



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 08:46 am BST

PDB ID : 1VVJ
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 bound to Codon CCC-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-05-24
Resolution : 3.44 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

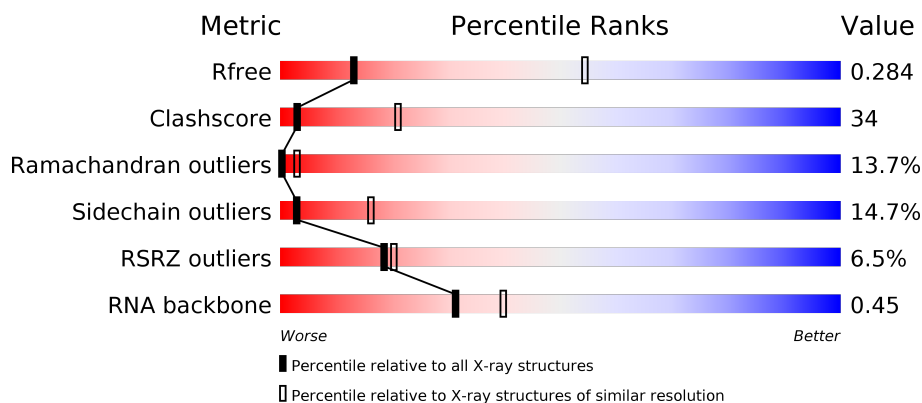
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)
RNA backbone	3102	1024 (3.92-2.96)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div>4%</div> <div>36%</div> <div>46%</div> <div>15%</div> <div>..</div> </div>
1	XA	1522	<div> <div>3%</div> <div>38%</div> <div>45%</div> <div>14%</div> <div>..</div> </div>
2	QB	256	<div> <div>12%</div> <div>16%</div> <div>59%</div> <div>16%</div> <div>7%</div> </div>
2	XB	256	<div> <div>9%</div> <div>16%</div> <div>60%</div> <div>16%</div> <div>7%</div> </div>

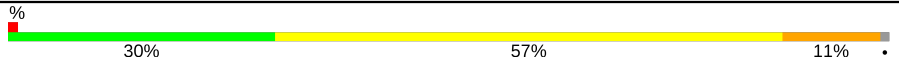
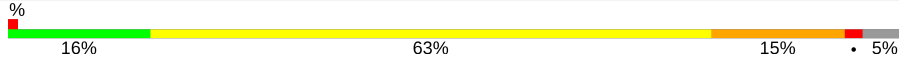
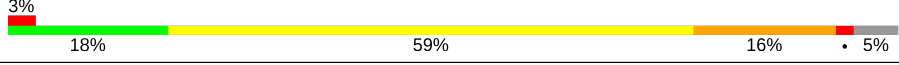
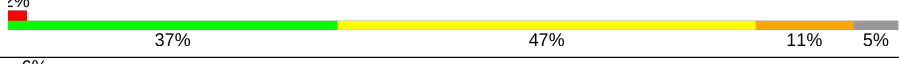
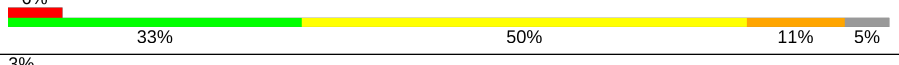
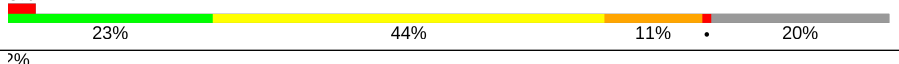
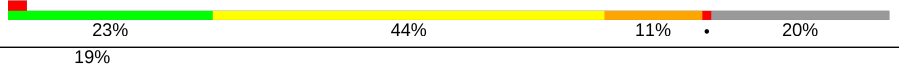
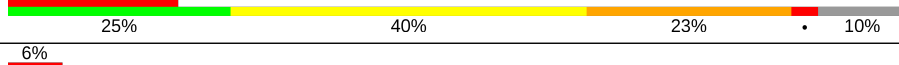
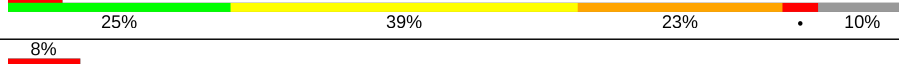
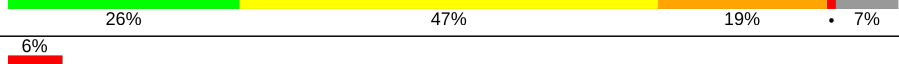
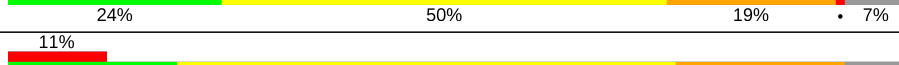
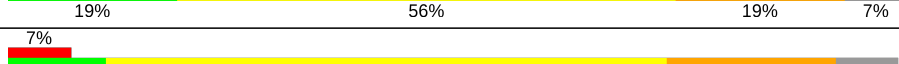
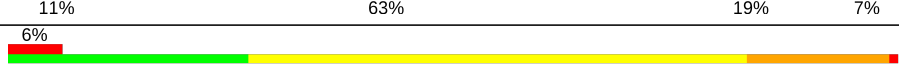
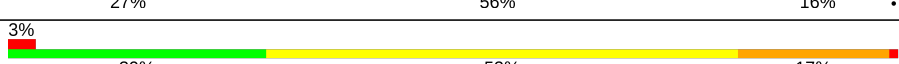
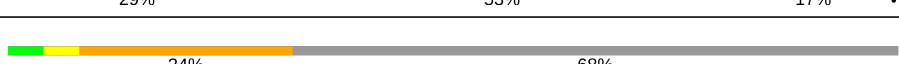
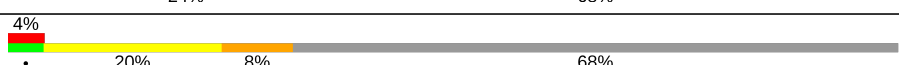
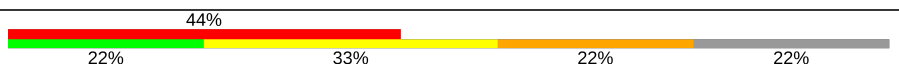
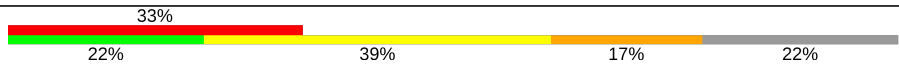
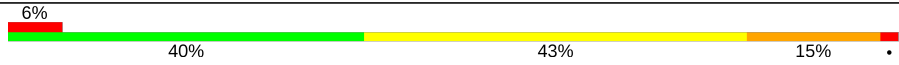


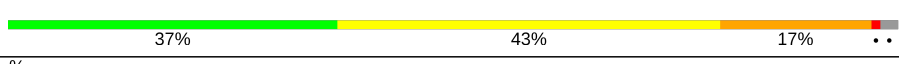
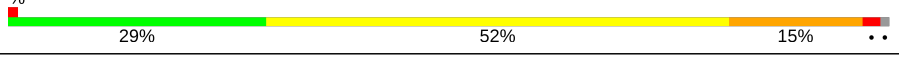
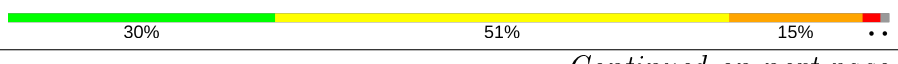

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

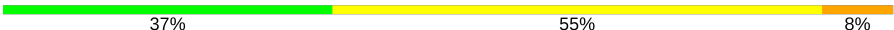


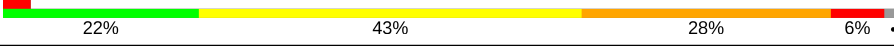
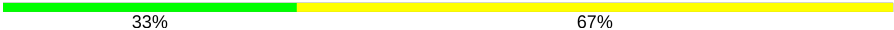

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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	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	Z6	3	
55	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
56	MG	QA	1615	-	-	-	X
56	MG	RA	3176	-	-	-	X
56	MG	RA	3202	-	-	-	X
56	MG	XA	1605	-	-	-	X
56	MG	YA	3012	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 291123 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	1501	Total	C	N	O	P	0	0	0
			32269	14363	5986	10420	1500			

- 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
			170	76	31	55	8			
23	XX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			

- 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	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			
25	YA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	3			
45	YZ	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	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 L32.

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 L33.

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 L34.

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 L35.

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 tRNA acceptor end mimic.

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 RNA chain called RNA (5'-R(*CP*CP*(PPU))-3').

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

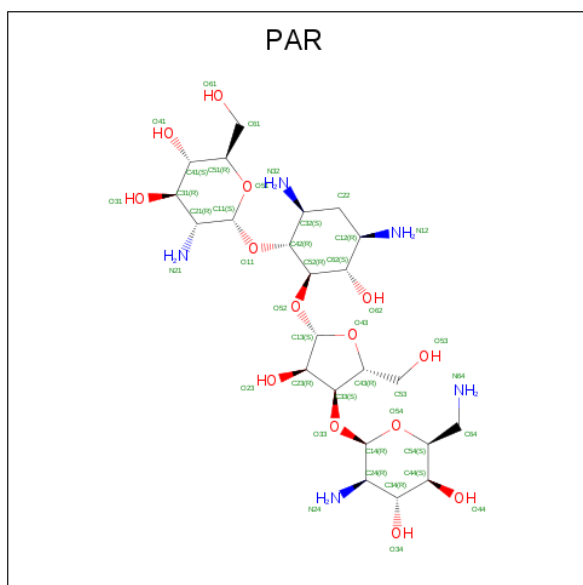
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RE	2	Total	Mg	0	0
			2	2		
56	YX	1	Total	Mg	0	0
			1	1		
56	XA	63	Total	Mg	0	0
			63	63		
56	QA	60	Total	Mg	0	0
			60	60		
56	Y5	1	Total	Mg	0	0
			1	1		
56	RP	1	Total	Mg	0	0
			1	1		
56	QX	2	Total	Mg	0	0
			2	2		
56	YA	242	Total	Mg	0	0
			242	242		
56	YB	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	QF	1	Total 1 Mg 1	0	0
56	QM	1	Total 1 Mg 1	0	0
56	R5	1	Total 1 Mg 1	0	0
56	RB	2	Total 2 Mg 2	0	0
56	RA	212	Total 212 Mg 212	0	0
56	XM	2	Total 2 Mg 2	0	0
56	QH	1	Total 1 Mg 1	0	0
56	XV	2	Total 2 Mg 2	0	0
56	RF	1	Total 1 Mg 1	0	0
56	QV	2	Total 2 Mg 2	0	0
56	YE	2	Total 2 Mg 2	0	0

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

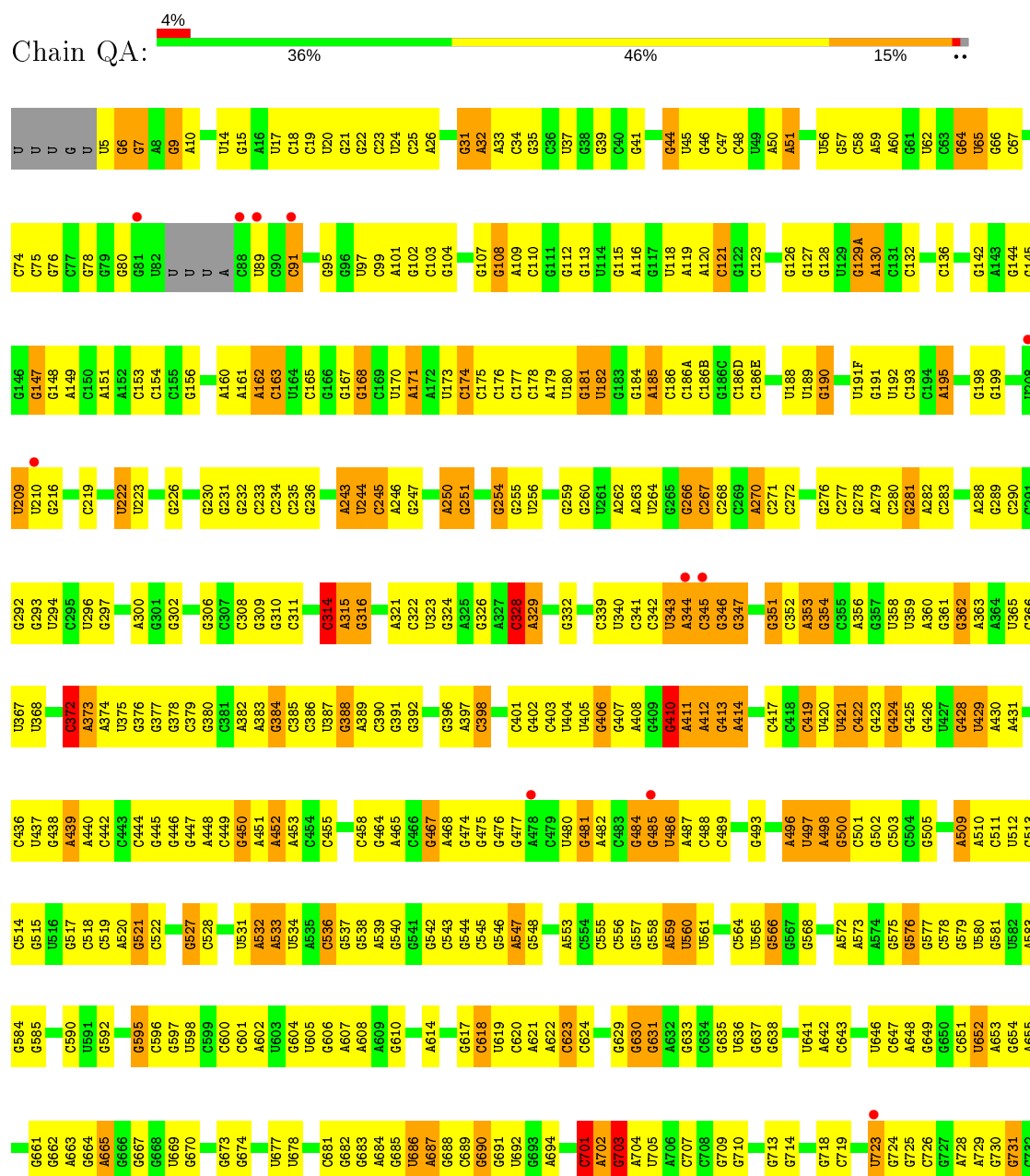
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

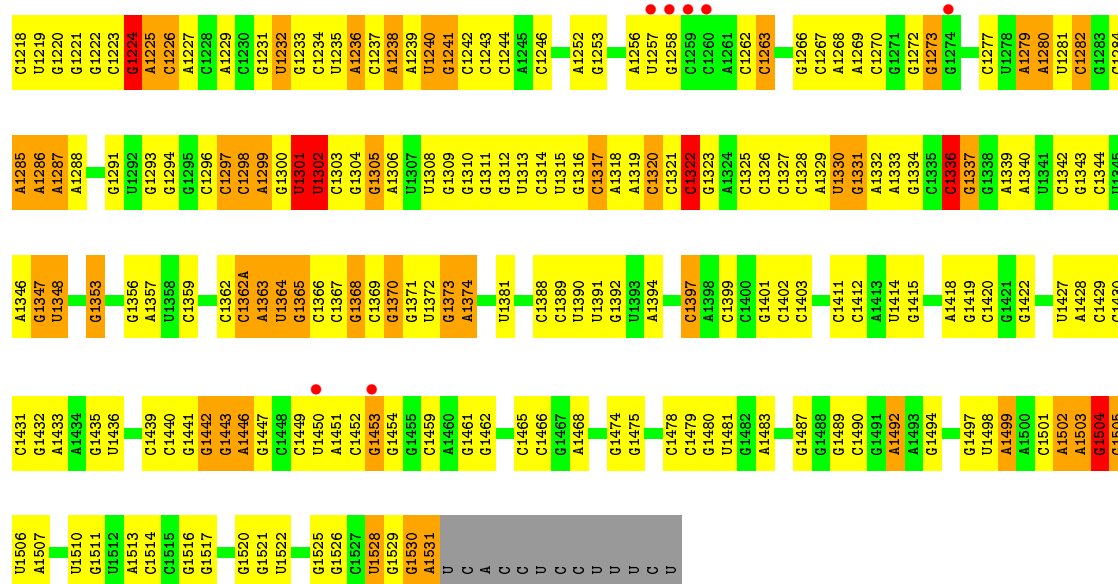
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

