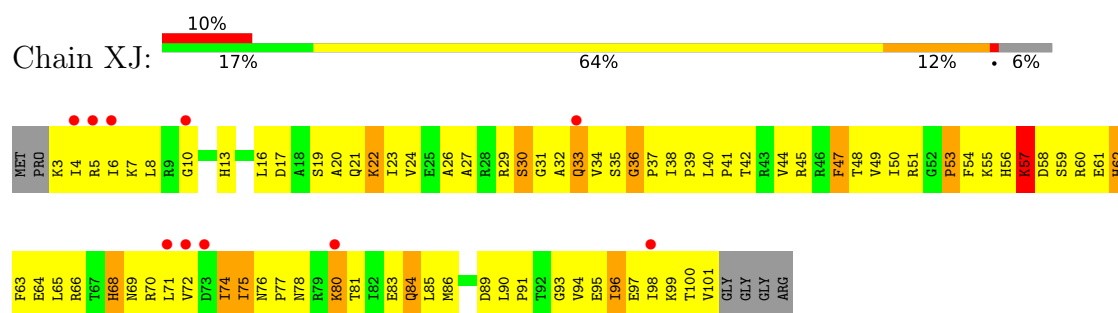
• Molecule 9: 30S ribosomal protein S9



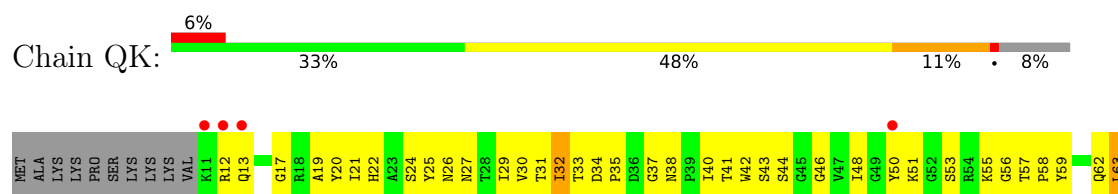
• Molecule 10: 30S ribosomal protein S10



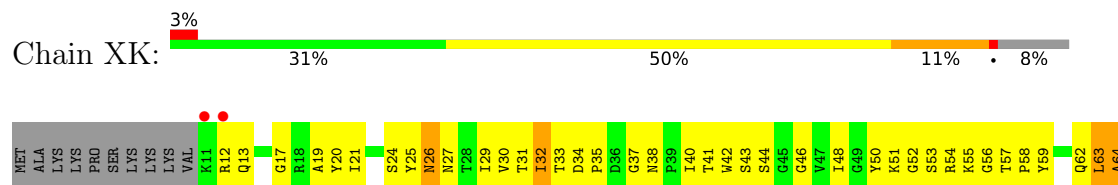
• Molecule 10: 30S ribosomal protein S10



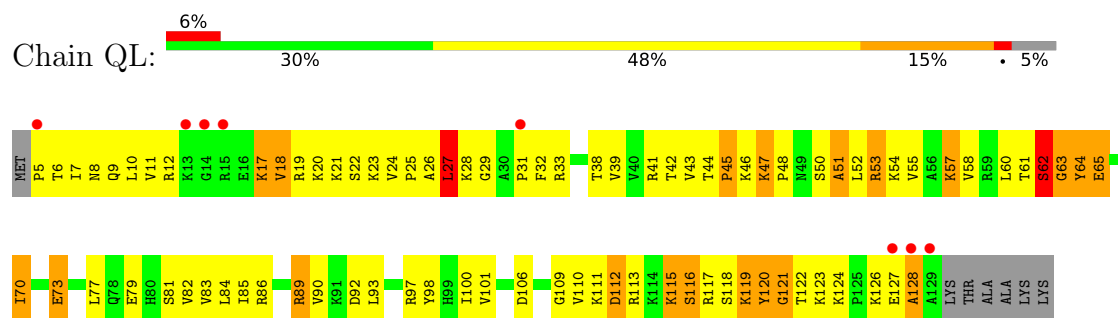
• Molecule 11: 30S ribosomal protein S11



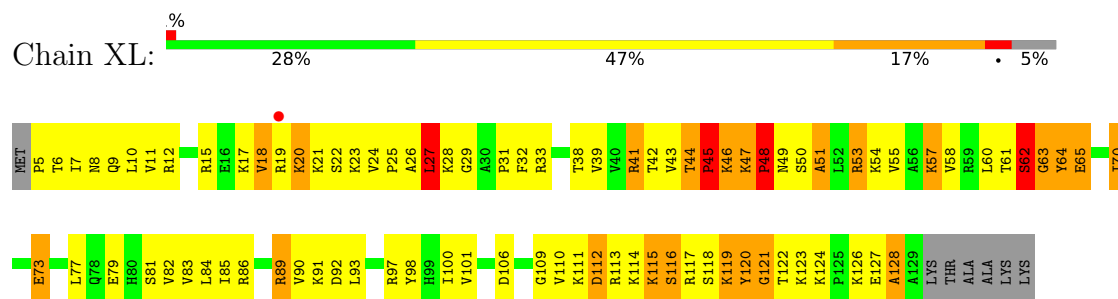
• Molecule 11: 30S ribosomal protein S11



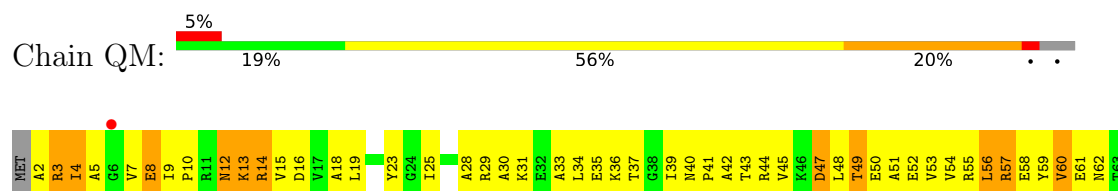
• Molecule 12: 30S ribosomal protein S12

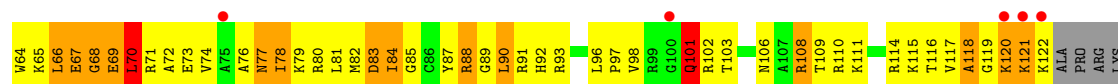


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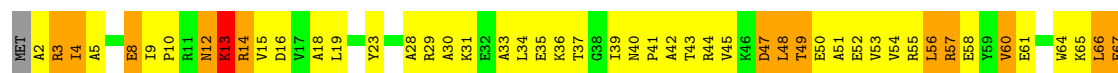


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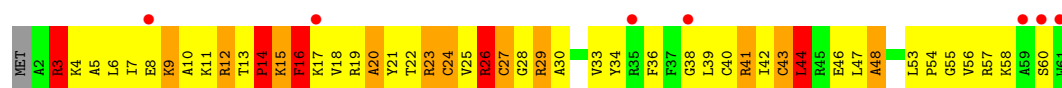




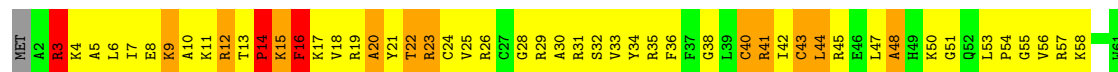
- Molecule 13: 30S ribosomal protein S13



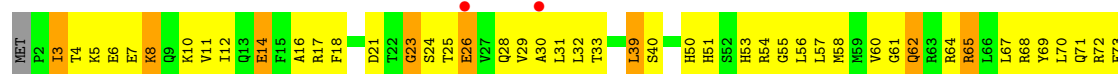
- Molecule 14: 30S ribosomal protein S14



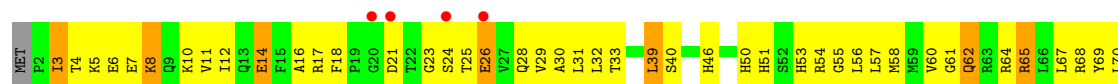
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

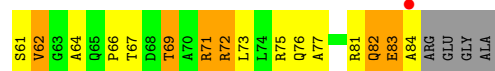
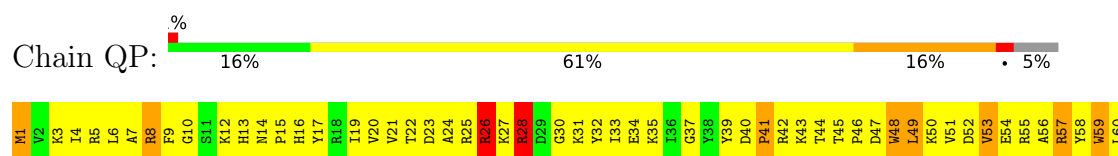


- Molecule 15: 30S ribosomal protein S15

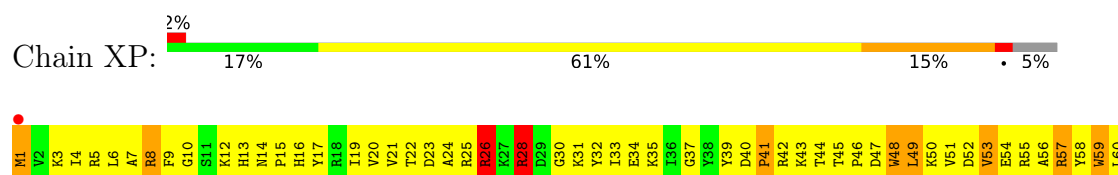


- Molecule 16: 30S ribosomal protein S16

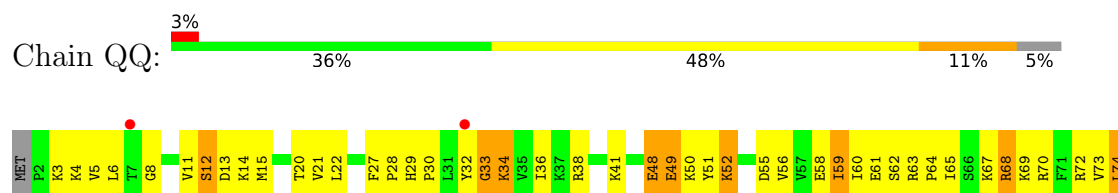




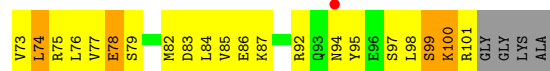
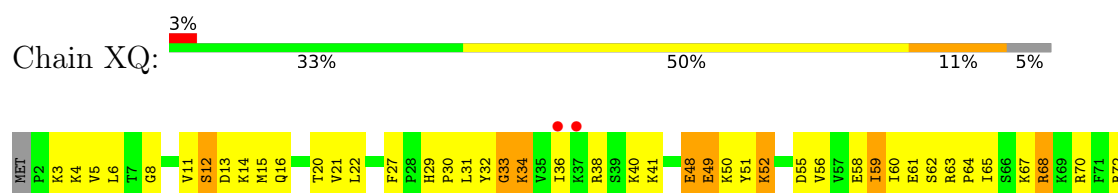
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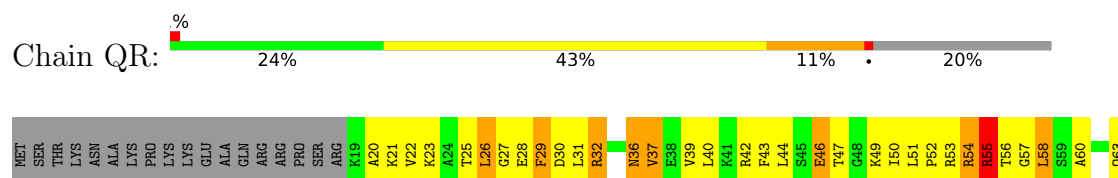
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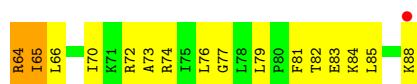


• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

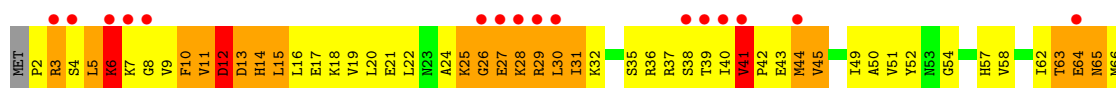
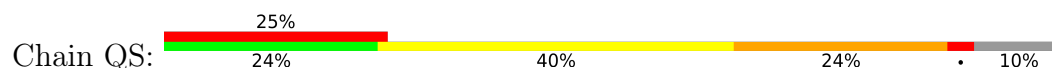




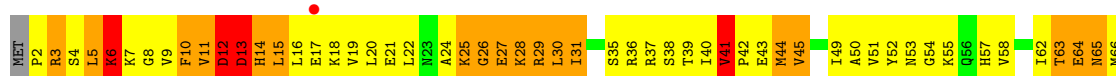
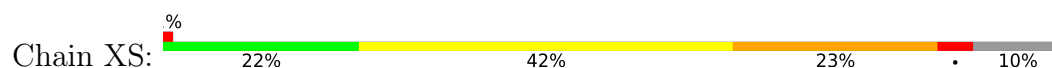
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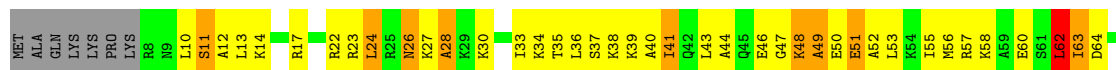
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

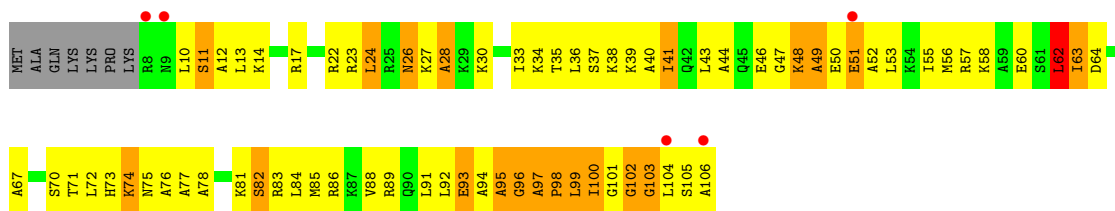


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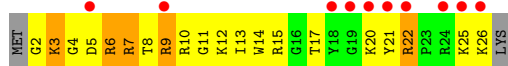


- Molecule 20: 30S ribosomal protein S20

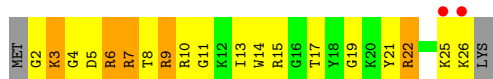
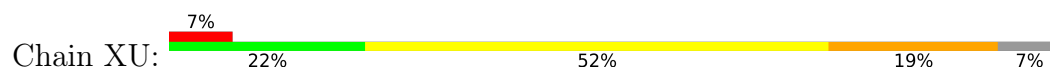




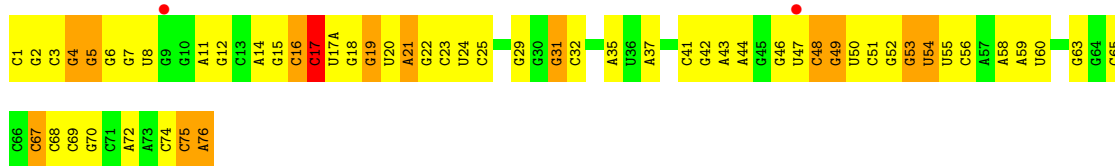
- Molecule 21: 30S ribosomal protein S21



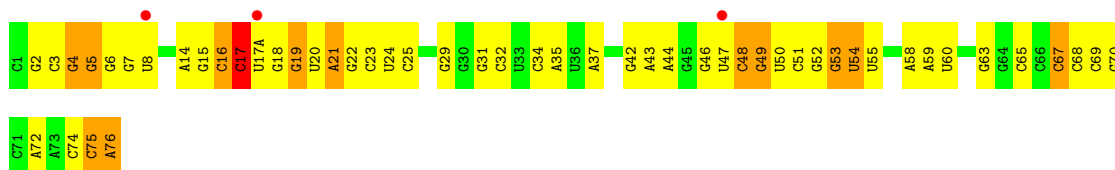
- Molecule 21: 30S ribosomal protein S21



- Molecule 22: P-site tRNA fMet



- Molecule 22: P-site tRNA fMet



- Molecule 23: A-site ASL SufA6



- Molecule 23: A-site ASL SufA6





G2193	G2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264												
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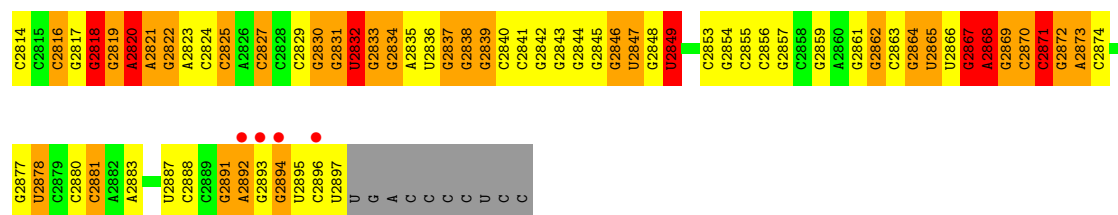




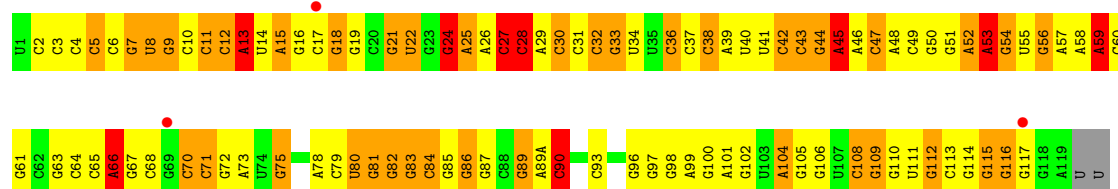
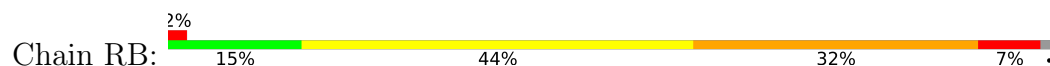


