



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:04 AM UTC

PDB ID : 8FON / pdb_00008fon
Title : Crystal structure of tRNA^{Lys}(SUU) bound to AUA codon in the ribosomal P site
Authors : Nguyen, H.A.; Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2023-01-02
Resolution : 3.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

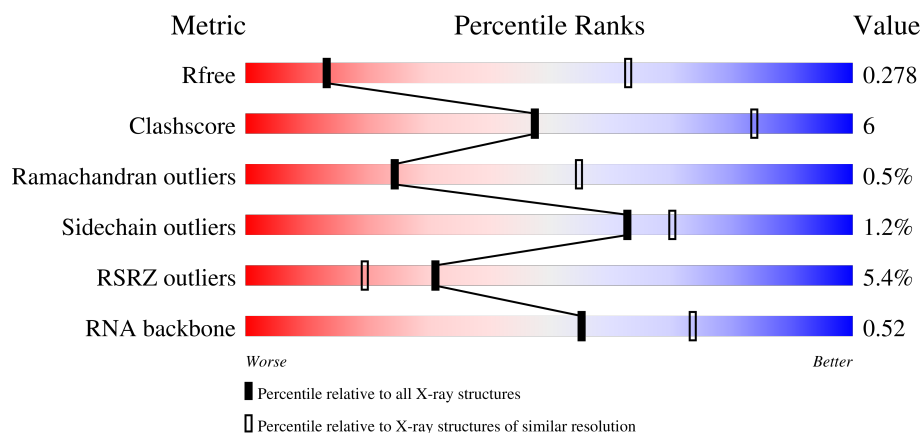
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)
RNA backbone	3983	1026 (4.22-3.06)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	3% 63% 31% . .
1	XA	1522	4% 61% 33% 5% .
2	QB	256	% 76% 15% . 8%
2	XB	256	2% 82% 10% 8%

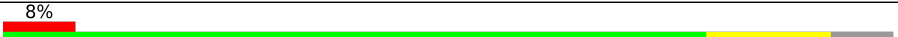
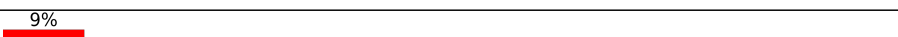
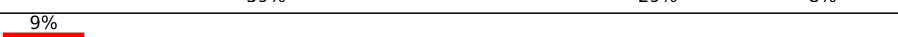
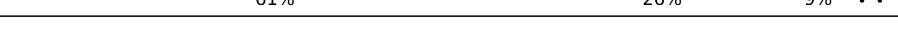
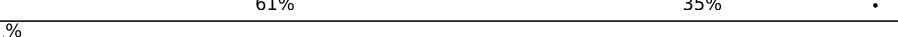
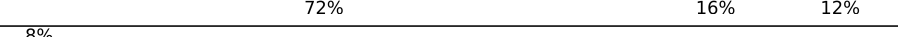
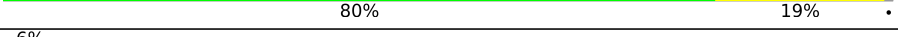
Continued on next page...

Continued from previous page...

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	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

Continued on next page...

Continued from previous page...

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	76	
22	XV	76	
23	QX	23	
23	XX	23	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	R4	71	83% 14% .
28	Y4	71	4% 82% 14% ..
29	R5	60	7% 92% 7% .
29	Y5	60	2% 90% 8% .
30	R6	54	15% 81% 17% .
30	Y6	54	9% 80% 19% .
31	R7	49	4% 84% 12% .
31	Y7	49	4% 90% 8% .
32	R8	65	5% 52% 31% 15% .
32	Y8	65	6% 77% 22% .
33	R9	37	24% 81% 19% .
33	Y9	37	5% 73% 27% .
34	RA	2915	5% 65% 29% ..
34	YA	2915	5% 65% 29% ..
35	RB	122	73% 24% ..
35	YB	122	7% 73% 23% ..
36	RD	276	4% 79% 19% .
36	YD	276	2% 83% 15% .
37	RE	206	12% 78% 20% .
37	YE	206	14% 87% 11% .
38	RF	210	10% 80% 16% .
38	YF	210	8% 86% 10% .
39	RG	182	4% 70% 26% ...
39	YG	182	5% 70% 27% ...
40	RH	180	14% 67% 26% ...

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	YH	180	
41	RI	148	
41	YI	148	
42	RN	140	
42	YN	140	
43	RO	122	
43	YO	122	
44	RP	150	
44	YP	150	
45	RQ	141	
45	YQ	141	
46	RR	118	
46	YR	118	
47	RS	112	
47	YS	112	
48	RT	146	
48	YT	146	
49	RU	118	
49	YU	118	
50	RV	101	
50	YV	101	
51	RW	113	
51	YW	113	
52	RX	96	
52	YX	96	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	RY	110	
53	YY	110	
54	RZ	206	
54	YZ	206	
55	XY	17	
56	Z6	3	
56	Z8	3	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292577 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	1511	Total	C	N	O	P	0	0	0
			32471	14454	6014	10493	1510			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	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	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- 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	126	Total	C	N	O		0	0	0
			998	633	193	172				

- 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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	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	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	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	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

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

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

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

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

- Molecule 22 is a RNA chain called P-site tRNA^{Lys}(SUU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	74	Total	C	N	O	P	0	0	0
			1584	710	278	523	73			
22	XV	74	Total	C	N	O	P	0	0	0
			1584	710	278	523	73			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
23	XX	23	Total	C	N	O	P	0	0	0
			499	223	96	157	23			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			
24	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
25	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
28	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
31	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RA	2881	Total	C	N	O	P	0	0	0
			62051	27618	11609	19944	2880			
34	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 35 is a RNA chain called 5S rRNA.

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

- Molecule 36 is a protein called 50S ribosomal protein L2.

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

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
37	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
40	YH	173	Total	C	N	O	S	0	0	0
			1330	845	250	234	1			

- Molecule 41 is a protein called 50S ribosomal protein L9.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
44	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			
46	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
53	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
54	YZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			

- Molecule 55 is a RNA chain called A-site ASL⁺Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	XY	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			

- Molecule 56 is a RNA chain called CC-puro.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	73	Total	Mg	0	0
			73	73		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QJ	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

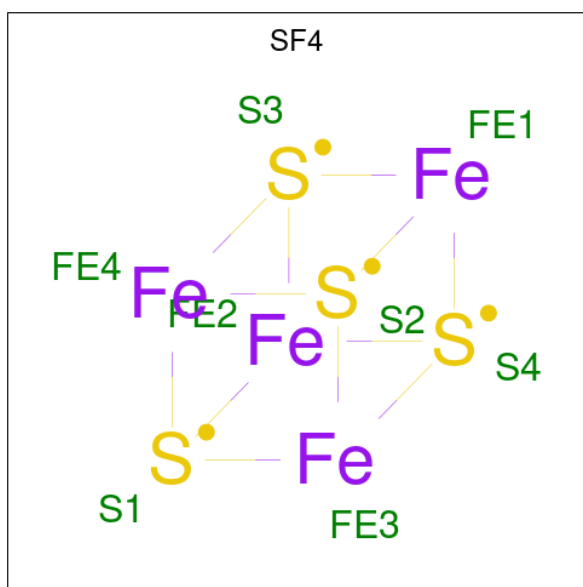
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R0	1	Total 1	Mg 1	0	0
57	R1	1	Total 1	Mg 1	0	0
57	R3	1	Total 1	Mg 1	0	0
57	RA	483	Total 483	Mg 483	0	0
57	RB	7	Total 7	Mg 7	0	0
57	RE	4	Total 4	Mg 4	0	0
57	RN	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	3	Total 3	Mg 3	0	0
57	RQ	3	Total 3	Mg 3	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RT	1	Total 1	Mg 1	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XA	73	Total 73	Mg 73	0	0
57	XE	1	Total 1	Mg 1	0	0
57	XK	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XQ	1	Total 1	Mg 1	0	0
57	XS	1	Total 1	Mg 1	0	0
57	Y0	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y1	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	Y8	1	Total 1	Mg 1	0	0
57	YA	538	Total 538	Mg 538	0	0
57	YB	13	Total 13	Mg 13	0	0
57	YD	3	Total 3	Mg 3	0	0
57	YE	4	Total 4	Mg 4	0	0
57	YN	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	3	Total 3	Mg 3	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YX	2	Total 2	Mg 2	0	0
57	YY	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	RY	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	Y5	1	Total	Zn	0	0
			1	1		
59	Y6	1	Total	Zn	0	0
			1	1		

Continued on next page...