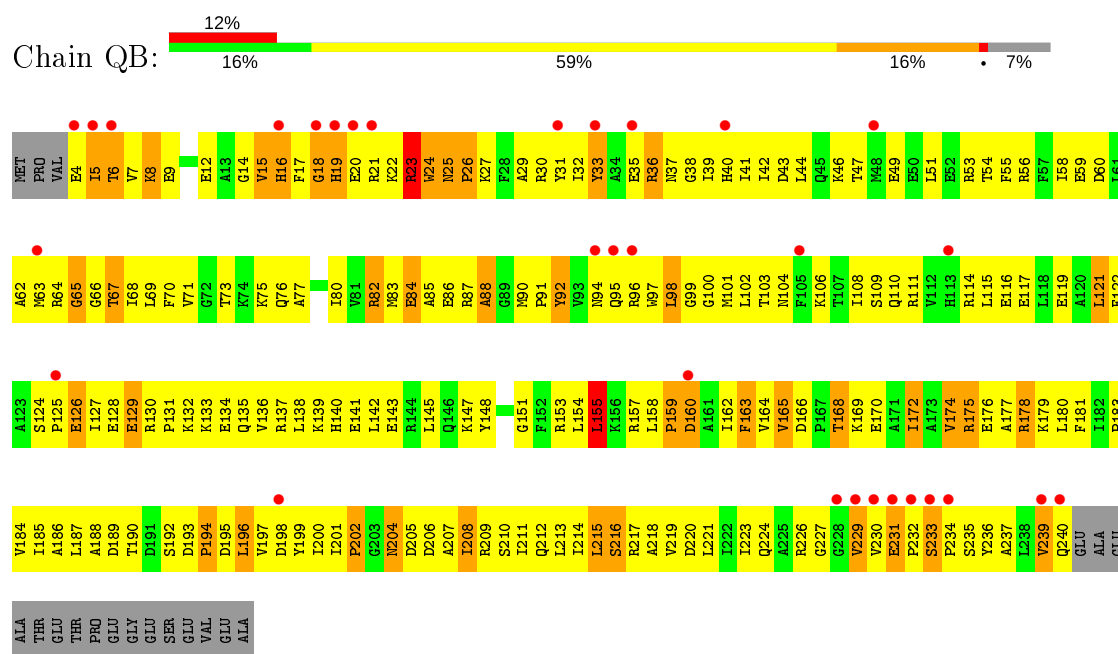




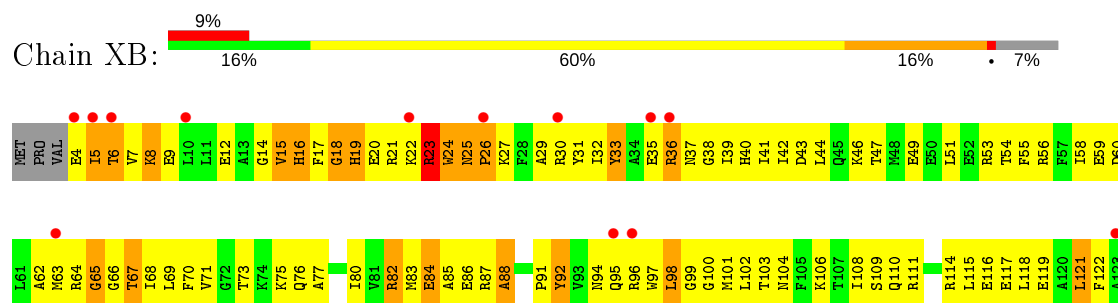


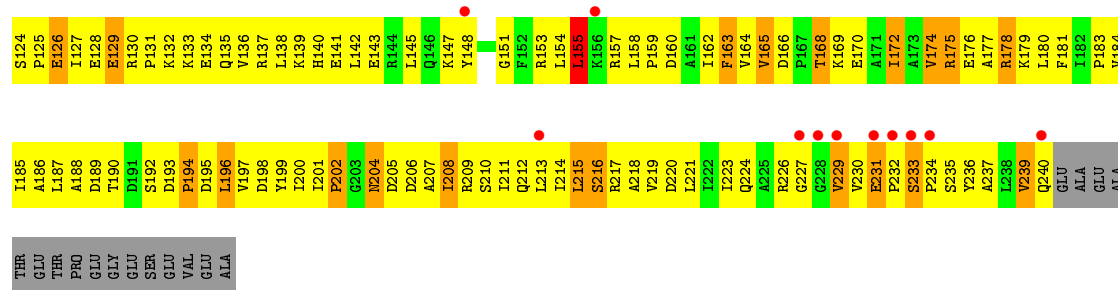


• Molecule 2: 30S ribosomal protein S2

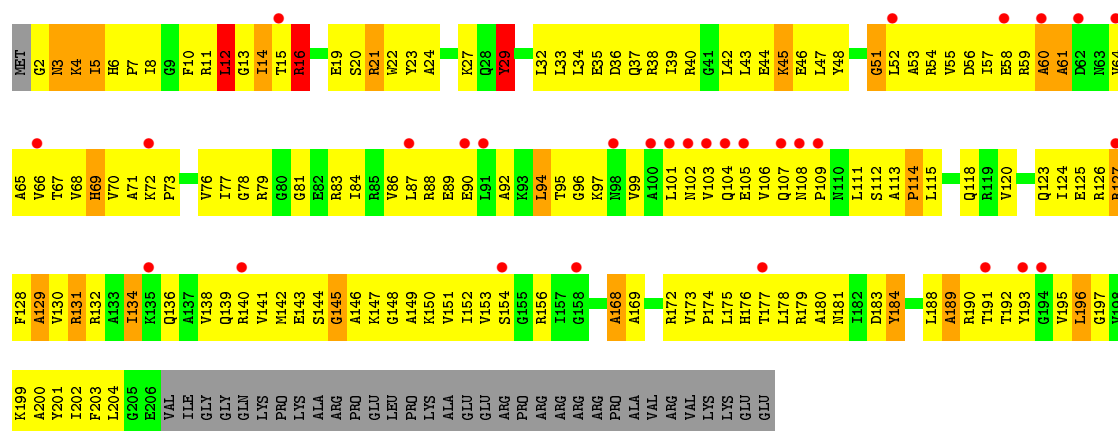


• Molecule 2: 30S ribosomal protein S2

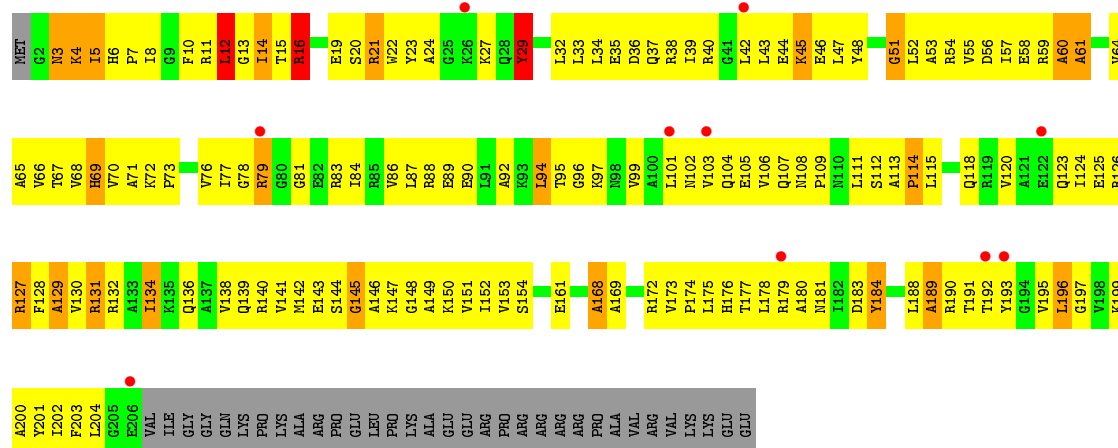




• Molecule 3: 30S ribosomal protein S3

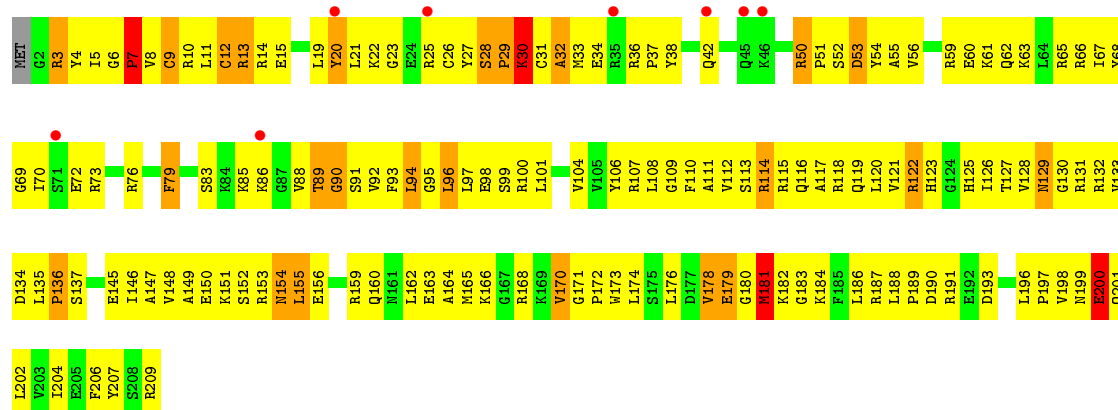


• Molecule 3: 30S ribosomal protein S3

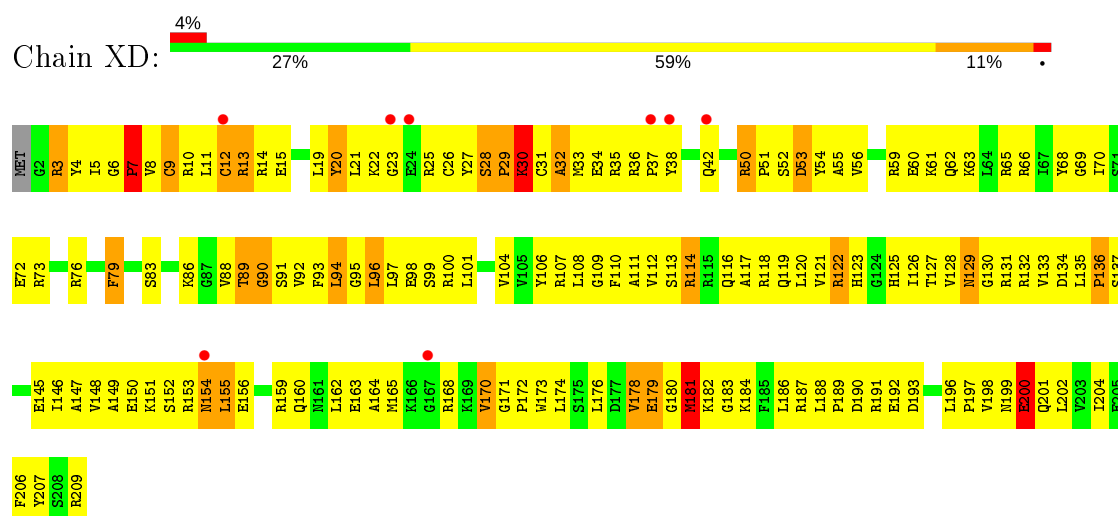


• Molecule 4: 30S ribosomal protein S4

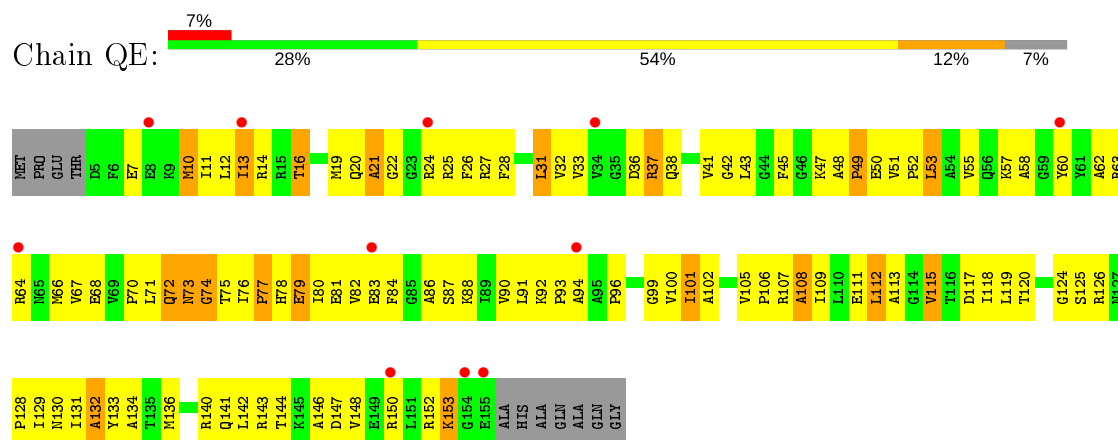




• Molecule 4: 30S ribosomal protein S4

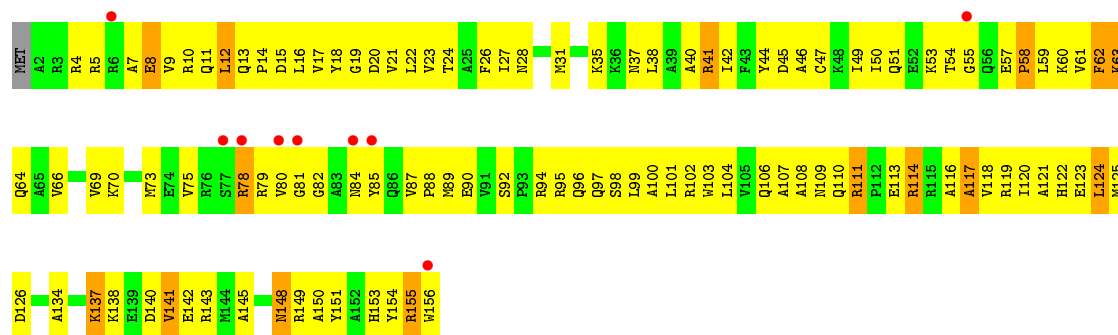


• Molecule 5: 30S ribosomal protein S5

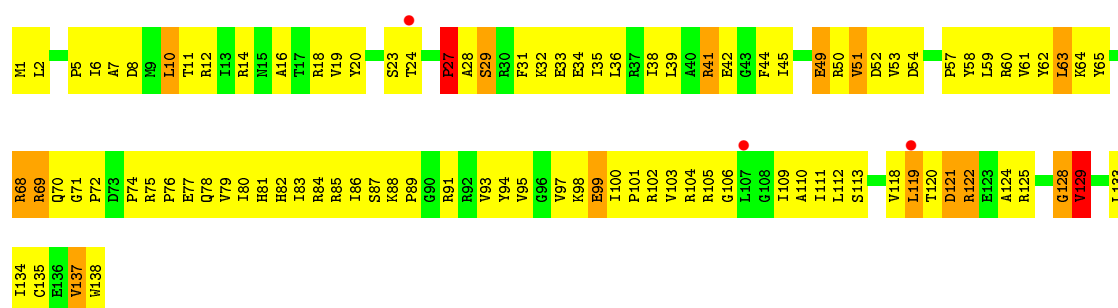


• Molecule 5: 30S ribosomal protein S5

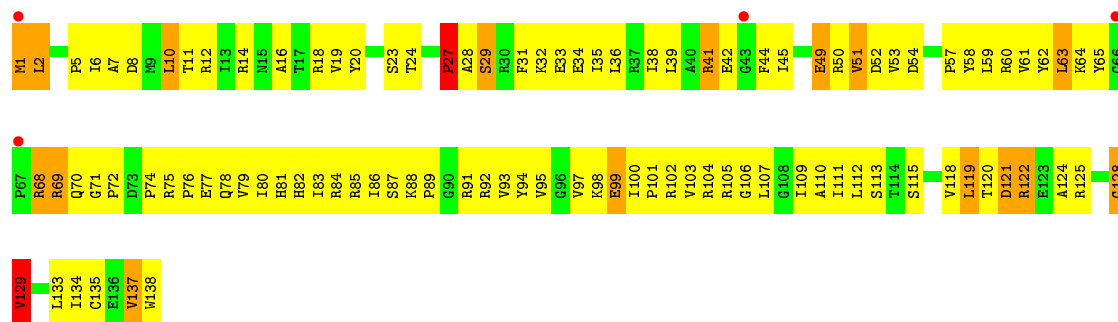




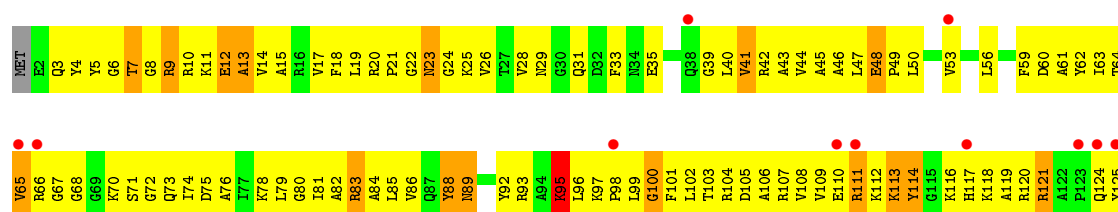
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

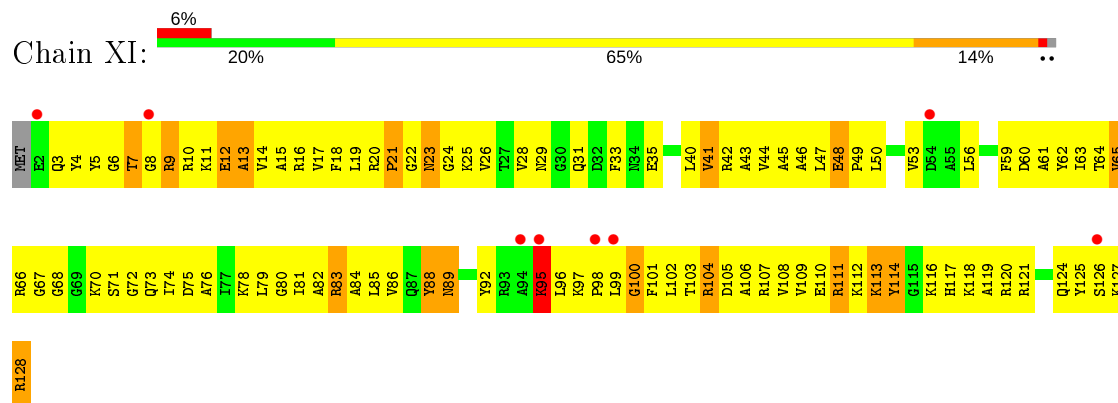


• Molecule 9: 30S ribosomal protein S9

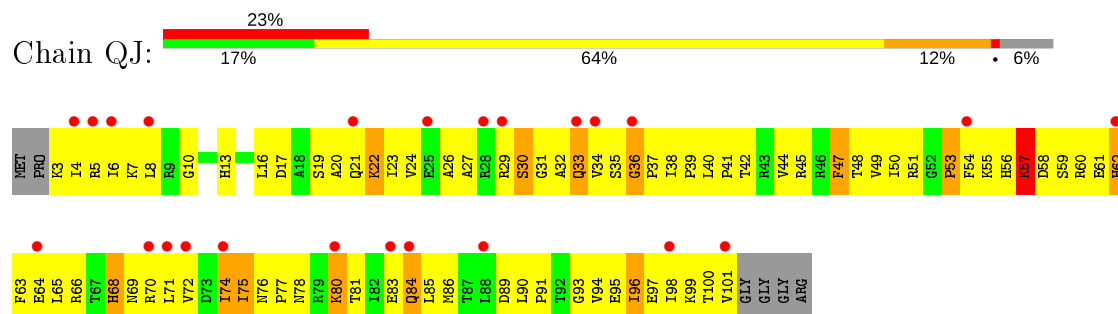




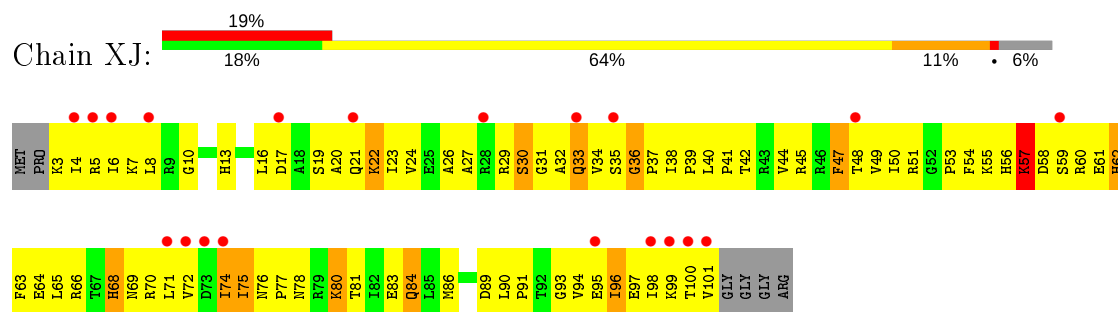
• Molecule 9: 30S ribosomal protein S9



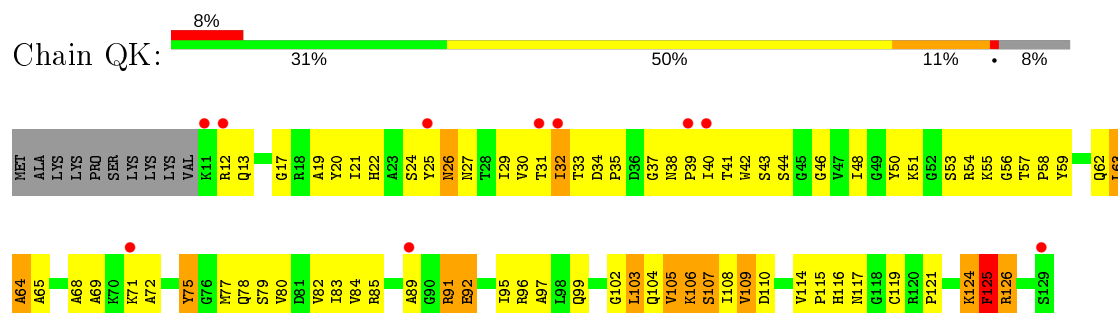
• Molecule 10: 30S ribosomal protein S10



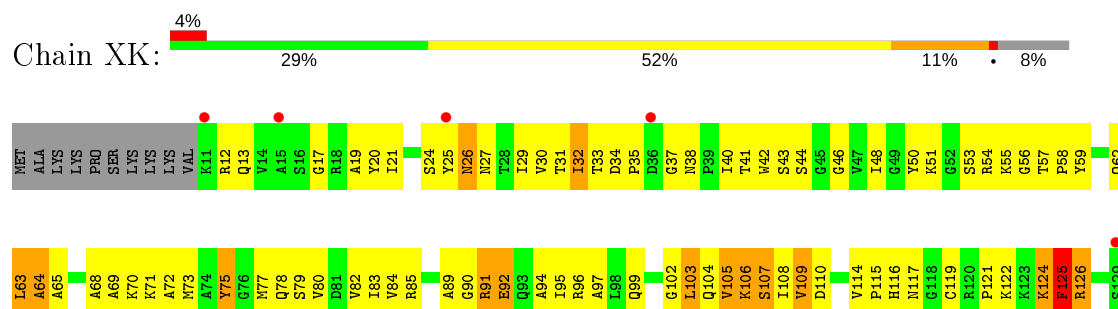
• Molecule 10: 30S ribosomal protein S10



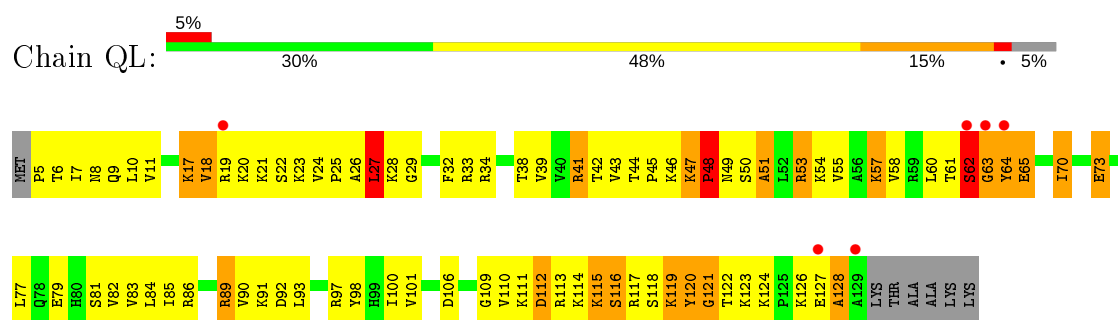
• Molecule 11: 30S ribosomal protein S11



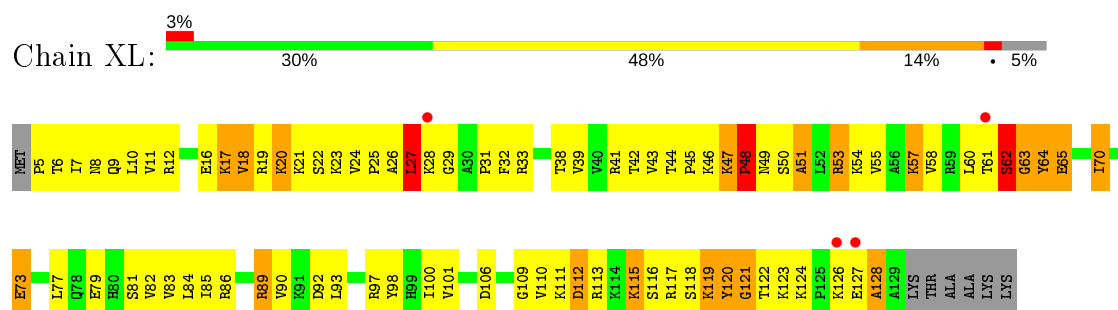
- Molecule 11: 30S ribosomal protein S11



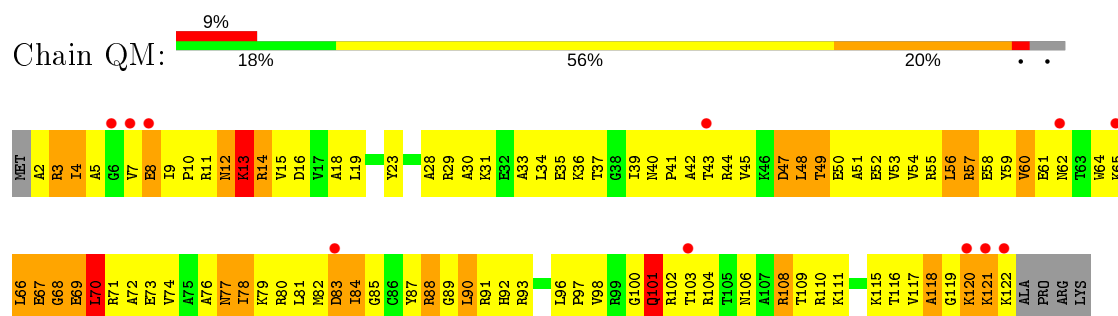
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

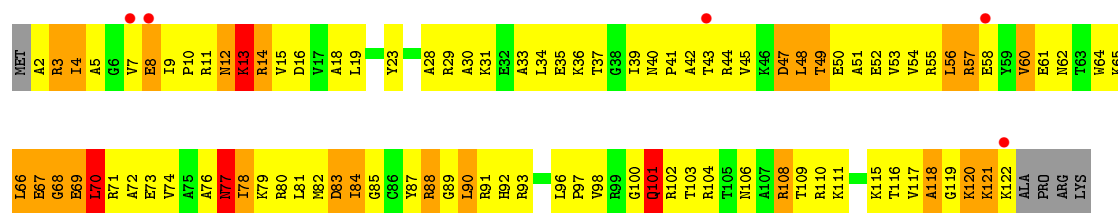


- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13





• Molecule 14: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15

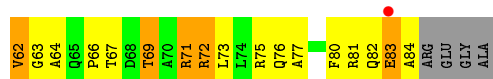


• Molecule 15: 30S ribosomal protein S15

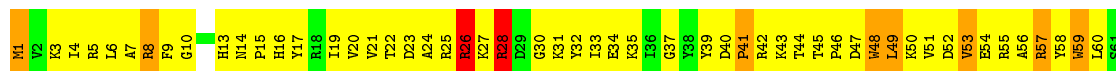


• Molecule 16: 30S ribosomal protein S16





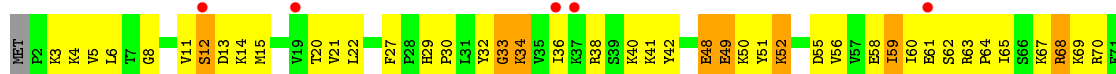
- Molecule 16: 30S ribosomal protein S16



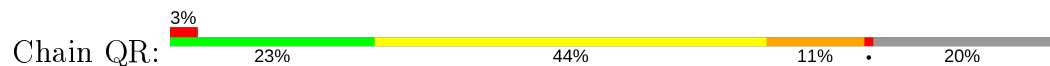
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

Chain XR:



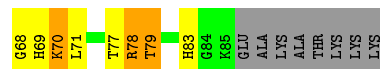
- Molecule 19: 30S ribosomal protein S19

Chain QS:



- Molecule 19: 30S ribosomal protein S19

Chain XS:



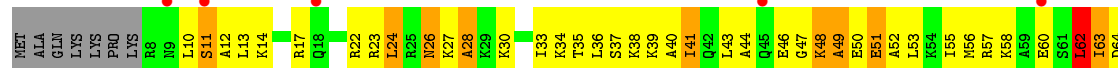
- Molecule 20: 30S ribosomal protein S20

Chain QT:



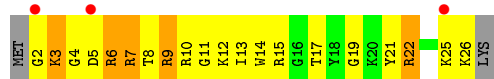
- Molecule 20: 30S ribosomal protein S20

Chain XT:

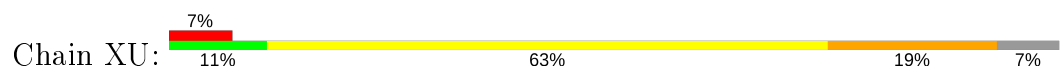




- Molecule 21: 30S ribosomal protein S21



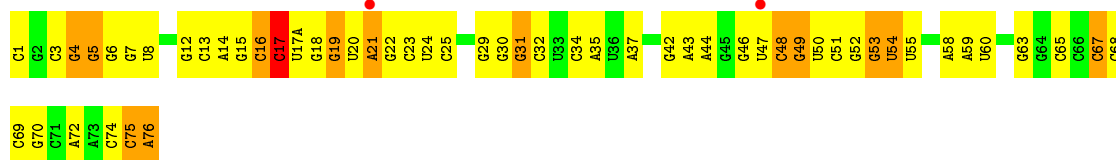
- Molecule 21: 30S ribosomal protein S21