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	G1756	G1674	C1611	A1546A	A1486	G1422	C1362	U1240	C1178	G1113	G1051
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		U1693	G1630	A1567	C1505	G1441	G1381	G1259	G1197	G1136	A1070
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		G1697	G1633	A1571	C1509	A1444A	G1385	G1264	C1200	C1140	C1075
		A1698	A1634	A1572	A1510	C1445	C1386	A1265	C1201	U1141	C1076
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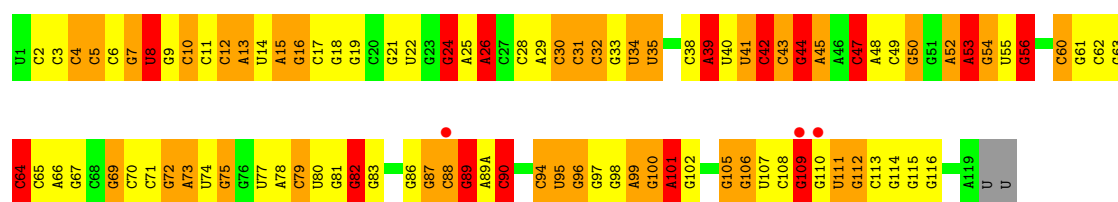
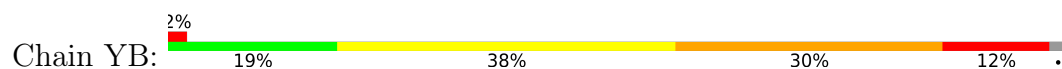
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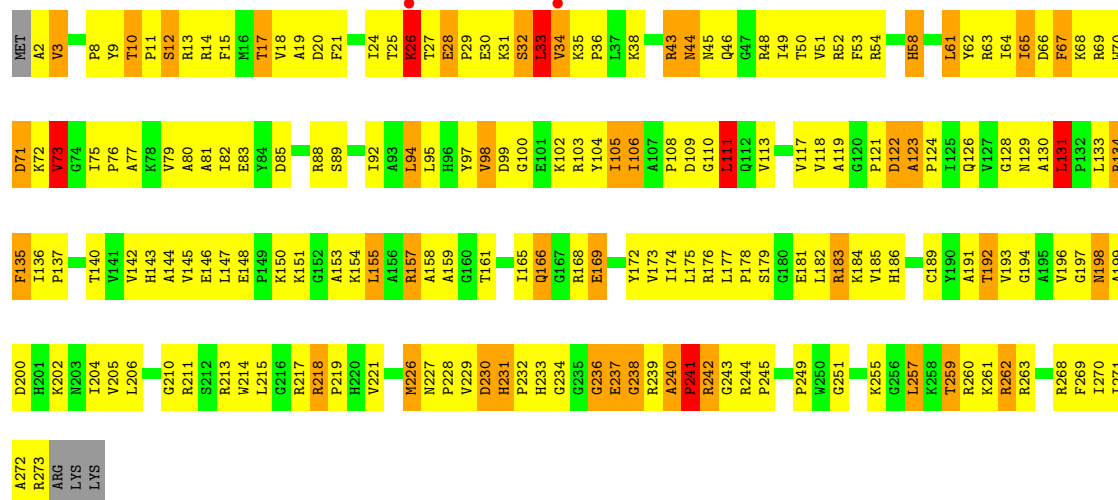
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA

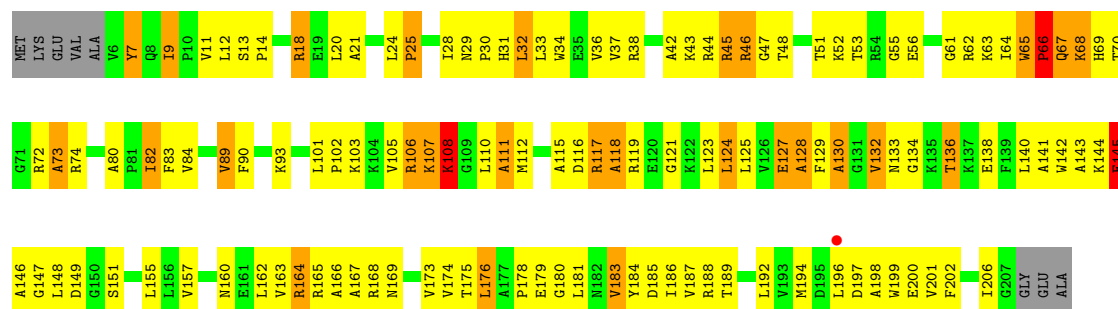


• Molecule 27: 50S ribosomal protein L2

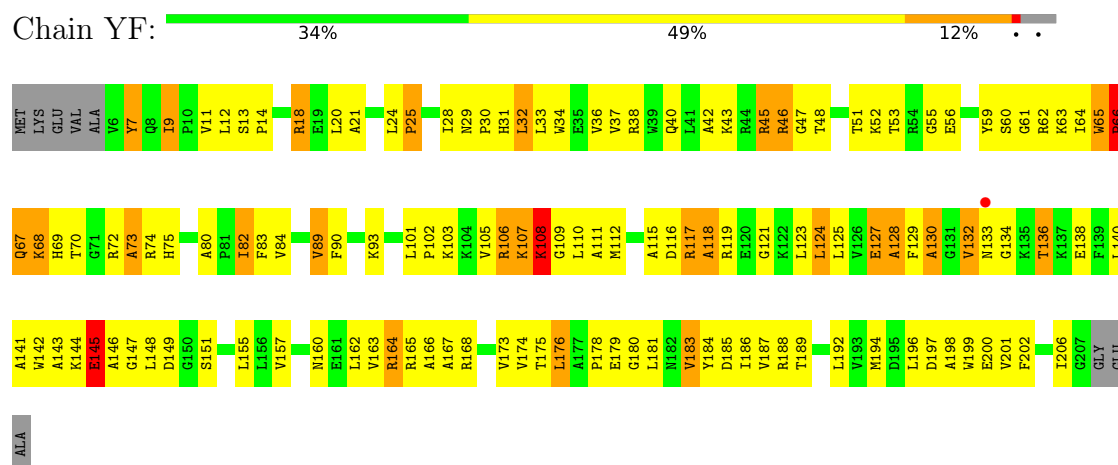


• Molecule 27: 50S ribosomal protein L2

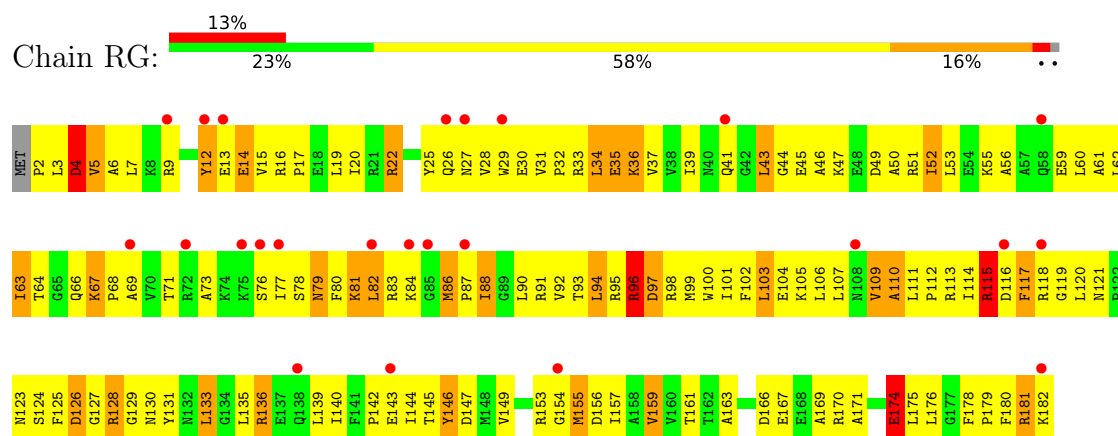




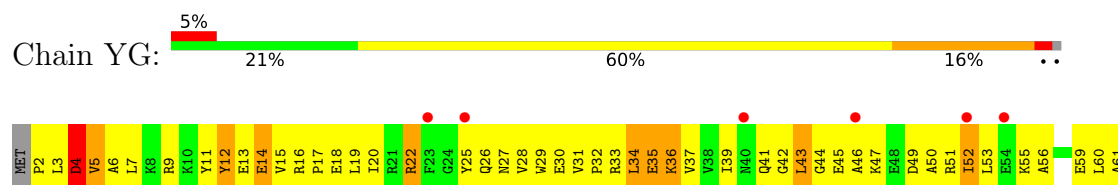
• Molecule 29: 50S ribosomal protein L4

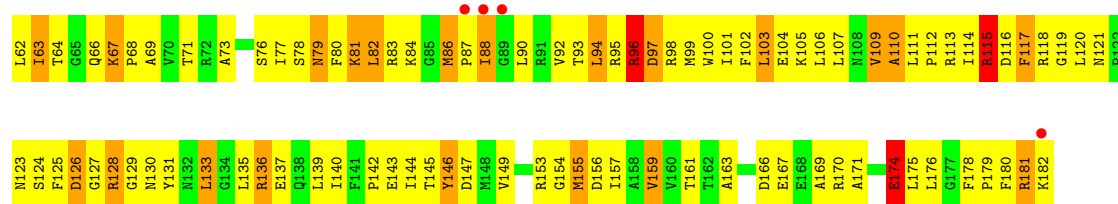


• Molecule 30: 50S ribosomal protein L5

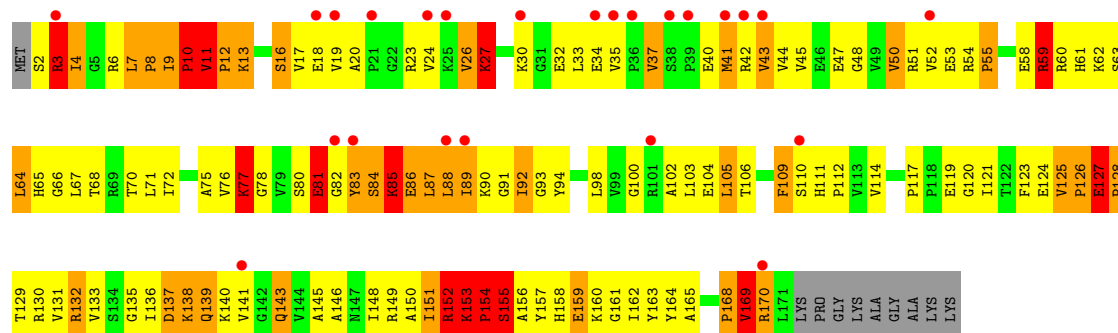
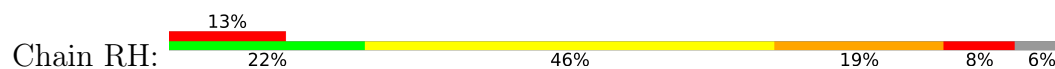


• Molecule 30: 50S ribosomal protein L5

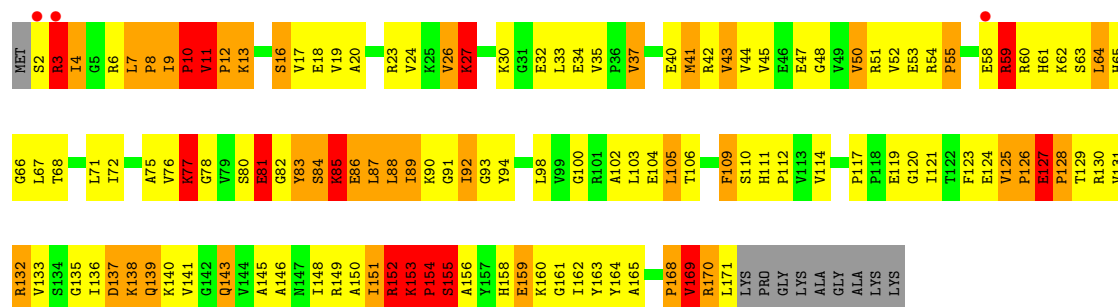
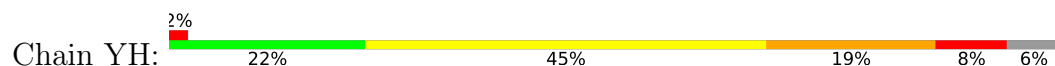




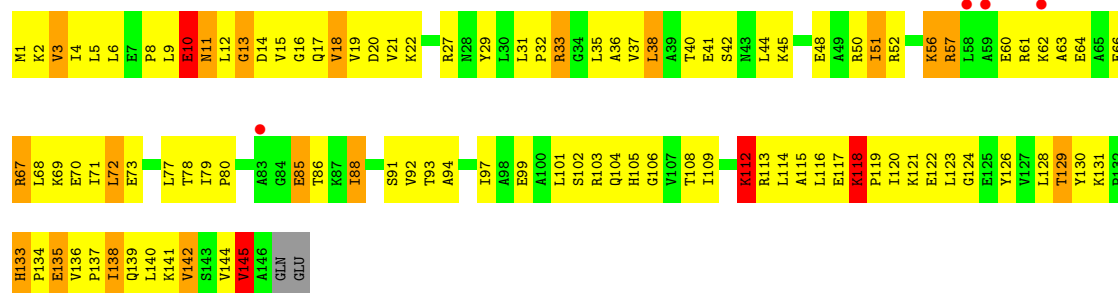
• Molecule 31: 50S ribosomal protein L6



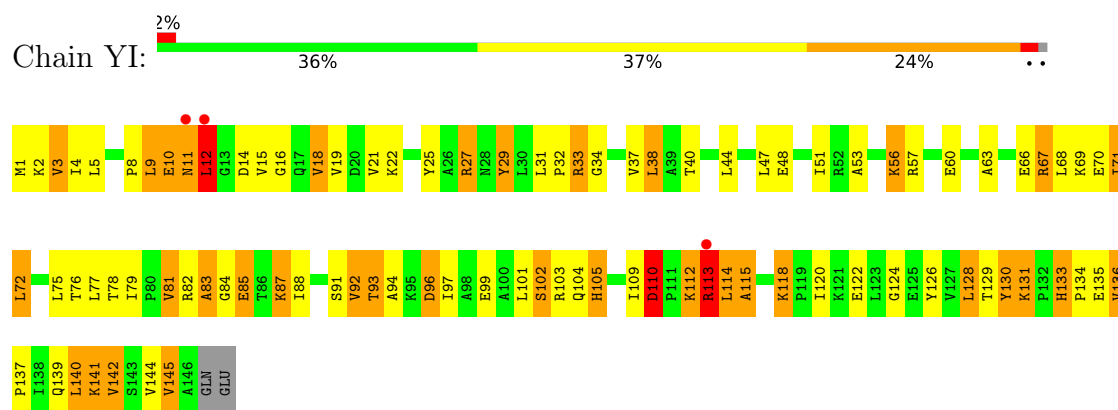
• Molecule 31: 50S ribosomal protein L6



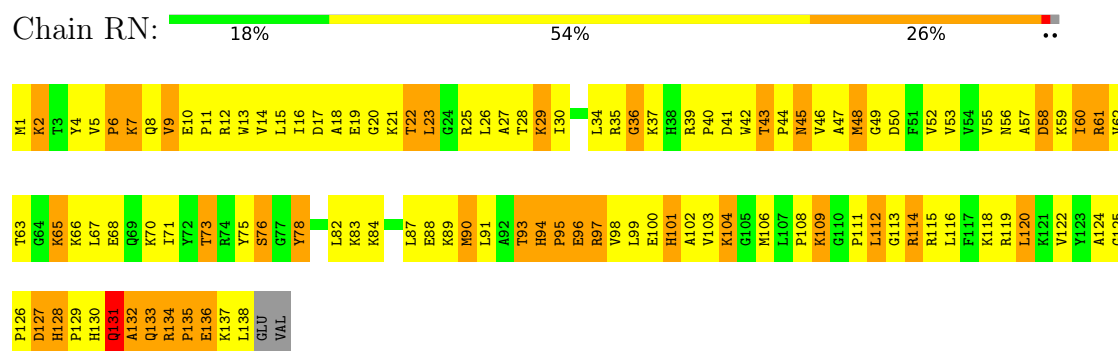
• Molecule 32: 50S ribosomal protein L9

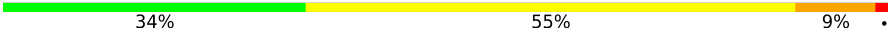


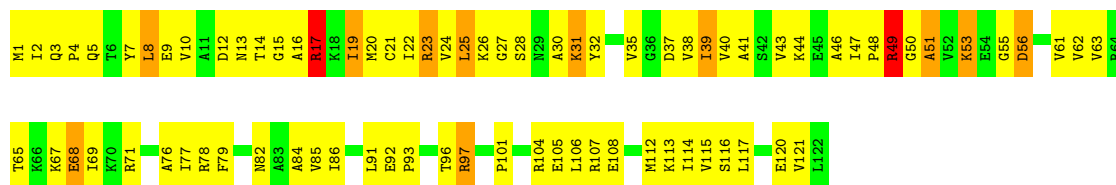
• Molecule 32: 50S ribosomal protein L9




- Molecule 33: 50S ribosomal protein L13

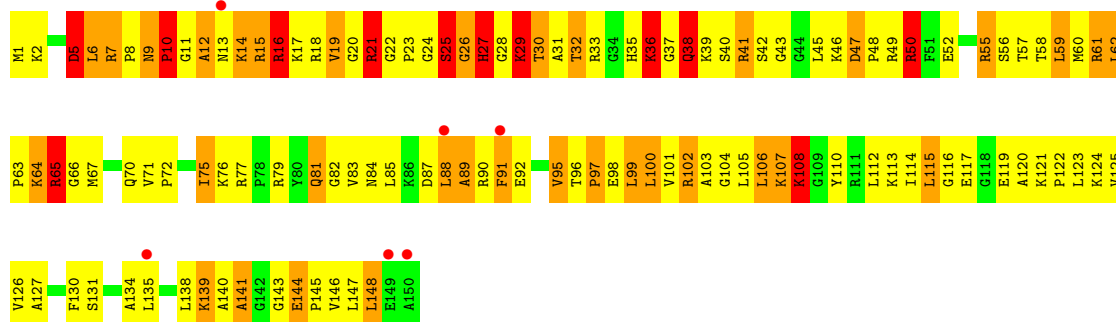


Chain YO:  34% 55% 9% 2%




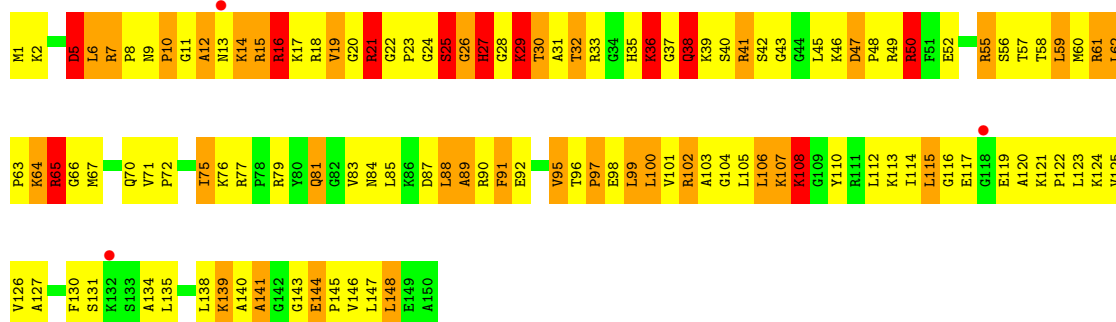
• Molecule 35: 50S ribosomal protein L15

Chain RP:  4% 19% 51% 23% 8%



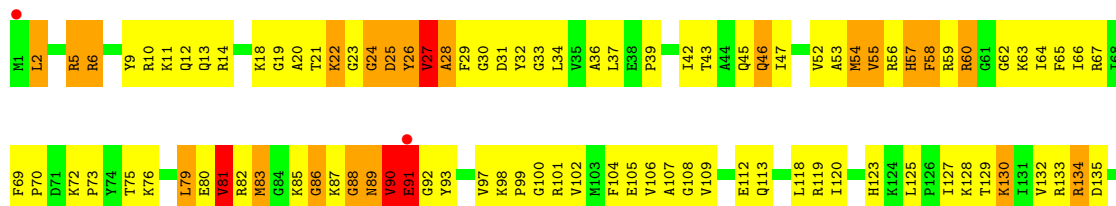
• Molecule 35: 50S ribosomal protein L15