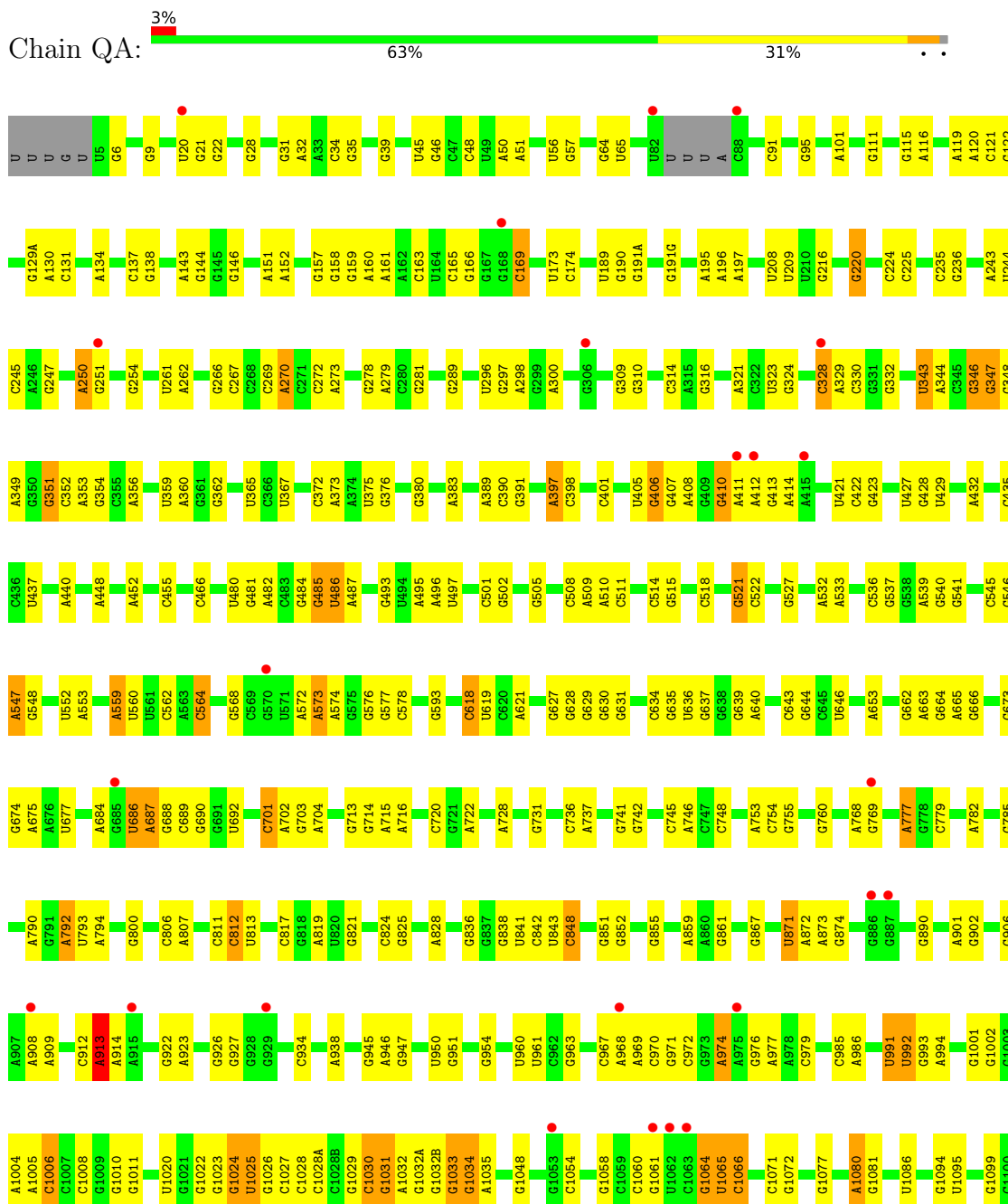
Continued from previous page...

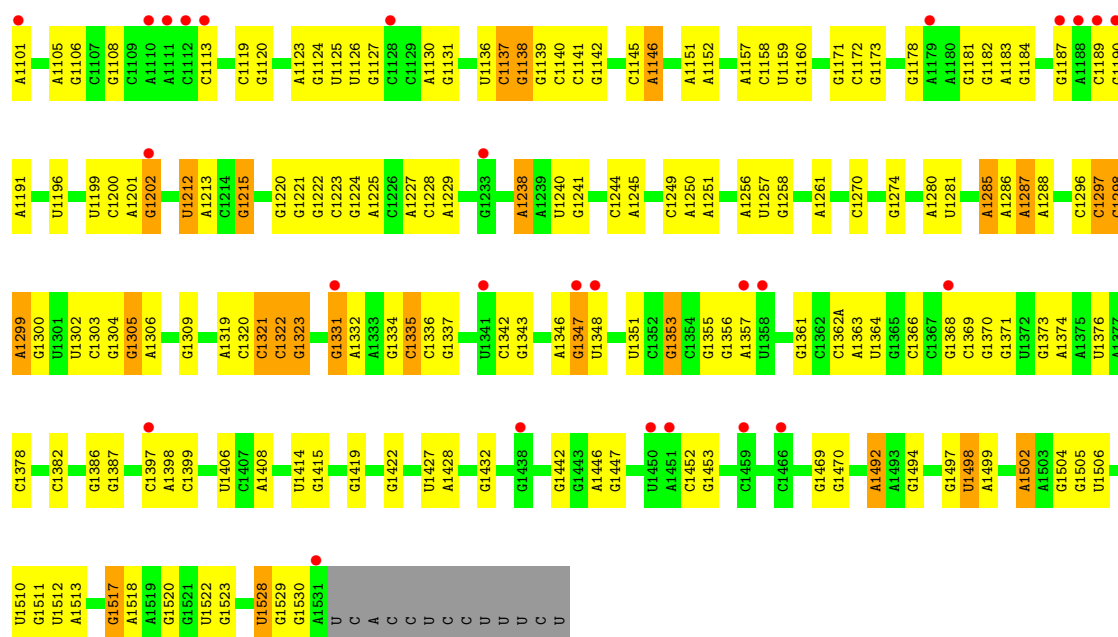
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total 1	Zn 1	0	0
59	YY	1	Total 1	Zn 1	0	0