- Molecule 22: P-site tRNA fMet



- Molecule 22: P-site tRNA fMet

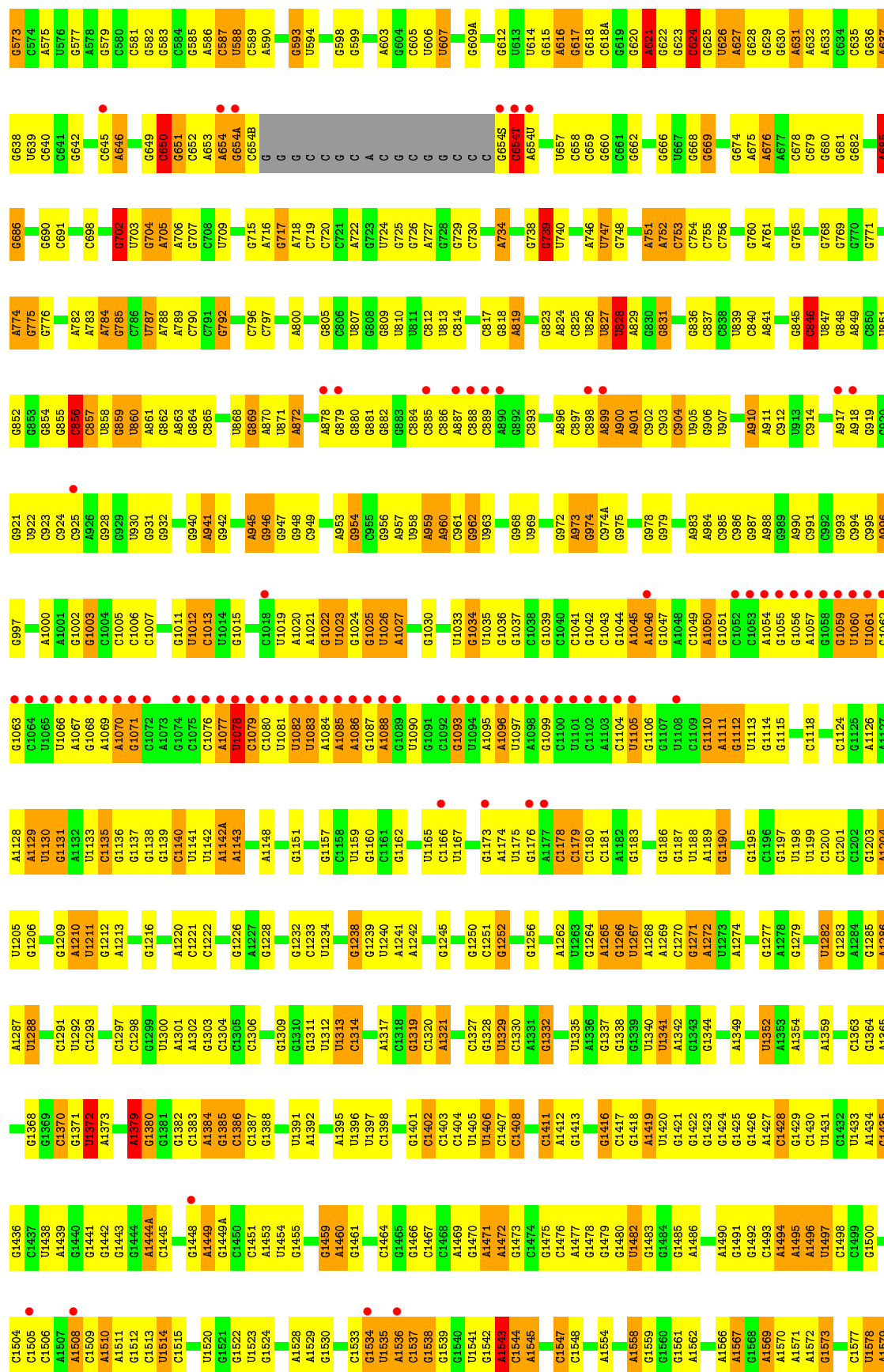


- Molecule 23: A-site ASL SufA6

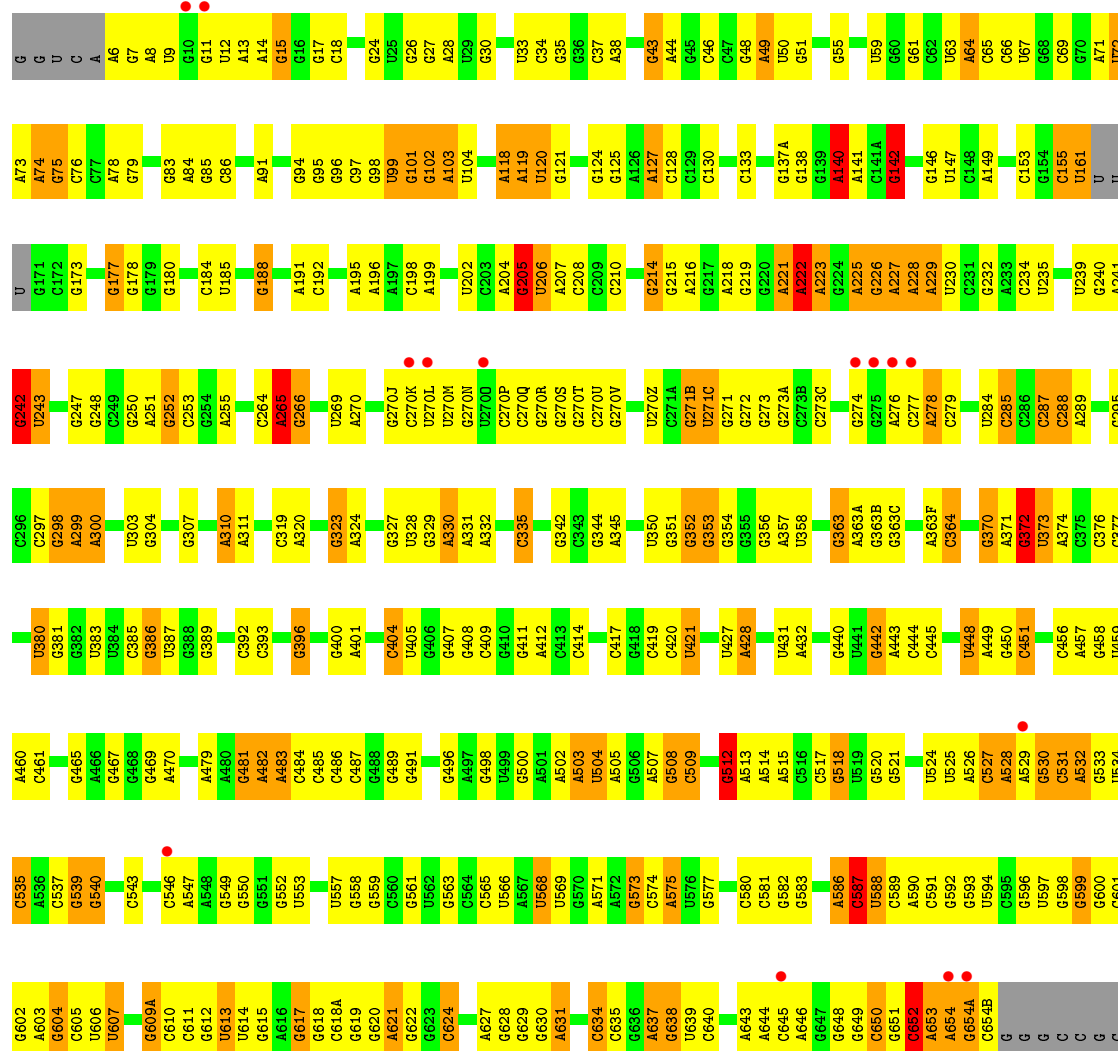


- Molecule 23: A-site ASL SufA6



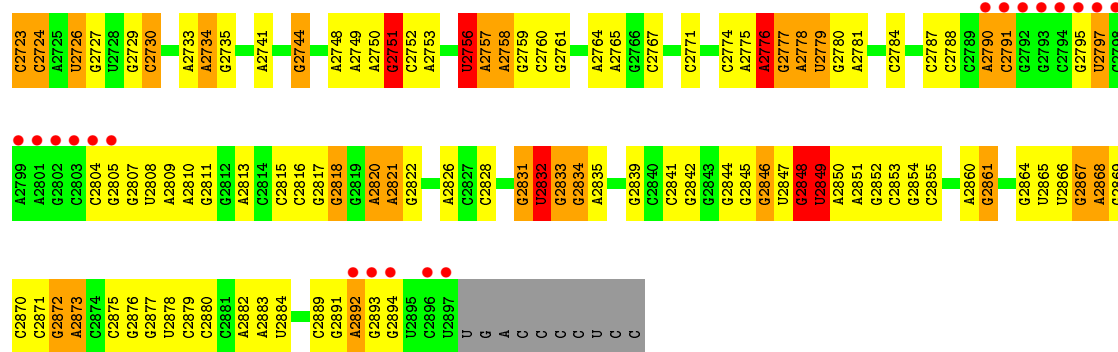


C2591	C2592	C2593	C2594	C2595	C2596	C2597	A2602	G2603	U2604	G2607	G2608	G2609	G2610	G2611	G2612	G2613	A2614	U2615	G2616	G2617	G2618	G2619	G2623	G2625	G2626	G2627	G2628	A2629	G2630	G2631	A2632	G2633	G2634	G2635	U2636	G2638	G2641	G2642	G2643	G2644	G2645	G2646	U2647	A2654	G2655	G2656	G2657	A2665																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G2444	G2445	A2446	A2448	A2449	A2450	A2451	U2457	G2458	A2459	U2460	G2466	G2467	G2468	G2469	G2470	A2471	G2472	U2475	G2476	A2477	G2481	G2482	G2483	G2484	G2485	G2486	G2487	U2488	G2489	G2490	G2494	G2495	G2496	A2497	G2498	G2499	G2502	A2503	U2504	G2505	G2506	G2507	G2508	U2511	G2517	U2518	G2519	G2520	C2521																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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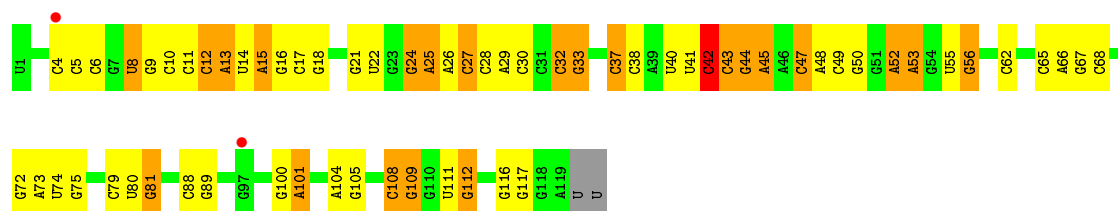


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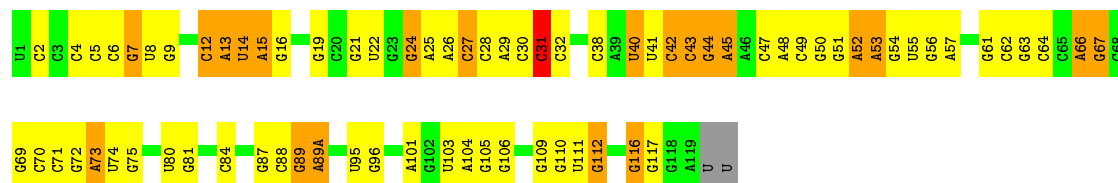
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		C2427	G2358	A2288	A2212	C2145		C1994	A1918					A1690
U2653	C2579	G2428	C2359	G2289	U2213	G2146	U2074	U1995	U1919	A1847			U1779	C1691
A2654	U2580	C2429	C2360	G2290	U2215	C2147		C1996	C1920	A1848			A1780	U1692
C2655	C2581	A2430	A2361	U2291	G2216	G2148		G1997		U1849			C1783	U1693
U2656	G2582		C2364	C2292	G2217	U2150	G2083	U1998	C1924	G1849			A1781	U1694
A2657	C2583	A2433	G2365	C2293	G2218	G2151	C2084	U1999	C1925	U1850			C1782	C1695
C2658	U2584	A2435	C2366	C2294	G2219	G2152	U2085	A2000		U1851			A1783	U1696
U2659	U2585		G2367	C2295	G2224	G2153	U2086	G2001	G1929	C1852			A1784	G1696
A2660				C2296	A2225	G2154	G2087	G2002	U1930	A1853			A1785	G1697
C2661	G2588	U2438	G2370	U2297	C2226	G2155		G2003	G1931	U1854			A1786	A1698
A2662		A2439	G2371	A2298	A2227	G2156	G2093		A1932	U1855			G1787	G1699
		C2440	G2372		G2228	U2157		G2009	G1933	U1856			C1788	A1700
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C2666	U2593	C2442	C2374	G2303		U2098	U2011	U2011	A1936	G1859			C1790	
	C2594		C2375	G2304	U2232	G2159	U2099	G2012	A1937	G1860			A1791	U1706
		G2445	G2376	A2305	U2233	G2160	G2100	A2013	A1938	U1861			C1793	
U2673		G2446	A2377	C2306	G2234	C2161	G2101	A2014	U1939	G1862			U1794	
		A2447	A2378	G2307		G2162	U2102	A2015		U1863			U1795	U1709
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C2678		U2449	G2380	G2310	G2239	C2164	U2104	U2017	C1942	G1869			C1797	
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C2680	A2602	A2450	C2382	G2312		G2166	C2106	A2020	U1944	A1871			G1718	
C2681		A2451	G2383	C2313	U2243	U2167	G2107	C2021	G1945	A1872			G1725	
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C2683	U2608	G2455	G2385	G2315	U2246	U2169	U2109	G2023	C1947	C1879			U1727	
			C2386	C2316		A2170	G2110	U2024		C1880			A1802	
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C2695	C2620	A2468	C2394	A2327	U2257	C2178	U2118	G2038	C1957	U1888			G1811	
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C2699	U2624	A2475	U2399		C2263	C2185	G2123	C2043	C1965				G1816	
C2700	C2625	U2476	C2401	G2334	U2263	G2186	G2124	C2044	A1966	C1895			G1817	
C2701		C2477	C2402	A2335	C2268	U2188	C2125	G2048	C1967	U1896			A1818	
U2702		A2478	C2403	A2336		C2189	A2126	G2049	G1968	G1897			A1819	
			C2404		A2268	U2190	G2127	C2050	A1969	U1898			U1820	
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C2710	C2630	C2483	G2407	C2343	A2274	U2193	U2130	G2052	A1972	A1901			G1824	
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		C2494	C2419	C2347	A2278	A2198	A2135	A2059	A1981	U1906			U1766	
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C2717			U2422	G2351	G2282	C2207	C2139	C2063		U1910			G1770	
G2718	C2641		A2422	C2351	G2282	U2207	C2140		C1988				G1771	
G2719	C2642		U2422	C2351	G2282	U2207	C2140		C1988				G1772	
U2720			U2422	C2351	G2282	U2207	C2140		C1988				G1772	
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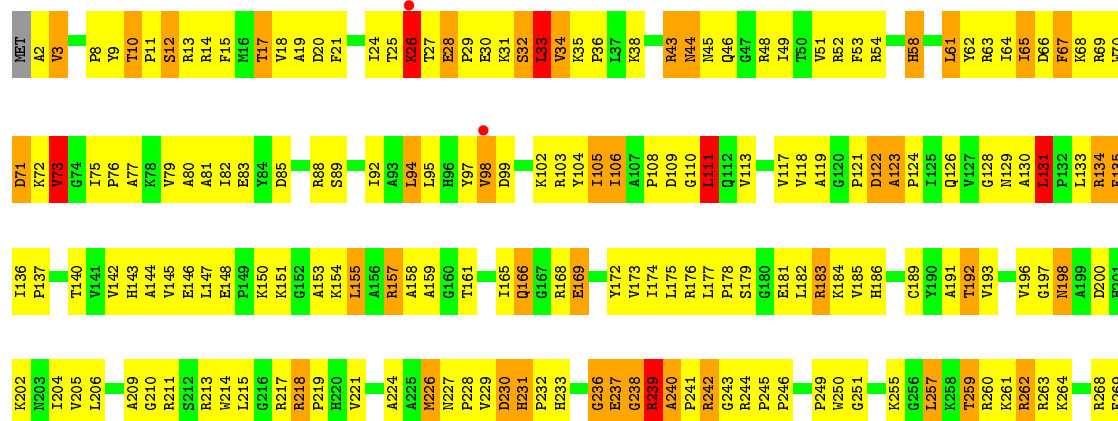
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA



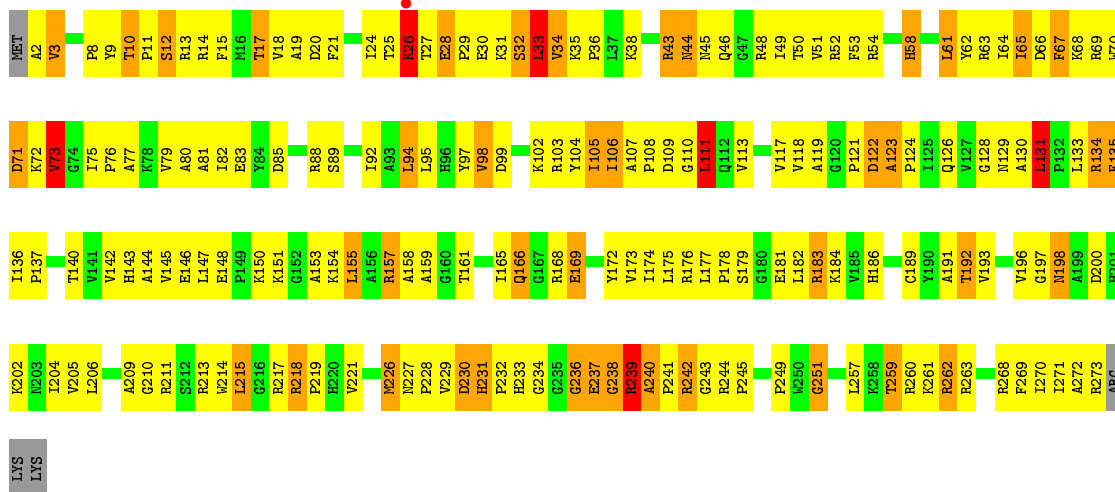
• Molecule 27: 50S ribosomal protein L2



L270
L271
A272
R273
ARG
LYS
LYS

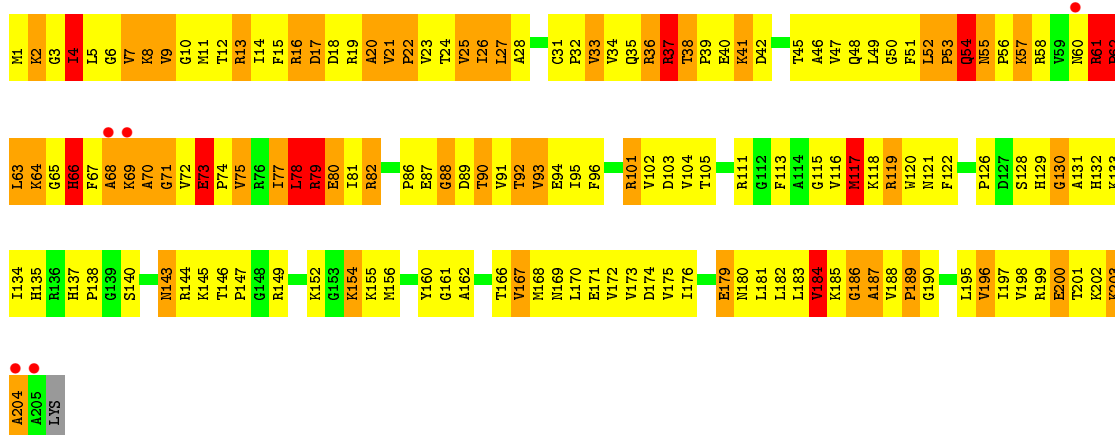
• Molecule 27: 50S ribosomal protein L2

Chain YD: 30% 51% 15% ..



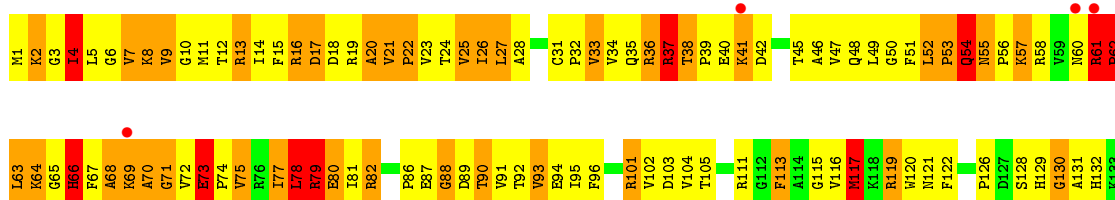
• Molecule 28: 50S ribosomal protein L3

Chain RE: 2% 22% 49% 24% 5%



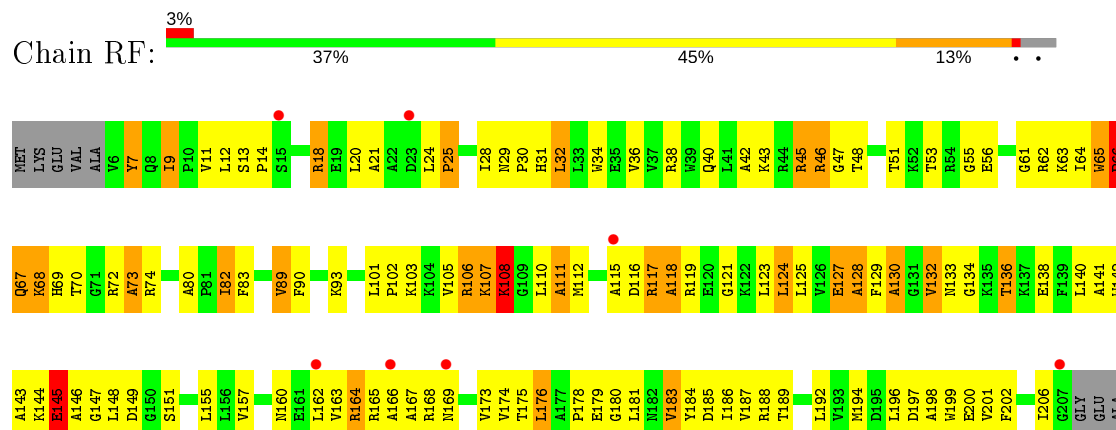
• Molecule 28: 50S ribosomal protein L3

Chain YE: 3% 24% 47% 24% 5%

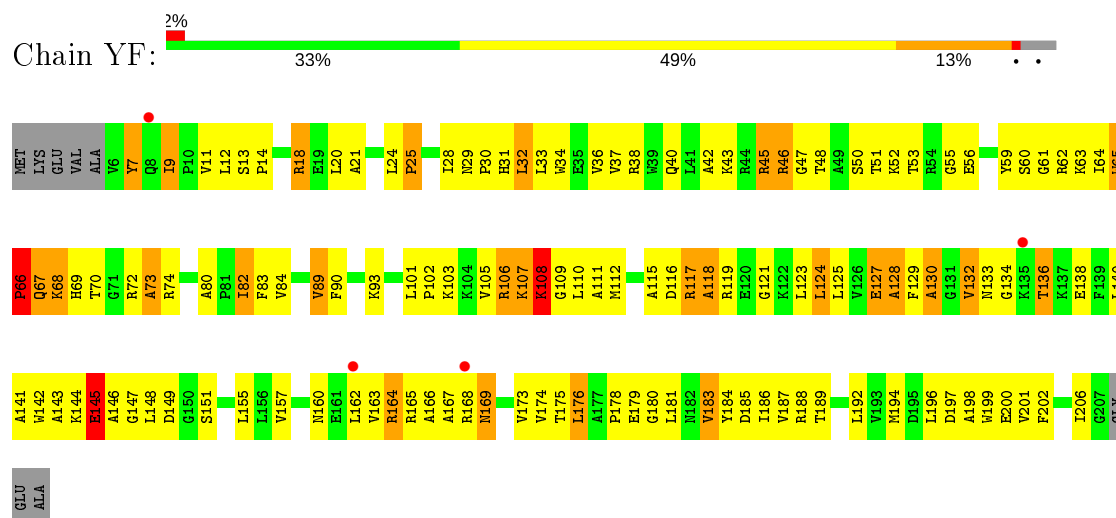




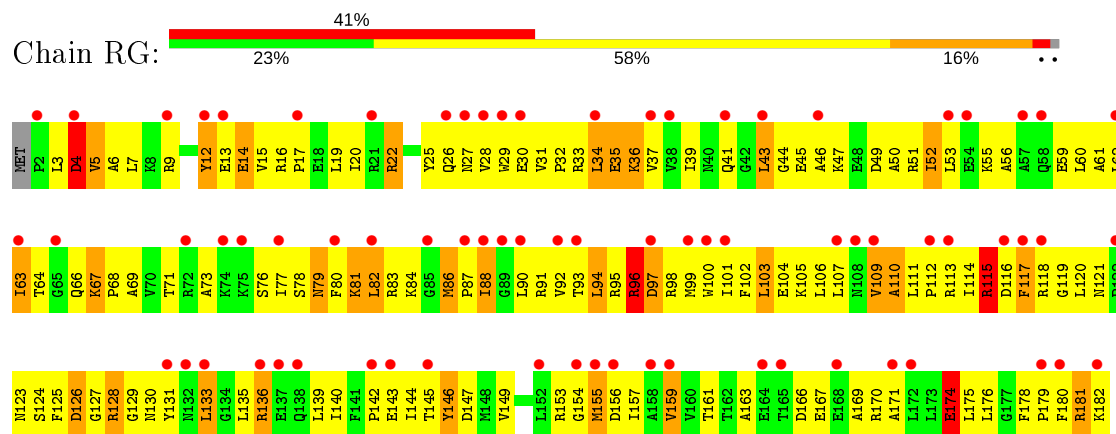
- Molecule 29: 50S ribosomal protein L4



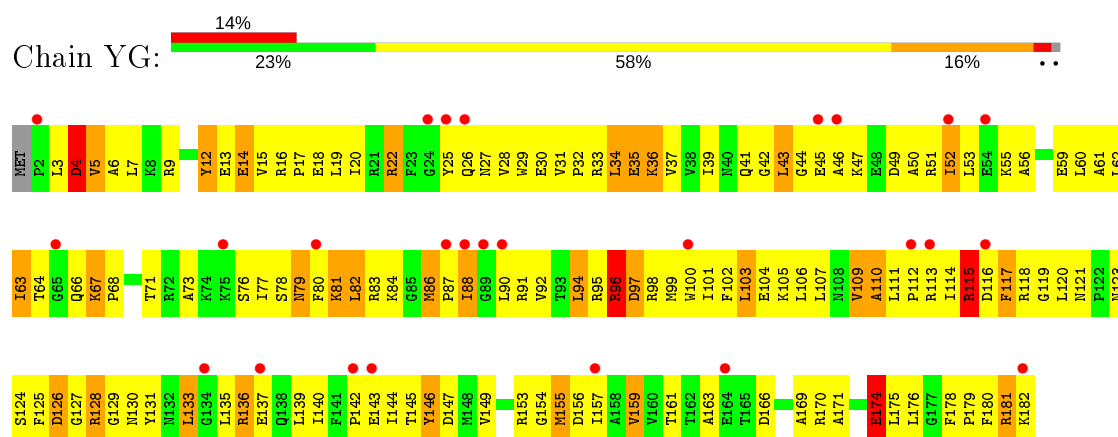
- Molecule 29: 50S ribosomal protein L4

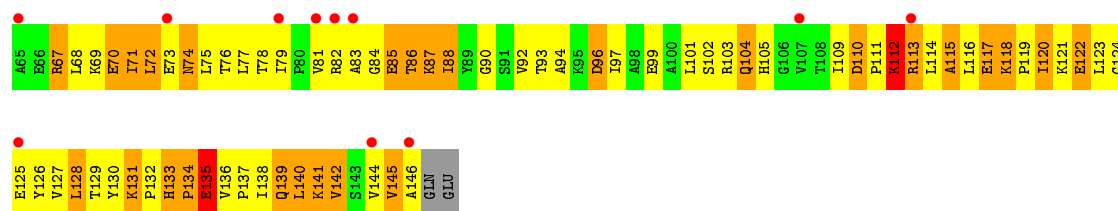


- Molecule 30: 50S ribosomal protein L5

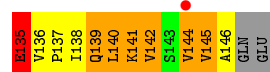
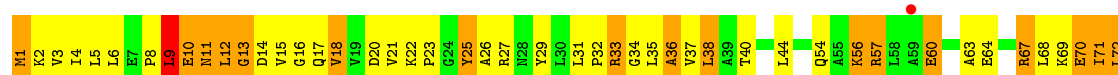
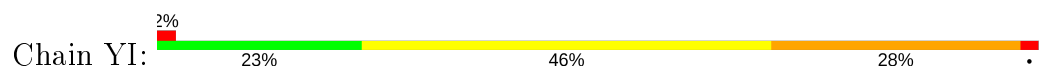