Chain YP:  2% 19% 51% 23% 7%



• Molecule 36: 50S ribosomal protein L16

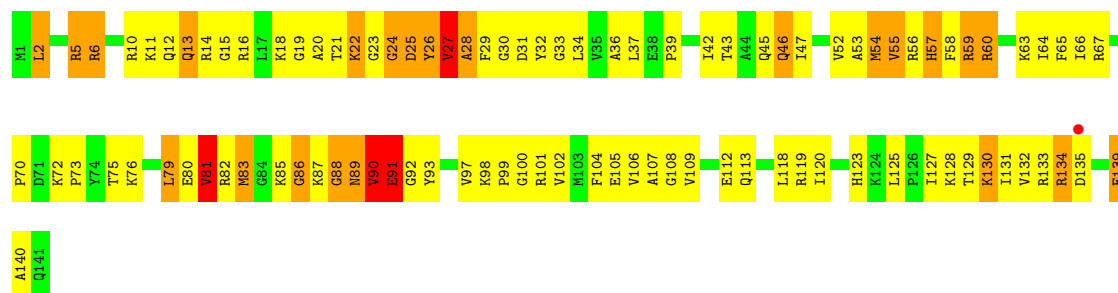
Chain RQ:  2% 30% 51% 16% 2%



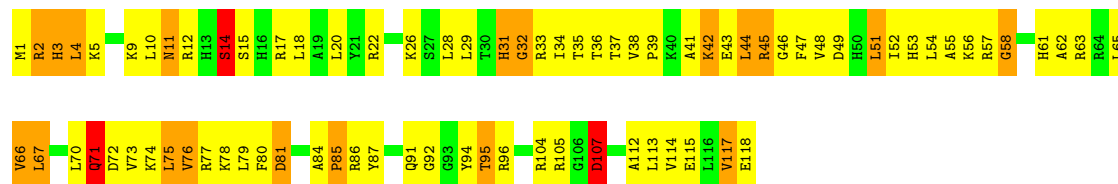




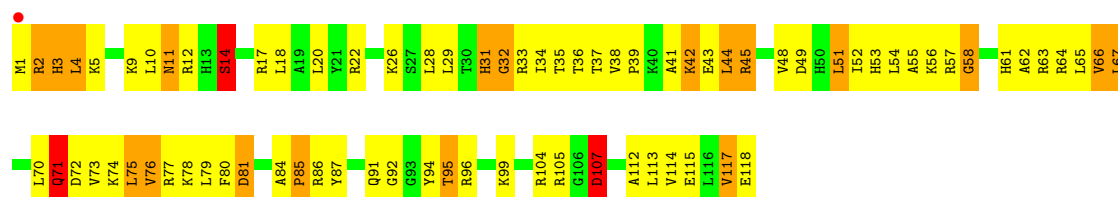
• Molecule 36: 50S ribosomal protein L16



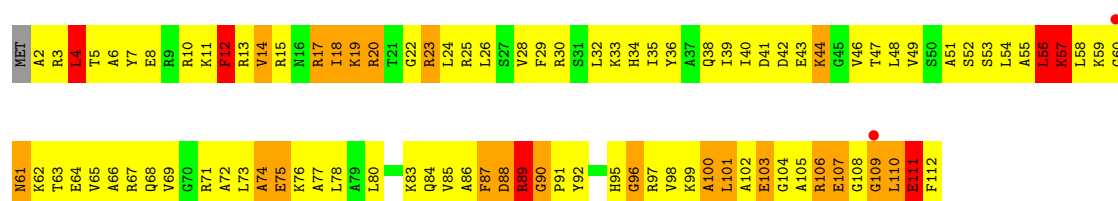
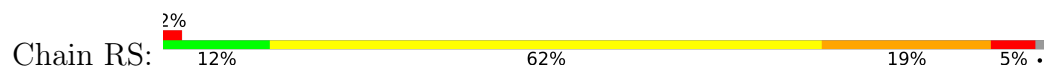
• Molecule 37: 50S ribosomal protein L17



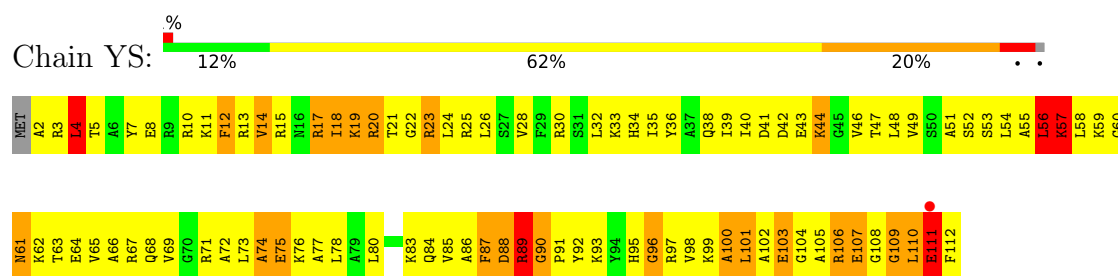
• Molecule 37: 50S ribosomal protein L17



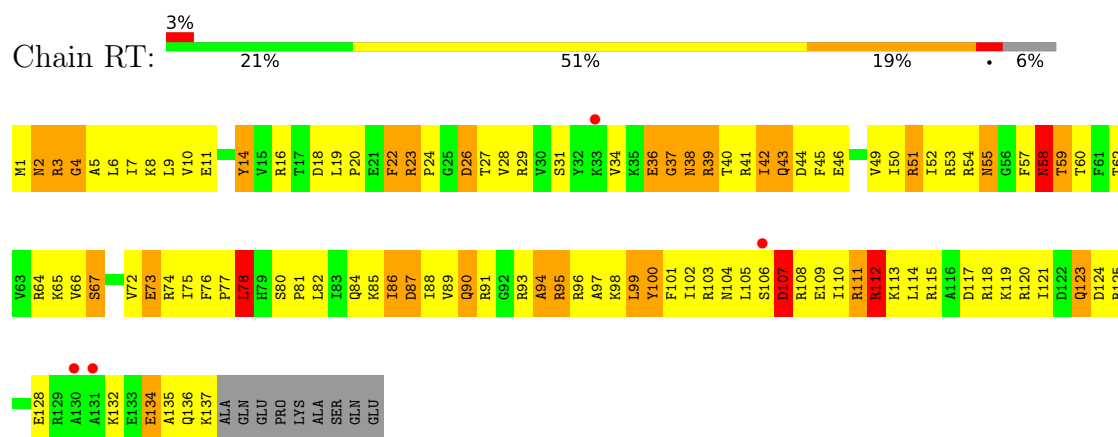
• Molecule 38: 50S ribosomal protein L18



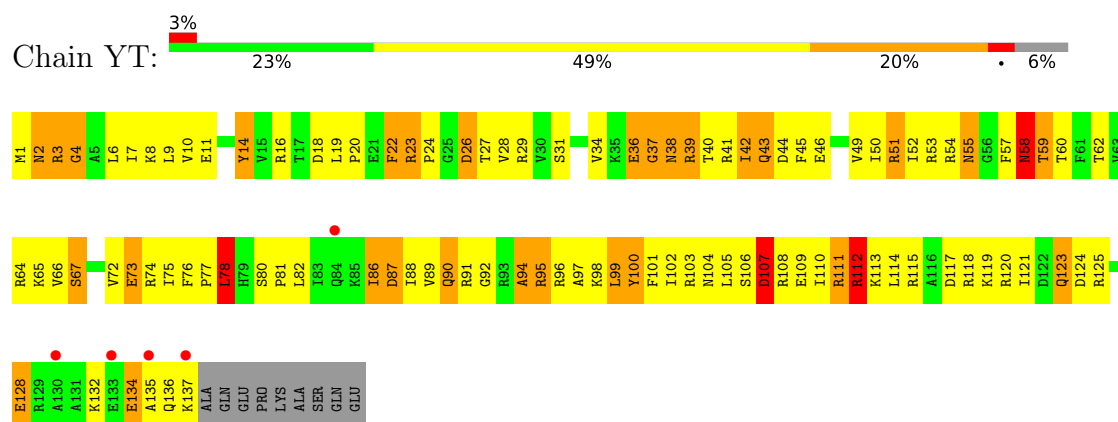
• Molecule 38: 50S ribosomal protein L18



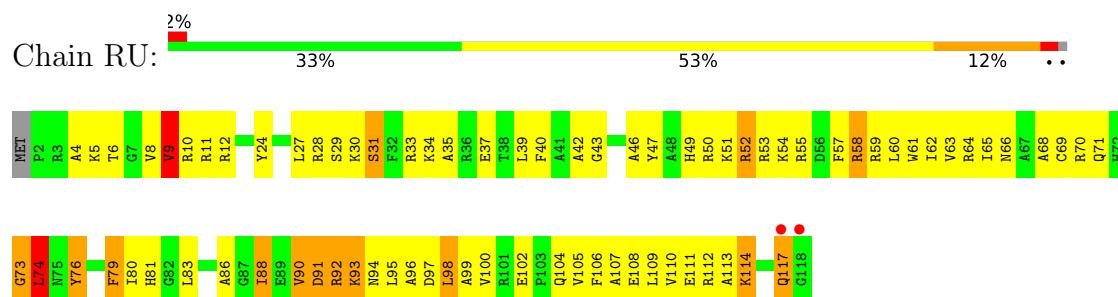
- Molecule 39: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L19

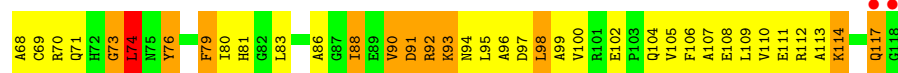


- Molecule 40: 50S ribosomal protein L20

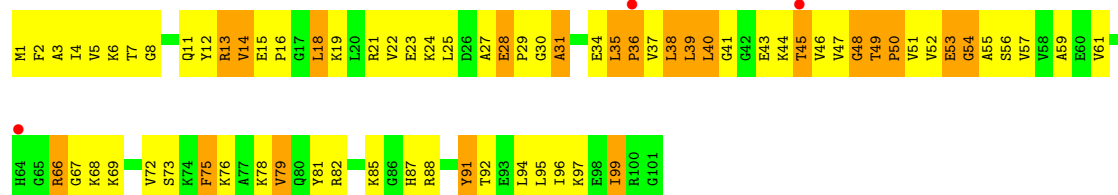


- Molecule 40: 50S ribosomal protein L20

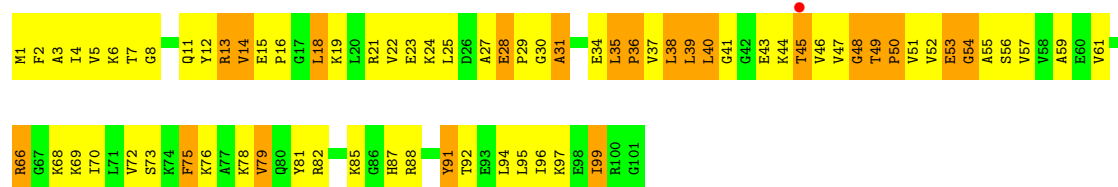




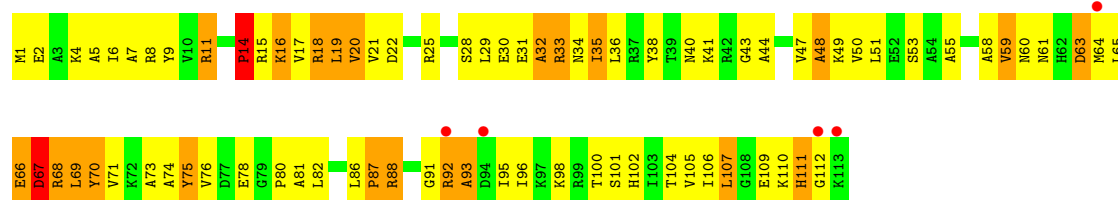
• Molecule 41: 50S ribosomal protein L21



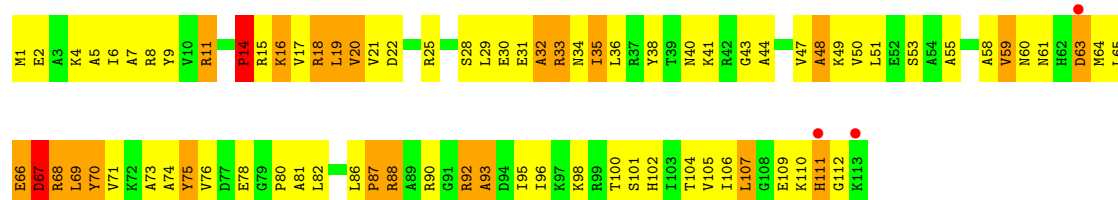
• Molecule 41: 50S ribosomal protein L21



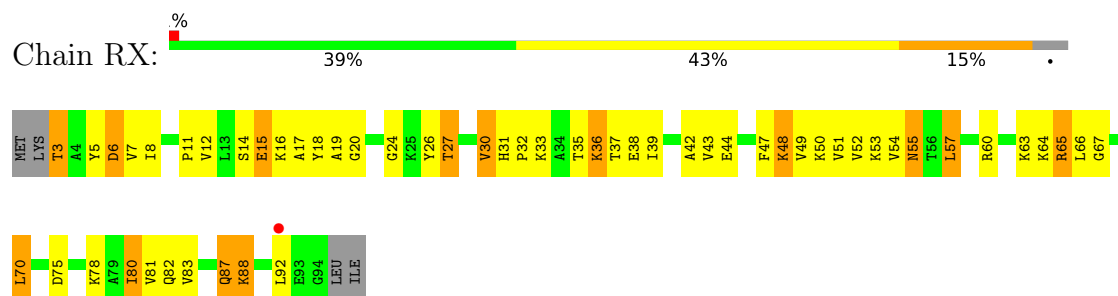
• Molecule 42: 50S ribosomal protein L22



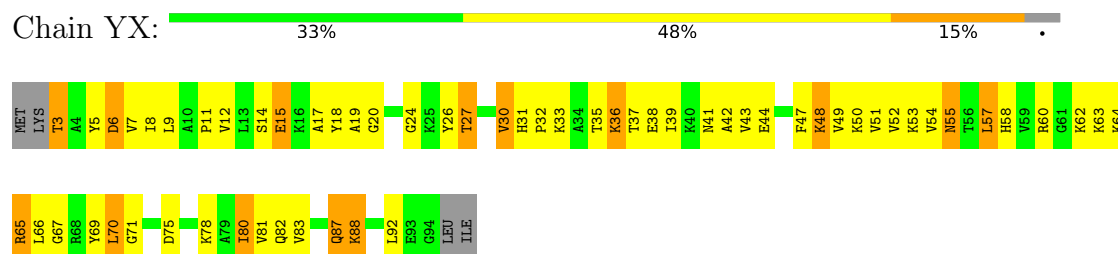
• Molecule 42: 50S ribosomal protein L22



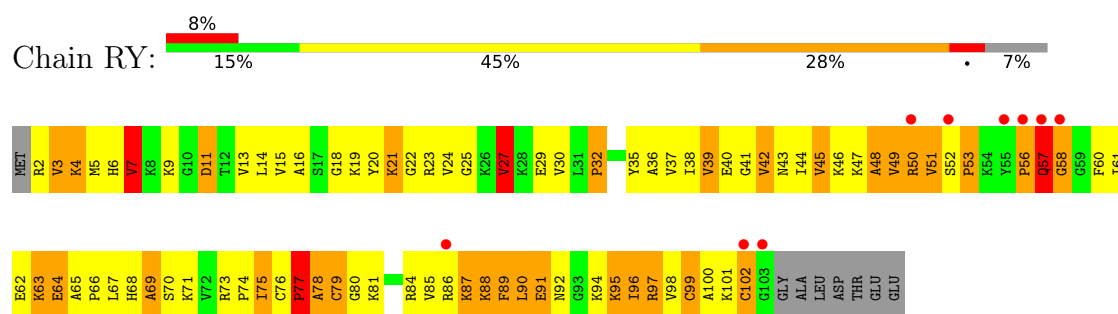
- Molecule 43: 50S ribosomal protein L23



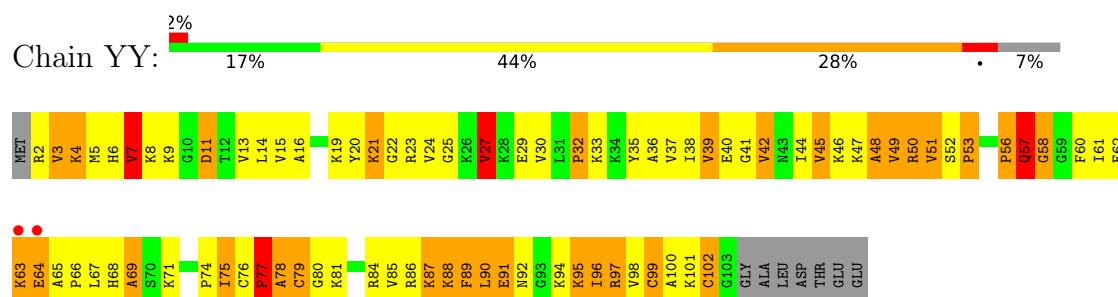
- Molecule 43: 50S ribosomal protein L23



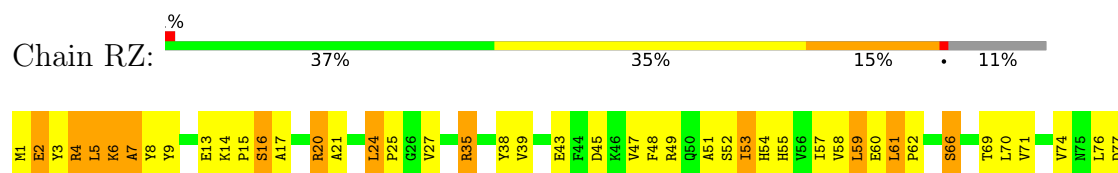
- Molecule 44: 50S ribosomal protein L24

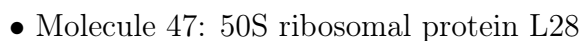


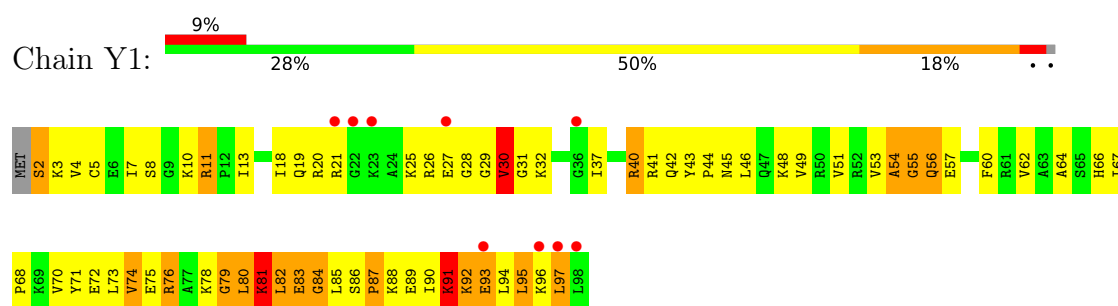
- Molecule 44: 50S ribosomal protein L24