3 Residue-property plots [i](#)

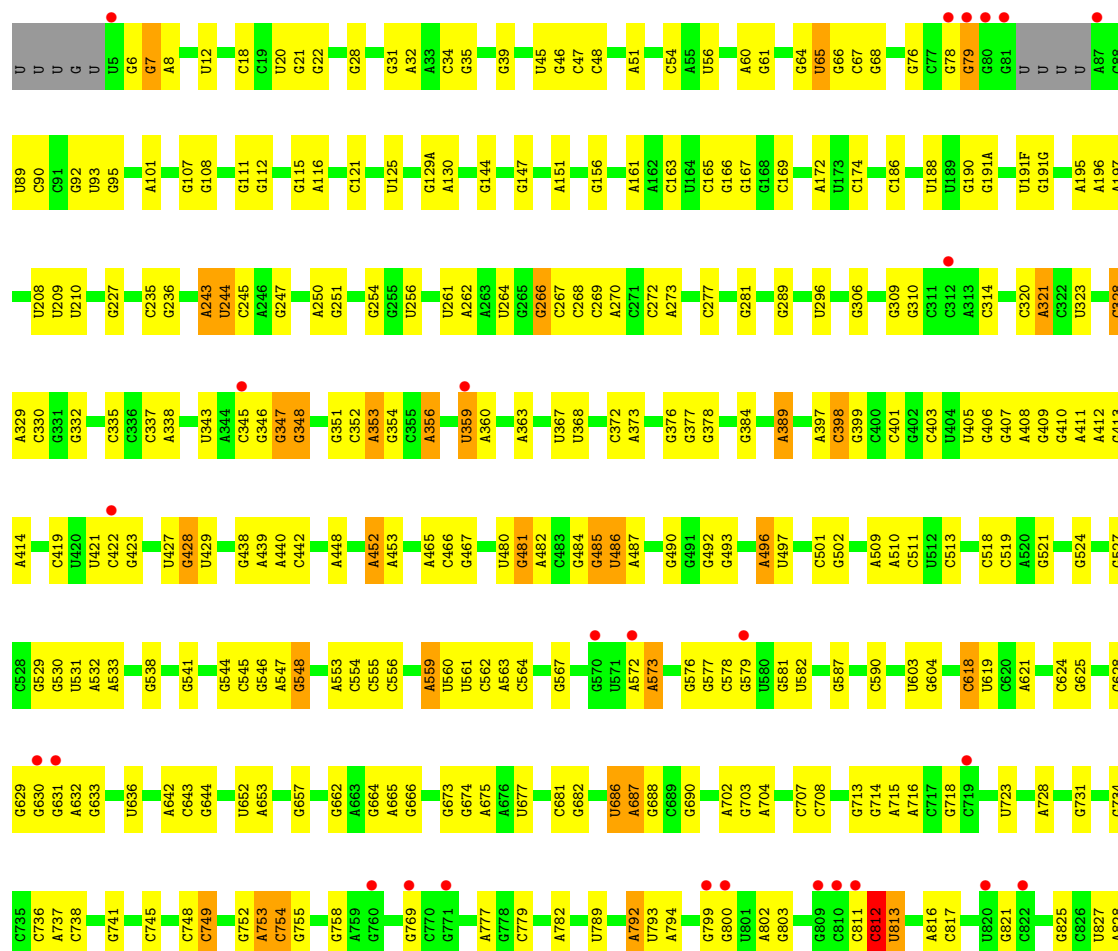
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

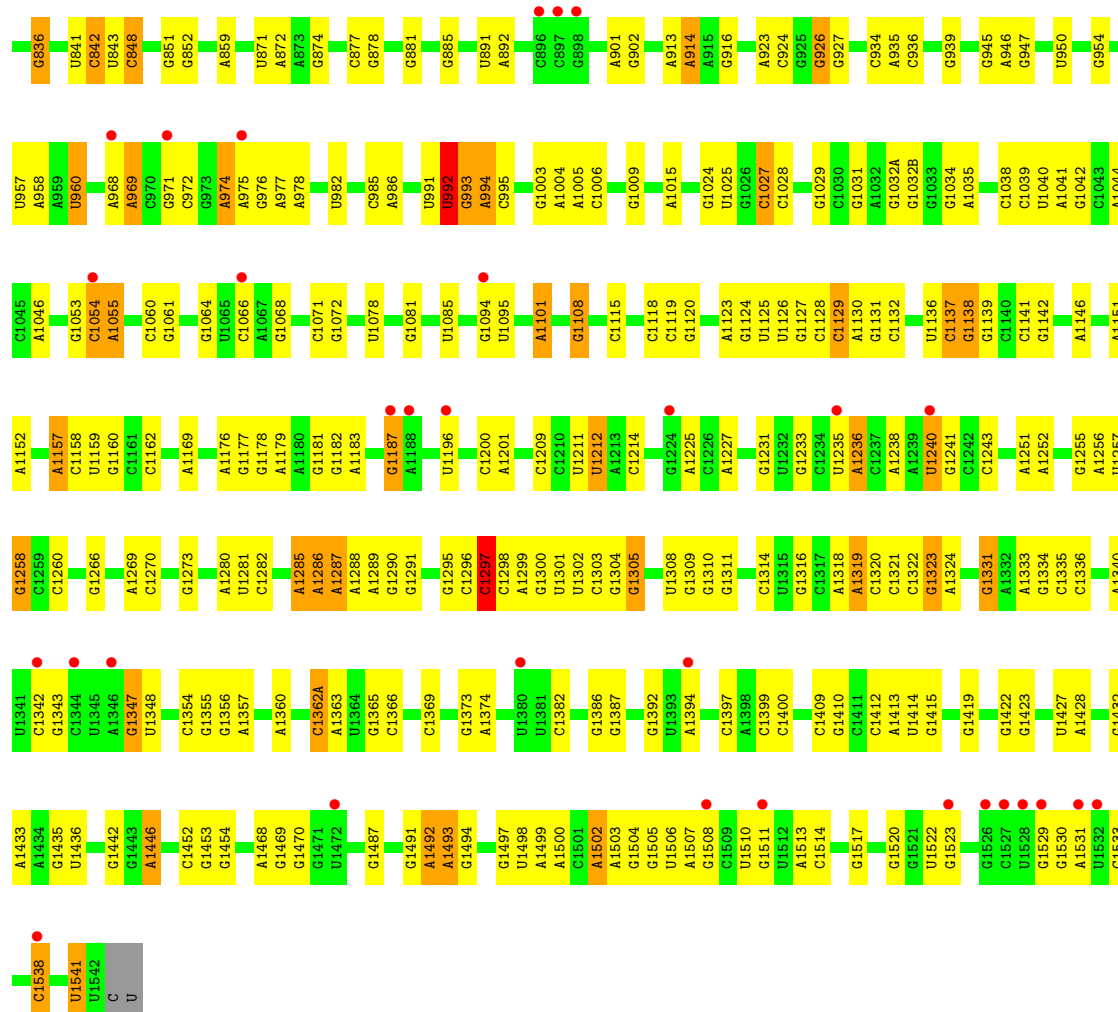
- Molecule 1: 16S rRNA



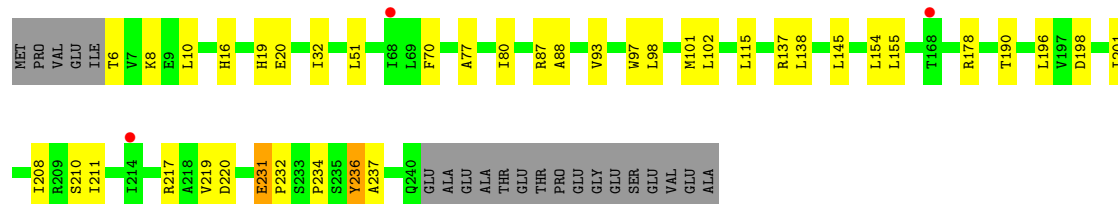
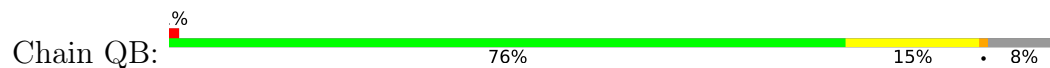