- Molecule 30: 50S ribosomal protein L5

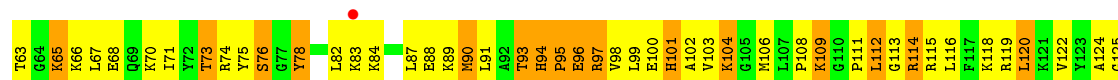
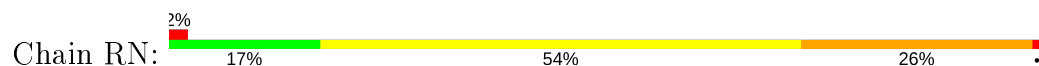




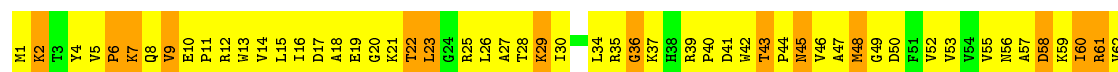
● Molecule 32: 50S ribosomal protein L9



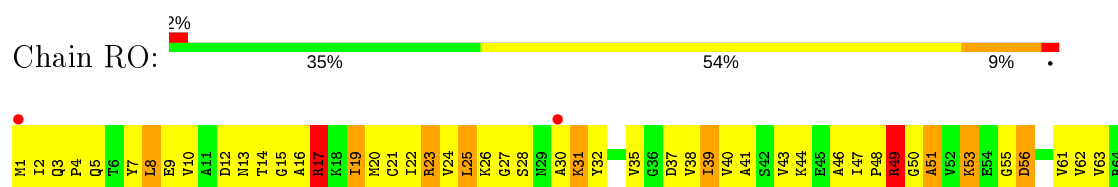
● Molecule 33: 50S ribosomal protein L13



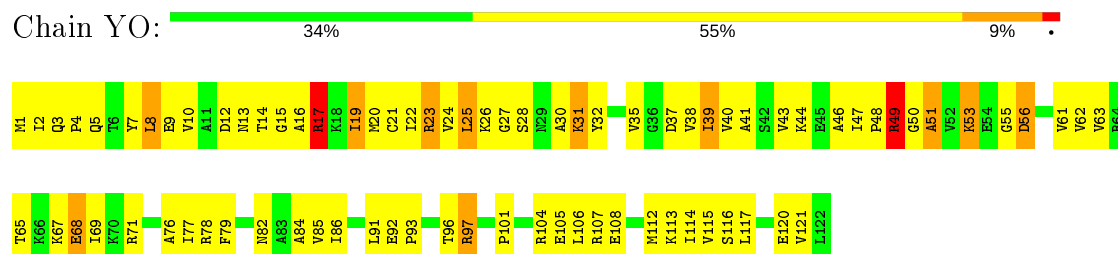
● Molecule 33: 50S ribosomal protein L13



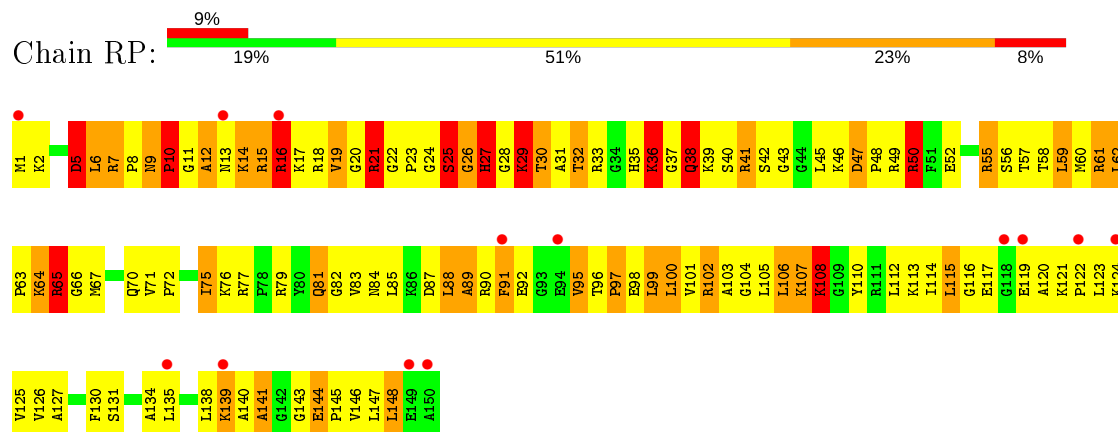
● Molecule 34: 50S ribosomal protein L14



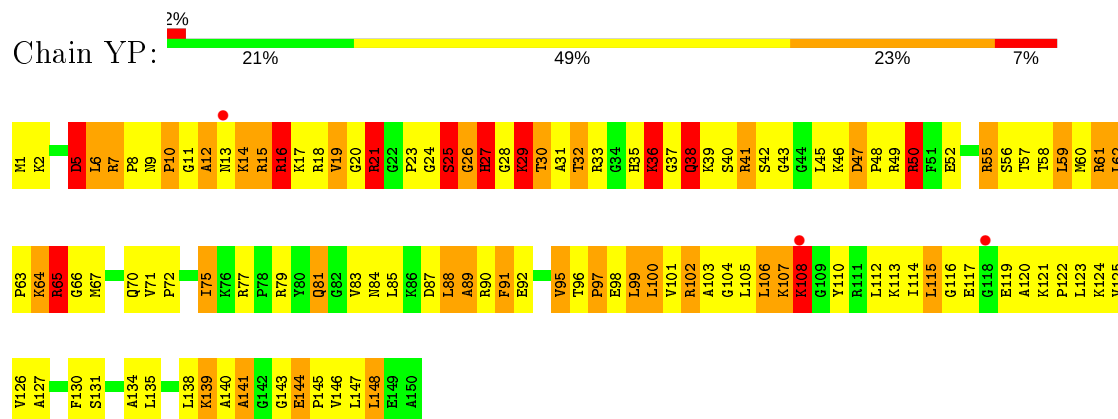
- Molecule 34: 50S ribosomal protein L14



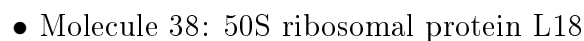
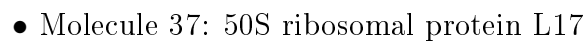
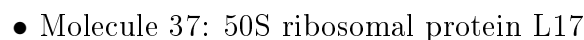
- Molecule 35: 50S ribosomal protein L15

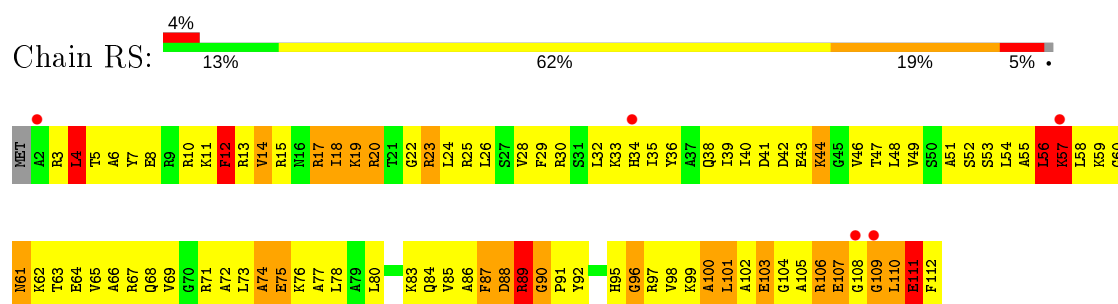


- Molecule 35: 50S ribosomal protein L15

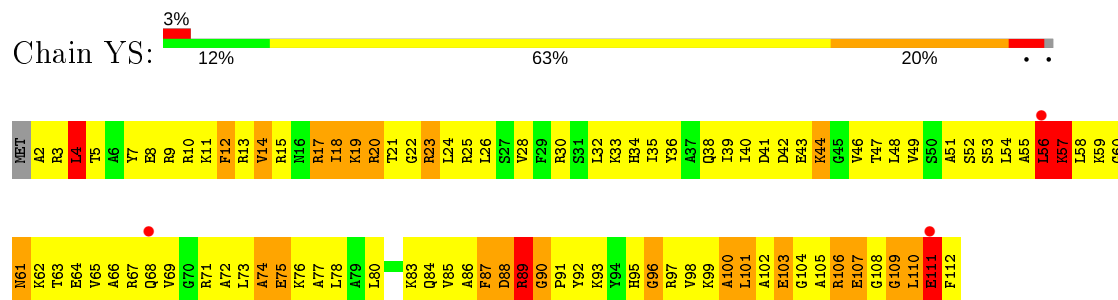


- Molecule 36: 50S ribosomal protein L16

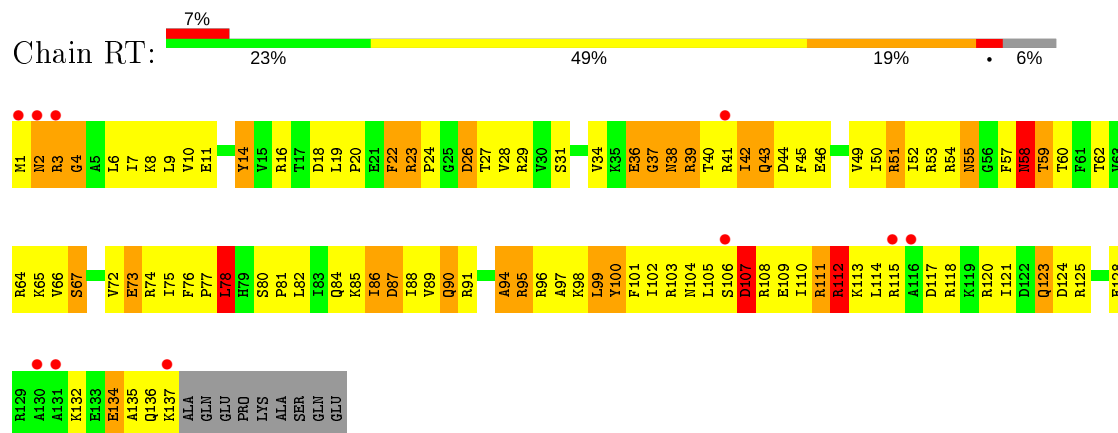




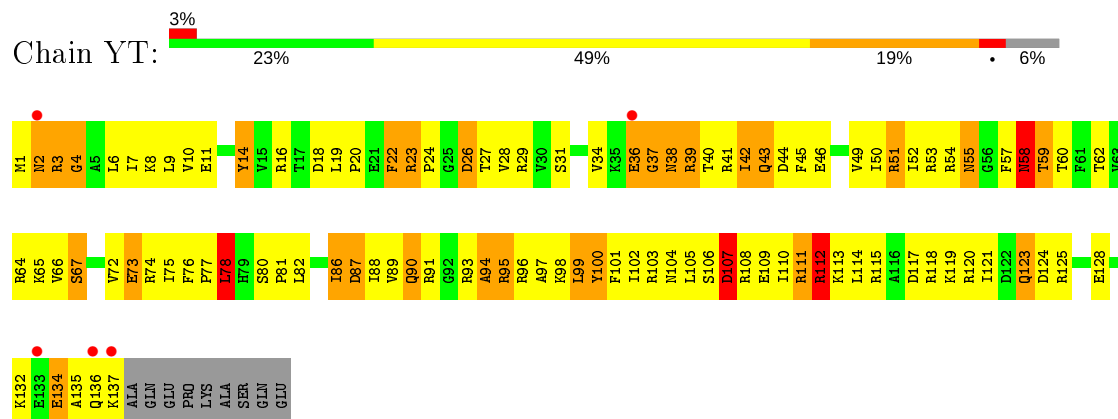
- Molecule 38: 50S ribosomal protein L18



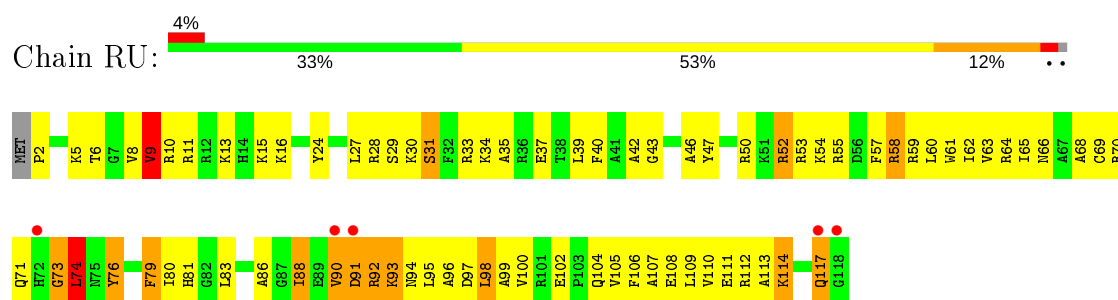
- Molecule 39: 50S ribosomal protein L19



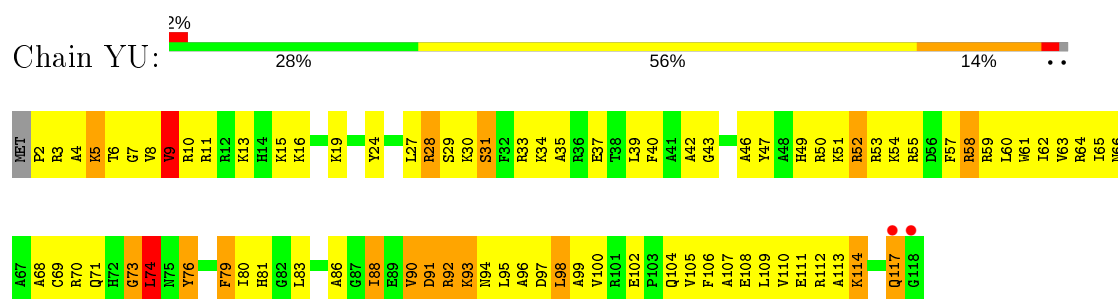
- Molecule 39: 50S ribosomal protein L19



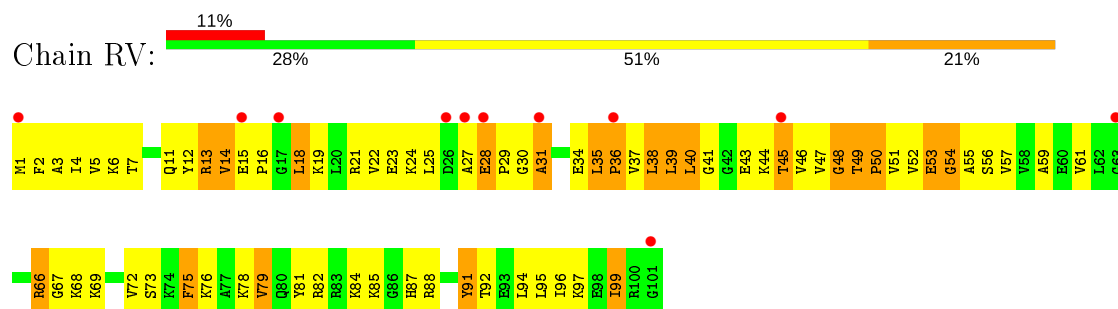
- Molecule 40: 50S ribosomal protein L20



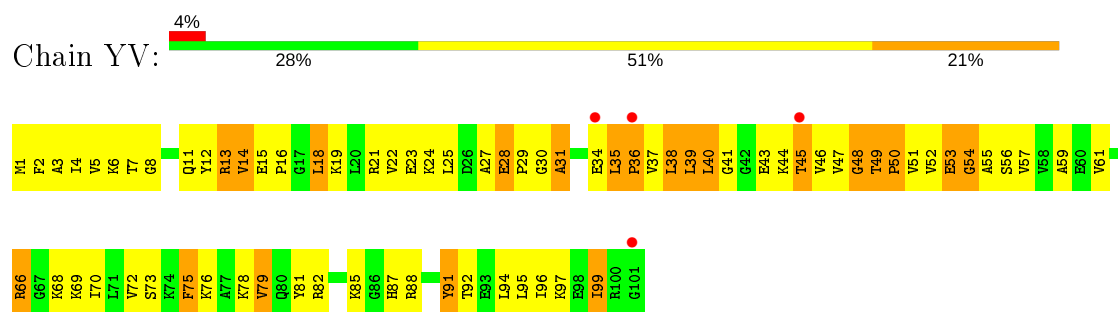
- Molecule 40: 50S ribosomal protein L20



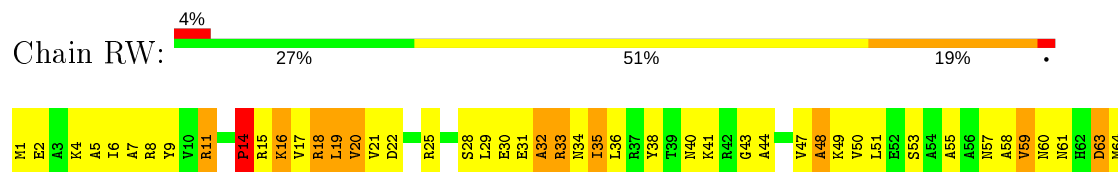
- Molecule 41: 50S ribosomal protein L21

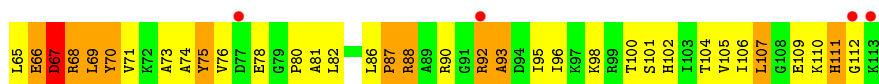


- Molecule 41: 50S ribosomal protein L21

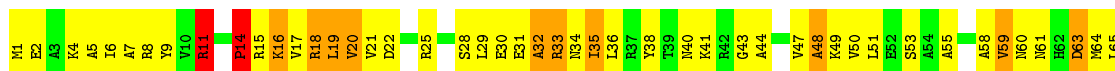


- Molecule 42: 50S ribosomal protein L22

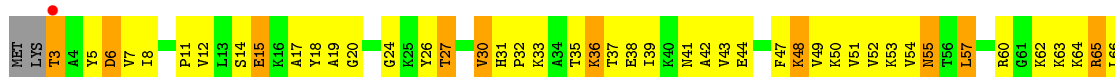




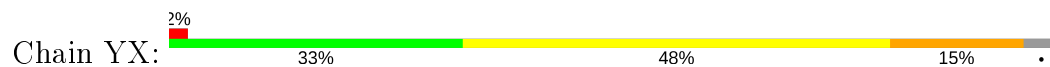
- Molecule 42: 50S ribosomal protein L22



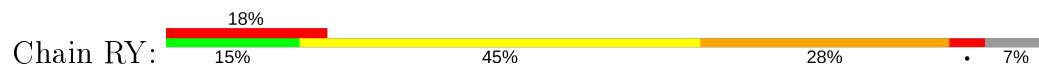
- Molecule 43: 50S ribosomal protein L23



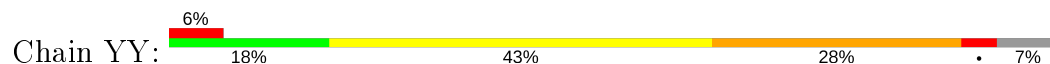
- Molecule 43: 50S ribosomal protein L23

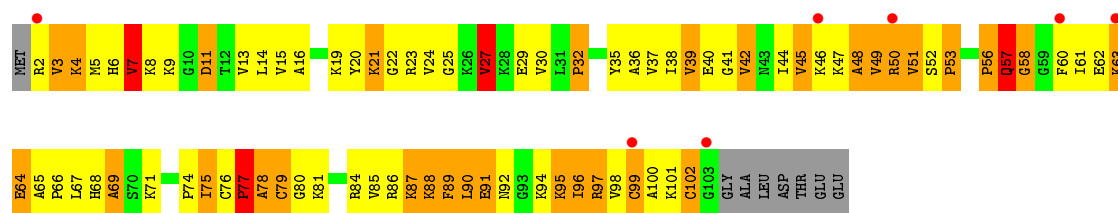


- Molecule 44: 50S ribosomal protein L24

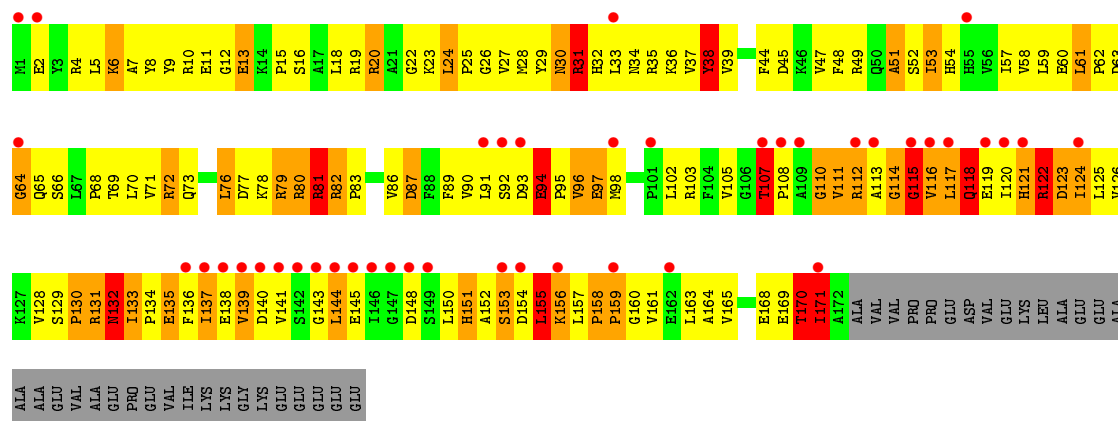
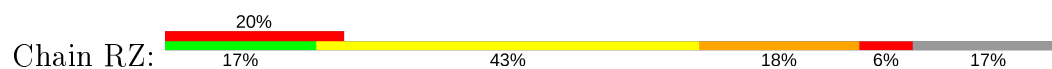