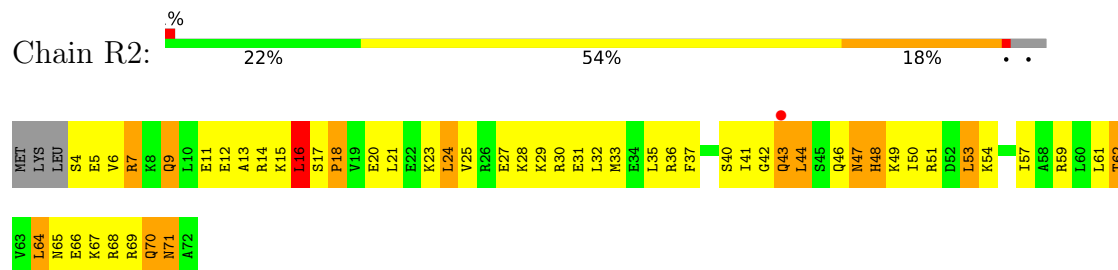
- Molecule 45: 50S ribosomal protein L25



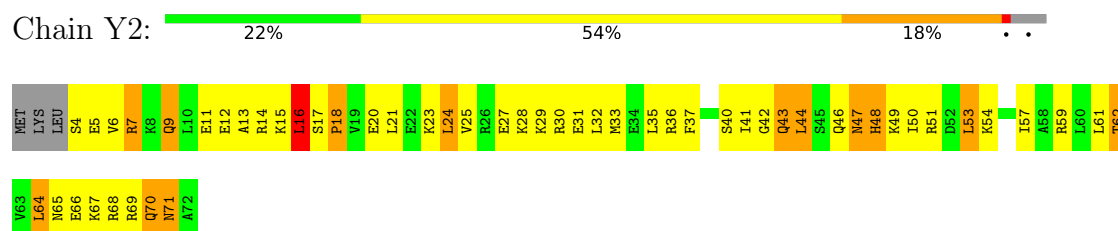




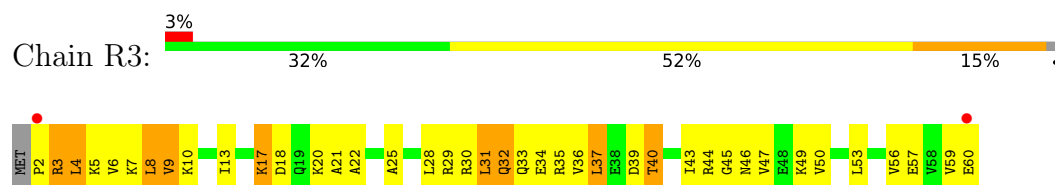
- Molecule 48: 50S ribosomal protein L29



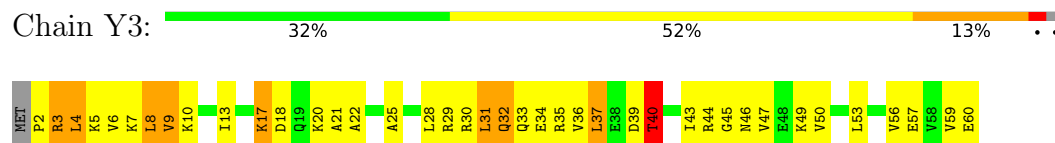
- Molecule 48: 50S ribosomal protein L29



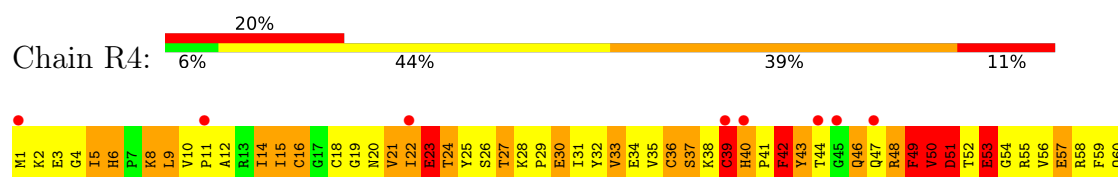
- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30

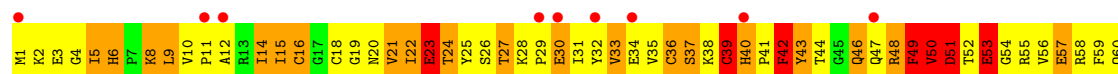


- Molecule 50: 50S ribosomal protein L31

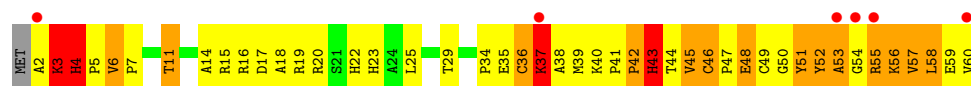
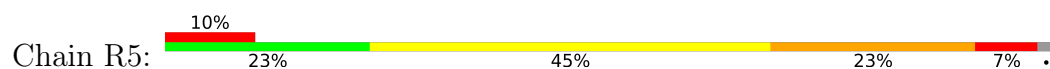




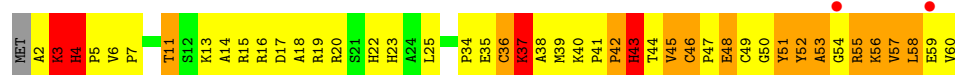
- Molecule 50: 50S ribosomal protein L31



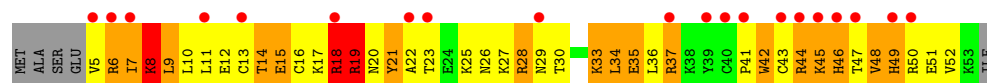
- Molecule 51: 50S ribosomal protein L32



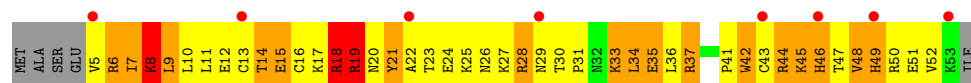
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



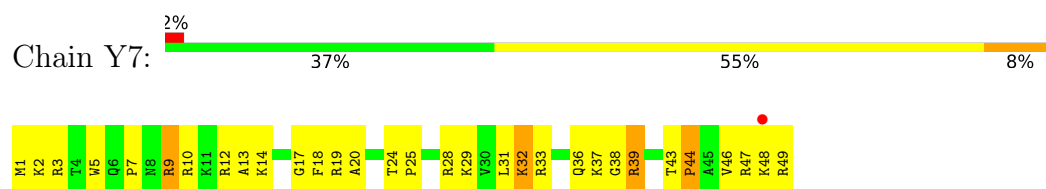
- Molecule 52: 50S ribosomal protein L33



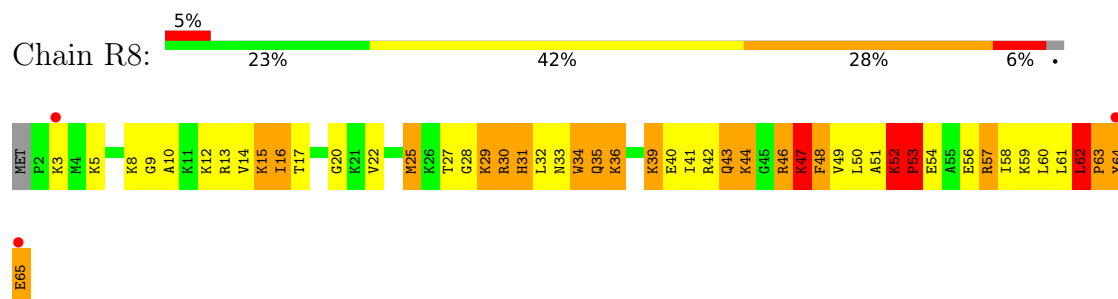
- Molecule 53: 50S ribosomal protein L34



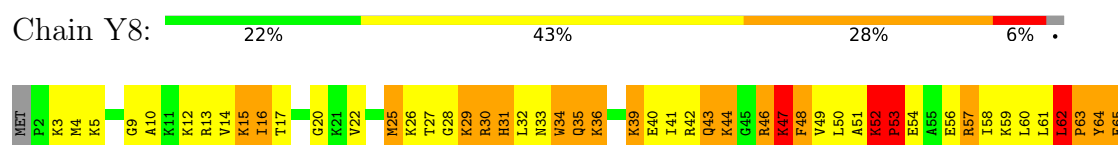
- Molecule 53: 50S ribosomal protein L34



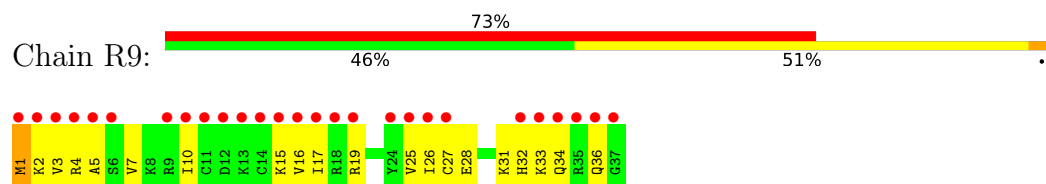
- Molecule 54: 50S ribosomal protein L35



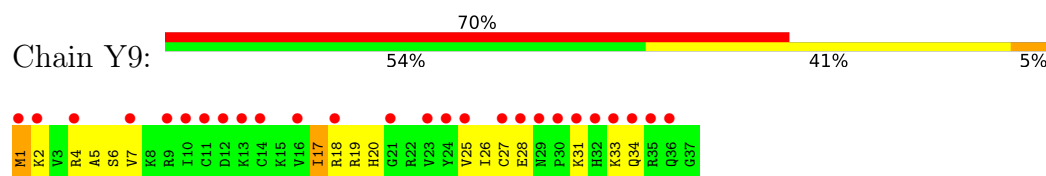
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.38Å 451.02Å 621.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 3.92 34.83 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.77-3.92) 99.8 (34.83-3.80)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	94.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	QA	0.84	19/36098 (0.1%)	1.59	747/56341 (1.3%)
1	XA	0.89	21/36101 (0.1%)	1.65	830/56346 (1.5%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.36	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.47	0/991	0.79	2/1327 (0.2%)
12	XL	0.52	1/991 (0.1%)	0.83	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.40	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.51	0/1836	1.00	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.39	0/185	0.71	0/285
23	XX	0.51	0/160	0.76	0/246
24	QY	0.52	0/311	0.87	0/483
24	XY	0.52	0/311	0.89	0/483
25	RA	1.03	104/69521 (0.1%)	1.85	2693/108529 (2.5%)
25	YA	1.19	254/69543 (0.4%)	1.98	3497/108563 (3.2%)
26	RB	0.82	1/2878 (0.0%)	1.59	60/4490 (1.3%)
26	YB	0.86	1/2878 (0.0%)	1.72	76/4490 (1.7%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.44	0/1151	0.77	1/1558 (0.1%)
32	YI	0.44	0/1151	0.76	0/1558
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.90	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YS	0.45	0/892	0.82	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.47	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.78	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.44	0/1493	0.70	0/2026
45	YZ	0.43	0/1493	0.70	0/2026
46	R0	0.52	0/657	0.73	0/874
46	Y0	0.55	0/657	0.80	1/874 (0.1%)
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.84	1/771 (0.1%)
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.71	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.59	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.78	0/40	1.78	1/60 (1.7%)
56	Z8	0.79	0/40	1.81	1/60 (1.7%)
All	All	0.89	404/316298 (0.1%)	1.59	7980/472872 (1.7%)

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 404 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	1201	A	C3'-C2'	12.06	1.66	1.52
1	XA	1054	C	C4'-C3'	11.40	1.65	1.53
25	YA	783	A	N7-C5	-11.18	1.32	1.39
25	YA	793	A	N7-C5	-10.74	1.32	1.39
25	YA	783	A	C5-C6	-10.48	1.31	1.41

The worst 5 of 7980 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	761	A	N1-C6-N6	19.13	130.07	118.60
25	RA	2490	G	C6-C5-N7	-18.87	119.08	130.40
25	RA	783	A	C6-C5-N7	-17.19	120.27	132.30
25	RA	783	A	N1-C6-N6	16.89	128.74	118.60
25	YA	783	A	N1-C6-N6	16.68	128.61	118.60

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	1130	0
1	XA	32249	0	16279	1064	1
2	QB	1924	0	1975	289	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	205	0
3	XC	1605	0	1668	211	0
4	QD	1703	0	1764	253	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1703	0	1765	214	0
5	QE	1155	0	1213	182	0
5	XE	1155	0	1213	147	0
6	QF	843	0	857	94	0
6	XF	843	0	857	99	0
7	QG	1257	0	1296	151	0
7	XG	1257	0	1294	142	0
8	QH	1116	0	1175	167	0
8	XH	1116	0	1177	150	0
9	QI	1010	0	1037	144	0
9	XI	1010	0	1037	152	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	132	0
11	QK	885	0	904	103	0
11	XK	885	0	904	107	0
12	QL	975	0	1062	100	0
12	XL	975	0	1062	111	0
13	QM	964	0	1034	169	0
13	XM	964	0	1034	163	0
14	QN	492	0	530	102	0
14	XN	492	0	530	99	0
15	QO	734	0	771	76	0
15	XO	734	0	771	78	0
16	QP	705	0	725	120	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	84	0
17	XQ	834	0	904	81	0
18	QR	574	0	644	66	0
18	XR	574	0	644	66	0
19	QS	674	0	699	109	0
19	XS	674	0	699	132	0
20	QT	763	0	860	108	0
20	XT	763	0	861	108	0
21	QU	217	0	234	30	0
21	XU	217	0	234	26	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	9	0
24	QY	303	0	154	11	0
24	XY	303	0	154	11	0
25	RA	62071	0	31285	1926	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	YA	62091	0	31293	1989	0
26	RB	2573	0	1306	121	0
26	YB	2573	0	1306	103	0
27	RD	2115	0	2195	324	0
27	YD	2115	0	2195	332	0
28	RE	1568	0	1634	270	0
28	YE	1568	0	1634	263	0
29	RF	1585	0	1632	178	0
29	YF	1585	0	1632	178	0
30	RG	1474	0	1535	201	0
30	YG	1474	0	1535	194	0
31	RH	1307	0	1382	226	0
31	YH	1307	0	1382	228	0
32	RI	1136	0	1223	79	1
32	YI	1136	0	1223	72	0
33	RN	1104	0	1180	200	0
33	YN	1104	0	1180	189	0
34	RO	933	0	996	126	0
34	YO	933	0	996	125	0
35	RP	1145	0	1228	256	0
35	YP	1145	0	1228	244	0
36	RQ	1122	0	1179	157	0
36	YQ	1122	0	1178	165	0
37	RR	968	0	1033	115	0
37	YR	968	0	1033	117	0
38	RS	882	0	943	166	0
38	YS	882	0	943	159	0
39	RT	1141	0	1202	151	0
39	YT	1141	0	1202	155	0
40	RU	964	0	1022	130	0
40	YU	964	0	1022	142	0
41	RV	779	0	852	130	0
41	YV	779	0	852	131	0
42	RW	900	0	964	100	0
42	YW	900	0	964	108	0
43	RX	725	0	778	70	0
43	YX	725	0	778	74	0
44	RY	785	0	878	167	0
44	YY	785	0	878	160	0
45	RZ	1461	0	1493	81	0
45	YZ	1461	0	1493	86	0
46	R0	648	0	671	55	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	142	0
47	Y1	763	0	848	142	0
48	R2	581	0	629	83	0
48	Y2	581	0	629	78	0
49	R3	469	0	518	41	0
49	Y3	469	0	518	46	0
50	R4	581	0	574	159	0
50	Y4	581	0	574	167	0
51	R5	459	0	480	73	0
51	Y5	459	0	480	76	0
52	R6	424	0	450	90	0
52	Y6	424	0	450	97	0
53	R7	430	0	480	42	0
53	Y7	430	0	480	40	0
54	R8	517	0	582	104	0
54	Y8	517	0	582	105	0
55	R9	307	0	335	23	0
55	Y9	307	0	336	24	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	17856	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 37.

The worst 5 of 17856 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	5
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	5
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	12
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	12
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	11
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	8
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	10
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	8
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	10
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	12
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	12
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	9
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	15
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	18
12	QL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	0	6
12	XL	123/132 (93%)	83 (68%)	24 (20%)	16 (13%)	0	5
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	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	17
15	XO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	17
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
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	2
21	QU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	3
21	XU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	3
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	17
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	17
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	10
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	10
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
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%)	1	13
32	YI	144/148 (97%)	93 (65%)	30 (21%)	21 (15%)	0	4
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	16
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16

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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	10
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	10
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	15
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	15
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
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	6
45	YZ	181/206 (88%)	128 (71%)	36 (20%)	17 (9%)	0	12
46	R0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	2	23
46	Y0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	2	23
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
48	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	4
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	4
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
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	19
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19
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	5

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%)	181 (88%)	24 (12%)	5	25
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5	25
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7	30
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7	30
4	QD	180/181 (99%)	160 (89%)	20 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	180/181 (99%)	165 (92%)	15 (8%)	11	39
5	QE	116/123 (94%)	107 (92%)	9 (8%)	12	41
5	XE	116/123 (94%)	107 (92%)	9 (8%)	12	41
6	QF	90/90 (100%)	76 (84%)	14 (16%)	2	17
6	XF	90/90 (100%)	76 (84%)	14 (16%)	2	17
7	QG	126/127 (99%)	115 (91%)	11 (9%)	10	37
7	XG	126/127 (99%)	115 (91%)	11 (9%)	10	37
8	QH	119/119 (100%)	106 (89%)	13 (11%)	6	28
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	28
9	QI	98/99 (99%)	87 (89%)	11 (11%)	6	27
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	27
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	35
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	9	35
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	30
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	30
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	22
12	XL	104/109 (95%)	89 (86%)	15 (14%)	3	19
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	15
13	XM	97/101 (96%)	81 (84%)	16 (16%)	2	15
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	11
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	30
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	42
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	42
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	23
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	23
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	26
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	26
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	18
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	68 (90%)	8 (10%)	7	29
20	XT	76/82 (93%)	68 (90%)	8 (10%)	7	29
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	53
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	53
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	13
27	YD	214/218 (98%)	178 (83%)	36 (17%)	2	15
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	6
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	6
29	RF	161/166 (97%)	140 (87%)	21 (13%)	4	22
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	22
30	RG	155/156 (99%)	130 (84%)	25 (16%)	2	16
30	YG	155/156 (99%)	130 (84%)	25 (16%)	2	16
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	9
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	9
32	RI	122/124 (98%)	94 (77%)	28 (23%)	1	6
32	YI	122/124 (98%)	92 (75%)	30 (25%)	0	5
33	RN	117/119 (98%)	98 (84%)	19 (16%)	2	16
33	YN	117/119 (98%)	98 (84%)	19 (16%)	2	16
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	30
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	30
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	5
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	5
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	15
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	15
38	RS	87/88 (99%)	74 (85%)	13 (15%)	3	18
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	18
39	RT	120/127 (94%)	97 (81%)	23 (19%)	1	10
39	YT	120/127 (94%)	97 (81%)	23 (19%)	1	10
40	RU	93/94 (99%)	80 (86%)	13 (14%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YU	93/94 (99%)	80 (86%)	13 (14%)	3	21
41	RV	82/82 (100%)	71 (87%)	11 (13%)	4	22
41	YV	82/82 (100%)	71 (87%)	11 (13%)	4	22
42	RW	92/92 (100%)	77 (84%)	15 (16%)	2	16
42	YW	92/92 (100%)	77 (84%)	15 (16%)	2	16
43	RX	74/78 (95%)	63 (85%)	11 (15%)	3	18
43	YX	74/78 (95%)	63 (85%)	11 (15%)	3	18
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	13
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	13
45	RZ	162/179 (90%)	133 (82%)	29 (18%)	2	12
45	YZ	162/179 (90%)	131 (81%)	31 (19%)	1	10
46	R0	65/67 (97%)	58 (89%)	7 (11%)	6	28
46	Y0	65/67 (97%)	58 (89%)	7 (11%)	6	28
47	R1	82/83 (99%)	67 (82%)	15 (18%)	1	11
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	11
48	R2	64/67 (96%)	57 (89%)	7 (11%)	6	28
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	28
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	6
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	6
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	2
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	5
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	7
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
53	R7	42/42 (100%)	39 (93%)	3 (7%)	14	44
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	44
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	3
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	49
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9702/10066 (96%)	8266 (85%)	1436 (15%)	<b>3</b> <b>18</b>