• Molecule 1: 16S rRNA

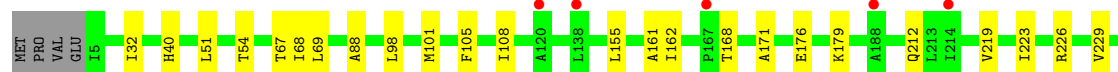
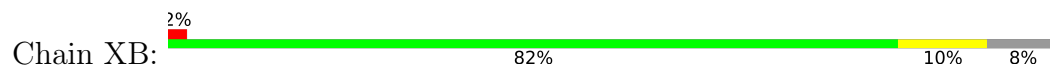


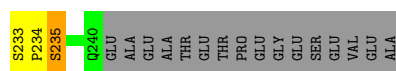


• Molecule 2: 30S ribosomal protein S2

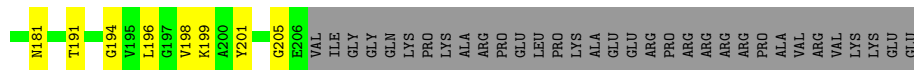
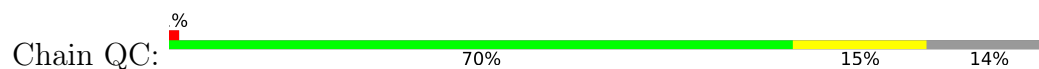


• Molecule 2: 30S ribosomal protein S2

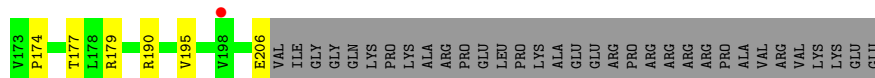
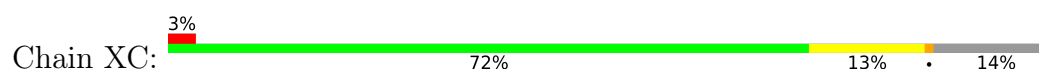




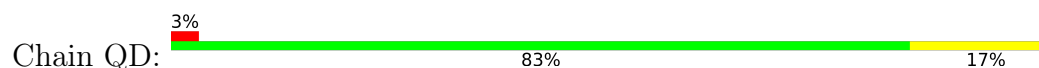
- Molecule 3: 30S ribosomal protein S3



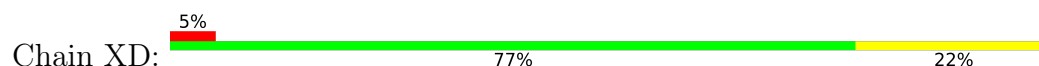
- Molecule 3: 30S ribosomal protein S3



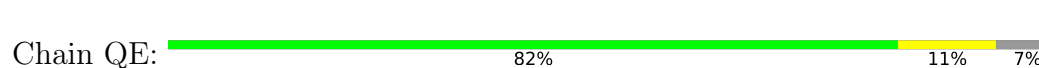
- Molecule 4: 30S ribosomal protein S4

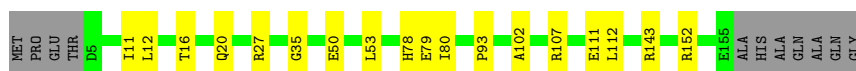


- Molecule 4: 30S ribosomal protein S4

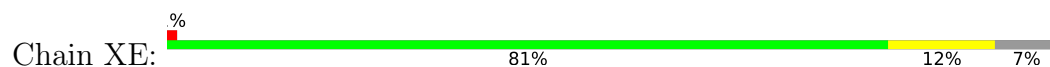


- Molecule 5: 30S ribosomal protein S5

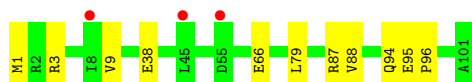
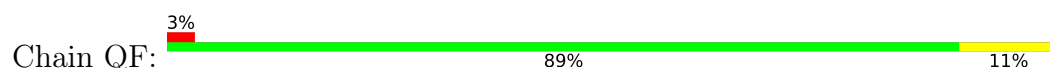




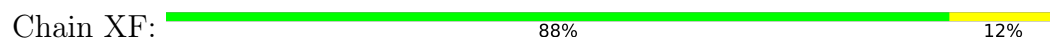
- Molecule 5: 30S ribosomal protein S5



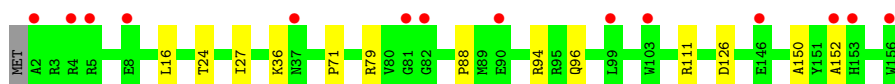
- Molecule 6: 30S ribosomal protein S6



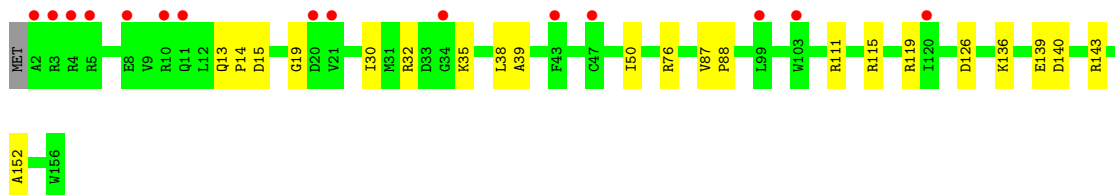
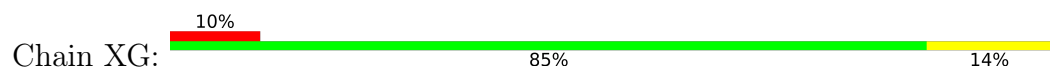
- Molecule 6: 30S ribosomal protein S6