- Molecule 44: 50S ribosomal protein L24

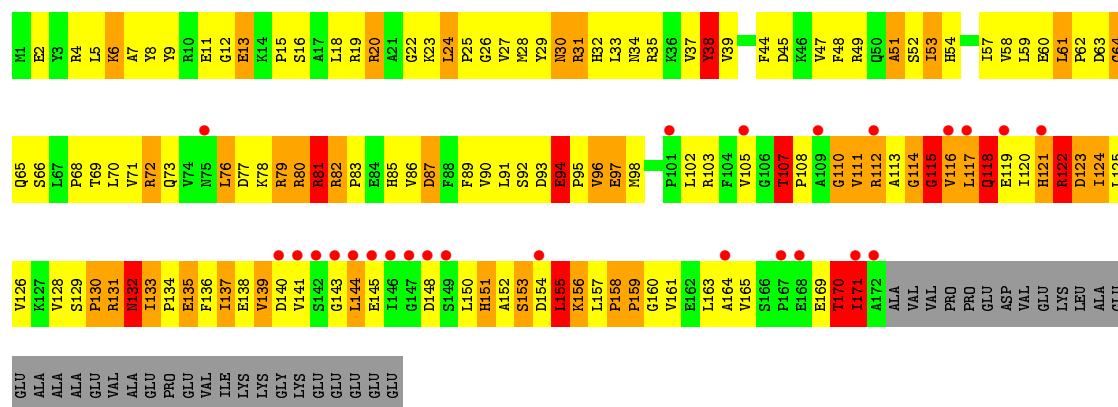
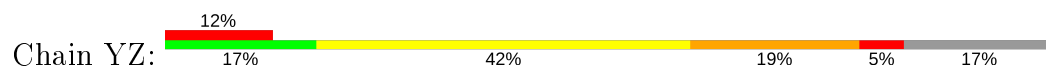




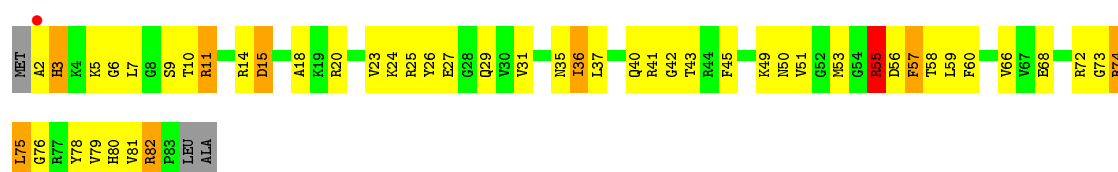
• Molecule 45: 50S ribosomal protein L25



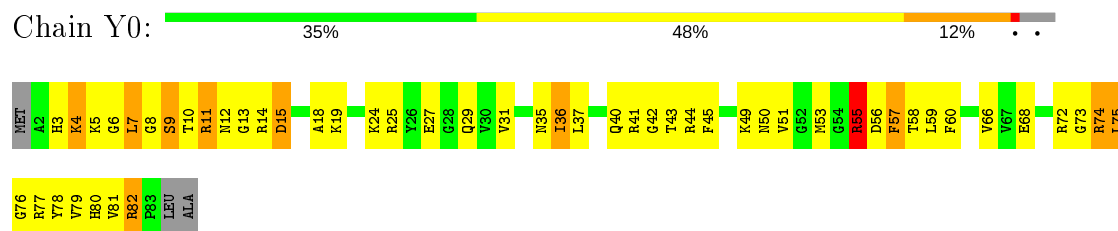
• Molecule 45: 50S ribosomal protein L25



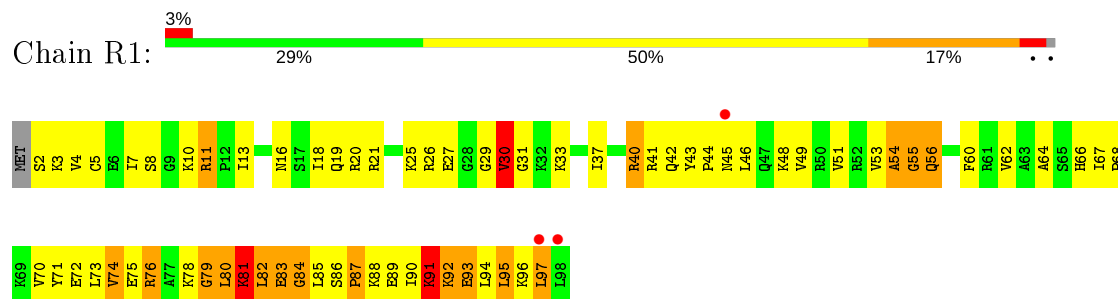
• Molecule 46: 50S ribosomal protein L27



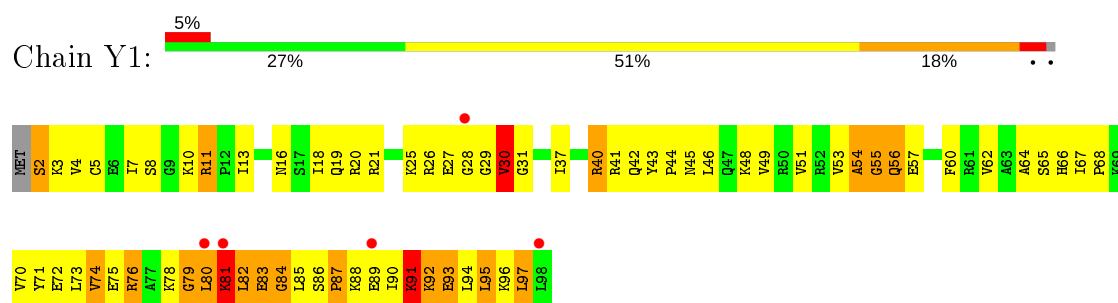
- Molecule 46: 50S ribosomal protein L27



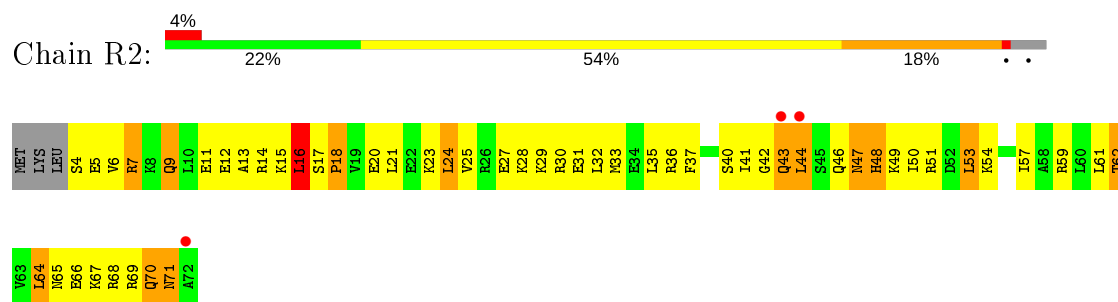
- Molecule 47: 50S ribosomal protein L28



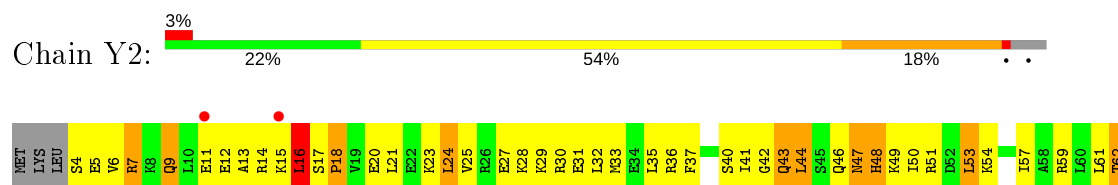
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29





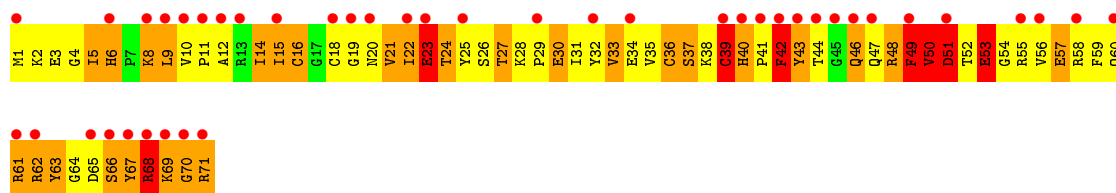
- Molecule 49: 50S ribosomal protein L30



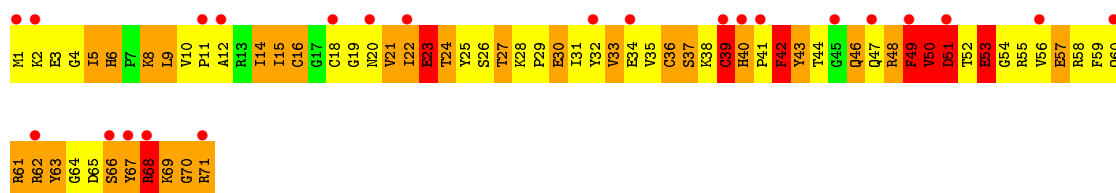
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L32



- Molecule 50: 50S ribosomal protein L32

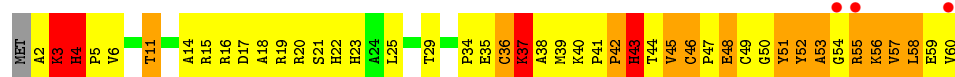


- Molecule 51: 50S ribosomal protein L33

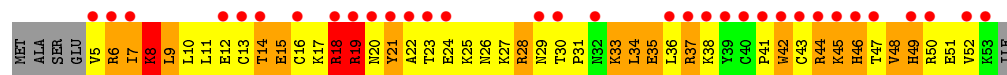


- Molecule 51: 50S ribosomal protein L33

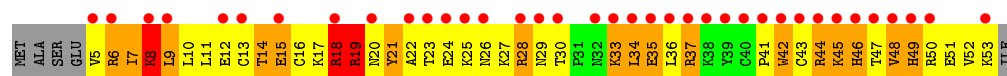




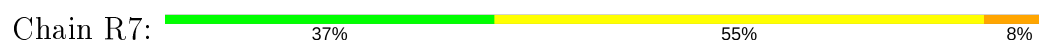
- Molecule 52: 50S ribosomal protein L34



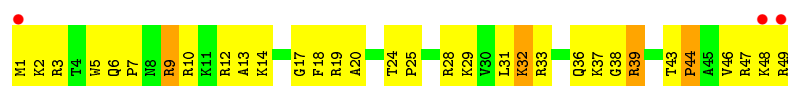
- Molecule 52: 50S ribosomal protein L34



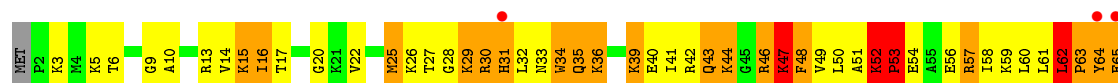
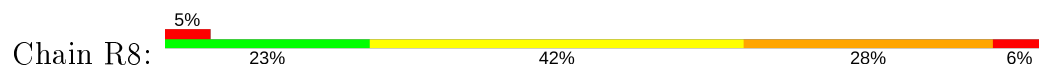
- Molecule 53: 50S ribosomal protein L35



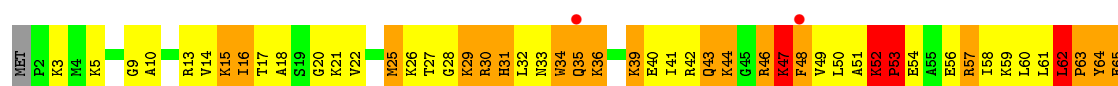
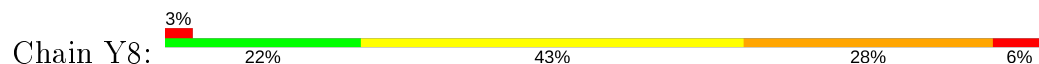
- Molecule 53: 50S ribosomal protein L35



- Molecule 54: tRNA acceptor end mimic



- Molecule 54: tRNA acceptor end mimic



- Molecule 55: RNA (5'-R(*CP*CP*(PPU))-3')





- Molecule 55: RNA (5'-R(*CP*CP*(PPU))-3')

Chain Z8: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.55Å 449.21Å 619.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.44 34.81 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.81-3.44) 98.2 (34.81-3.26)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.243 , 0.285 0.243 , 0.284	Depositor DCC
R_{free} test set	40944 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	291123	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	QA	0.42	0/36098	0.97	58/56341 (0.1%)
1	XA	0.45	0/36123	1.00	71/56380 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.42	0/1733	0.69	1/2318 (0.0%)
4	XD	0.42	0/1733	0.70	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	0.61	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	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.45	0/991	1.00	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	0.43	0/501	0.70	1/664 (0.2%)
14	XN	0.43	0/501	0.70	1/664 (0.2%)
15	QO	0.39	0/745	0.66	0/992
15	XO	0.39	0/745	0.66	0/992
16	QP	0.37	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	0.38	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	0.73	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	0.34	0/765	0.69	0/1007
20	XT	0.33	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.62	0/288
22	QV	0.52	0/1836	0.99	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.40	0/189	0.75	0/292
23	XX	0.66	0/189	1.09	2/292 (0.7%)
24	QY	0.51	0/311	0.88	0/483
24	XY	0.52	0/311	0.89	0/483
25	RA	0.52	2/69543 (0.0%)	1.06	149/108563 (0.1%)
25	YA	0.59	2/69521 (0.0%)	1.10	200/108529 (0.2%)
26	RB	0.44	0/2878	1.04	7/4490 (0.2%)
26	YB	0.46	0/2878	1.03	2/4490 (0.0%)
27	RD	0.62	2/2165 (0.1%)	0.90	3/2919 (0.1%)
27	YD	0.62	2/2165 (0.1%)	0.90	3/2919 (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	4/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.40	0/1151	0.80	1/1558 (0.1%)
32	YI	0.40	0/1151	0.79	1/1558 (0.1%)
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	0.53	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.94	3/1544 (0.2%)
35	YP	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.53	0/1143	0.89	3/1527 (0.2%)
36	YQ	0.53	0/1143	0.89	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	0.78	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	0.47	0/1408	0.77	1/1908 (0.1%)
45	YZ	0.47	0/1408	0.77	1/1908 (0.1%)
46	R0	0.57	0/657	0.80	0/874
46	Y0	0.60	0/657	0.85	0/874
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	0.50	0/583	0.83	1/771 (0.1%)
48	Y2	0.50	0/583	0.84	1/771 (0.1%)
49	R3	0.43	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	Z6	0.82	0/40	1.81	1/60 (1.7%)
55	Z8	0.80	0/40	1.80	1/60 (1.7%)
All	All	0.50	8/315563 (0.0%)	0.98	571/471909 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	236	GLY	C-N	8.59	1.53	1.34
27	RD	236	GLY	C-N	8.55	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	239	ARG	CA-C	-6.77	1.35	1.52
27	RD	239	ARG	CA-C	-6.76	1.35	1.52
25	YA	783	A	N7-C5	-5.95	1.35	1.39

The worst 5 of 571 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	QL	47	LYS	C-N-CD	-20.50	75.51	120.60
12	XL	47	LYS	C-N-CD	-20.46	75.58	120.60
25	YA	761	A	N1-C6-N6	12.76	126.25	118.60
25	YA	945	A	N9-C1'-C2'	12.75	130.58	114.00
22	QV	17	C	C2-N1-C1'	11.85	131.84	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16275	828	0
1	XA	32269	0	16289	816	0
2	QB	1924	0	1975	291	0
2	XB	1924	0	1975	301	0
3	QC	1605	0	1668	208	0
3	XC	1605	0	1668	209	1
4	QD	1703	0	1762	240	0
4	XD	1703	0	1763	215	0
5	QE	1155	0	1213	147	0
5	XE	1155	0	1213	142	0
6	QF	843	0	857	93	0
6	XF	843	0	857	99	0
7	QG	1257	0	1296	149	0
7	XG	1257	0	1296	147	0
8	QH	1116	0	1176	155	0
8	XH	1116	0	1177	164	0
9	QI	1010	0	1037	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	XI	1010	0	1037	160	0
10	QJ	801	0	849	138	0
10	XJ	801	0	849	136	0
11	QK	885	0	904	108	1
11	XK	885	0	904	118	0
12	QL	975	0	1062	109	0
12	XL	975	0	1062	113	0
13	QM	964	0	1034	171	0
13	XM	964	0	1034	180	0
14	QN	492	0	531	89	0
14	XN	492	0	529	87	0
15	QO	734	0	771	75	0
15	XO	734	0	771	74	0
16	QP	705	0	725	114	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	84	0
17	XQ	834	0	904	82	0
18	QR	574	0	644	68	0
18	XR	574	0	644	67	0
19	QS	674	0	699	104	0
19	XS	674	0	699	143	0
20	QT	763	0	860	108	0
20	XT	763	0	861	102	0
21	QU	217	0	234	30	0
21	XU	217	0	234	29	0
22	QV	1644	0	836	41	0
22	XV	1644	0	836	40	0
23	QX	170	0	87	16	0
23	XX	170	0	88	10	0
24	QY	303	0	154	13	0
24	XY	303	0	154	17	0
25	RA	62091	0	31301	1401	0
25	YA	62071	0	31286	1351	0
26	RB	2573	0	1306	70	0
26	YB	2573	0	1306	61	0
27	RD	2115	0	2195	324	0
27	YD	2115	0	2195	350	0
28	RE	1568	0	1634	277	0
28	YE	1568	0	1634	266	0
29	RF	1585	0	1632	174	0
29	YF	1585	0	1632	182	0
30	RG	1474	0	1535	212	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	YG	1474	0	1535	206	0
31	RH	1307	0	1382	217	0
31	YH	1307	0	1382	219	1
32	RI	1136	0	1223	179	0
32	YI	1136	0	1223	176	0
33	RN	1104	0	1180	194	0
33	YN	1104	0	1180	186	0
34	RO	933	0	996	123	0
34	YO	933	0	996	124	0
35	RP	1145	0	1228	248	0
35	YP	1145	0	1228	247	0
36	RQ	1122	0	1179	168	0
36	YQ	1122	0	1179	168	0
37	RR	968	0	1033	115	0
37	YR	968	0	1033	112	0
38	RS	882	0	943	158	0
38	YS	882	0	943	163	0
39	RT	1141	0	1202	152	0
39	YT	1141	0	1202	156	0
40	RU	964	0	1022	130	0
40	YU	964	0	1022	138	0
41	RV	779	0	852	132	0
41	YV	779	0	852	130	1
42	RW	900	0	964	101	0
42	YW	900	0	964	108	0
43	RX	725	0	778	68	0
43	YX	725	0	778	82	0
44	RY	785	0	878	163	0
44	YY	785	0	878	154	1
45	RZ	1378	0	1407	227	0
45	YZ	1378	0	1407	227	0
46	R0	648	0	672	88	0
46	Y0	648	0	672	85	0
47	R1	763	0	848	141	0
47	Y1	763	0	848	145	0
48	R2	581	0	629	80	0
48	Y2	581	0	629	75	0
49	R3	469	0	518	40	0
49	Y3	469	0	518	41	0
50	R4	581	0	574	159	0
50	Y4	581	0	574	180	0
51	R5	459	0	480	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Y5	459	0	480	75	1
52	R6	424	0	450	93	0
52	Y6	424	0	450	90	0
53	R7	430	0	480	47	0
53	Y7	430	0	480	42	0
54	R8	517	0	582	106	0
54	Y8	517	0	582	100	0
55	Z6	74	0	51	10	0
55	Z8	74	0	51	4	0
56	QA	60	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	2	0	0	0	0
56	QX	2	0	0	0	0
56	R5	1	0	0	0	0
56	RA	212	0	0	0	0
56	RB	2	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RP	1	0	0	0	0
56	XA	63	0	0	0	0
56	XM	2	0	0	0	0
56	XV	2	0	0	0	0
56	Y5	1	0	0	0	0
56	YA	242	0	0	0	0
56	YB	2	0	0	0	0
56	YE	2	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	4	0
57	XA	42	0	45	1	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
All	All	291123	0	197505	16608	3

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 34.