5 of 1436 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	XT	24	LEU
35	YP	27	HIS
27	YD	157	ARG
20	XT	11	SER
30	YG	88	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
52	R6	32	ASN
10	XJ	78	ASN
43	YX	87	GLN
2	XB	135	GLN
5	XE	78	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	385 (25%)	49 (3%)
1	XA	1498/1522 (98%)	378 (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%)	835 (29%)	82 (2%)
25	YA	2880/2916 (98%)	865 (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%)	2615 (28%)	294 (3%)

5 of 2615 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	$\# Z  > 2$
24	1MG	QY	37	24	18,26,27	2.28	2 (11%)	19,39,42	1.55	3 (15%)
56	PPU	Z8	76	56,25	32,40,41	2.54	6 (18%)	33,57,60	2.15	5 (15%)
24	1MG	XY	37	24	18,26,27	2.29	2 (11%)	19,39,42	1.55	2 (10%)
56	PPU	Z6	76	56,25	32,40,41	2.55	5 (15%)	33,57,60	2.16	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	QY	37	24	-	0/3/25/26	0/3/3/3
56	PPU	Z8	76	56,25	-	2/21/43/44	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	XY	37	24	-	0/3/25/26	0/3/3/3
56	PPU	Z6	76	56,25	-	2/21/43/44	0/4/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.25	1.41	1.23
56	Z8	76	PPU	O-C	9.21	1.41	1.23
24	XY	37	1MG	C2-N2	7.86	1.48	1.34
24	QY	37	1MG	C2-N2	7.81	1.48	1.34
56	Z6	76	PPU	C9-N6	-5.88	1.32	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.65	110.17	123.21
56	Z8	76	PPU	C3'-N3'-C	-8.63	110.20	123.21
56	Z8	76	PPU	N3-C2-N1	-4.67	121.38	128.68
56	Z6	76	PPU	N3-C2-N1	-4.66	121.39	128.68
24	QY	37	1MG	C8-N7-C5	4.16	110.91	102.99

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
24	QY	37	1MG	1	0
56	Z8	76	PPU	10	0
24	XY	37	1MG	1	0
56	Z6	76	PPU	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	-	18,24,25	0.70	0	18,35,38	1.45	2 (11%)

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	-	-	1/3/25/26	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	XX	101	AMP	C5-C6-N6	4.34	126.94	120.35
59	XX	101	AMP	C1'-N9-C4	3.22	132.29	126.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

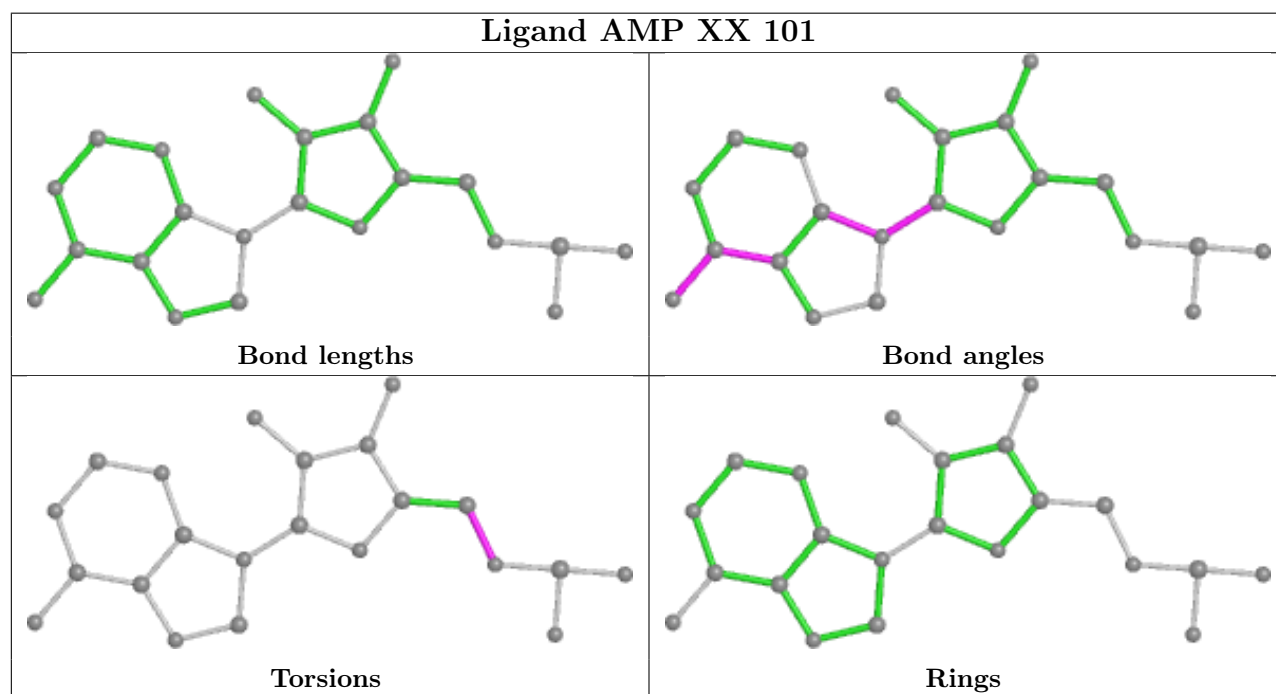
Mol	Chain	Res	Type	Atoms
59	XX	101	AMP	C4'-C5'-O5'-P

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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	QA	1500/1522 (98%)	0.06	50 (3%) 46 37	3, 59, 153, 236	0
1	XA	1500/1522 (98%)	0.01	41 (2%) 54 44	1, 53, 148, 240	0
2	QB	237/256 (92%)	0.31	18 (7%) 13 11	41, 113, 151, 177	0
2	XB	237/256 (92%)	0.11	9 (3%) 40 32	21, 96, 142, 157	0
3	QC	205/239 (85%)	0.36	20 (9%) 7 7	22, 104, 139, 161	0
3	XC	205/239 (85%)	-0.13	4 (1%) 65 56	22, 79, 122, 161	0
4	QD	208/209 (99%)	-0.14	2 (0%) 82 75	8, 69, 116, 153	0
4	XD	208/209 (99%)	0.01	4 (1%) 66 58	16, 74, 114, 158	0
5	QE	151/162 (93%)	0.35	6 (3%) 38 31	32, 95, 133, 161	0
5	XE	151/162 (93%)	-0.21	0 100 100	20, 63, 108, 140	0
6	QF	101/101 (100%)	-0.10	3 (2%) 50 39	15, 68, 105, 139	0
6	XF	101/101 (100%)	0.17	6 (5%) 22 18	4, 66, 107, 134	0
7	QG	155/156 (99%)	0.16	9 (5%) 23 19	26, 89, 133, 154	0
7	XG	155/156 (99%)	0.10	9 (5%) 23 19	28, 83, 124, 148	0
8	QH	138/138 (100%)	-0.10	1 (0%) 87 82	21, 79, 122, 132	0
8	XH	138/138 (100%)	-0.18	2 (1%) 75 66	14, 68, 108, 133	0
9	QI	127/128 (99%)	0.48	12 (9%) 8 8	49, 102, 138, 161	0
9	XI	127/128 (99%)	0.10	4 (3%) 49 38	13, 91, 134, 162	0
10	QJ	99/105 (94%)	0.87	19 (19%) 1 1	57, 108, 148, 192	0
10	XJ	99/105 (94%)	0.52	10 (10%) 7 7	40, 94, 140, 165	0
11	QK	119/129 (92%)	0.31	8 (6%) 17 14	25, 72, 127, 150	0
11	XK	119/129 (92%)	-0.02	4 (3%) 45 36	4, 59, 109, 129	0
12	QL	125/132 (94%)	0.14	8 (6%) 19 15	15, 64, 124, 159	0
12	XL	125/132 (94%)	-0.10	1 (0%) 86 80	6, 48, 102, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	0.18	6 (4%) 28 25	48, 101, 151, 159	0
13	XM	121/126 (96%)	-0.04	1 (0%) 86 80	38, 85, 119, 158	0
14	QN	60/61 (98%)	0.67	7 (11%) 4 5	52, 108, 148, 159	0
14	XN	60/61 (98%)	-0.09	0 100 100	33, 72, 116, 130	0
15	QO	88/89 (98%)	-0.10	3 (3%) 45 36	17, 71, 119, 151	0
15	XO	88/89 (98%)	0.03	4 (4%) 33 28	7, 59, 102, 127	0
16	QP	84/88 (95%)	-0.13	1 (1%) 79 70	14, 59, 114, 134	0
16	XP	84/88 (95%)	-0.13	2 (2%) 59 49	28, 68, 122, 176	0
17	QQ	100/105 (95%)	0.06	3 (3%) 50 39	30, 70, 116, 148	0
17	XQ	100/105 (95%)	0.03	3 (3%) 50 39	19, 71, 106, 144	0
18	QR	70/88 (79%)	0.03	1 (1%) 75 66	22, 70, 125, 150	0
18	XR	70/88 (79%)	-0.07	1 (1%) 75 66	9, 65, 106, 140	0
19	QS	84/93 (90%)	1.05	23 (27%) 0 0	69, 116, 148, 161	0
19	XS	84/93 (90%)	0.09	1 (1%) 79 70	48, 87, 132, 145	0
20	QT	99/106 (93%)	0.13	2 (2%) 65 56	16, 73, 113, 135	0
20	XT	99/106 (93%)	0.24	5 (5%) 28 24	23, 77, 124, 157	0
21	QU	25/27 (92%)	1.63	10 (40%) 0 0	31, 92, 141, 158	0
21	XU	25/27 (92%)	0.90	2 (8%) 12 11	32, 83, 121, 143	0
22	QV	77/77 (100%)	0.29	2 (2%) 56 46	21, 85, 147, 180	0
22	XV	77/77 (100%)	0.27	3 (3%) 39 31	6, 64, 119, 169	0
23	QX	8/25 (32%)	0.72	1 (12%) 3 5	50, 74, 138, 138	0
23	XX	7/25 (28%)	0.86	0 100 100	18, 51, 81, 90	0
24	QY	13/18 (72%)	1.86	4 (30%) 0 0	106, 175, 223, 238	0
24	XY	13/18 (72%)	2.22	4 (30%) 0 0	55, 149, 189, 217	0
25	RA	2882/2916 (98%)	0.03	137 (4%) 30 26	0, 30, 174, 252	0
25	YA	2883/2916 (98%)	-0.07	108 (3%) 41 33	0, 20, 159, 242	0
26	RB	120/122 (98%)	0.24	3 (2%) 57 48	39, 82, 133, 170	0
26	YB	120/122 (98%)	0.10	3 (2%) 57 48	16, 68, 104, 146	0
27	RD	272/276 (98%)	-0.25	2 (0%) 87 82	0, 34, 82, 147	0
27	YD	272/276 (98%)	-0.37	0 100 100	0, 18, 64, 125	0
28	RE	205/206 (99%)	-0.19	2 (0%) 82 75	1, 49, 112, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YE	205/206 (99%)	-0.18	4 (1%) 65 56	0, 47, 104, 155	0
29	RF	202/210 (96%)	-0.29	1 (0%) 91 85	0, 55, 108, 143	0
29	YF	202/210 (96%)	-0.33	1 (0%) 91 85	0, 32, 96, 124	0
30	RG	181/182 (99%)	0.82	24 (13%) 3 3	39, 113, 160, 177	0
30	YG	181/182 (99%)	0.24	10 (5%) 25 22	18, 92, 131, 177	0
31	RH	170/180 (94%)	0.89	24 (14%) 2 3	45, 112, 156, 177	0
31	YH	170/180 (94%)	-0.09	3 (1%) 68 60	11, 66, 116, 131	0
32	RI	146/148 (98%)	-0.12	4 (2%) 54 44	3, 77, 124, 177	0
32	YI	146/148 (98%)	-0.21	3 (2%) 63 54	3, 64, 125, 140	0
33	RN	138/140 (98%)	-0.04	0 100 100	6, 61, 118, 144	0
33	YN	138/140 (98%)	-0.33	0 100 100	4, 45, 98, 131	0
34	RO	122/122 (100%)	-0.28	0 100 100	2, 42, 80, 107	0
34	YO	122/122 (100%)	-0.28	0 100 100	2, 41, 82, 126	0
35	RP	150/150 (100%)	-0.02	6 (4%) 38 31	1, 58, 130, 158	0
35	YP	150/150 (100%)	-0.16	3 (2%) 65 56	1, 46, 101, 160	0
36	RQ	141/141 (100%)	-0.08	3 (2%) 63 54	3, 58, 103, 133	0
36	YQ	141/141 (100%)	-0.27	1 (0%) 87 82	0, 47, 97, 115	0
37	RR	118/118 (100%)	-0.38	0 100 100	1, 34, 87, 136	0
37	YR	118/118 (100%)	-0.32	1 (0%) 86 80	2, 38, 98, 136	0
38	RS	111/112 (99%)	-0.03	2 (1%) 68 60	23, 83, 117, 138	0
38	YS	111/112 (99%)	0.04	1 (0%) 84 77	13, 73, 115, 168	0
39	RT	137/146 (93%)	-0.02	4 (2%) 51 41	8, 58, 130, 152	0
39	YT	137/146 (93%)	-0.13	5 (3%) 42 34	9, 56, 122, 170	0
40	RU	117/118 (99%)	-0.14	2 (1%) 70 61	1, 49, 113, 166	0
40	YU	117/118 (99%)	-0.42	2 (1%) 70 61	1, 31, 97, 145	0
41	RV	101/101 (100%)	-0.10	3 (2%) 50 39	1, 68, 120, 193	0
41	YV	101/101 (100%)	-0.19	1 (0%) 82 75	1, 45, 97, 171	0
42	RW	113/113 (100%)	-0.06	5 (4%) 34 29	2, 34, 95, 131	0
42	YW	113/113 (100%)	-0.16	3 (2%) 54 44	1, 24, 84, 155	0
43	RX	92/96 (95%)	-0.19	1 (1%) 80 73	4, 44, 91, 131	0
43	YX	92/96 (95%)	-0.09	0 100 100	1, 25, 64, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RY	102/110 (92%)	0.40	9 (8%) 10 9	10, 84, 138, 174	0
44	YY	102/110 (92%)	-0.31	2 (1%) 65 56	2, 50, 106, 160	0
45	RZ	183/206 (88%)	0.02	3 (1%) 72 62	20, 88, 136, 160	0
45	YZ	183/206 (88%)	-0.08	6 (3%) 46 37	20, 78, 137, 167	0
46	R0	82/85 (96%)	-0.39	1 (1%) 79 70	6, 44, 83, 137	0
46	Y0	82/85 (96%)	-0.39	0 100 100	2, 32, 70, 88	0
47	R1	97/98 (98%)	0.27	6 (6%) 20 17	2, 47, 126, 202	0
47	Y1	97/98 (98%)	0.13	9 (9%) 8 8	0, 32, 114, 142	0
48	R2	69/72 (95%)	-0.17	1 (1%) 75 66	8, 72, 116, 128	0
48	Y2	69/72 (95%)	-0.31	0 100 100	0, 39, 97, 137	0
49	R3	59/60 (98%)	-0.11	2 (3%) 45 36	7, 60, 126, 152	0
49	Y3	59/60 (98%)	-0.41	0 100 100	3, 40, 87, 128	0
50	R4	71/71 (100%)	1.03	14 (19%) 1 1	78, 145, 193, 235	0
50	Y4	71/71 (100%)	0.52	11 (15%) 2 2	69, 122, 166, 194	0
51	R5	59/60 (98%)	0.16	6 (10%) 6 7	4, 39, 139, 166	0
51	Y5	59/60 (98%)	0.06	2 (3%) 45 36	1, 40, 132, 156	0
52	R6	49/54 (90%)	1.93	20 (40%) 0 0	48, 122, 152, 191	0
52	Y6	49/54 (90%)	0.99	8 (16%) 1 2	47, 108, 148, 175	0
53	R7	49/49 (100%)	-0.20	1 (2%) 65 56	1, 27, 75, 161	0
53	Y7	49/49 (100%)	-0.13	1 (2%) 65 56	1, 15, 84, 140	0
54	R8	64/65 (98%)	0.00	3 (4%) 31 26	4, 41, 94, 153	0
54	Y8	64/65 (98%)	-0.09	0 100 100	2, 34, 85, 138	0
55	R9	37/37 (100%)	3.10	27 (72%) 0 0	53, 103, 154, 162	0
55	Y9	37/37 (100%)	2.81	26 (70%) 0 0	60, 98, 136, 154	0
56	Z6	2/3 (66%)	0.66	0 100 100	17, 17, 17, 30	0
56	Z8	2/3 (66%)	0.70	0 100 100	19, 19, 19, 22	0
All	All	20870/21494 (97%)	0.03	869 (4%) 36 30	0, 55, 139, 252	0

The worst 5 of 869 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	2173	A	14.2
25	RA	1084	A	12.3

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Mol	Chain	Res	Type	RSRZ
25	RA	1094	U	11.8
25	RA	1058	G	11.5
40	RU	118	GLY	11.0