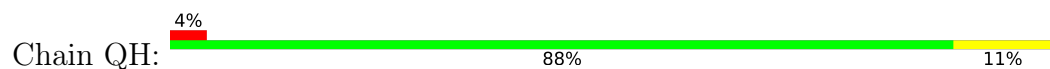
- Molecule 7: 30S ribosomal protein S7



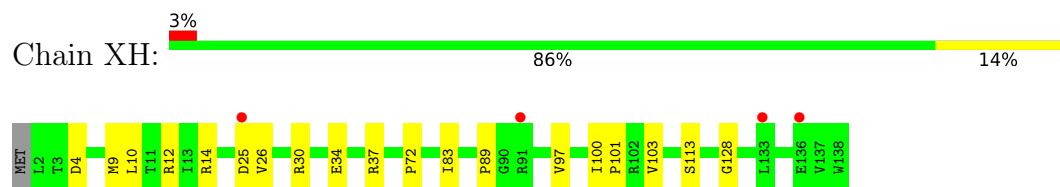
- Molecule 7: 30S ribosomal protein S7



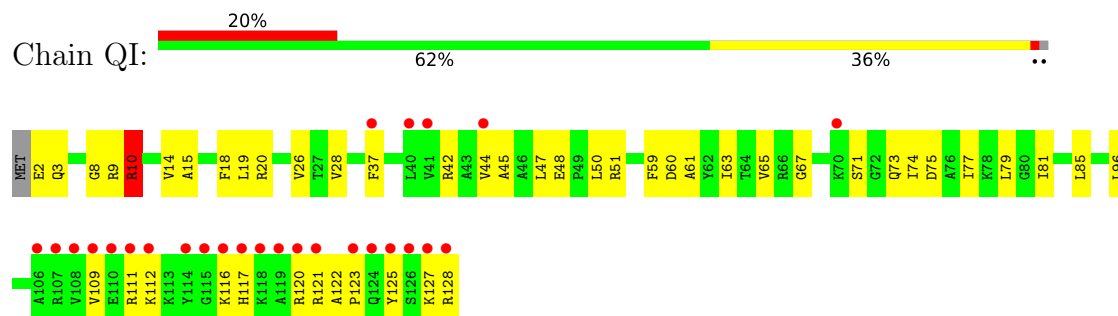
- Molecule 8: 30S ribosomal protein S8



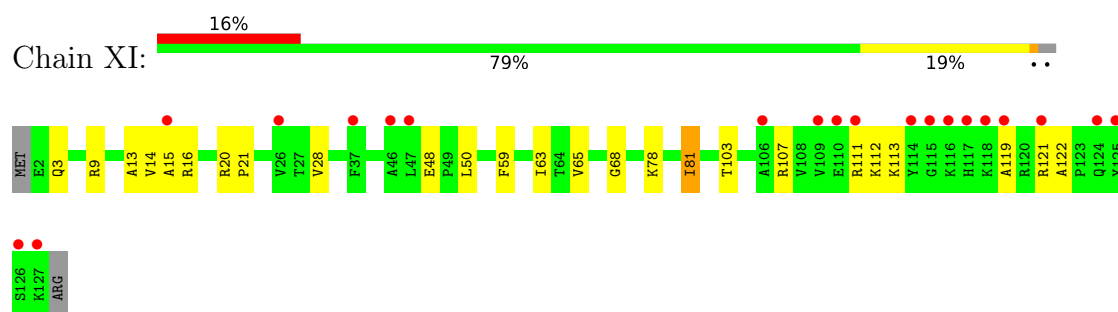
- Molecule 8: 30S ribosomal protein S8



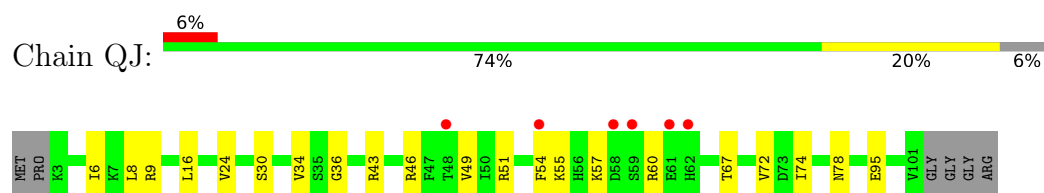
- Molecule 9: 30S ribosomal protein S9



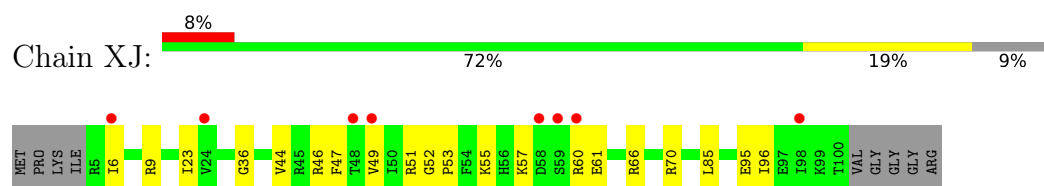
- Molecule 9: 30S ribosomal protein S9



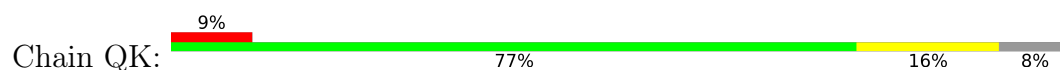
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

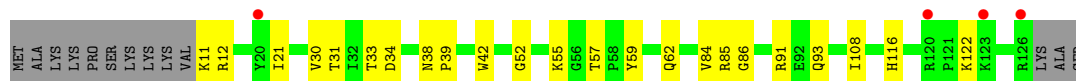
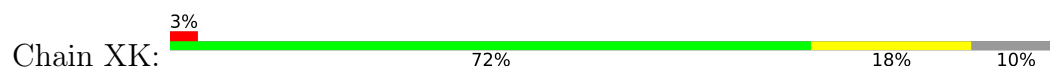


- Molecule 11: 30S ribosomal protein S11

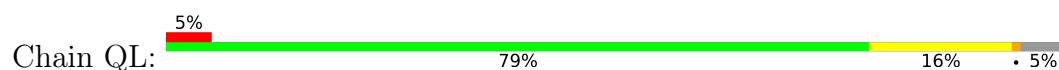




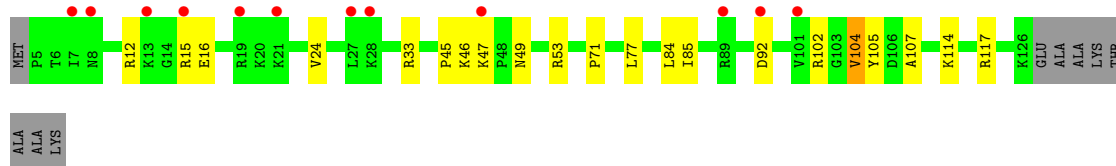
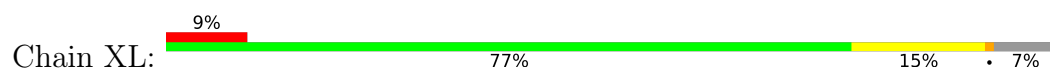
- Molecule 11: 30S ribosomal protein S11



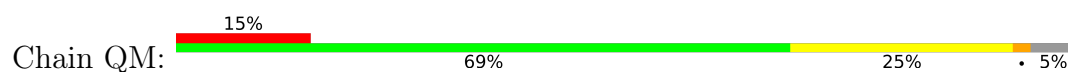
- Molecule 12: 30S ribosomal protein S12



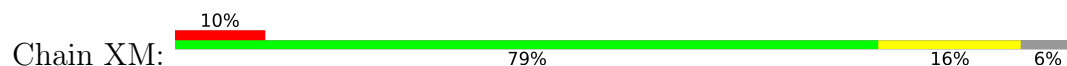
- Molecule 12: 30S ribosomal protein S12



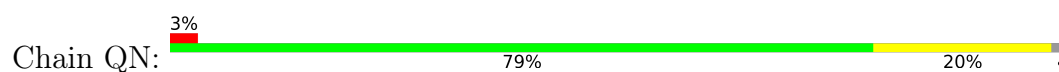
- Molecule 13: 30S ribosomal protein S13

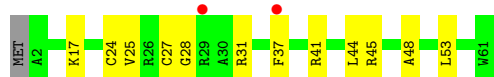


- Molecule 13: 30S ribosomal protein S13

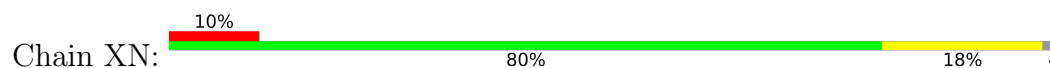


- Molecule 14: 30S ribosomal protein S14 type Z

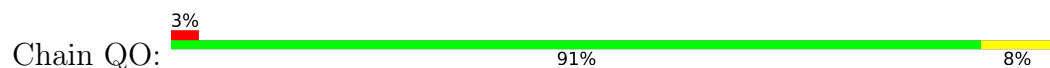




- Molecule 14: 30S ribosomal protein S14 type Z



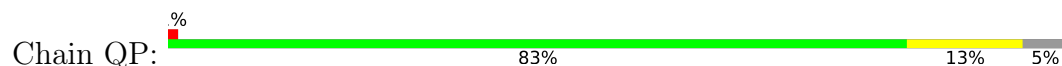
- Molecule 15: 30S ribosomal protein S15



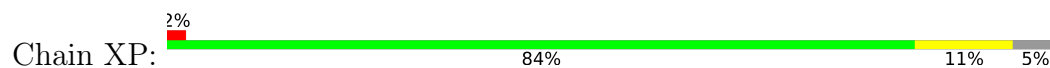
- Molecule 15: 30S ribosomal protein S15



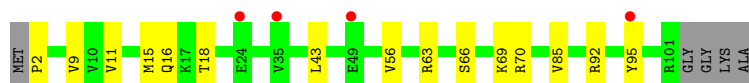
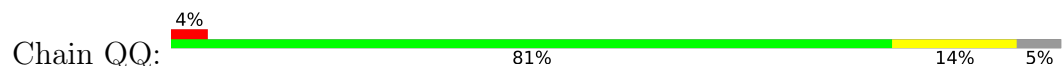
- Molecule 16: 30S ribosomal protein S16