The worst 5 of 16608 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:QN:39:LEU:HD22	14:QN:43:CYS:SG	1.33	1.63
36:YQ:81:VAL:HG23	46:Y0:7:LEU:CD2	1.21	1.60
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.54
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
19:QS:5:LEU:HD22	50:R4:67:TYR:CE2	1.45	1.51

All (3) 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)
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.98	0.22
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.04	0.16
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	4
2	XB	235/256 (92%)	152 (65%)	53 (23%)	30 (13%)	0	4
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	7
3	XC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	7
4	QD	206/209 (99%)	133 (65%)	51 (25%)	22 (11%)	0	6
4	XD	206/209 (99%)	133 (65%)	50 (24%)	23 (11%)	0	5
5	QE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	6
5	XE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	6
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	7
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	7
7	QG	153/156 (98%)	102 (67%)	37 (24%)	14 (9%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	XG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	6
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	4
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	4
10	QJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	6
10	XJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	7
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	9
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	9
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	5
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	5
13	QM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	1
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	1
14	QN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	2
14	XN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	11
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	11
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	9
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	9
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	5
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	5
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	1
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	1
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
27	RD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1	10
27	YD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	6
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	6
30	RG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	5
30	YG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	5
31	RH	168/180 (93%)	94 (56%)	35 (21%)	39 (23%)	0	1
31	YH	168/180 (93%)	95 (56%)	35 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	83 (58%)	33 (23%)	28 (19%)	0	1
32	YI	144/148 (97%)	85 (59%)	32 (22%)	27 (19%)	0	1
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	10
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	10
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%)	94 (68%)	30 (22%)	15 (11%)	0	5
36	YQ	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	0	5
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	2
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	2
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	9
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	9
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	6
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	6
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	16
44	RY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
45	RZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
45	YZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
46	R0	80/85 (94%)	61 (76%)	14 (18%)	5 (6%)	1	13
46	Y0	80/85 (94%)	62 (78%)	12 (15%)	6 (8%)	1	10
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	16
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	16
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
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	0
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
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	13
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	13
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1
All	All	11378/12054 (94%)	7461 (66%)	2359 (21%)	1558 (14%)	0	3

5 of 1558 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	24
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5	24
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7	31
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7	31
4	QD	180/181 (99%)	164 (91%)	16 (9%)	9	36
4	XD	180/181 (99%)	164 (91%)	16 (9%)	9	36
5	QE	116/123 (94%)	107 (92%)	9 (8%)	12	42
5	XE	116/123 (94%)	108 (93%)	8 (7%)	15	47
6	QF	90/90 (100%)	77 (86%)	13 (14%)	3	17
6	XF	90/90 (100%)	77 (86%)	13 (14%)	3	17
7	QG	126/127 (99%)	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	26
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	26
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	36
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	9	36
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	31
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	31
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	19
12	XL	104/109 (95%)	90 (86%)	14 (14%)	4	19
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	11
13	XM	97/101 (96%)	80 (82%)	17 (18%)	2	9
14	QN	49/50 (98%)	45 (92%)	4 (8%)	11	40
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	43
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	43
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	21
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	21
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	18	50
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	50
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	25
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	25
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	15
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	15
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	57
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	57
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	10
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	10
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	3
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	3
29	RF	161/166 (97%)	140 (87%)	21 (13%)	4	20
29	YF	161/166 (97%)	139 (86%)	22 (14%)	3	18
30	RG	155/156 (99%)	130 (84%)	25 (16%)	2	13
30	YG	155/156 (99%)	131 (84%)	24 (16%)	2	14
31	RH	142/148 (96%)	115 (81%)	27 (19%)	1	6
31	YH	142/148 (96%)	115 (81%)	27 (19%)	1	6
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1	5
32	YI	122/124 (98%)	97 (80%)	25 (20%)	1	5
33	RN	117/119 (98%)	98 (84%)	19 (16%)	2	12
33	YN	117/119 (98%)	98 (84%)	19 (16%)	2	12
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	31
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	31
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	3
36	RQ	111/111 (100%)	92 (83%)	19 (17%)	2	10
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	10
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	11
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	11
38	RS	87/88 (99%)	74 (85%)	13 (15%)	3	16
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	16
39	RT	120/127 (94%)	97 (81%)	23 (19%)	1	6
39	YT	120/127 (94%)	97 (81%)	23 (19%)	1	6
40	RU	93/94 (99%)	80 (86%)	13 (14%)	3	17
40	YU	93/94 (99%)	80 (86%)	13 (14%)	3	17
41	RV	82/82 (100%)	71 (87%)	11 (13%)	4	19
41	YV	82/82 (100%)	71 (87%)	11 (13%)	4	19
42	RW	92/92 (100%)	77 (84%)	15 (16%)	2	12
42	YW	92/92 (100%)	77 (84%)	15 (16%)	2	12
43	RX	74/78 (95%)	63 (85%)	11 (15%)	3	16
43	YX	74/78 (95%)	63 (85%)	11 (15%)	3	16
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	9
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	9
45	RZ	152/179 (85%)	124 (82%)	28 (18%)	1	7
45	YZ	152/179 (85%)	124 (82%)	28 (18%)	1	7
46	R0	65/67 (97%)	55 (85%)	10 (15%)	2	14
46	Y0	65/67 (97%)	56 (86%)	9 (14%)	3	18
47	R1	82/83 (99%)	67 (82%)	15 (18%)	1	7
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	7
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	4
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	4
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	2
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	3
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	3
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	5
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	5
53	R7	42/42 (100%)	39 (93%)	3 (7%)	14	46
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	46
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	2
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	2
All	All	9614/9998 (96%)	8197 (85%)	1417 (15%)	3	16

5 of 1417 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	17	LYS
7	XG	148	ASN
45	YZ	132	ASN
50	R4	53	GLU
2	XB	94	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
47	R1	56	GLN
5	XE	78	HIS
43	YX	87	GLN
48	R2	9	GLN
2	XB	135	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	343 (22%)	51 (3%)
1	XA	1499/1522 (98%)	333 (22%)	55 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	6 (85%)	1 (14%)
23	XX	7/25 (28%)	2 (28%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	QY	13/18 (72%)	6 (46%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2880/2916 (98%)	734 (25%)	76 (2%)
25	YA	2879/2916 (98%)	747 (25%)	75 (2%)
26	RB	119/122 (97%)	30 (25%)	2 (1%)
26	YB	119/122 (97%)	38 (31%)	1 (0%)
55	Z6	1/3 (33%)	0	0
55	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	2304 (25%)	265 (2%)

5 of 2304 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	32	A
1	QA	39	G

5 of 265 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2566	A
1	XA	481	G
25	YA	2198	A
25	RA	2689	U
1	XA	64	G

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
55	PPU	Z6	76	55,25	32,40,41	2.55	6 (18%)	33,57,60	2.14	5 (15%)
24	1MG	QY	37	24	18,26,27	2.82	3 (16%)	19,39,42	1.47	4 (21%)
24	1MG	XY	37	24	18,26,27	2.79	3 (16%)	19,39,42	1.48	4 (21%)
55	PPU	Z8	76	55,25	32,40,41	2.54	6 (18%)	33,57,60	2.14	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PPU	Z6	76	55,25	-	2/21/43/44	0/4/4/4
24	1MG	QY	37	24	-	0/3/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/3/25/26	0/3/3/3
55	PPU	Z8	76	55,25	-	2/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Z6	76	PPU	O-C	9.21	1.41	1.23
55	Z8	76	PPU	O-C	9.21	1.41	1.23
24	QY	37	1MG	C4-N3	8.79	1.49	1.35
24	XY	37	1MG	C4-N3	8.64	1.49	1.35
24	QY	37	1MG	C2-N2	7.17	1.48	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	Z8	76	PPU	C3'-N3'-C	-8.58	110.27	123.21
55	Z6	76	PPU	C3'-N3'-C	-8.58	110.28	123.21
55	Z6	76	PPU	N3-C2-N1	-4.69	121.35	128.68
55	Z8	76	PPU	N3-C2-N1	-4.67	121.38	128.68
24	QY	37	1MG	N2-C2-N1	4.23	123.79	118.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	Z6	76	PPU	10	0
24	XY	37	1MG	1	0
55	Z8	76	PPU	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 607 ligands modelled in this entry, 605 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	PAR	XA	1664	-	45,45,45	1.46	7 (15%)	64,67,67	1.33	7 (10%)
57	PAR	QA	1661	-	45,45,45	1.43	7 (15%)	64,67,67	1.36	8 (12%)

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
57	PAR	XA	1664	-	-	4/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	QA	1661	-	-	7/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	QA	1661	PAR	C64-C54	4.85	1.58	1.52
57	XA	1664	PAR	C64-C54	4.83	1.58	1.52
57	XA	1664	PAR	C52-C42	3.02	1.58	1.52
57	XA	1664	PAR	C11-C21	2.98	1.58	1.52
57	QA	1661	PAR	C52-C42	2.97	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	XA	1664	PAR	O33-C14-C24	4.33	115.67	108.22
57	QA	1661	PAR	C14-O54-C54	4.20	121.94	113.69
57	XA	1664	PAR	C14-O54-C54	4.06	121.65	113.69
57	QA	1661	PAR	O33-C14-C24	3.79	114.74	108.22
57	QA	1661	PAR	O52-C13-C23	3.79	115.81	107.96

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1661	PAR	C44-C54-C64-N64
57	QA	1661	PAR	O54-C54-C64-N64
57	XA	1664	PAR	O51-C51-C61-O61
57	XA	1664	PAR	C41-C51-C61-O61
57	QA	1661	PAR	O51-C51-C61-O61

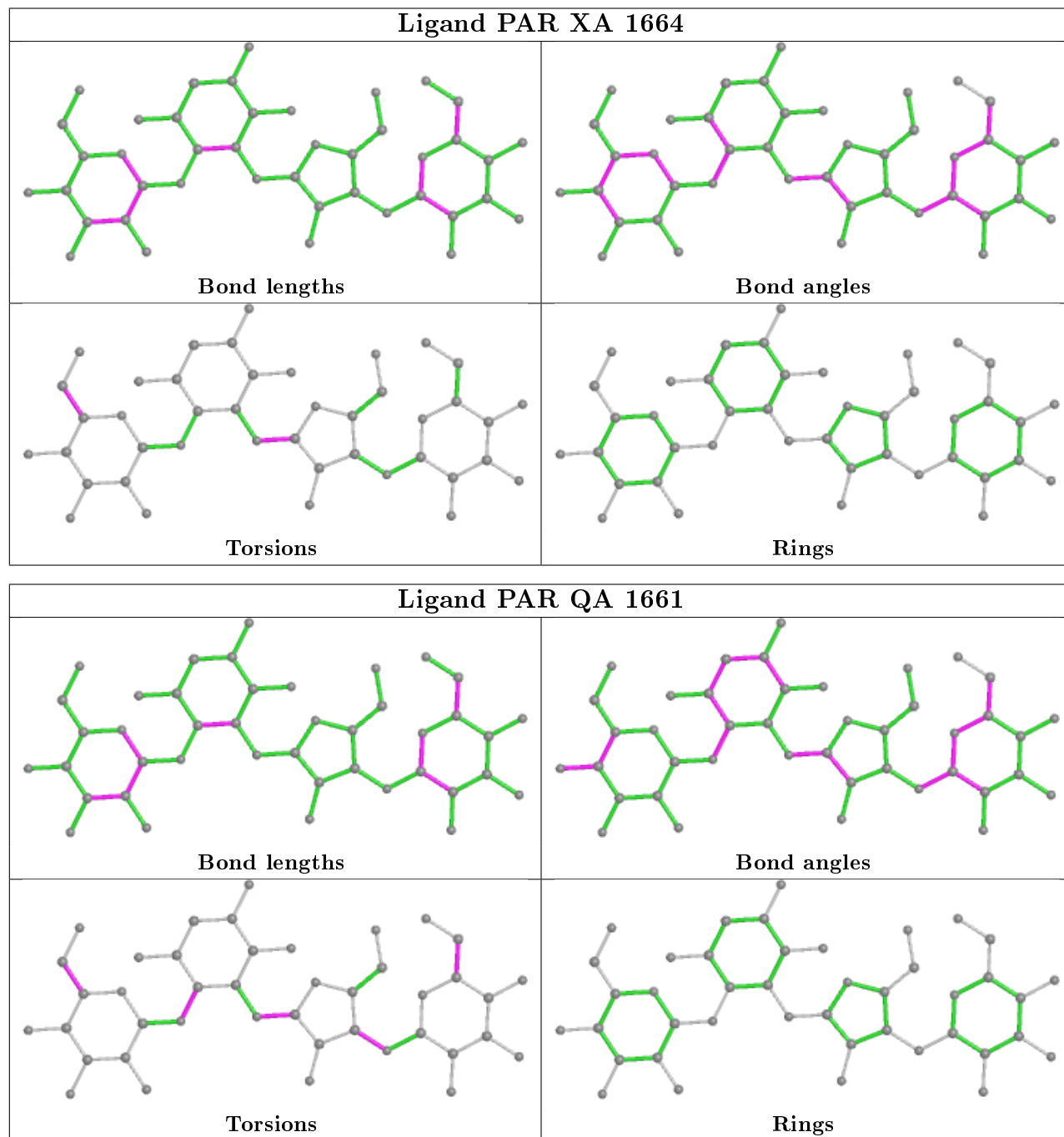
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1664	PAR	1	0
57	QA	1661	PAR	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.19	57 (3%) 40 39	30, 83, 175, 356	0
1	XA	1501/1522 (98%)	0.06	50 (3%) 46 45	30, 76, 171, 324	0
2	QB	237/256 (92%)	0.84	31 (13%) 3 5	56, 138, 222, 266	0
2	XB	237/256 (92%)	0.50	24 (10%) 7 9	55, 126, 194, 238	0
3	QC	205/239 (85%)	0.69	30 (14%) 2 3	54, 122, 199, 216	0
3	XC	205/239 (85%)	0.25	10 (4%) 29 30	39, 95, 158, 217	0
4	QD	208/209 (99%)	0.17	8 (3%) 40 39	44, 92, 154, 184	0
4	XD	208/209 (99%)	0.30	8 (3%) 40 39	39, 95, 161, 234	0
5	QE	151/162 (93%)	0.57	11 (7%) 15 17	29, 104, 175, 237	0
5	XE	151/162 (93%)	0.12	4 (2%) 56 54	34, 79, 149, 229	0
6	QF	101/101 (100%)	0.11	3 (2%) 50 48	44, 86, 125, 222	0
6	XF	101/101 (100%)	0.10	3 (2%) 50 48	36, 86, 144, 209	0
7	QG	155/156 (99%)	0.50	15 (9%) 7 10	51, 106, 181, 215	0
7	XG	155/156 (99%)	0.28	9 (5%) 23 24	46, 103, 177, 230	0
8	QH	138/138 (100%)	0.25	3 (2%) 62 60	48, 108, 167, 204	0
8	XH	138/138 (100%)	0.18	4 (2%) 51 50	48, 96, 158, 208	0
9	QI	127/128 (99%)	0.69	14 (11%) 5 8	53, 124, 188, 214	0
9	XI	127/128 (99%)	0.55	8 (6%) 20 21	43, 116, 194, 219	0
10	QJ	99/105 (94%)	1.30	24 (24%) 0 1	67, 145, 212, 246	0
10	XJ	99/105 (94%)	0.90	20 (20%) 1 1	37, 119, 193, 210	0
11	QK	119/129 (92%)	0.52	10 (8%) 11 14	42, 92, 152, 199	0
11	XK	119/129 (92%)	0.31	5 (4%) 36 35	39, 89, 165, 204	0
12	QL	125/132 (94%)	0.39	6 (4%) 30 31	42, 84, 176, 269	0
12	XL	125/132 (94%)	0.08	4 (3%) 47 46	30, 66, 131, 242	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.53	11 (9%) 9 11	43, 124, 197, 254	0
13	XM	121/126 (96%)	0.24	5 (4%) 37 36	44, 98, 183, 264	0
14	QN	60/61 (98%)	1.05	9 (15%) 2 3	61, 128, 195, 227	0
14	XN	60/61 (98%)	0.09	1 (1%) 70 68	47, 87, 134, 161	0
15	QO	88/89 (98%)	0.44	7 (7%) 12 15	42, 97, 165, 235	0
15	XO	88/89 (98%)	-0.07	1 (1%) 80 77	39, 79, 130, 178	0
16	QP	84/88 (95%)	0.28	1 (1%) 79 76	41, 79, 136, 206	0
16	XP	84/88 (95%)	0.38	3 (3%) 42 42	54, 92, 151, 203	0
17	QQ	100/105 (95%)	0.27	2 (2%) 65 63	53, 102, 165, 210	0
17	XQ	100/105 (95%)	0.42	6 (6%) 21 23	38, 101, 159, 213	0
18	QR	70/88 (79%)	0.12	3 (4%) 35 34	34, 90, 156, 213	0
18	XR	70/88 (79%)	0.10	2 (2%) 51 50	30, 88, 138, 206	0
19	QS	84/93 (90%)	1.23	18 (21%) 0 1	87, 149, 204, 237	0
19	XS	84/93 (90%)	0.56	6 (7%) 16 18	55, 105, 176, 244	0
20	QT	99/106 (93%)	0.53	9 (9%) 9 11	48, 101, 192, 233	0
20	XT	99/106 (93%)	0.25	6 (6%) 21 23	50, 107, 163, 197	0
21	QU	25/27 (92%)	1.03	3 (12%) 4 6	41, 100, 139, 189	0
21	XU	25/27 (92%)	0.72	2 (8%) 12 15	52, 96, 135, 165	0
22	QV	77/77 (100%)	0.46	5 (6%) 18 20	40, 91, 151, 170	0
22	XV	77/77 (100%)	0.18	2 (2%) 56 54	34, 77, 126, 180	0
23	QX	8/25 (32%)	0.64	0 100 100	61, 82, 137, 169	0
23	XX	8/25 (32%)	0.65	1 (12%) 3 6	39, 67, 104, 175	0
24	QY	13/18 (72%)	4.04	8 (61%) 0 0	93, 213, 294, 312	0
24	XY	13/18 (72%)	2.83	6 (46%) 0 0	69, 188, 276, 278	0
25	RA	2883/2916 (98%)	0.12	174 (6%) 21 23	24, 57, 221, 389	0
25	YA	2882/2916 (98%)	-0.00	158 (5%) 25 26	17, 48, 215, 377	0
26	RB	120/122 (98%)	0.11	2 (1%) 70 68	52, 91, 141, 150	0
26	YB	120/122 (98%)	-0.12	0 100 100	44, 74, 109, 158	0
27	RD	272/276 (98%)	0.06	2 (0%) 87 85	19, 60, 98, 243	0
27	YD	272/276 (98%)	-0.12	1 (0%) 92 91	13, 50, 85, 221	0
28	RE	205/206 (99%)	0.16	5 (2%) 59 57	24, 78, 165, 260	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.19	6 (2%)	51	50	22, 76, 161, 238	0
29	RF	202/210 (96%)	0.21	7 (3%)	44	43	21, 82, 158, 250	0
29	YF	202/210 (96%)	0.04	4 (1%)	65	63	13, 64, 130, 197	0
30	RG	181/182 (99%)	1.89	74 (40%)	0	0	58, 164, 258, 303	0
30	YG	181/182 (99%)	0.90	26 (14%)	2	4	59, 108, 186, 248	0
31	RH	170/180 (94%)	1.29	37 (21%)	0	1	78, 171, 239, 267	0
31	YH	170/180 (94%)	0.46	10 (5%)	22	24	39, 100, 156, 260	0
32	RI	146/148 (98%)	0.66	16 (10%)	5	8	56, 118, 204, 240	0
32	YI	146/148 (98%)	0.24	3 (2%)	63	62	40, 104, 169, 214	0
33	RN	138/140 (98%)	0.08	3 (2%)	62	60	32, 84, 153, 194	0
33	YN	138/140 (98%)	-0.06	1 (0%)	87	85	31, 78, 128, 166	0
34	RO	122/122 (100%)	0.04	3 (2%)	57	55	24, 71, 133, 170	0
34	YO	122/122 (100%)	0.08	0	100	100	23, 66, 114, 153	0
35	RP	150/150 (100%)	0.35	13 (8%)	10	13	15, 79, 185, 232	0
35	YP	150/150 (100%)	0.12	3 (2%)	65	63	5, 68, 135, 230	0
36	RQ	141/141 (100%)	0.31	7 (4%)	28	29	38, 85, 149, 219	0
36	YQ	141/141 (100%)	0.02	2 (1%)	75	72	27, 66, 118, 196	0
37	RR	118/118 (100%)	-0.09	0	100	100	28, 68, 107, 171	0
37	YR	118/118 (100%)	-0.08	0	100	100	20, 64, 114, 153	0
38	RS	111/112 (99%)	0.26	5 (4%)	33	32	40, 90, 146, 203	0
38	YS	111/112 (99%)	0.07	3 (2%)	54	52	36, 77, 134, 207	0
39	RT	137/146 (93%)	0.31	10 (7%)	15	17	39, 90, 189, 221	0
39	YT	137/146 (93%)	0.27	5 (3%)	42	42	41, 78, 176, 220	0
40	RU	117/118 (99%)	0.14	5 (4%)	35	34	27, 73, 155, 249	0
40	YU	117/118 (99%)	-0.05	2 (1%)	70	68	20, 59, 129, 212	0
41	RV	101/101 (100%)	0.46	11 (10%)	5	8	28, 88, 167, 278	0
41	YV	101/101 (100%)	0.16	4 (3%)	38	37	25, 82, 143, 255	0
42	RW	113/113 (100%)	0.09	4 (3%)	44	43	28, 63, 127, 241	0
42	YW	113/113 (100%)	-0.10	0	100	100	22, 60, 109, 204	0
43	RX	92/96 (95%)	0.00	1 (1%)	80	77	31, 65, 108, 137	0
43	YX	92/96 (95%)	0.12	2 (2%)	62	60	21, 50, 92, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.94	20 (19%) 1 1	46, 106, 214, 270	0
44	YY	102/110 (92%)	0.34	7 (6%) 16 19	25, 85, 144, 243	0
45	RZ	172/206 (83%)	1.50	42 (24%) 0 1	62, 130, 264, 332	0
45	YZ	172/206 (83%)	0.89	25 (14%) 2 4	33, 111, 243, 361	0
46	R0	82/85 (96%)	0.25	1 (1%) 79 76	35, 72, 105, 143	0
46	Y0	82/85 (96%)	0.03	0 100 100	28, 63, 99, 116	0
47	R1	97/98 (98%)	0.40	3 (3%) 49 48	24, 67, 167, 259	0
47	Y1	97/98 (98%)	0.27	5 (5%) 27 28	20, 65, 161, 211	0
48	R2	69/72 (95%)	0.07	3 (4%) 35 34	34, 82, 149, 217	0
48	Y2	69/72 (95%)	0.11	2 (2%) 51 50	22, 72, 138, 203	0
49	R3	59/60 (98%)	0.24	1 (1%) 70 68	35, 81, 147, 173	0
49	Y3	59/60 (98%)	0.05	2 (3%) 45 44	33, 67, 108, 178	0
50	R4	71/71 (100%)	3.14	42 (59%) 0 0	102, 207, 283, 352	0
50	Y4	71/71 (100%)	1.83	23 (32%) 0 0	88, 160, 251, 277	0
51	R5	59/60 (98%)	0.49	7 (11%) 4 6	12, 64, 224, 264	0
51	Y5	59/60 (98%)	-0.07	3 (5%) 28 28	20, 71, 220, 229	0
52	R6	49/54 (90%)	4.18	33 (67%) 0 0	119, 196, 290, 297	0
52	Y6	49/54 (90%)	3.70	37 (75%) 0 0	120, 182, 235, 265	0
53	R7	49/49 (100%)	-0.25	0 100 100	19, 44, 100, 216	0
53	Y7	49/49 (100%)	-0.06	3 (6%) 21 23	15, 37, 100, 216	0
54	R8	64/65 (98%)	0.22	3 (4%) 31 31	18, 62, 156, 228	0
54	Y8	64/65 (98%)	0.23	2 (3%) 49 48	20, 61, 116, 173	0
55	Z6	2/3 (66%)	0.38	0 100 100	49, 49, 49, 51	0
55	Z8	2/3 (66%)	0.22	0 100 100	36, 36, 36, 37	0
All	All	20776/21420 (96%)	0.27	1351 (6%) 18 20	5, 78, 195, 389	0