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	1MG	QY	37	24/25	0.88	0.23	130,130,130,130	0
24	1MG	XY	37	24/25	0.90	0.26	56,56,56,56	0
56	PPU	Z8	76	37/38	0.91	0.39	10,10,10,10	0
56	PPU	Z6	76	37/38	0.95	0.32	14,14,14,14	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	RA	3219	1/1	0.43	0.72	40,40,40,40	0
57	MG	QF	201	1/1	0.45	1.08	36,36,36,36	0
57	MG	RA	3166	1/1	0.49	0.29	34,34,34,34	0
57	MG	RA	3213	1/1	0.50	0.50	8,8,8,8	0
57	MG	RA	3062	1/1	0.51	1.84	50,50,50,50	0
57	MG	RA	3138	1/1	0.53	0.76	29,29,29,29	0
57	MG	RA	3226	1/1	0.55	0.37	9,9,9,9	0
57	MG	YA	3207	1/1	0.55	0.97	7,7,7,7	0
57	MG	RA	3227	1/1	0.59	0.56	22,22,22,22	0
57	MG	QA	1620	1/1	0.60	0.32	6,6,6,6	0
57	MG	YA	3196	1/1	0.61	0.51	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1661	1/1	0.61	0.33	64,64,64,64	0
57	MG	YA	3236	1/1	0.61	0.28	5,5,5,5	0
57	MG	QA	1629	1/1	0.64	0.85	0,0,0,0	0
57	MG	RA	3239	1/1	0.65	0.49	14,14,14,14	0
57	MG	YA	3183	1/1	0.66	0.55	16,16,16,16	0
57	MG	YA	3131	1/1	0.66	0.41	3,3,3,3	0
57	MG	YA	3254	1/1	0.67	0.63	2,2,2,2	0
57	MG	QA	1631	1/1	0.69	0.42	26,26,26,26	0
57	MG	YA	3076	1/1	0.69	1.29	50,50,50,50	0
57	MG	YA	3176	1/1	0.70	0.51	6,6,6,6	0
57	MG	RA	3153	1/1	0.70	0.34	15,15,15,15	0
57	MG	RA	3225	1/1	0.71	0.25	10,10,10,10	0
57	MG	YA	3100	1/1	0.72	0.91	6,6,6,6	0
57	MG	YA	3219	1/1	0.72	0.17	7,7,7,7	0
57	MG	R8	101	1/1	0.73	0.37	0,0,0,0	0
57	MG	RA	3003	1/1	0.74	0.93	5,5,5,5	0
57	MG	XA	1667	1/1	0.75	0.27	17,17,17,17	0
57	MG	RA	3206	1/1	0.76	0.37	3,3,3,3	0
57	MG	RA	3049	1/1	0.76	1.01	13,13,13,13	0
57	MG	YA	3184	1/1	0.76	0.32	7,7,7,7	0
57	MG	YA	3242	1/1	0.76	0.79	4,4,4,4	0
57	MG	YA	3250	1/1	0.76	1.17	11,11,11,11	0
57	MG	RA	3203	1/1	0.76	0.38	24,24,24,24	0
57	MG	RA	3191	1/1	0.77	0.31	67,67,67,67	0
57	MG	RA	3199	1/1	0.77	0.73	6,6,6,6	0
57	MG	RA	3157	1/1	0.77	0.55	0,0,0,0	0
57	MG	YA	3152	1/1	0.77	0.66	5,5,5,5	0
57	MG	YA	3166	1/1	0.77	0.30	4,4,4,4	0
57	MG	YA	3172	1/1	0.77	1.39	1,1,1,1	0
57	MG	XA	1642	1/1	0.77	0.72	5,5,5,5	0
57	MG	RA	3007	1/1	0.77	0.41	16,16,16,16	0
59	AMP	XX	101	22/23	0.77	0.30	91,91,91,91	0
57	MG	YA	3030	1/1	0.78	0.95	5,5,5,5	0
57	MG	RP	201	1/1	0.78	1.36	21,21,21,21	0
57	MG	RA	3173	1/1	0.78	0.50	48,48,48,48	0
57	MG	YA	3121	1/1	0.79	0.42	62,62,62,62	0
57	MG	RA	3224	1/1	0.79	0.39	5,5,5,5	0
57	MG	YA	3063	1/1	0.80	0.29	11,11,11,11	0
57	MG	RA	3046	1/1	0.80	0.87	50,50,50,50	0
57	MG	YA	3080	1/1	0.80	1.46	50,50,50,50	0
57	MG	QA	1632	1/1	0.80	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3210	1/1	0.80	0.51	3,3,3,3	0
57	MG	QX	101	1/1	0.80	0.41	4,4,4,4	0
57	MG	RA	3179	1/1	0.80	0.38	4,4,4,4	0
57	MG	QA	1650	1/1	0.80	0.61	11,11,11,11	0
57	MG	XA	1656	1/1	0.80	1.10	10,10,10,10	0
57	MG	RA	3197	1/1	0.80	0.65	3,3,3,3	0
57	MG	QA	1623	1/1	0.80	0.42	14,14,14,14	0
57	MG	RA	3172	1/1	0.81	0.48	4,4,4,4	0
57	MG	XA	1627	1/1	0.81	0.27	14,14,14,14	0
57	MG	YA	3167	1/1	0.81	0.52	2,2,2,2	0
57	MG	RA	3063	1/1	0.81	0.81	3,3,3,3	0
57	MG	XA	1655	1/1	0.81	0.29	9,9,9,9	0
57	MG	RD	301	1/1	0.81	0.47	1,1,1,1	0
57	MG	XA	1663	1/1	0.81	0.54	15,15,15,15	0
57	MG	YB	201	1/1	0.81	0.31	7,7,7,7	0
57	MG	RA	3221	1/1	0.81	0.33	22,22,22,22	0
57	MG	YA	3145	1/1	0.82	0.33	9,9,9,9	0
57	MG	XA	1646	1/1	0.82	0.28	7,7,7,7	0
57	MG	RA	3130	1/1	0.82	0.61	2,2,2,2	0
57	MG	YA	3114	1/1	0.82	0.33	13,13,13,13	0
57	MG	RA	3207	1/1	0.82	0.27	11,11,11,11	0
57	MG	RA	3009	1/1	0.82	0.36	10,10,10,10	0
57	MG	XB	301	1/1	0.83	0.33	2,2,2,2	0
57	MG	YA	3012	1/1	0.83	1.55	50,50,50,50	0
57	MG	XA	1629	1/1	0.83	0.17	8,8,8,8	0
57	MG	YA	3159	1/1	0.83	0.20	6,6,6,6	0
57	MG	QA	1601	1/1	0.83	0.35	9,9,9,9	0
57	MG	RA	3137	1/1	0.83	0.44	10,10,10,10	0
57	MG	RA	3022	1/1	0.83	0.36	4,4,4,4	0
57	MG	R0	101	1/1	0.83	0.30	0,0,0,0	0
57	MG	QA	1638	1/1	0.83	0.64	34,34,34,34	0
57	MG	YP	201	1/1	0.83	0.15	94,94,94,94	0
57	MG	RA	3202	1/1	0.83	0.15	16,16,16,16	0
57	MG	XA	1650	1/1	0.84	0.28	18,18,18,18	0
57	MG	YA	3039	1/1	0.84	0.28	6,6,6,6	0
57	MG	RA	3069	1/1	0.84	0.82	4,4,4,4	0
57	MG	RA	3070	1/1	0.84	0.90	0,0,0,0	0
57	MG	QA	1637	1/1	0.84	0.31	0,0,0,0	0
57	MG	YA	3246	1/1	0.84	0.35	7,7,7,7	0
57	MG	QA	1618	1/1	0.84	0.51	3,3,3,3	0
57	MG	YA	3252	1/1	0.84	0.75	8,8,8,8	0
57	MG	QA	1649	1/1	0.84	0.41	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	3260	1/1	0.84	0.97	50,50,50,50	0
57	MG	RA	3176	1/1	0.84	0.31	3,3,3,3	0
57	MG	YA	3014	1/1	0.84	1.25	50,50,50,50	0
57	MG	YA	3140	1/1	0.84	0.25	12,12,12,12	0
57	MG	YA	3238	1/1	0.85	0.29	11,11,11,11	0
57	MG	YA	3117	1/1	0.85	0.99	6,6,6,6	0
57	MG	RA	3169	1/1	0.85	0.24	16,16,16,16	0
57	MG	YA	3248	1/1	0.85	0.44	0,0,0,0	0
57	MG	XA	1662	1/1	0.85	0.88	11,11,11,11	0
57	MG	YA	3049	1/1	0.85	0.89	50,50,50,50	0
57	MG	XA	1638	1/1	0.85	0.33	20,20,20,20	0
57	MG	QA	1624	1/1	0.85	0.65	0,0,0,0	0
57	MG	QA	1662	1/1	0.85	0.27	37,37,37,37	0
57	MG	QA	1664	1/1	0.85	0.41	54,54,54,54	0
57	MG	RA	3168	1/1	0.85	0.47	1,1,1,1	0
57	MG	XA	1607	1/1	0.86	0.38	16,16,16,16	0
57	MG	RA	3071	1/1	0.86	0.23	1,1,1,1	0
57	MG	YA	3175	1/1	0.86	0.24	9,9,9,9	0
57	MG	YA	3045	1/1	0.86	0.53	13,13,13,13	0
57	MG	RA	3076	1/1	0.86	0.53	7,7,7,7	0
57	MG	RA	3220	1/1	0.86	0.28	26,26,26,26	0
57	MG	YA	3193	1/1	0.86	0.19	3,3,3,3	0
57	MG	RA	3039	1/1	0.86	0.36	10,10,10,10	0
57	MG	RA	3222	1/1	0.86	0.34	14,14,14,14	0
57	MG	YA	3085	1/1	0.86	0.61	13,13,13,13	0
57	MG	YA	3212	1/1	0.86	0.25	8,8,8,8	0
57	MG	RA	3006	1/1	0.86	0.97	50,50,50,50	0
57	MG	YA	3230	1/1	0.86	0.16	8,8,8,8	0
57	MG	RA	3048	1/1	0.86	0.21	3,3,3,3	0
57	MG	YA	3237	1/1	0.86	0.32	7,7,7,7	0
57	MG	QA	1646	1/1	0.86	0.53	10,10,10,10	0
57	MG	QA	1626	1/1	0.86	0.40	57,57,57,57	0
57	MG	YA	3122	1/1	0.86	0.40	3,3,3,3	0
57	MG	YA	3247	1/1	0.86	0.39	14,14,14,14	0
57	MG	YA	3128	1/1	0.86	0.57	12,12,12,12	0
57	MG	RA	3159	1/1	0.86	0.26	6,6,6,6	0
57	MG	QA	1615	1/1	0.86	0.78	4,4,4,4	0
57	MG	RA	3025	1/1	0.86	0.14	3,3,3,3	0
57	MG	YA	3001	1/1	0.86	1.21	50,50,50,50	0
57	MG	RA	3032	1/1	0.86	1.18	50,50,50,50	0
57	MG	YB	202	1/1	0.86	0.67	24,24,24,24	0
57	MG	YA	3165	1/1	0.86	0.23	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	3208	1/1	0.86	0.65	15,15,15,15	0
57	MG	RA	3141	1/1	0.87	0.24	2,2,2,2	0
57	MG	RA	3192	1/1	0.87	0.27	21,21,21,21	0
57	MG	XA	1665	1/1	0.87	0.49	7,7,7,7	0
57	MG	RA	3142	1/1	0.87	0.49	36,36,36,36	0
57	MG	YA	3243	1/1	0.87	0.42	32,32,32,32	0
57	MG	RA	3229	1/1	0.87	1.51	50,50,50,50	0
57	MG	RA	3121	1/1	0.87	0.77	5,5,5,5	0
58	ZN	QN	101	1/1	0.87	0.13	104,104,104,104	0
57	MG	RA	3132	1/1	0.87	0.16	3,3,3,3	0
57	MG	QA	1655	1/1	0.88	0.67	20,20,20,20	0
57	MG	YA	3119	1/1	0.88	0.78	8,8,8,8	0
57	MG	RA	3234	1/1	0.88	0.34	9,9,9,9	0
57	MG	RA	3085	1/1	0.88	0.81	5,5,5,5	0
57	MG	YA	3245	1/1	0.88	0.30	2,2,2,2	0
57	MG	RA	3209	1/1	0.88	0.33	17,17,17,17	0
57	MG	XA	1664	1/1	0.88	0.29	8,8,8,8	0
57	MG	YA	3188	1/1	0.88	0.51	1,1,1,1	0
57	MG	QA	1603	1/1	0.88	0.93	14,14,14,14	0
57	MG	RA	3193	1/1	0.88	0.33	22,22,22,22	0
57	MG	YA	3151	1/1	0.88	0.17	5,5,5,5	0
57	MG	XA	1671	1/1	0.88	0.22	3,3,3,3	0
57	MG	YA	3155	1/1	0.88	0.33	7,7,7,7	0
57	MG	YA	3218	1/1	0.88	0.36	5,5,5,5	0
57	MG	XA	1647	1/1	0.88	0.37	1,1,1,1	0
57	MG	Y7	101	1/1	0.88	0.73	15,15,15,15	0
57	MG	XA	1648	1/1	0.88	0.57	3,3,3,3	0
57	MG	RA	3195	1/1	0.88	0.26	24,24,24,24	0
57	MG	RA	3233	1/1	0.89	0.64	2,2,2,2	0
57	MG	RA	3083	1/1	0.89	0.39	6,6,6,6	0
57	MG	QA	1636	1/1	0.89	0.12	16,16,16,16	0
57	MG	YA	3224	1/1	0.89	0.38	0,0,0,0	0
57	MG	YA	3146	1/1	0.89	0.44	0,0,0,0	0
57	MG	RA	3088	1/1	0.89	0.61	15,15,15,15	0
57	MG	RA	3114	1/1	0.89	0.33	1,1,1,1	0
57	MG	RA	3033	1/1	0.89	0.58	50,50,50,50	0
57	MG	YA	3066	1/1	0.89	0.59	7,7,7,7	0
57	MG	YA	3074	1/1	0.89	0.18	11,11,11,11	0
57	MG	YA	3075	1/1	0.89	0.26	0,0,0,0	0
57	MG	XA	1657	1/1	0.89	0.42	8,8,8,8	0
57	MG	R5	101	1/1	0.89	0.52	5,5,5,5	0
57	MG	YA	3084	1/1	0.89	0.27	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3125	1/1	0.89	0.52	1,1,1,1	0
57	MG	XA	1603	1/1	0.89	0.62	8,8,8,8	0
57	MG	RA	3155	1/1	0.89	0.39	10,10,10,10	0
57	MG	RA	3177	1/1	0.89	0.79	7,7,7,7	0
57	MG	YA	3263	1/1	0.89	0.76	4,4,4,4	0
57	MG	YA	3269	1/1	0.89	0.78	1,1,1,1	0
57	MG	RA	3052	1/1	0.89	0.87	50,50,50,50	0
57	MG	XA	1630	1/1	0.89	0.64	10,10,10,10	0
57	MG	YA	3200	1/1	0.89	0.92	4,4,4,4	0
57	MG	RA	3182	1/1	0.89	0.21	4,4,4,4	0
57	MG	YA	3209	1/1	0.89	0.28	15,15,15,15	0
57	MG	RA	3185	1/1	0.89	0.18	9,9,9,9	0
57	MG	RE	302	1/1	0.90	0.25	1,1,1,1	0
57	MG	QH	201	1/1	0.90	0.21	47,47,47,47	0
57	MG	RR	202	1/1	0.90	0.34	0,0,0,0	0
57	MG	XA	1652	1/1	0.90	0.33	66,66,66,66	0
57	MG	RA	3175	1/1	0.90	0.12	1,1,1,1	0
57	MG	YA	3071	1/1	0.90	0.19	28,28,28,28	0
57	MG	RA	3162	1/1	0.90	0.23	2,2,2,2	0
57	MG	YA	3160	1/1	0.90	0.49	1,1,1,1	0
57	MG	YA	3239	1/1	0.90	0.20	5,5,5,5	0
57	MG	RA	3117	1/1	0.90	0.15	25,25,25,25	0
57	MG	RA	3178	1/1	0.90	0.25	1,1,1,1	0
57	MG	XA	1605	1/1	0.90	0.57	3,3,3,3	0
57	MG	RA	3026	1/1	0.90	0.63	50,50,50,50	0
57	MG	YA	3173	1/1	0.90	0.30	35,35,35,35	0
57	MG	YA	3174	1/1	0.90	0.22	40,40,40,40	0
57	MG	RA	3005	1/1	0.90	0.62	12,12,12,12	0
57	MG	RA	3170	1/1	0.90	1.02	5,5,5,5	0
57	MG	YA	3101	1/1	0.90	0.59	2,2,2,2	0
57	MG	YA	3256	1/1	0.90	0.39	7,7,7,7	0
57	MG	YA	3103	1/1	0.90	0.14	5,5,5,5	0
57	MG	YA	3185	1/1	0.90	0.14	2,2,2,2	0
57	MG	RA	3187	1/1	0.90	0.48	3,3,3,3	0
57	MG	XA	1631	1/1	0.90	0.20	31,31,31,31	0
57	MG	XV	102	1/1	0.90	0.66	9,9,9,9	0
57	MG	XA	1636	1/1	0.90	0.38	3,3,3,3	0
57	MG	RA	3188	1/1	0.90	0.34	5,5,5,5	0
57	MG	RA	3171	1/1	0.90	0.19	12,12,12,12	0
57	MG	RA	3140	1/1	0.90	0.73	9,9,9,9	0
57	MG	RA	3223	1/1	0.91	0.30	47,47,47,47	0
57	MG	XA	1609	1/1	0.91	0.52	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	3044	1/1	0.91	0.85	10,10,10,10	0
57	MG	RA	3198	1/1	0.91	0.18	12,12,12,12	0
57	MG	XA	1653	1/1	0.91	0.35	8,8,8,8	0
57	MG	YA	3099	1/1	0.91	0.76	10,10,10,10	0
57	MG	YA	3192	1/1	0.91	0.52	11,11,11,11	0
57	MG	YA	3153	1/1	0.91	0.41	20,20,20,20	0
57	MG	QA	1657	1/1	0.91	0.14	7,7,7,7	0
57	MG	YA	3156	1/1	0.91	0.58	2,2,2,2	0
57	MG	YA	3201	1/1	0.91	0.56	9,9,9,9	0
57	MG	YA	3202	1/1	0.91	0.25	1,1,1,1	0
57	MG	YA	3203	1/1	0.91	0.15	53,53,53,53	0
57	MG	RA	3214	1/1	0.91	0.34	5,5,5,5	0
57	MG	XA	1635	1/1	0.91	0.57	4,4,4,4	0
57	MG	YA	3265	1/1	0.91	1.06	4,4,4,4	0
57	MG	YA	3268	1/1	0.91	0.53	6,6,6,6	0
57	MG	RA	3018	1/1	0.91	0.73	6,6,6,6	0
57	MG	RA	3001	1/1	0.91	0.59	3,3,3,3	0
57	MG	XA	1641	1/1	0.91	1.19	21,21,21,21	0
57	MG	YA	3169	1/1	0.91	0.16	6,6,6,6	0
57	MG	RA	3194	1/1	0.91	0.28	6,6,6,6	0
58	ZN	QD	301	1/1	0.91	0.35	50,50,50,50	0
57	MG	XA	1666	1/1	0.91	0.32	50,50,50,50	0
58	ZN	Y9	101	1/1	0.91	0.47	138,138,138,138	0
57	MG	QA	1628	1/1	0.91	0.21	8,8,8,8	0
57	MG	RA	3174	1/1	0.92	0.52	4,4,4,4	0
57	MG	XA	1621	1/1	0.92	0.33	3,3,3,3	0
57	MG	YA	3194	1/1	0.92	0.17	0,0,0,0	0
57	MG	XA	1624	1/1	0.92	0.59	3,3,3,3	0
57	MG	YA	3198	1/1	0.92	0.25	51,51,51,51	0
57	MG	QA	1643	1/1	0.92	0.29	33,33,33,33	0
57	MG	RA	3028	1/1	0.92	0.46	14,14,14,14	0
57	MG	XM	201	1/1	0.92	0.11	85,85,85,85	0
57	MG	YA	3127	1/1	0.92	0.29	2,2,2,2	0
57	MG	RA	3101	1/1	0.92	0.45	11,11,11,11	0
57	MG	RA	3230	1/1	0.92	0.74	5,5,5,5	0
57	MG	YA	3133	1/1	0.92	0.13	1,1,1,1	0
57	MG	YA	3135	1/1	0.92	0.25	6,6,6,6	0
57	MG	YA	3002	1/1	0.92	1.06	50,50,50,50	0
57	MG	YA	3141	1/1	0.92	0.53	0,0,0,0	0
57	MG	YA	3222	1/1	0.92	0.19	8,8,8,8	0
57	MG	YA	3006	1/1	0.92	0.56	3,3,3,3	0
57	MG	YA	3225	1/1	0.92	0.24	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	3110	1/1	0.92	0.48	3,3,3,3	0
57	MG	YA	3234	1/1	0.92	0.53	17,17,17,17	0
57	MG	YA	3149	1/1	0.92	0.20	15,15,15,15	0
57	MG	RA	3055	1/1	0.92	0.93	5,5,5,5	0
57	MG	YA	3016	1/1	0.92	0.22	6,6,6,6	0
57	MG	YA	3024	1/1	0.92	0.54	50,50,50,50	0
57	MG	YA	3154	1/1	0.92	0.23	1,1,1,1	0
57	MG	RA	3235	1/1	0.92	0.62	1,1,1,1	0
57	MG	RA	3116	1/1	0.92	0.46	9,9,9,9	0
57	MG	YA	3157	1/1	0.92	0.63	0,0,0,0	0
57	MG	QA	1612	1/1	0.92	0.46	7,7,7,7	0
57	MG	RE	301	1/1	0.92	0.27	12,12,12,12	0
57	MG	YA	3050	1/1	0.92	0.45	50,50,50,50	0
57	MG	QA	1613	1/1	0.92	0.68	15,15,15,15	0
57	MG	RA	3036	1/1	0.92	0.78	6,6,6,6	0
57	MG	XA	1649	1/1	0.92	0.20	0,0,0,0	0
57	MG	YA	3171	1/1	0.92	0.40	13,13,13,13	0
57	MG	YA	3261	1/1	0.92	0.30	4,4,4,4	0
57	MG	RA	3216	1/1	0.92	0.52	7,7,7,7	0
57	MG	RA	3129	1/1	0.92	0.21	31,31,31,31	0
57	MG	QA	1614	1/1	0.92	0.51	9,9,9,9	0
57	MG	RA	3131	1/1	0.92	0.68	9,9,9,9	0
57	MG	QA	1609	1/1	0.92	0.72	4,4,4,4	0
57	MG	YA	3179	1/1	0.92	0.24	0,0,0,0	0
57	MG	YB	203	1/1	0.92	0.23	37,37,37,37	0
57	MG	YA	3181	1/1	0.92	0.34	3,3,3,3	0
57	MG	QA	1640	1/1	0.92	0.35	9,9,9,9	0
57	MG	XA	1606	1/1	0.92	0.56	10,10,10,10	0
57	MG	QA	1642	1/1	0.92	0.49	16,16,16,16	0
58	ZN	R9	101	1/1	0.92	0.40	145,145,145,145	0
57	MG	YA	3186	1/1	0.92	0.62	11,11,11,11	0
57	MG	XA	1608	1/1	0.92	0.13	37,37,37,37	0
57	MG	RA	3041	1/1	0.93	0.44	4,4,4,4	0
57	MG	XA	1654	1/1	0.93	0.29	26,26,26,26	0
57	MG	YA	3028	1/1	0.93	0.37	6,6,6,6	0
57	MG	RA	3238	1/1	0.93	0.49	16,16,16,16	0
57	MG	QA	1619	1/1	0.93	0.45	4,4,4,4	0
57	MG	XA	1625	1/1	0.93	0.17	5,5,5,5	0
57	MG	XA	1661	1/1	0.93	0.16	2,2,2,2	0
57	MG	YA	3132	1/1	0.93	0.10	5,5,5,5	0
57	MG	RB	201	1/1	0.93	0.13	8,8,8,8	0
57	MG	YA	3053	1/1	0.93	0.53	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	3054	1/1	0.93	0.31	1,1,1,1	0
57	MG	RA	3089	1/1	0.93	0.57	11,11,11,11	0
57	MG	YA	3189	1/1	0.93	0.55	6,6,6,6	0
57	MG	YA	3142	1/1	0.93	0.66	19,19,19,19	0
57	MG	RA	3045	1/1	0.93	0.12	1,1,1,1	0
57	MG	YA	3069	1/1	0.93	0.51	2,2,2,2	0
57	MG	YA	3259	1/1	0.93	0.72	8,8,8,8	0
57	MG	RA	3067	1/1	0.93	0.25	2,2,2,2	0
57	MG	QA	1602	1/1	0.93	0.81	12,12,12,12	0
57	MG	QA	1656	1/1	0.93	0.14	30,30,30,30	0
57	MG	QA	1622	1/1	0.93	0.33	14,14,14,14	0