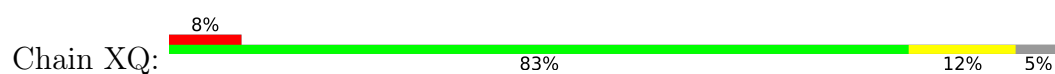
- Molecule 16: 30S ribosomal protein S16



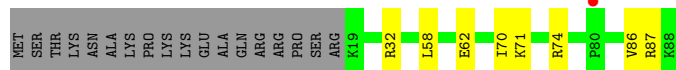
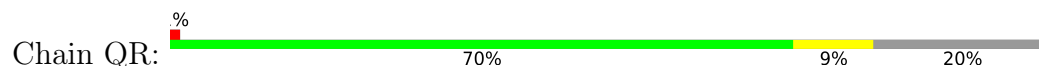
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



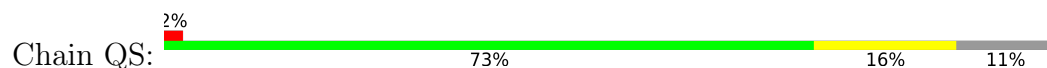
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



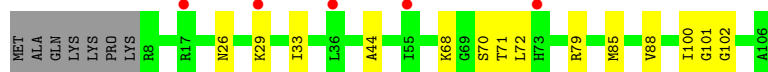
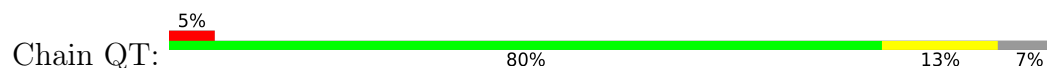
- Molecule 19: 30S ribosomal protein S19



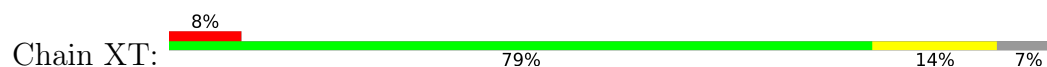
- Molecule 19: 30S ribosomal protein S19



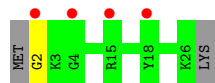
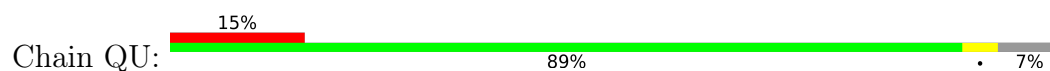
- Molecule 20: 30S ribosomal protein S20



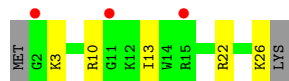
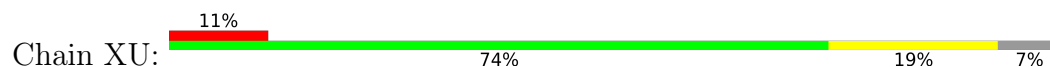
- Molecule 20: 30S ribosomal protein S20



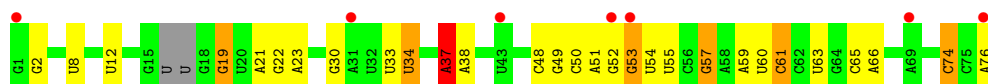
- Molecule 21: 30S ribosomal protein Thx



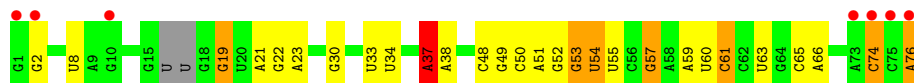
- Molecule 21: 30S ribosomal protein Thx



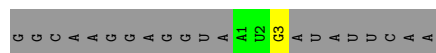
- Molecule 22: P-site tRNA^{Lys}(SUU)



- Molecule 22: P-site tRNA^{Lys}(SUU)



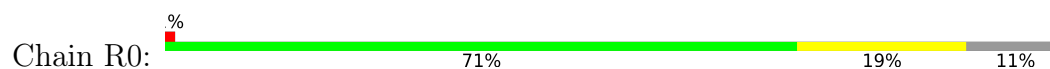
- Molecule 23: mRNA



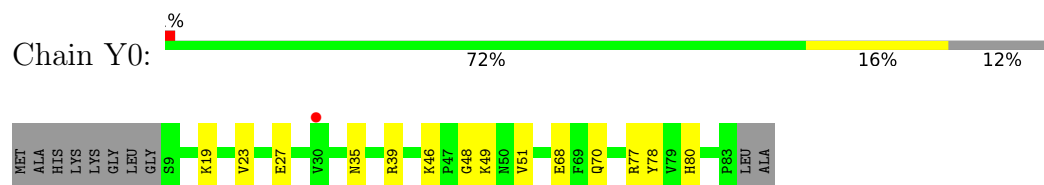
- Molecule 23: mRNA



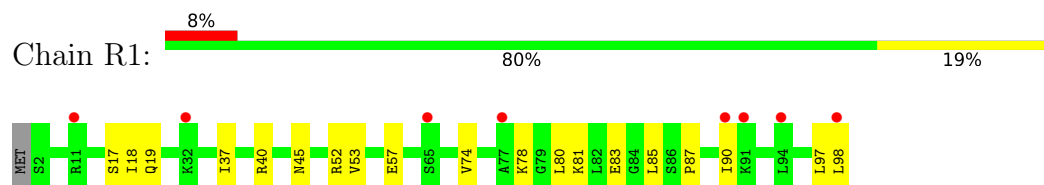
- Molecule 24: 50S ribosomal protein L27



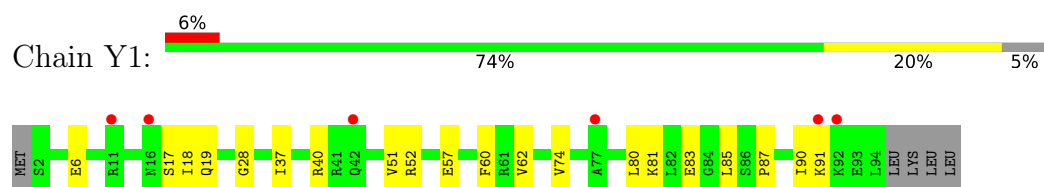
- Molecule 24: 50S ribosomal protein L27



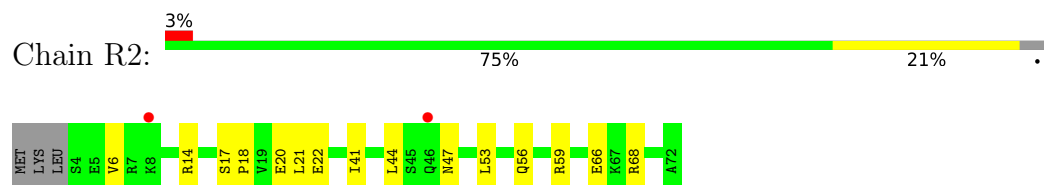
- Molecule 25: 50S ribosomal protein L28



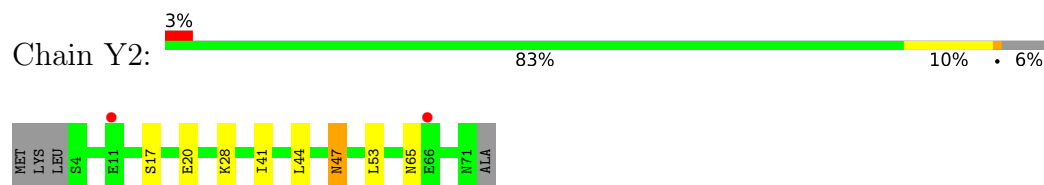
- Molecule 25: 50S ribosomal protein L28