The worst 5 of 1351 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	2173	A	16.7
25	RA	2116	G	15.6
52	R6	43	CYS	15.1
25	YA	2175	C	15.0
24	QY	32	U	14.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	1MG	QY	37	24/25	0.83	0.24	124,124,124,124	0
24	1MG	XY	37	24/25	0.93	0.15	89,89,89,89	0
55	PPU	Z6	76	37/38	0.94	0.28	53,53,53,53	0
55	PPU	Z8	76	37/38	0.95	0.25	40,40,40,40	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	RA	3203	1/1	0.57	0.27	73,73,73,73	0
56	MG	QH	201	1/1	0.63	0.31	124,124,124,124	0
56	MG	QA	1639	1/1	0.64	0.13	44,44,44,44	0
56	MG	XA	1605	1/1	0.65	0.41	126,126,126,126	0
56	MG	QA	1615	1/1	0.67	0.76	46,46,46,46	0
56	MG	YA	3173	1/1	0.67	0.20	43,43,43,43	0
56	MG	XA	1648	1/1	0.68	0.32	25,25,25,25	0
56	MG	YA	3012	1/1	0.70	1.51	80,80,80,80	0
56	MG	RA	3176	1/1	0.71	0.53	71,71,71,71	0
56	MG	XM	202	1/1	0.72	0.32	43,43,43,43	0
56	MG	RA	3201	1/1	0.72	0.34	22,22,22,22	0
56	MG	YA	3171	1/1	0.72	0.30	72,72,72,72	0
56	MG	RA	3141	1/1	0.73	0.37	43,43,43,43	0
56	MG	YA	3236	1/1	0.74	0.24	57,57,57,57	0
56	MG	YA	3172	1/1	0.75	0.17	55,55,55,55	0
58	ZN	QN	101	1/1	0.76	0.13	155,155,155,155	0
56	MG	RA	3173	1/1	0.76	0.18	71,71,71,71	0
56	MG	XA	1619	1/1	0.76	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3177	1/1	0.76	0.17	35,35,35,35	0
56	MG	RA	3202	1/1	0.77	0.41	84,84,84,84	0
56	MG	YA	3169	1/1	0.78	0.21	84,84,84,84	0
56	MG	YE	302	1/1	0.79	0.19	13,13,13,13	0
56	MG	YA	3156	1/1	0.80	0.15	33,33,33,33	0
56	MG	YA	3239	1/1	0.81	0.44	48,48,48,48	0
56	MG	YA	3176	1/1	0.81	0.17	54,54,54,54	0
56	MG	YA	3120	1/1	0.81	0.23	36,36,36,36	0
56	MG	YA	3084	1/1	0.83	0.19	23,23,23,23	0
56	MG	YA	3158	1/1	0.83	0.12	20,20,20,20	0
56	MG	YA	3105	1/1	0.83	0.22	16,16,16,16	0
56	MG	RA	3187	1/1	0.83	0.49	68,68,68,68	0
56	MG	XA	1647	1/1	0.84	0.52	58,58,58,58	0
56	MG	QA	1620	1/1	0.84	0.50	40,40,40,40	0
56	MG	RA	3096	1/1	0.84	0.16	8,8,8,8	0
56	MG	RA	3192	1/1	0.84	0.29	56,56,56,56	0
56	MG	RA	3175	1/1	0.84	0.25	99,99,99,99	0
56	MG	QA	1627	1/1	0.84	0.36	57,57,57,57	0
56	MG	XA	1644	1/1	0.84	0.28	59,59,59,59	0
56	MG	YA	3240	1/1	0.84	0.14	45,45,45,45	0
56	MG	YA	3181	1/1	0.84	0.28	51,51,51,51	0
56	MG	YA	3165	1/1	0.84	0.24	42,42,42,42	0
56	MG	QA	1643	1/1	0.84	0.20	24,24,24,24	0
56	MG	QA	1613	1/1	0.84	0.33	56,56,56,56	0
56	MG	RA	3200	1/1	0.84	0.23	58,58,58,58	0
56	MG	YA	3116	1/1	0.85	0.20	28,28,28,28	0
56	MG	RA	3167	1/1	0.85	0.19	35,35,35,35	0
56	MG	XA	1638	1/1	0.86	0.21	55,55,55,55	0
56	MG	YA	3164	1/1	0.86	0.30	25,25,25,25	0
56	MG	QA	1614	1/1	0.86	0.25	38,38,38,38	0
56	MG	RA	3186	1/1	0.86	0.22	90,90,90,90	0
56	MG	YA	3183	1/1	0.86	0.12	36,36,36,36	0
56	MG	RA	3208	1/1	0.86	0.14	47,47,47,47	0
56	MG	XA	1618	1/1	0.86	0.14	24,24,24,24	0
56	MG	RA	3162	1/1	0.86	0.28	56,56,56,56	0
56	MG	YA	3133	1/1	0.86	0.73	43,43,43,43	0
56	MG	QF	201	1/1	0.86	0.17	56,56,56,56	0
56	MG	XA	1642	1/1	0.86	0.27	49,49,49,49	0
56	MG	RA	3083	1/1	0.87	0.20	26,26,26,26	0
56	MG	YA	3207	1/1	0.87	0.30	66,66,66,66	0
56	MG	RA	3163	1/1	0.87	0.18	38,38,38,38	0
56	MG	RA	3122	1/1	0.87	0.24	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3117	1/1	0.87	0.24	42,42,42,42	0
56	MG	YA	3228	1/1	0.87	0.17	45,45,45,45	0
56	MG	YA	3122	1/1	0.87	0.17	35,35,35,35	0
56	MG	RA	3210	1/1	0.87	0.34	38,38,38,38	0
56	MG	RA	3196	1/1	0.88	0.23	53,53,53,53	0
56	MG	RA	3197	1/1	0.88	0.15	50,50,50,50	0
56	MG	YA	3227	1/1	0.88	0.14	22,22,22,22	0
56	MG	YA	3162	1/1	0.88	0.27	34,34,34,34	0
56	MG	QA	1657	1/1	0.88	0.10	76,76,76,76	0
56	MG	RA	3205	1/1	0.88	0.23	54,54,54,54	0
56	MG	RA	3195	1/1	0.88	0.25	28,28,28,28	0
56	MG	RA	3144	1/1	0.88	0.18	36,36,36,36	0
56	MG	YA	3039	1/1	0.88	0.20	30,30,30,30	0
56	MG	RA	3209	1/1	0.88	0.25	49,49,49,49	0
56	MG	RA	3207	1/1	0.88	0.12	51,51,51,51	0
56	MG	YA	3190	1/1	0.88	0.24	51,51,51,51	0
56	MG	YA	3186	1/1	0.88	0.28	50,50,50,50	0
56	MG	RA	3190	1/1	0.88	0.18	50,50,50,50	0
56	MG	RA	3180	1/1	0.89	0.21	28,28,28,28	0
56	MG	RA	3080	1/1	0.89	0.27	44,44,44,44	0
56	MG	RA	3147	1/1	0.89	0.41	49,49,49,49	0
56	MG	XA	1645	1/1	0.89	0.19	31,31,31,31	0
56	MG	RA	3108	1/1	0.89	0.17	26,26,26,26	0
56	MG	XA	1641	1/1	0.89	0.13	24,24,24,24	0
56	MG	XA	1626	1/1	0.89	0.32	27,27,27,27	0
56	MG	RA	3056	1/1	0.89	0.15	26,26,26,26	0
56	MG	YA	3016	1/1	0.89	0.14	19,19,19,19	0
56	MG	RA	3106	1/1	0.89	0.50	24,24,24,24	0
56	MG	RA	3169	1/1	0.89	0.14	23,23,23,23	0
56	MG	YA	3234	1/1	0.89	0.22	34,34,34,34	0
56	MG	XA	1621	1/1	0.89	0.15	22,22,22,22	0
56	MG	QA	1625	1/1	0.89	0.14	66,66,66,66	0
56	MG	YA	3188	1/1	0.89	0.20	38,38,38,38	0
56	MG	QA	1640	1/1	0.89	0.18	54,54,54,54	0
56	MG	YA	3107	1/1	0.89	0.22	25,25,25,25	0
56	MG	RA	3133	1/1	0.89	0.13	32,32,32,32	0
56	MG	XA	1654	1/1	0.89	0.12	50,50,50,50	0
56	MG	QA	1660	1/1	0.90	0.19	45,45,45,45	0
56	MG	QA	1618	1/1	0.90	0.16	41,41,41,41	0
56	MG	XA	1658	1/1	0.90	0.28	50,50,50,50	0
56	MG	QA	1644	1/1	0.90	0.19	23,23,23,23	0
56	MG	RA	3152	1/1	0.90	0.18	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3185	1/1	0.90	0.37	44,44,44,44	0
56	MG	RA	3191	1/1	0.90	0.17	62,62,62,62	0
57	PAR	QA	1661	42/42	0.90	0.23	75,75,75,75	0
56	MG	RA	3206	1/1	0.90	0.28	38,38,38,38	0
56	MG	YA	3139	1/1	0.90	0.22	32,32,32,32	0
56	MG	RA	3130	1/1	0.90	0.31	44,44,44,44	0
56	MG	YA	3130	1/1	0.90	0.19	16,16,16,16	0
56	MG	XA	1652	1/1	0.90	0.16	64,64,64,64	0
56	MG	RA	3097	1/1	0.90	0.21	24,24,24,24	0
56	MG	RA	3183	1/1	0.90	0.33	49,49,49,49	0
56	MG	RA	3072	1/1	0.90	0.27	24,24,24,24	0
56	MG	YA	3192	1/1	0.90	0.28	40,40,40,40	0
56	MG	YA	3056	1/1	0.90	0.19	9,9,9,9	0
56	MG	RA	3174	1/1	0.90	0.39	68,68,68,68	0
56	MG	QA	1632	1/1	0.90	0.24	41,41,41,41	0
56	MG	RF	301	1/1	0.90	0.24	45,45,45,45	0
56	MG	QA	1652	1/1	0.90	0.16	36,36,36,36	0
56	MG	QA	1622	1/1	0.90	0.27	60,60,60,60	0
56	MG	XA	1656	1/1	0.90	0.18	37,37,37,37	0
56	MG	XA	1631	1/1	0.91	0.32	45,45,45,45	0
56	MG	RA	3027	1/1	0.91	0.74	80,80,80,80	0
56	MG	XA	1653	1/1	0.91	0.22	44,44,44,44	0
56	MG	YX	101	1/1	0.91	0.09	28,28,28,28	0
56	MG	YA	3003	1/1	0.91	0.13	13,13,13,13	0
56	MG	XA	1663	1/1	0.91	0.29	85,85,85,85	0
56	MG	RA	3103	1/1	0.91	0.61	48,48,48,48	0
56	MG	YA	3151	1/1	0.91	0.51	26,26,26,26	0
56	MG	RA	3171	1/1	0.91	0.33	49,49,49,49	0
56	MG	QA	1601	1/1	0.91	0.23	27,27,27,27	0
57	PAR	XA	1664	42/42	0.91	0.25	57,57,57,57	0
56	MG	QA	1638	1/1	0.91	0.31	53,53,53,53	0
56	MG	RA	3098	1/1	0.91	0.13	11,11,11,11	0
56	MG	RA	3101	1/1	0.91	0.11	50,50,50,50	0
56	MG	YA	3200	1/1	0.91	0.12	15,15,15,15	0
56	MG	YA	3182	1/1	0.91	0.24	30,30,30,30	0
56	MG	RA	3111	1/1	0.91	0.30	52,52,52,52	0
56	MG	YA	3065	1/1	0.91	0.13	12,12,12,12	0
56	MG	RA	3159	1/1	0.91	0.42	26,26,26,26	0
56	MG	QA	1637	1/1	0.91	0.17	49,49,49,49	0
56	MG	YA	3117	1/1	0.91	0.34	60,60,60,60	0
56	MG	YA	3194	1/1	0.91	0.30	42,42,42,42	0
56	MG	RA	3181	1/1	0.91	0.28	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3201	1/1	0.91	0.10	122,122,122,122	0
56	MG	QA	1659	1/1	0.92	0.26	79,79,79,79	0
56	MG	YA	3152	1/1	0.92	0.39	38,38,38,38	0
56	MG	RA	3146	1/1	0.92	0.30	44,44,44,44	0
56	MG	RA	3066	1/1	0.92	0.24	12,12,12,12	0
56	MG	RA	3091	1/1	0.92	0.17	21,21,21,21	0
56	MG	RA	3033	1/1	0.92	0.21	62,62,62,62	0
56	MG	RA	3164	1/1	0.92	0.15	52,52,52,52	0
56	MG	RA	3095	1/1	0.92	0.14	31,31,31,31	0
56	MG	XA	1651	1/1	0.92	0.14	18,18,18,18	0
56	MG	YA	3150	1/1	0.92	0.19	54,54,54,54	0
56	MG	RA	3123	1/1	0.92	0.14	32,32,32,32	0
56	MG	QV	102	1/1	0.92	0.19	8,8,8,8	0
56	MG	YB	202	1/1	0.92	0.16	42,42,42,42	0
56	MG	YA	3071	1/1	0.92	0.14	18,18,18,18	0
56	MG	RA	3075	1/1	0.92	0.35	4,4,4,4	0
56	MG	XA	1614	1/1	0.92	0.11	14,14,14,14	0
56	MG	YA	3061	1/1	0.92	0.12	35,35,35,35	0
56	MG	YA	3230	1/1	0.92	0.39	43,43,43,43	0
56	MG	RA	3115	1/1	0.92	0.26	59,59,59,59	0
56	MG	QA	1611	1/1	0.92	0.08	32,32,32,32	0
56	MG	YA	3098	1/1	0.92	0.18	49,49,49,49	0
56	MG	RA	3015	1/1	0.92	0.15	15,15,15,15	0
56	MG	QA	1634	1/1	0.92	0.10	48,48,48,48	0
56	MG	RA	3178	1/1	0.92	0.25	62,62,62,62	0
56	MG	RA	3153	1/1	0.92	0.16	36,36,36,36	0
56	MG	RA	3092	1/1	0.92	0.10	18,18,18,18	0
56	MG	RA	3188	1/1	0.92	0.28	58,58,58,58	0
56	MG	QA	1610	1/1	0.92	0.21	33,33,33,33	0
56	MG	YA	3063	1/1	0.92	0.12	6,6,6,6	0
56	MG	RA	3073	1/1	0.92	0.38	5,5,5,5	0
56	MG	RA	3158	1/1	0.93	0.16	14,14,14,14	0
56	MG	RA	3102	1/1	0.93	0.25	32,32,32,32	0
56	MG	RA	3157	1/1	0.93	0.38	20,20,20,20	0
56	MG	YE	301	1/1	0.93	0.11	1,1,1,1	0
56	MG	RA	3193	1/1	0.93	0.15	49,49,49,49	0
56	MG	RA	3120	1/1	0.93	0.11	10,10,10,10	0
56	MG	YA	3178	1/1	0.93	0.22	68,68,68,68	0
56	MG	YA	3082	1/1	0.93	0.15	13,13,13,13	0
56	MG	QA	1645	1/1	0.93	0.17	22,22,22,22	0
56	MG	RA	3114	1/1	0.93	0.11	30,30,30,30	0
56	MG	YA	3242	1/1	0.93	0.32	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3007	1/1	0.93	0.13	8,8,8,8	0
56	MG	YA	3198	1/1	0.93	0.26	32,32,32,32	0
56	MG	YA	3208	1/1	0.93	0.21	53,53,53,53	0
56	MG	XA	1632	1/1	0.93	0.19	11,11,11,11	0
56	MG	QA	1635	1/1	0.93	0.18	31,31,31,31	0
56	MG	QA	1633	1/1	0.93	0.36	50,50,50,50	0
56	MG	XA	1655	1/1	0.93	0.21	33,33,33,33	0
56	MG	RA	3012	1/1	0.93	0.37	26,26,26,26	0
56	MG	RA	3150	1/1	0.93	0.25	26,26,26,26	0
56	MG	YA	3168	1/1	0.93	0.29	65,65,65,65	0
56	MG	RA	3143	1/1	0.93	0.47	16,16,16,16	0
56	MG	XA	1646	1/1	0.93	0.18	23,23,23,23	0
56	MG	YA	3124	1/1	0.93	0.22	22,22,22,22	0
56	MG	RA	3134	1/1	0.93	0.21	18,18,18,18	0
56	MG	YA	3142	1/1	0.93	0.16	30,30,30,30	0
56	MG	YA	3160	1/1	0.93	0.19	37,37,37,37	0
56	MG	QA	1619	1/1	0.93	0.29	48,48,48,48	0
56	MG	RA	3168	1/1	0.93	0.10	31,31,31,31	0
56	MG	QA	1631	1/1	0.93	0.15	55,55,55,55	0
56	MG	XV	102	1/1	0.93	0.12	22,22,22,22	0
56	MG	YA	3141	1/1	0.93	0.48	43,43,43,43	0
56	MG	YA	3226	1/1	0.93	0.15	14,14,14,14	0
56	MG	RA	3139	1/1	0.93	0.13	31,31,31,31	0
56	MG	YA	3196	1/1	0.94	0.13	33,33,33,33	0
56	MG	YA	3191	1/1	0.94	0.13	24,24,24,24	0
56	MG	QA	1623	1/1	0.94	0.15	28,28,28,28	0
56	MG	YA	3005	1/1	0.94	0.12	19,19,19,19	0
56	MG	RA	3009	1/1	0.94	0.17	21,21,21,21	0
56	MG	YA	3212	1/1	0.94	0.10	21,21,21,21	0
56	MG	RA	3040	1/1	0.94	0.13	9,9,9,9	0
56	MG	RA	3131	1/1	0.94	0.20	77,77,77,77	0
56	MG	YA	3170	1/1	0.94	0.35	10,10,10,10	0
56	MG	YA	3205	1/1	0.94	0.15	28,28,28,28	0
56	MG	RA	3127	1/1	0.94	0.18	47,47,47,47	0
56	MG	RA	3199	1/1	0.94	0.18	47,47,47,47	0
56	MG	YA	3149	1/1	0.94	0.30	26,26,26,26	0
56	MG	RA	3160	1/1	0.94	0.17	25,25,25,25	0
56	MG	RA	3082	1/1	0.94	0.14	13,13,13,13	0
56	MG	YA	3066	1/1	0.94	0.48	18,18,18,18	0
56	MG	YA	3175	1/1	0.94	0.12	12,12,12,12	0
56	MG	QA	1656	1/1	0.94	0.22	53,53,53,53	0
56	MG	RA	3069	1/1	0.94	0.30	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3131	1/1	0.94	0.14	20,20,20,20	0
56	MG	RA	3128	1/1	0.94	0.20	27,27,27,27	0
56	MG	RA	3189	1/1	0.94	0.23	34,34,34,34	0
56	MG	RA	3078	1/1	0.94	0.19	15,15,15,15	0
56	MG	YA	3241	1/1	0.94	0.28	33,33,33,33	0
56	MG	YA	3211	1/1	0.94	0.18	42,42,42,42	0
56	MG	RA	3149	1/1	0.94	0.18	48,48,48,48	0
56	MG	YA	3174	1/1	0.94	0.19	29,29,29,29	0
56	MG	XA	1625	1/1	0.94	0.14	20,20,20,20	0
56	MG	RA	3104	1/1	0.94	0.24	44,44,44,44	0
56	MG	YA	3197	1/1	0.94	0.16	33,33,33,33	0
56	MG	RA	3161	1/1	0.94	0.16	32,32,32,32	0
56	MG	YA	3184	1/1	0.94	0.17	33,33,33,33	0
56	MG	QX	102	1/1	0.94	0.09	42,42,42,42	0
56	MG	YA	3223	1/1	0.94	0.09	30,30,30,30	0
56	MG	XA	1662	1/1	0.94	0.24	27,27,27,27	0
56	MG	YA	3018	1/1	0.94	0.32	24,24,24,24	0
56	MG	YA	3214	1/1	0.94	0.15	42,42,42,42	0
56	MG	YA	3215	1/1	0.94	0.15	51,51,51,51	0
56	MG	RA	3057	1/1	0.94	0.06	22,22,22,22	0
56	MG	YA	3127	1/1	0.94	0.53	44,44,44,44	0
56	MG	XM	201	1/1	0.94	0.12	28,28,28,28	0
56	MG	YA	3199	1/1	0.94	0.21	42,42,42,42	0
56	MG	YA	3067	1/1	0.94	0.14	15,15,15,15	0
56	MG	RA	3121	1/1	0.94	0.65	35,35,35,35	0
56	MG	YA	3088	1/1	0.94	0.26	20,20,20,20	0
56	MG	XA	1650	1/1	0.94	0.26	39,39,39,39	0
56	MG	RA	3179	1/1	0.94	0.21	22,22,22,22	0
56	MG	XA	1636	1/1	0.94	0.15	58,58,58,58	0
56	MG	YA	3159	1/1	0.94	0.30	43,43,43,43	0
56	MG	RA	3137	1/1	0.94	0.17	36,36,36,36	0
56	MG	YA	3231	1/1	0.94	0.29	32,32,32,32	0
56	MG	YA	3126	1/1	0.94	0.18	27,27,27,27	0
56	MG	YA	3033	1/1	0.94	0.24	6,6,6,6	0
56	MG	RA	3135	1/1	0.94	0.27	32,32,32,32	0
56	MG	YA	3121	1/1	0.94	0.16	23,23,23,23	0
56	MG	RA	3094	1/1	0.95	0.12	19,19,19,19	0
56	MG	RA	3099	1/1	0.95	0.13	21,21,21,21	0
56	MG	RA	3048	1/1	0.95	0.22	13,13,13,13	0
56	MG	YA	3154	1/1	0.95	0.16	15,15,15,15	0
56	MG	YA	3155	1/1	0.95	0.24	22,22,22,22	0
56	MG	XA	1609	1/1	0.95	0.24	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3148	1/1	0.95	0.11	25,25,25,25	0
56	MG	RA	3166	1/1	0.95	0.23	56,56,56,56	0
56	MG	YA	3070	1/1	0.95	0.13	22,22,22,22	0
56	MG	QA	1617	1/1	0.95	0.22	41,41,41,41	0
56	MG	XA	1637	1/1	0.95	0.11	39,39,39,39	0
56	MG	RA	3119	1/1	0.95	0.39	34,34,34,34	0
56	MG	XA	1660	1/1	0.95	0.08	61,61,61,61	0
56	MG	XA	1639	1/1	0.95	0.17	32,32,32,32	0
56	MG	RB	202	1/1	0.95	0.07	31,31,31,31	0
56	MG	YA	3085	1/1	0.95	0.10	41,41,41,41	0
56	MG	XA	1627	1/1	0.95	0.29	31,31,31,31	0
56	MG	YA	3224	1/1	0.95	0.18	18,18,18,18	0
56	MG	QA	1650	1/1	0.95	0.14	36,36,36,36	0
56	MG	YA	3185	1/1	0.95	0.09	10,10,10,10	0
56	MG	YA	3232	1/1	0.95	0.29	43,43,43,43	0
56	MG	RA	3148	1/1	0.95	0.20	21,21,21,21	0
56	MG	QA	1629	1/1	0.95	0.17	68,68,68,68	0
56	MG	YA	3128	1/1	0.95	0.21	23,23,23,23	0
56	MG	RA	3136	1/1	0.95	0.24	49,49,49,49	0
56	MG	RA	3065	1/1	0.95	0.28	21,21,21,21	0
56	MG	RA	3116	1/1	0.95	0.22	69,69,69,69	0
56	MG	YA	3045	1/1	0.95	0.37	22,22,22,22	0
56	MG	QA	1649	1/1	0.95	0.34	45,45,45,45	0
56	MG	RA	3125	1/1	0.95	0.32	24,24,24,24	0
56	MG	QA	1655	1/1	0.95	0.36	50,50,50,50	0
56	MG	YA	3220	1/1	0.95	0.14	18,18,18,18	0
56	MG	YA	3221	1/1	0.95	0.21	26,26,26,26	0
56	MG	YA	3145	1/1	0.95	0.15	42,42,42,42	0
56	MG	RA	3047	1/1	0.95	0.23	7,7,7,7	0
56	MG	YA	3134	1/1	0.95	0.10	29,29,29,29	0
56	MG	XA	1661	1/1	0.95	0.20	38,38,38,38	0
56	MG	RA	3005	1/1	0.95	0.26	8,8,8,8	0
56	MG	YA	3004	1/1	0.95	0.23	13,13,13,13	0
56	MG	RA	3023	1/1	0.95	0.29	24,24,24,24	0
56	MG	RA	3018	1/1	0.95	0.22	6,6,6,6	0
56	MG	RP	201	1/1	0.95	0.34	37,37,37,37	0
56	MG	XA	1617	1/1	0.96	0.14	26,26,26,26	0
56	MG	RA	3090	1/1	0.96	0.11	14,14,14,14	0
56	MG	YA	3074	1/1	0.96	0.17	28,28,28,28	0
56	MG	YA	3225	1/1	0.96	0.16	32,32,32,32	0
56	MG	YA	3060	1/1	0.96	0.23	13,13,13,13	0
56	MG	XA	1615	1/1	0.96	0.24	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1612	1/1	0.96	0.31	21,21,21,21	0
56	MG	YA	3008	1/1	0.96	0.27	17,17,17,17	0
56	MG	XA	1620	1/1	0.96	0.10	55,55,55,55	0
56	MG	RA	3184	1/1	0.96	0.30	33,33,33,33	0
56	MG	QA	1653	1/1	0.96	0.26	39,39,39,39	0
56	MG	QA	1626	1/1	0.96	0.34	77,77,77,77	0
56	MG	YA	3100	1/1	0.96	0.32	1,1,1,1	0
56	MG	RA	3034	1/1	0.96	0.28	16,16,16,16	0
56	MG	YA	3163	1/1	0.96	0.20	40,40,40,40	0
56	MG	YA	3102	1/1	0.96	0.25	5,5,5,5	0
56	MG	RA	3044	1/1	0.96	0.29	21,21,21,21	0
56	MG	RA	3051	1/1	0.96	0.40	1,1,1,1	0
56	MG	RA	3041	1/1	0.96	0.17	5,5,5,5	0
56	MG	QA	1612	1/1	0.96	0.07	37,37,37,37	0
56	MG	YA	3097	1/1	0.96	0.24	19,19,19,19	0
56	MG	RA	3140	1/1	0.96	0.20	45,45,45,45	0
56	MG	YA	3187	1/1	0.96	0.36	58,58,58,58	0
56	MG	RA	3052	1/1	0.96	0.42	24,24,24,24	0
56	MG	RA	3020	1/1	0.96	0.27	29,29,29,29	0
56	MG	QA	1602	1/1	0.96	0.34	19,19,19,19	0
56	MG	RA	3004	1/1	0.96	0.11	5,5,5,5	0
56	MG	RE	302	1/1	0.96	0.38	22,22,22,22	0
58	ZN	QD	301	1/1	0.96	0.19	59,59,59,59	0
56	MG	RA	3001	1/1	0.96	0.19	36,36,36,36	0
56	MG	RA	3063	1/1	0.96	0.20	27,27,27,27	0
56	MG	YA	3179	1/1	0.96	0.41	31,31,31,31	0
56	MG	RA	3016	1/1	0.96	0.26	2,2,2,2	0
56	MG	RA	3124	1/1	0.96	0.33	21,21,21,21	0
56	MG	YA	3210	1/1	0.96	0.11	35,35,35,35	0
56	MG	RA	3038	1/1	0.96	0.15	14,14,14,14	0
56	MG	YA	3219	1/1	0.96	0.26	29,29,29,29	0
56	MG	RA	3008	1/1	0.96	0.20	13,13,13,13	0
56	MG	YA	3119	1/1	0.96	0.37	35,35,35,35	0
56	MG	YA	3083	1/1	0.96	0.42	21,21,21,21	0
56	MG	YA	3123	1/1	0.96	0.12	15,15,15,15	0
56	MG	RA	3003	1/1	0.96	0.23	17,17,17,17	0
56	MG	QA	1604	1/1	0.96	0.10	33,33,33,33	0
56	MG	YA	3203	1/1	0.96	0.13	24,24,24,24	0
56	MG	QA	1616	1/1	0.96	0.09	42,42,42,42	0
56	MG	YA	3009	1/1	0.96	0.45	27,27,27,27	0
56	MG	RA	3177	1/1	0.96	0.15	59,59,59,59	0
56	MG	XA	1659	1/1	0.96	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1657	1/1	0.96	0.13	28,28,28,28	0
56	MG	YA	3144	1/1	0.96	0.16	13,13,13,13	0
56	MG	YA	3034	1/1	0.96	0.19	3,3,3,3	0
56	MG	RA	3212	1/1	0.96	0.28	18,18,18,18	0
56	MG	YA	3115	1/1	0.96	0.14	21,21,21,21	0
56	MG	YA	3125	1/1	0.96	0.13	18,18,18,18	0
56	MG	QA	1624	1/1	0.96	0.34	24,24,24,24	0
56	MG	YA	3202	1/1	0.96	0.07	21,21,21,21	0
56	MG	RA	3088	1/1	0.96	0.17	24,24,24,24	0
56	MG	RA	3087	1/1	0.96	0.11	9,9,9,9	0
56	MG	QA	1606	1/1	0.97	0.16	7,7,7,7	0
56	MG	R5	101	1/1	0.97	0.14	27,27,27,27	0
56	MG	RA	3129	1/1	0.97	0.20	26,26,26,26	0
56	MG	YA	3106	1/1	0.97	0.29	32,32,32,32	0
56	MG	YA	3110	1/1	0.97	0.08	10,10,10,10	0
56	MG	YA	3019	1/1	0.97	0.39	21,21,21,21	0
56	MG	RA	3077	1/1	0.97	0.32	14,14,14,14	0
56	MG	YA	3233	1/1	0.97	0.38	44,44,44,44	0
56	MG	YA	3193	1/1	0.97	0.14	39,39,39,39	0
56	MG	YA	3054	1/1	0.97	0.14	14,14,14,14	0
56	MG	XA	1633	1/1	0.97	0.23	32,32,32,32	0
56	MG	YA	3035	1/1	0.97	0.20	10,10,10,10	0
56	MG	YA	3040	1/1	0.97	0.12	1,1,1,1	0
56	MG	YA	3090	1/1	0.97	0.39	11,11,11,11	0
56	MG	QA	1647	1/1	0.97	0.10	41,41,41,41	0
56	MG	RA	3132	1/1	0.97	0.21	12,12,12,12	0
56	MG	YA	3051	1/1	0.97	0.22	4,4,4,4	0
56	MG	YA	3118	1/1	0.97	0.17	12,12,12,12	0
56	MG	YA	3143	1/1	0.97	0.13	33,33,33,33	0
56	MG	RA	3155	1/1	0.97	0.21	12,12,12,12	0
56	MG	RA	3085	1/1	0.97	0.11	15,15,15,15	0
56	MG	RA	3074	1/1	0.97	0.32	8,8,8,8	0
56	MG	YA	3189	1/1	0.97	0.11	31,31,31,31	0
56	MG	XA	1623	1/1	0.97	0.39	31,31,31,31	0
56	MG	YA	3020	1/1	0.97	0.34	8,8,8,8	0
56	MG	RA	3026	1/1	0.97	0.22	6,6,6,6	0
56	MG	XA	1610	1/1	0.97	0.17	37,37,37,37	0
56	MG	RA	3002	1/1	0.97	0.24	8,8,8,8	0
56	MG	YA	3157	1/1	0.97	0.16	29,29,29,29	0
56	MG	QA	1608	1/1	0.97	0.18	27,27,27,27	0
56	MG	RA	3100	1/1	0.97	0.16	44,44,44,44	0
56	MG	XA	1649	1/1	0.97	0.36	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1605	1/1	0.97	0.17	51,51,51,51	0
56	MG	YA	3113	1/1	0.97	0.27	21,21,21,21	0
56	MG	YA	3112	1/1	0.97	0.11	41,41,41,41	0
56	MG	RA	3118	1/1	0.97	0.14	14,14,14,14	0
56	MG	YA	3081	1/1	0.97	0.30	18,18,18,18	0
56	MG	YA	3069	1/1	0.97	0.16	16,16,16,16	0
56	MG	YA	3180	1/1	0.97	0.11	53,53,53,53	0
56	MG	XA	1602	1/1	0.97	0.15	15,15,15,15	0
56	MG	RA	3081	1/1	0.97	0.47	28,28,28,28	0
56	MG	RA	3068	1/1	0.97	0.13	16,16,16,16	0
56	MG	RA	3105	1/1	0.97	0.12	50,50,50,50	0
56	MG	YA	3014	1/1	0.97	0.39	12,12,12,12	0
56	MG	YA	3047	1/1	0.97	0.26	6,6,6,6	0
56	MG	RA	3093	1/1	0.97	0.08	24,24,24,24	0
56	MG	YA	3129	1/1	0.97	0.07	22,22,22,22	0
56	MG	XA	1640	1/1	0.97	0.19	47,47,47,47	0
56	MG	YA	3136	1/1	0.97	0.15	4,4,4,4	0
56	MG	YA	3059	1/1	0.97	0.15	74,74,74,74	0
56	MG	RA	3076	1/1	0.97	0.40	22,22,22,22	0
56	MG	YA	3072	1/1	0.97	0.14	10,10,10,10	0
56	MG	YA	3132	1/1	0.97	0.11	13,13,13,13	0
56	MG	YA	3101	1/1	0.97	0.27	5,5,5,5	0
56	MG	XA	1629	1/1	0.97	0.13	49,49,49,49	0
56	MG	YA	3026	1/1	0.97	0.40	9,9,9,9	0
56	MG	QA	1630	1/1	0.97	0.12	66,66,66,66	0
56	MG	RA	3071	1/1	0.97	0.19	32,32,32,32	0
56	MG	QX	101	1/1	0.97	0.10	24,24,24,24	0
56	MG	RE	301	1/1	0.97	0.12	22,22,22,22	0
56	MG	RA	3060	1/1	0.97	0.22	25,25,25,25	0
56	MG	RA	3211	1/1	0.97	0.27	13,13,13,13	0
56	MG	YA	3055	1/1	0.97	0.22	16,16,16,16	0
56	MG	RA	3198	1/1	0.97	0.09	53,53,53,53	0
56	MG	YA	3218	1/1	0.97	0.11	19,19,19,19	0
56	MG	YA	3041	1/1	0.97	0.28	6,6,6,6	0
56	MG	YA	3216	1/1	0.97	0.09	42,42,42,42	0
56	MG	QA	1642	1/1	0.97	0.09	49,49,49,49	0
56	MG	XA	1634	1/1	0.97	0.29	28,28,28,28	0
56	MG	RA	3037	1/1	0.97	0.26	10,10,10,10	0
56	MG	QV	101	1/1	0.97	0.19	17,17,17,17	0
56	MG	YA	3092	1/1	0.97	0.16	11,11,11,11	0
56	MG	RA	3204	1/1	0.97	0.12	30,30,30,30	0
56	MG	RA	3138	1/1	0.97	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1609	1/1	0.97	0.28	34,34,34,34	0
56	MG	QA	1607	1/1	0.97	0.14	22,22,22,22	0
56	MG	RA	3145	1/1	0.97	0.22	37,37,37,37	0
56	MG	YA	3077	1/1	0.97	0.15	8,8,8,8	0
56	MG	RA	3151	1/1	0.97	0.23	23,23,23,23	0
56	MG	YA	3057	1/1	0.97	0.49	22,22,22,22	0
56	MG	RA	3172	1/1	0.97	0.21	29,29,29,29	0
56	MG	XA	1643	1/1	0.97	0.17	47,47,47,47	0
56	MG	YA	3030	1/1	0.97	0.27	24,24,24,24	0
56	MG	RA	3021	1/1	0.97	0.42	27,27,27,27	0
56	MG	YA	3146	1/1	0.97	0.11	50,50,50,50	0
56	MG	YA	3138	1/1	0.97	0.16	15,15,15,15	0
56	MG	YA	3080	1/1	0.97	0.30	3,3,3,3	0
56	MG	RA	3170	1/1	0.97	0.09	41,41,41,41	0
56	MG	YA	3140	1/1	0.97	0.29	2,2,2,2	0
56	MG	RA	3042	1/1	0.97	0.20	11,11,11,11	0
56	MG	YA	3213	1/1	0.97	0.13	41,41,41,41	0
56	MG	QA	1636	1/1	0.97	0.08	15,15,15,15	0
56	MG	YA	3029	1/1	0.97	0.35	17,17,17,17	0
56	MG	YA	3167	1/1	0.97	0.06	12,12,12,12	0
56	MG	QA	1621	1/1	0.97	0.18	48,48,48,48	0
56	MG	XA	1628	1/1	0.98	0.17	24,24,24,24	0
56	MG	RA	3022	1/1	0.98	0.33	3,3,3,3	0
56	MG	YA	3050	1/1	0.98	0.18	2,2,2,2	0
56	MG	RA	3045	1/1	0.98	0.29	12,12,12,12	0
56	MG	YA	3038	1/1	0.98	0.13	12,12,12,12	0
56	MG	RA	3058	1/1	0.98	0.20	13,13,13,13	0
56	MG	XA	1601	1/1	0.98	0.12	15,15,15,15	0
56	MG	YA	3052	1/1	0.98	0.23	17,17,17,17	0
56	MG	YA	3195	1/1	0.98	0.09	55,55,55,55	0
56	MG	RA	3079	1/1	0.98	0.20	32,32,32,32	0
56	MG	YA	3091	1/1	0.98	0.13	23,23,23,23	0
56	MG	YA	3049	1/1	0.98	0.27	15,15,15,15	0
56	MG	YA	3064	1/1	0.98	0.18	23,23,23,23	0
56	MG	YB	201	1/1	0.98	0.15	21,21,21,21	0
56	MG	YA	3217	1/1	0.98	0.09	35,35,35,35	0
56	MG	RA	3035	1/1	0.98	0.12	21,21,21,21	0
56	MG	YA	3073	1/1	0.98	0.25	24,24,24,24	0
56	MG	RA	3062	1/1	0.98	0.38	21,21,21,21	0
56	MG	QA	1628	1/1	0.98	0.28	14,14,14,14	0
56	MG	XA	1606	1/1	0.98	0.25	17,17,17,17	0
56	MG	YA	3036	1/1	0.98	0.23	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3039	1/1	0.98	0.26	18,18,18,18	0
56	MG	YA	3103	1/1	0.98	0.08	12,12,12,12	0
56	MG	YA	3025	1/1	0.98	0.18	6,6,6,6	0
56	MG	YA	3209	1/1	0.98	0.18	41,41,41,41	0
56	MG	RA	3142	1/1	0.98	0.11	15,15,15,15	0
56	MG	XA	1630	1/1	0.98	0.14	39,39,39,39	0
56	MG	RA	3089	1/1	0.98	0.28	26,26,26,26	0
56	MG	YA	3094	1/1	0.98	0.29	10,10,10,10	0
56	MG	YA	3068	1/1	0.98	0.31	12,12,12,12	0
56	MG	RA	3165	1/1	0.98	0.09	5,5,5,5	0
56	MG	RB	201	1/1	0.98	0.05	13,13,13,13	0
56	MG	YA	3166	1/1	0.98	0.19	51,51,51,51	0
56	MG	RA	3110	1/1	0.98	0.12	51,51,51,51	0
56	MG	YA	3238	1/1	0.98	0.26	34,34,34,34	0
58	ZN	XD	301	1/1	0.98	0.23	49,49,49,49	0
56	MG	YA	3079	1/1	0.98	0.26	18,18,18,18	0
56	MG	YA	3022	1/1	0.98	0.21	6,6,6,6	0
56	MG	QA	1641	1/1	0.98	0.17	25,25,25,25	0
56	MG	XV	101	1/1	0.98	0.21	14,14,14,14	0
56	MG	YA	3024	1/1	0.98	0.19	10,10,10,10	0
56	MG	QM	201	1/1	0.98	0.15	34,34,34,34	0
56	MG	QA	1646	1/1	0.98	0.25	14,14,14,14	0
56	MG	YA	3032	1/1	0.98	0.21	9,9,9,9	0
56	MG	RA	3064	1/1	0.98	0.40	25,25,25,25	0
56	MG	RA	3061	1/1	0.98	0.21	28,28,28,28	0
56	MG	RA	3067	1/1	0.98	0.06	7,7,7,7	0
56	MG	YA	3006	1/1	0.98	0.24	0,0,0,0	0
56	MG	QA	1658	1/1	0.98	0.08	68,68,68,68	0
56	MG	YA	3137	1/1	0.98	0.08	15,15,15,15	0
56	MG	XA	1622	1/1	0.98	0.07	40,40,40,40	0
56	MG	RA	3030	1/1	0.98	0.28	15,15,15,15	0
56	MG	RA	3010	1/1	0.98	0.36	4,4,4,4	0
56	MG	YA	3044	1/1	0.98	0.22	9,9,9,9	0
56	MG	Y5	101	1/1	0.98	0.15	25,25,25,25	0
56	MG	QA	1654	1/1	0.98	0.15	14,14,14,14	0
56	MG	YA	3237	1/1	0.98	0.08	15,15,15,15	0
56	MG	RA	3028	1/1	0.98	0.19	12,12,12,12	0
56	MG	YA	3010	1/1	0.98	0.15	3,3,3,3	0
56	MG	YA	3021	1/1	0.98	0.32	12,12,12,12	0
56	MG	RA	3084	1/1	0.98	0.30	17,17,17,17	0
56	MG	YA	3076	1/1	0.98	0.37	7,7,7,7	0
56	MG	RA	3194	1/1	0.98	0.14	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3126	1/1	0.98	0.24	27,27,27,27	0
56	MG	YA	3087	1/1	0.98	0.24	7,7,7,7	0
56	MG	XA	1611	1/1	0.98	0.17	29,29,29,29	0
56	MG	RA	3031	1/1	0.98	0.29	26,26,26,26	0
56	MG	YA	3001	1/1	0.98	0.43	13,13,13,13	0
56	MG	YA	3086	1/1	0.98	0.14	3,3,3,3	0
56	MG	YA	3078	1/1	0.98	0.39	25,25,25,25	0
58	ZN	XN	101	1/1	0.98	0.12	107,107,107,107	0
56	MG	YA	3099	1/1	0.98	0.34	11,11,11,11	0
56	MG	YA	3017	1/1	0.98	0.11	16,16,16,16	0
56	MG	RA	3043	1/1	0.98	0.11	30,30,30,30	0
56	MG	RA	3070	1/1	0.98	0.31	37,37,37,37	0
56	MG	YA	3048	1/1	0.98	0.16	4,4,4,4	0
56	MG	YA	3153	1/1	0.98	0.22	26,26,26,26	0
56	MG	YA	3161	1/1	0.98	0.09	30,30,30,30	0
56	MG	YA	3027	1/1	0.98	0.11	5,5,5,5	0
56	MG	RA	3113	1/1	0.98	0.27	24,24,24,24	0
56	MG	RA	3046	1/1	0.98	0.35	31,31,31,31	0
56	MG	YA	3075	1/1	0.98	0.10	14,14,14,14	0
56	MG	YA	3109	1/1	0.98	0.25	25,25,25,25	0
56	MG	XA	1608	1/1	0.98	0.16	7,7,7,7	0
56	MG	RA	3182	1/1	0.98	0.34	25,25,25,25	0
56	MG	RA	3154	1/1	0.98	0.13	12,12,12,12	0
56	MG	RA	3029	1/1	0.98	0.15	2,2,2,2	0
56	MG	YA	3043	1/1	0.98	0.39	9,9,9,9	0
56	MG	YA	3015	1/1	0.98	0.43	10,10,10,10	0
56	MG	RA	3019	1/1	0.98	0.16	10,10,10,10	0
56	MG	RA	3112	1/1	0.98	0.28	50,50,50,50	0
56	MG	RA	3086	1/1	0.98	0.22	33,33,33,33	0
56	MG	YA	3222	1/1	0.98	0.05	9,9,9,9	0
56	MG	XA	1603	1/1	0.98	0.07	23,23,23,23	0
56	MG	YA	3229	1/1	0.98	0.10	52,52,52,52	0
56	MG	YA	3206	1/1	0.98	0.10	24,24,24,24	0
56	MG	QA	1651	1/1	0.98	0.21	70,70,70,70	0
56	MG	YA	3095	1/1	0.99	0.29	5,5,5,5	0
56	MG	RA	3017	1/1	0.99	0.12	13,13,13,13	0
56	MG	YA	3007	1/1	0.99	0.17	6,6,6,6	0
56	MG	XA	1613	1/1	0.99	0.13	45,45,45,45	0
56	MG	QA	1603	1/1	0.99	0.05	28,28,28,28	0
56	MG	RA	3024	1/1	0.99	0.45	4,4,4,4	0
56	MG	XA	1624	1/1	0.99	0.13	35,35,35,35	0
56	MG	RA	3049	1/1	0.99	0.15	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3156	1/1	0.99	0.16	22,22,22,22	0
56	MG	YA	3235	1/1	0.99	0.13	26,26,26,26	0
56	MG	YA	3135	1/1	0.99	0.10	33,33,33,33	0
56	MG	YA	3108	1/1	0.99	0.11	5,5,5,5	0
56	MG	YA	3204	1/1	0.99	0.16	43,43,43,43	0
56	MG	RA	3059	1/1	0.99	0.27	21,21,21,21	0
56	MG	YA	3093	1/1	0.99	0.14	18,18,18,18	0
56	MG	RA	3014	1/1	0.99	0.24	10,10,10,10	0
56	MG	XA	1607	1/1	0.99	0.07	5,5,5,5	0
56	MG	RA	3109	1/1	0.99	0.07	26,26,26,26	0
56	MG	QA	1648	1/1	0.99	0.03	100,100,100,100	0
56	MG	YA	3013	1/1	0.99	0.31	3,3,3,3	0
56	MG	YA	3111	1/1	0.99	0.23	30,30,30,30	0
56	MG	YA	3089	1/1	0.99	0.23	2,2,2,2	0
56	MG	XA	1635	1/1	0.99	0.07	36,36,36,36	0
56	MG	YA	3011	1/1	0.99	0.26	13,13,13,13	0
56	MG	RA	3050	1/1	0.99	0.14	0,0,0,0	0
56	MG	RA	3013	1/1	0.99	0.22	10,10,10,10	0
56	MG	YA	3046	1/1	0.99	0.13	4,4,4,4	0
56	MG	RA	3107	1/1	0.99	0.28	21,21,21,21	0
56	MG	YA	3023	1/1	0.99	0.26	4,4,4,4	0
56	MG	XA	1604	1/1	0.99	0.07	31,31,31,31	0
56	MG	YA	3031	1/1	0.99	0.35	6,6,6,6	0
56	MG	RA	3006	1/1	0.99	0.17	3,3,3,3	0
56	MG	RA	3055	1/1	0.99	0.15	12,12,12,12	0
56	MG	YA	3062	1/1	0.99	0.11	6,6,6,6	0
56	MG	RA	3036	1/1	0.99	0.33	10,10,10,10	0
56	MG	RA	3025	1/1	0.99	0.14	9,9,9,9	0
56	MG	YA	3114	1/1	0.99	0.24	6,6,6,6	0
56	MG	YA	3147	1/1	0.99	0.11	11,11,11,11	0
56	MG	RA	3032	1/1	0.99	0.16	17,17,17,17	0
56	MG	RA	3054	1/1	0.99	0.23	5,5,5,5	0
56	MG	YA	3058	1/1	0.99	0.30	16,16,16,16	0
56	MG	YA	3028	1/1	0.99	0.18	23,23,23,23	0
56	MG	YA	3037	1/1	0.99	0.20	3,3,3,3	0
56	MG	XA	1616	1/1	0.99	0.11	20,20,20,20	0
56	MG	YA	3053	1/1	0.99	0.15	4,4,4,4	0
56	MG	RA	3011	1/1	0.99	0.17	30,30,30,30	0
56	MG	YA	3096	1/1	0.99	0.22	15,15,15,15	0
56	MG	RA	3053	1/1	0.99	0.17	5,5,5,5	0
56	MG	YA	3104	1/1	0.99	0.24	6,6,6,6	0
56	MG	YA	3042	1/1	0.99	0.31	28,28,28,28	0