57	MG	YA	3267	1/1	0.93	0.41	4,4,4,4	0
57	MG	RA	3152	1/1	0.93	0.14	4,4,4,4	0
57	MG	RA	3050	1/1	0.93	0.56	11,11,11,11	0
57	MG	XA	1601	1/1	0.93	0.95	1,1,1,1	0
57	MG	YA	3088	1/1	0.93	0.58	50,50,50,50	0
57	MG	YA	3094	1/1	0.93	0.91	11,11,11,11	0
57	MG	RA	3079	1/1	0.93	0.68	5,5,5,5	0
57	MG	RA	3231	1/1	0.93	0.30	14,14,14,14	0
57	MG	RA	3232	1/1	0.93	0.39	13,13,13,13	0
57	MG	QA	1627	1/1	0.93	0.21	10,10,10,10	0
57	MG	RA	3218	1/1	0.93	0.32	23,23,23,23	0
57	MG	YA	3115	1/1	0.93	0.32	4,4,4,4	0
57	MG	YA	3229	1/1	0.93	0.24	3,3,3,3	0
57	MG	YA	3150	1/1	0.94	0.41	4,4,4,4	0
57	MG	RB	202	1/1	0.94	0.08	4,4,4,4	0
57	MG	YA	3211	1/1	0.94	0.60	7,7,7,7	0
57	MG	QA	1651	1/1	0.94	0.22	9,9,9,9	0
57	MG	QA	1644	1/1	0.94	0.26	4,4,4,4	0
57	MG	XA	1634	1/1	0.94	0.55	0,0,0,0	0
57	MG	YA	3221	1/1	0.94	0.50	18,18,18,18	0
57	MG	RA	3112	1/1	0.94	0.17	6,6,6,6	0
57	MG	XA	1668	1/1	0.94	0.23	18,18,18,18	0
57	MG	XA	1670	1/1	0.94	0.17	43,43,43,43	0
57	MG	RA	3164	1/1	0.94	0.16	4,4,4,4	0
57	MG	XA	1637	1/1	0.94	0.43	25,25,25,25	0
57	MG	YA	3164	1/1	0.94	0.46	8,8,8,8	0
57	MG	YA	3086	1/1	0.94	0.78	6,6,6,6	0
57	MG	QA	1633	1/1	0.94	0.58	4,4,4,4	0
57	MG	XV	101	1/1	0.94	0.45	14,14,14,14	0
57	MG	YA	3168	1/1	0.94	0.29	41,41,41,41	0
57	MG	YA	3240	1/1	0.94	0.17	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3183	1/1	0.94	0.33	57,57,57,57	0
57	MG	QA	1648	1/1	0.94	0.32	12,12,12,12	0
57	MG	RA	3186	1/1	0.94	0.23	8,8,8,8	0
57	MG	YA	3004	1/1	0.94	0.40	12,12,12,12	0
57	MG	YA	3106	1/1	0.94	0.34	8,8,8,8	0
57	MG	RA	3010	1/1	0.94	0.51	14,14,14,14	0
57	MG	YA	3011	1/1	0.94	0.32	0,0,0,0	0
57	MG	YA	3251	1/1	0.94	0.17	9,9,9,9	0
57	MG	RA	3211	1/1	0.94	0.24	2,2,2,2	0
57	MG	YA	3253	1/1	0.94	0.59	6,6,6,6	0
57	MG	YA	3180	1/1	0.94	0.41	38,38,38,38	0
57	MG	RA	3013	1/1	0.94	0.53	4,4,4,4	0
57	MG	YA	3258	1/1	0.94	0.52	1,1,1,1	0
57	MG	YA	3015	1/1	0.94	1.11	50,50,50,50	0
57	MG	RA	3143	1/1	0.94	0.30	7,7,7,7	0
57	MG	YA	3124	1/1	0.94	0.21	9,9,9,9	0
57	MG	XA	1651	1/1	0.94	0.27	25,25,25,25	0
57	MG	RA	3215	1/1	0.94	0.17	27,27,27,27	0
57	MG	YA	3266	1/1	0.94	0.27	2,2,2,2	0
57	MG	RA	3145	1/1	0.94	0.47	3,3,3,3	0
57	MG	YA	3032	1/1	0.94	0.28	1,1,1,1	0
57	MG	RA	3236	1/1	0.94	0.44	0,0,0,0	0
57	MG	YA	3043	1/1	0.94	1.15	2,2,2,2	0
57	MG	XA	1620	1/1	0.94	0.16	2,2,2,2	0
57	MG	RA	3237	1/1	0.94	1.23	1,1,1,1	0
57	MG	YE	301	1/1	0.94	0.18	0,0,0,0	0
57	MG	QA	1607	1/1	0.94	0.11	13,13,13,13	0
57	MG	YA	3144	1/1	0.94	0.13	4,4,4,4	0
57	MG	XA	1658	1/1	0.94	0.43	9,9,9,9	0
57	MG	QA	1639	1/1	0.94	0.19	3,3,3,3	0
57	MG	YA	3205	1/1	0.94	0.14	10,10,10,10	0
57	MG	RA	3004	1/1	0.94	0.96	10,10,10,10	0
57	MG	YA	3208	1/1	0.94	0.21	15,15,15,15	0
57	MG	YA	3215	1/1	0.95	0.18	14,14,14,14	0
57	MG	RA	3014	1/1	0.95	0.28	13,13,13,13	0
57	MG	YA	3078	1/1	0.95	0.36	2,2,2,2	0
57	MG	RA	3190	1/1	0.95	0.20	16,16,16,16	0
57	MG	RA	3120	1/1	0.95	0.22	1,1,1,1	0
57	MG	RA	3047	1/1	0.95	0.62	5,5,5,5	0
57	MG	RA	3029	1/1	0.95	0.37	1,1,1,1	0
57	MG	YA	3227	1/1	0.95	0.28	0,0,0,0	0
57	MG	RA	3015	1/1	0.95	0.69	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3161	1/1	0.95	0.20	1,1,1,1	0
57	MG	YA	3163	1/1	0.95	0.21	4,4,4,4	0
57	MG	RA	3016	1/1	0.95	0.39	8,8,8,8	0
57	MG	YA	3096	1/1	0.95	0.52	3,3,3,3	0
57	MG	YA	3007	1/1	0.95	0.17	7,7,7,7	0
57	MG	QA	1625	1/1	0.95	0.30	0,0,0,0	0
57	MG	RA	3020	1/1	0.95	0.73	50,50,50,50	0
57	MG	RA	3134	1/1	0.95	0.13	25,25,25,25	0
57	MG	RA	3135	1/1	0.95	0.17	7,7,7,7	0
57	MG	YA	3111	1/1	0.95	0.21	15,15,15,15	0
57	MG	RA	3058	1/1	0.95	0.74	3,3,3,3	0
57	MG	YA	3019	1/1	0.95	0.47	5,5,5,5	0
57	MG	XA	1611	1/1	0.95	0.31	7,7,7,7	0
57	MG	YA	3118	1/1	0.95	0.28	14,14,14,14	0
57	MG	YA	3026	1/1	0.95	1.12	1,1,1,1	0
57	MG	YA	3120	1/1	0.95	0.60	8,8,8,8	0
57	MG	RA	3204	1/1	0.95	0.27	18,18,18,18	0
57	MG	RA	3092	1/1	0.95	0.53	7,7,7,7	0
57	MG	YA	3255	1/1	0.95	1.32	0,0,0,0	0
57	MG	YA	3123	1/1	0.95	0.19	18,18,18,18	0
57	MG	XA	1622	1/1	0.95	0.13	7,7,7,7	0
57	MG	YA	3125	1/1	0.95	0.41	12,12,12,12	0
57	MG	YA	3033	1/1	0.95	0.45	4,4,4,4	0
57	MG	XA	1660	1/1	0.95	0.14	24,24,24,24	0
57	MG	YA	3190	1/1	0.95	0.24	21,21,21,21	0
57	MG	YA	3264	1/1	0.95	0.17	9,9,9,9	0
57	MG	RA	3093	1/1	0.95	0.59	10,10,10,10	0
57	MG	RA	3094	1/1	0.95	0.47	0,0,0,0	0
57	MG	QA	1641	1/1	0.95	0.23	7,7,7,7	0
57	MG	YA	3134	1/1	0.95	0.78	11,11,11,11	0
57	MG	XA	1628	1/1	0.95	0.54	10,10,10,10	0
57	MG	YA	3136	1/1	0.95	0.12	21,21,21,21	0
57	MG	YA	3052	1/1	0.95	0.70	14,14,14,14	0
57	MG	RA	3102	1/1	0.95	0.27	4,4,4,4	0
57	MG	RA	3181	1/1	0.95	0.20	3,3,3,3	0
57	MG	RA	3043	1/1	0.95	0.21	10,10,10,10	0
57	MG	RA	3111	1/1	0.95	0.46	11,11,11,11	0
57	MG	QA	1605	1/1	0.95	1.07	7,7,7,7	0
57	MG	RA	3068	1/1	0.95	0.12	6,6,6,6	0
57	MG	YA	3072	1/1	0.95	0.21	2,2,2,2	0
57	MG	XA	1672	1/1	0.95	0.41	0,0,0,0	0
57	MG	QA	1611	1/1	0.95	0.31	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	RA	3189	1/1	0.96	0.27	4,4,4,4	0
57	MG	XA	1643	1/1	0.96	0.37	5,5,5,5	0
57	MG	RA	3149	1/1	0.96	0.15	20,20,20,20	0
57	MG	YA	3204	1/1	0.96	0.10	11,11,11,11	0
57	MG	RA	3150	1/1	0.96	0.32	37,37,37,37	0
57	MG	RA	3151	1/1	0.96	0.41	9,9,9,9	0
57	MG	YA	3034	1/1	0.96	0.54	2,2,2,2	0
57	MG	YA	3035	1/1	0.96	0.33	9,9,9,9	0
57	MG	RA	3031	1/1	0.96	0.74	5,5,5,5	0
57	MG	YA	3041	1/1	0.96	0.73	0,0,0,0	0
57	MG	YA	3139	1/1	0.96	0.40	7,7,7,7	0
57	MG	QA	1604	1/1	0.96	0.27	0,0,0,0	0
57	MG	RA	3154	1/1	0.96	0.18	11,11,11,11	0
57	MG	RA	3019	1/1	0.96	0.38	8,8,8,8	0
57	MG	YA	3143	1/1	0.96	0.15	8,8,8,8	0
57	MG	RA	3074	1/1	0.96	0.12	8,8,8,8	0
57	MG	RA	3035	1/1	0.96	0.41	11,11,11,11	0
57	MG	RA	3201	1/1	0.96	0.77	10,10,10,10	0
57	MG	RF	301	1/1	0.96	0.39	2,2,2,2	0
57	MG	RA	3160	1/1	0.96	0.33	4,4,4,4	0
57	MG	RA	3161	1/1	0.96	0.13	1,1,1,1	0
57	MG	YA	3232	1/1	0.96	0.41	2,2,2,2	0
57	MG	YA	3068	1/1	0.96	0.51	2,2,2,2	0
57	MG	XA	1659	1/1	0.96	0.32	0,0,0,0	0
57	MG	YA	3070	1/1	0.96	0.40	15,15,15,15	0
57	MG	RA	3119	1/1	0.96	0.39	3,3,3,3	0
57	MG	RA	3205	1/1	0.96	0.31	12,12,12,12	0
57	MG	RA	3077	1/1	0.96	0.55	0,0,0,0	0
57	MG	YA	3158	1/1	0.96	0.27	6,6,6,6	0
57	MG	RA	3051	1/1	0.96	0.47	7,7,7,7	0
57	MG	RA	3167	1/1	0.96	0.23	3,3,3,3	0
57	MG	RA	3122	1/1	0.96	0.56	5,5,5,5	0
57	MG	QA	1645	1/1	0.96	0.13	38,38,38,38	0
57	MG	YA	3082	1/1	0.96	0.23	3,3,3,3	0
57	MG	RA	3126	1/1	0.96	0.44	2,2,2,2	0
57	MG	RA	3084	1/1	0.96	0.16	4,4,4,4	0
57	MG	RA	3053	1/1	0.96	0.16	2,2,2,2	0
57	MG	QA	1621	1/1	0.96	0.11	5,5,5,5	0
57	MG	YA	3089	1/1	0.96	0.43	5,5,5,5	0
57	MG	XA	1618	1/1	0.96	0.50	3,3,3,3	0
57	MG	YA	3095	1/1	0.96	0.48	2,2,2,2	0
57	MG	RA	3217	1/1	0.96	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3097	1/1	0.96	0.65	5,5,5,5	0
57	MG	RA	3024	1/1	0.96	0.23	16,16,16,16	0
57	MG	RA	3090	1/1	0.96	0.15	75,75,75,75	0
57	MG	YA	3178	1/1	0.96	0.13	2,2,2,2	0
57	MG	RA	3091	1/1	0.96	0.44	9,9,9,9	0
57	MG	XX	102	1/1	0.96	0.09	50,50,50,50	0
57	MG	YA	3104	1/1	0.96	0.59	10,10,10,10	0
57	MG	RA	3136	1/1	0.96	0.37	0,0,0,0	0
57	MG	RA	3061	1/1	0.96	0.16	53,53,53,53	0
57	MG	QA	1616	1/1	0.96	0.09	29,29,29,29	0
57	MG	RA	3180	1/1	0.96	0.11	6,6,6,6	0
57	MG	YA	3116	1/1	0.96	0.42	3,3,3,3	0
57	MG	RA	3139	1/1	0.96	0.24	2,2,2,2	0
57	MG	QA	1663	1/1	0.96	0.10	47,47,47,47	0
57	MG	RA	3095	1/1	0.96	0.80	1,1,1,1	0
57	MG	YQ	201	1/1	0.96	0.21	99,99,99,99	0
57	MG	RA	3184	1/1	0.96	0.26	8,8,8,8	0
57	MG	RA	3064	1/1	0.96	0.18	5,5,5,5	0
57	MG	YA	3195	1/1	0.96	0.39	9,9,9,9	0
57	MG	RA	3008	1/1	0.96	0.46	0,0,0,0	0
57	MG	RA	3017	1/1	0.96	0.39	11,11,11,11	0
57	MG	RA	3147	1/1	0.96	0.23	9,9,9,9	0
57	MG	YA	3199	1/1	0.97	0.11	55,55,55,55	0
57	MG	YA	3129	1/1	0.97	0.70	15,15,15,15	0
57	MG	YA	3130	1/1	0.97	0.21	20,20,20,20	0
57	MG	YA	3058	1/1	0.97	0.52	15,15,15,15	0
57	MG	YA	3059	1/1	0.97	0.32	5,5,5,5	0
57	MG	YA	3061	1/1	0.97	0.12	17,17,17,17	0
57	MG	QA	1654	1/1	0.97	0.13	17,17,17,17	0
57	MG	YA	3064	1/1	0.97	0.35	8,8,8,8	0
57	MG	RA	3002	1/1	0.97	0.89	6,6,6,6	0
57	MG	YA	3137	1/1	0.97	0.21	10,10,10,10	0
57	MG	YA	3138	1/1	0.97	0.12	0,0,0,0	0
57	MG	QA	1617	1/1	0.97	0.20	4,4,4,4	0
57	MG	RA	3115	1/1	0.97	0.44	6,6,6,6	0
57	MG	XA	1644	1/1	0.97	0.14	5,5,5,5	0
57	MG	YA	3217	1/1	0.97	0.17	35,35,35,35	0
57	MG	XA	1645	1/1	0.97	0.23	1,1,1,1	0
57	MG	RA	3086	1/1	0.97	0.24	0,0,0,0	0
57	MG	YA	3003	1/1	0.97	0.17	2,2,2,2	0
57	MG	RA	3012	1/1	0.97	0.50	4,4,4,4	0
57	MG	YA	3223	1/1	0.97	0.42	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3005	1/1	0.97	0.25	3,3,3,3	0
57	MG	YA	3077	1/1	0.97	0.30	2,2,2,2	0
57	MG	RA	3144	1/1	0.97	0.26	0,0,0,0	0
57	MG	YA	3228	1/1	0.97	0.50	17,17,17,17	0
57	MG	RA	3200	1/1	0.97	0.14	1,1,1,1	0
57	MG	YA	3081	1/1	0.97	0.50	9,9,9,9	0
57	MG	YA	3010	1/1	0.97	0.40	5,5,5,5	0
57	MG	YA	3233	1/1	0.97	0.22	7,7,7,7	0
57	MG	YA	3083	1/1	0.97	0.50	9,9,9,9	0
57	MG	RA	3118	1/1	0.97	0.22	2,2,2,2	0
57	MG	RA	3146	1/1	0.97	0.13	5,5,5,5	0
57	MG	XA	1610	1/1	0.97	0.23	3,3,3,3	0
57	MG	YA	3087	1/1	0.97	0.68	11,11,11,11	0
57	MG	RA	3065	1/1	0.97	0.37	7,7,7,7	0
57	MG	XA	1614	1/1	0.97	0.15	26,26,26,26	0
57	MG	YA	3093	1/1	0.97	0.36	7,7,7,7	0
57	MG	YA	3162	1/1	0.97	0.18	0,0,0,0	0
57	MG	RA	3021	1/1	0.97	0.22	2,2,2,2	0
57	MG	YA	3021	1/1	0.97	0.43	12,12,12,12	0
57	MG	RA	3034	1/1	0.97	0.86	9,9,9,9	0
57	MG	QA	1647	1/1	0.97	0.26	33,33,33,33	0
57	MG	YA	3098	1/1	0.97	0.29	1,1,1,1	0
57	MG	RA	3124	1/1	0.97	0.34	10,10,10,10	0
57	MG	QA	1635	1/1	0.97	0.41	13,13,13,13	0
57	MG	YA	3170	1/1	0.97	0.20	8,8,8,8	0
57	MG	QA	1659	1/1	0.97	0.23	4,4,4,4	0
57	MG	YA	3102	1/1	0.97	0.48	14,14,14,14	0
57	MG	XA	1626	1/1	0.97	0.16	6,6,6,6	0
57	MG	RA	3040	1/1	0.97	0.37	14,14,14,14	0
57	MG	RA	3097	1/1	0.97	0.47	2,2,2,2	0
57	MG	RA	3054	1/1	0.97	0.28	3,3,3,3	0
57	MG	YA	3262	1/1	0.97	0.55	8,8,8,8	0
57	MG	YA	3112	1/1	0.97	0.13	21,21,21,21	0
57	MG	YA	3113	1/1	0.97	0.20	1,1,1,1	0
57	MG	YA	3040	1/1	0.97	0.55	10,10,10,10	0
57	MG	QA	1652	1/1	0.97	0.16	12,12,12,12	0
57	MG	RA	3103	1/1	0.97	0.48	9,9,9,9	0
57	MG	XA	1632	1/1	0.97	0.81	14,14,14,14	0
57	MG	YA	3046	1/1	0.97	0.40	3,3,3,3	0
57	MG	YA	3047	1/1	0.97	0.60	3,3,3,3	0
57	MG	YA	3048	1/1	0.97	0.22	4,4,4,4	0
57	MG	RA	3106	1/1	0.97	0.36	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1669	1/1	0.97	0.19	38,38,38,38	0
57	MG	YA	3191	1/1	0.97	0.05	7,7,7,7	0
57	MG	RA	3163	1/1	0.97	1.01	12,12,12,12	0
57	MG	RA	3108	1/1	0.97	0.09	0,0,0,0	0
57	MG	RA	3027	1/1	0.97	0.49	13,13,13,13	0
57	MG	YA	3126	1/1	0.97	0.35	7,7,7,7	0
57	MG	YA	3055	1/1	0.97	0.26	0,0,0,0	0
57	MG	YA	3197	1/1	0.97	0.15	1,1,1,1	0
57	MG	YA	3056	1/1	0.97	0.18	5,5,5,5	0
57	MG	YA	3060	1/1	0.98	0.59	10,10,10,10	0
57	MG	RA	3075	1/1	0.98	0.19	3,3,3,3	0
57	MG	RA	3123	1/1	0.98	0.12	7,7,7,7	0
57	MG	RA	3096	1/1	0.98	0.58	4,4,4,4	0
57	MG	RR	201	1/1	0.98	0.24	13,13,13,13	0
57	MG	YA	3206	1/1	0.98	0.34	26,26,26,26	0
57	MG	XA	1640	1/1	0.98	0.12	75,75,75,75	0
57	MG	RA	3059	1/1	0.98	0.44	11,11,11,11	0
57	MG	RA	3156	1/1	0.98	0.13	9,9,9,9	0
57	MG	RA	3098	1/1	0.98	0.63	14,14,14,14	0
57	MG	YA	3008	1/1	0.98	0.32	10,10,10,10	0
57	MG	YA	3073	1/1	0.98	0.25	1,1,1,1	0
57	MG	YA	3213	1/1	0.98	0.13	19,19,19,19	0
57	MG	YA	3009	1/1	0.98	0.73	8,8,8,8	0
57	MG	YA	3216	1/1	0.98	0.16	19,19,19,19	0
57	MG	RA	3099	1/1	0.98	0.24	10,10,10,10	0
57	MG	RA	3100	1/1	0.98	0.14	2,2,2,2	0
57	MG	RA	3060	1/1	0.98	0.30	6,6,6,6	0
57	MG	YA	3220	1/1	0.98	0.66	33,33,33,33	0
57	MG	YA	3013	1/1	0.98	0.54	5,5,5,5	0
57	MG	YA	3079	1/1	0.98	0.23	4,4,4,4	0
57	MG	YA	3147	1/1	0.98	0.57	4,4,4,4	0
57	MG	YA	3148	1/1	0.98	0.14	7,7,7,7	0
57	MG	XA	1604	1/1	0.98	0.96	10,10,10,10	0
57	MG	YA	3226	1/1	0.98	0.38	1,1,1,1	0
57	MG	QV	101	1/1	0.98	0.26	1,1,1,1	0
57	MG	RA	3133	1/1	0.98	0.16	0,0,0,0	0
57	MG	YA	3017	1/1	0.98	0.17	1,1,1,1	0
57	MG	YA	3018	1/1	0.98	0.69	3,3,3,3	0
57	MG	YA	3231	1/1	0.98	0.11	45,45,45,45	0
57	MG	RA	3080	1/1	0.98	0.34	21,21,21,21	0
57	MG	RA	3105	1/1	0.98	0.47	11,11,11,11	0
57	MG	RA	3081	1/1	0.98	0.71	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3235	1/1	0.98	0.37	3,3,3,3	0
57	MG	YA	3025	1/1	0.98	0.19	4,4,4,4	0
57	MG	RA	3196	1/1	0.98	0.18	0,0,0,0	0
57	MG	YA	3090	1/1	0.98	0.43	1,1,1,1	0
57	MG	YA	3091	1/1	0.98	0.39	13,13,13,13	0
57	MG	YA	3092	1/1	0.98	0.25	12,12,12,12	0
57	MG	YA	3241	1/1	0.98	0.18	5,5,5,5	0
57	MG	YA	3027	1/1	0.98	0.10	1,1,1,1	0
57	MG	RA	3228	1/1	0.98	0.51	11,11,11,11	0
57	MG	YA	3029	1/1	0.98	0.81	10,10,10,10	0
57	MG	XA	1612	1/1	0.98	0.17	19,19,19,19	0
57	MG	YA	3031	1/1	0.98	0.60	0,0,0,0	0
57	MG	RA	3037	1/1	0.98	0.51	5,5,5,5	0
57	MG	YA	3249	1/1	0.98	0.31	10,10,10,10	0
57	MG	XA	1615	1/1	0.98	0.28	6,6,6,6	0
57	MG	XA	1616	1/1	0.98	0.31	1,1,1,1	0
57	MG	XA	1617	1/1	0.98	0.22	15,15,15,15	0
57	MG	YA	3036	1/1	0.98	0.32	2,2,2,2	0
57	MG	YA	3038	1/1	0.98	0.16	7,7,7,7	0
57	MG	RA	3109	1/1	0.98	0.23	8,8,8,8	0
57	MG	YA	3105	1/1	0.98	0.18	4,4,4,4	0
57	MG	XA	1619	1/1	0.98	0.28	5,5,5,5	0
57	MG	YA	3107	1/1	0.98	0.46	15,15,15,15	0
57	MG	YA	3108	1/1	0.98	0.49	1,1,1,1	0
57	MG	YA	3109	1/1	0.98	0.31	2,2,2,2	0
57	MG	QA	1608	1/1	0.98	0.09	10,10,10,10	0
57	MG	YA	3042	1/1	0.98	0.57	2,2,2,2	0
57	MG	RA	3030	1/1	0.98	0.36	5,5,5,5	0
57	MG	YA	3044	1/1	0.98	0.31	6,6,6,6	0
57	MG	RA	3023	1/1	0.98	0.32	16,16,16,16	0
57	MG	XA	1623	1/1	0.98	0.16	14,14,14,14	0
57	MG	YA	3187	1/1	0.98	0.13	2,2,2,2	0
57	MG	RA	3113	1/1	0.98	0.11	0,0,0,0	0
57	MG	RA	3087	1/1	0.98	0.93	11,11,11,11	0
57	MG	RA	3042	1/1	0.98	0.18	2,2,2,2	0
57	MG	RA	3011	1/1	0.98	0.18	6,6,6,6	0
57	MG	YA	3051	1/1	0.98	0.44	3,3,3,3	0
57	MG	QA	1630	1/1	0.98	0.15	7,7,7,7	0
57	MG	QA	1634	1/1	0.98	0.18	7,7,7,7	0
57	MG	Y5	101	1/1	0.98	0.36	6,6,6,6	0
57	MG	RA	3056	1/1	0.98	0.36	5,5,5,5	0
57	MG	RA	3072	1/1	0.98	0.41	3,3,3,3	0