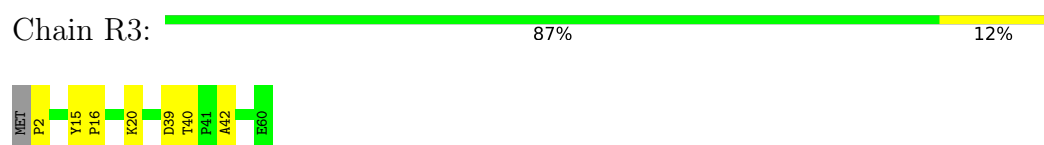
- Molecule 26: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

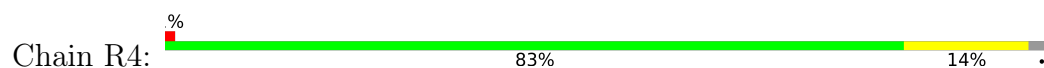


- Molecule 27: 50S ribosomal protein L30

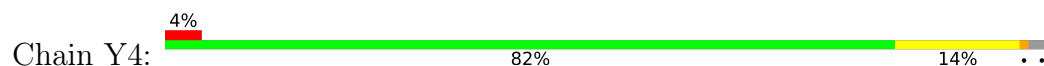




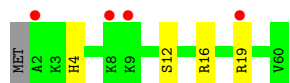
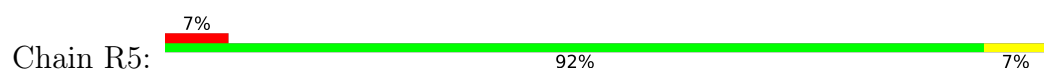
- Molecule 28: 50S ribosomal protein L31



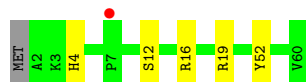
- Molecule 28: 50S ribosomal protein L31



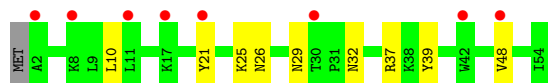
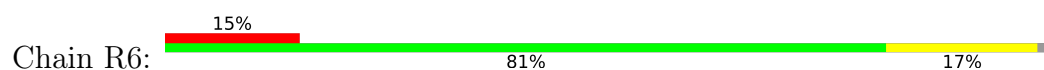
- Molecule 29: 50S ribosomal protein L32



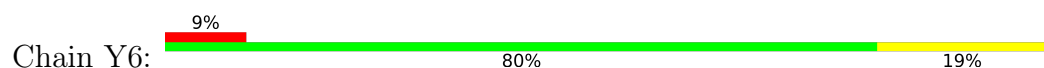
- Molecule 29: 50S ribosomal protein L32



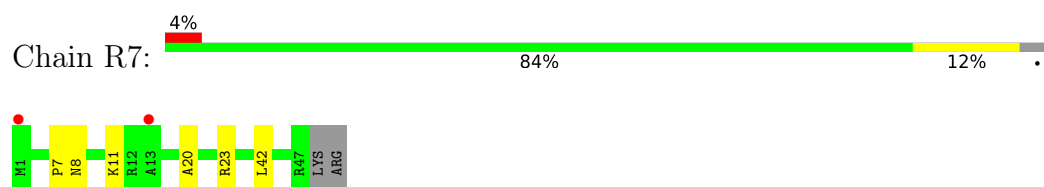
- Molecule 30: 50S ribosomal protein L33



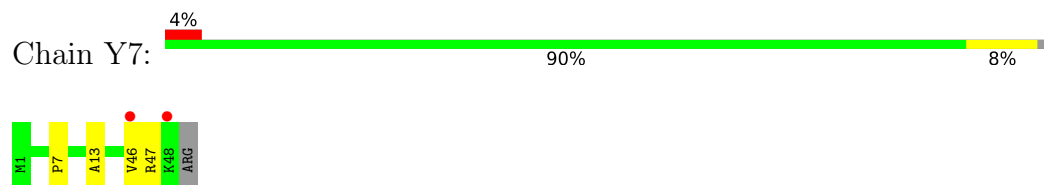
- Molecule 30: 50S ribosomal protein L33



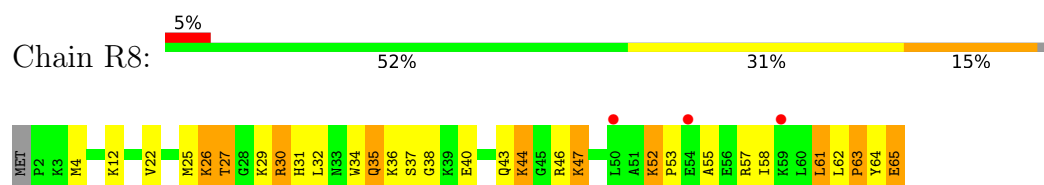
- Molecule 31: 50S ribosomal protein L34



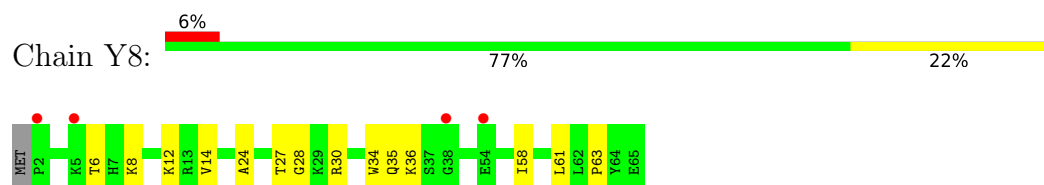
- Molecule 31: 50S ribosomal protein L34



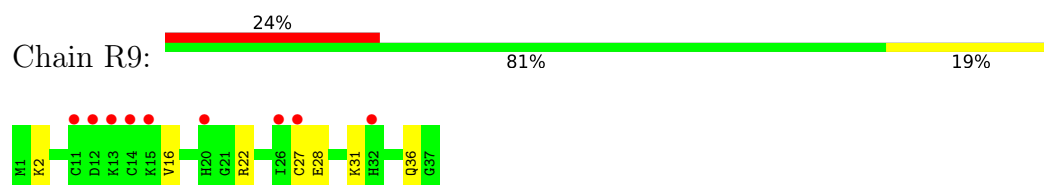
- Molecule 32: 50S ribosomal protein L35



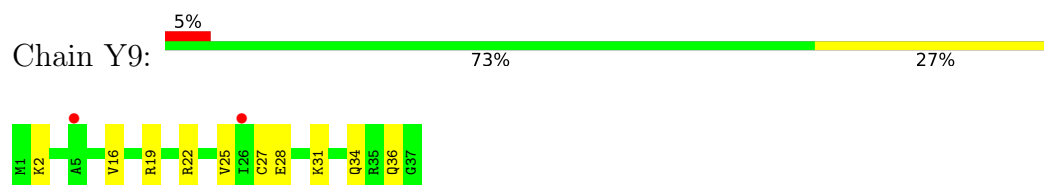
- Molecule 32: 50S ribosomal protein L35



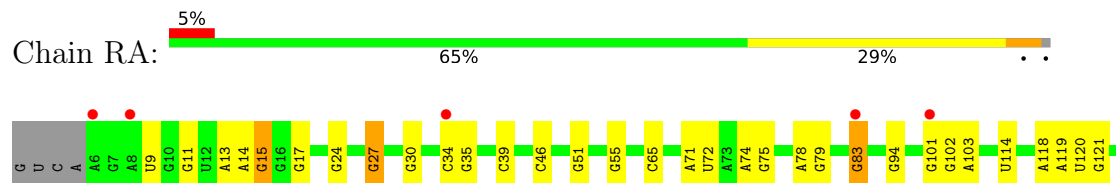
- Molecule 33: 50S ribosomal protein L36