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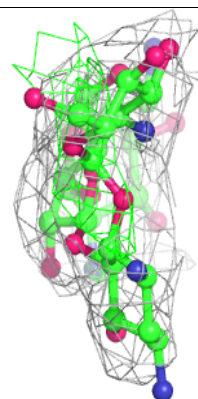
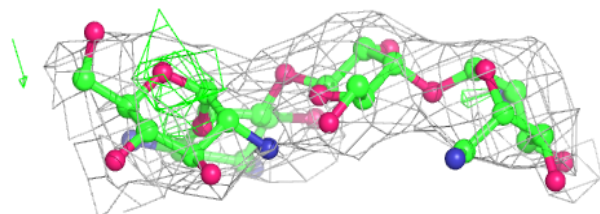
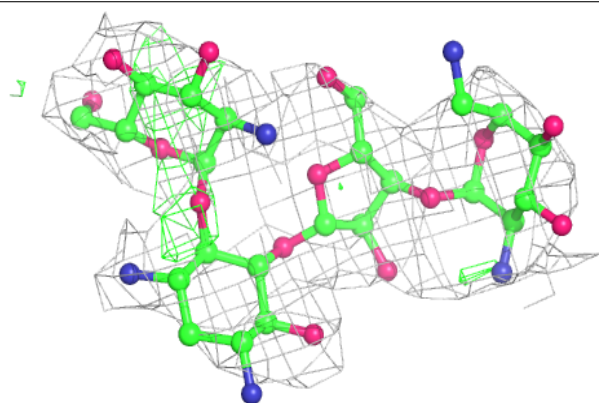
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3002	1/1	1.00	0.38	15,15,15,15	0

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

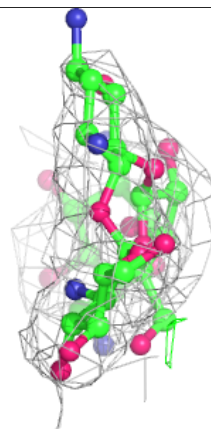
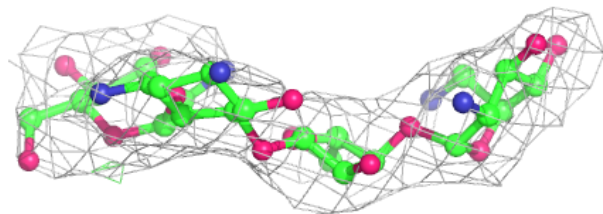
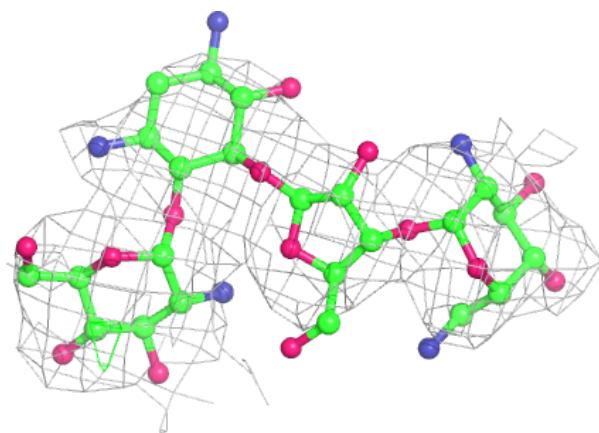
Electron density around PAR QA 1661:

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



Electron density around PAR XA 1664:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.