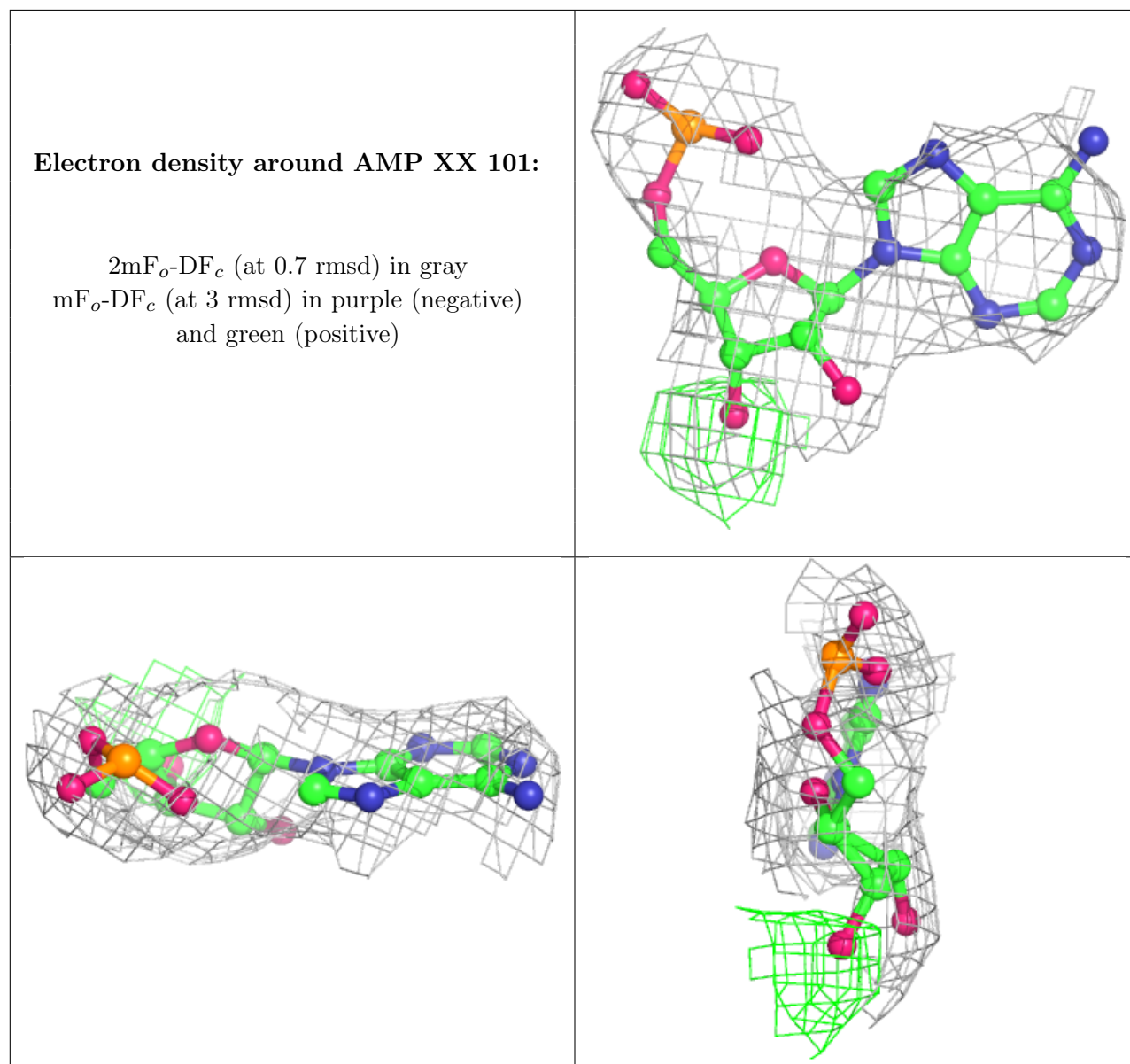
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1606	1/1	0.98	0.13	16,16,16,16	0
57	MG	YA	3057	1/1	0.98	0.88	4,4,4,4	0
58	ZN	XN	101	1/1	0.98	0.20	84,84,84,84	0
57	MG	XA	1633	1/1	0.98	0.21	3,3,3,3	0
57	MG	RA	3212	1/1	0.98	0.51	1,1,1,1	0
57	MG	YA	3062	1/1	0.99	0.39	6,6,6,6	0
57	MG	RA	3127	1/1	0.99	0.22	0,0,0,0	0
57	MG	YA	3037	1/1	0.99	0.25	13,13,13,13	0
57	MG	YA	3065	1/1	0.99	0.15	5,5,5,5	0
57	MG	XA	1602	1/1	0.99	0.20	7,7,7,7	0
57	MG	YA	3067	1/1	0.99	0.34	5,5,5,5	0
57	MG	RA	3128	1/1	0.99	0.44	7,7,7,7	0
57	MG	YA	3257	1/1	0.99	0.23	3,3,3,3	0
57	MG	QA	1653	1/1	0.99	0.07	67,67,67,67	0
57	MG	QA	1658	1/1	0.99	0.24	16,16,16,16	0
57	MG	RA	3038	1/1	0.99	0.32	8,8,8,8	0
57	MG	RA	3104	1/1	0.99	0.21	3,3,3,3	0
57	MG	RA	3165	1/1	0.99	0.48	13,13,13,13	0
57	MG	RA	3148	1/1	0.99	0.34	5,5,5,5	0
57	MG	YA	3020	1/1	0.99	0.86	0,0,0,0	0
57	MG	RA	3082	1/1	0.99	0.30	0,0,0,0	0
57	MG	YA	3022	1/1	0.99	0.28	1,1,1,1	0
57	MG	YA	3023	1/1	0.99	0.32	2,2,2,2	0
57	MG	RA	3057	1/1	0.99	0.30	2,2,2,2	0
57	MG	RA	3107	1/1	0.99	0.19	10,10,10,10	0
57	MG	YA	3110	1/1	0.99	0.12	2,2,2,2	0
57	MG	XA	1613	1/1	0.99	0.08	0,0,0,0	0
57	MG	RA	3073	1/1	0.99	0.35	2,2,2,2	0
57	MG	QM	201	1/1	0.99	0.14	44,44,44,44	0
57	MG	RA	3066	1/1	0.99	0.53	6,6,6,6	0
57	MG	QA	1610	1/1	0.99	0.23	7,7,7,7	0
57	MG	XA	1639	1/1	0.99	0.12	5,5,5,5	0
57	MG	YA	3177	1/1	0.99	0.21	3,3,3,3	0
57	MG	RA	3210	1/1	0.99	0.17	45,45,45,45	0
57	MG	QA	1660	1/1	0.99	0.75	2,2,2,2	0
57	MG	RA	3078	1/1	0.99	0.35	3,3,3,3	0
58	ZN	XD	301	1/1	0.99	0.42	50,50,50,50	0
57	MG	RA	3158	1/1	0.99	0.27	15,15,15,15	0
57	MG	YA	3214	1/1	0.99	0.20	2,2,2,2	0
57	MG	YA	3182	1/1	0.99	0.13	8,8,8,8	0
57	MG	YA	3244	1/1	1.00	0.10	9,9,9,9	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 ⓘ

There are no such residues in this entry.