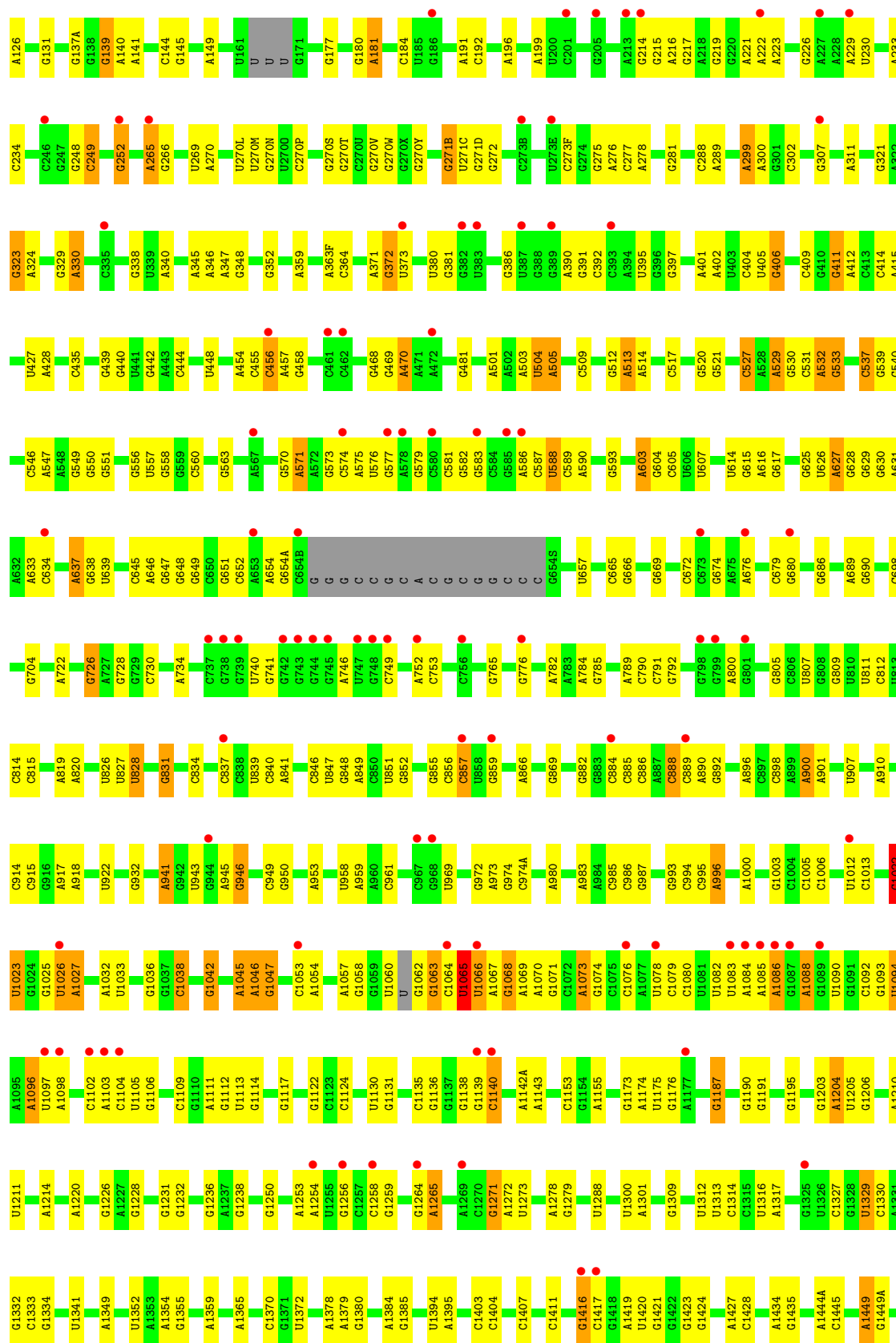


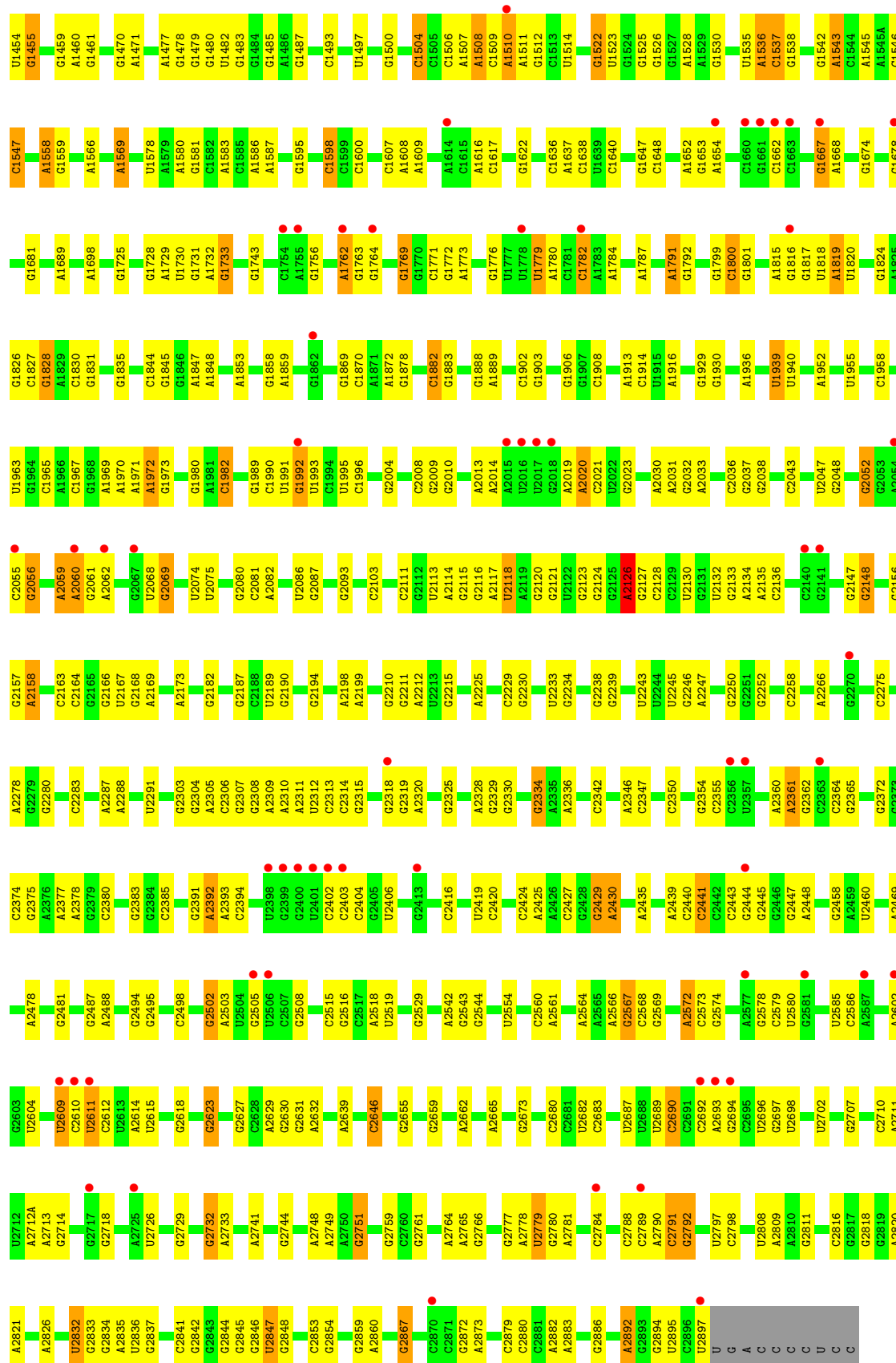
- Molecule 33: 50S ribosomal protein L36

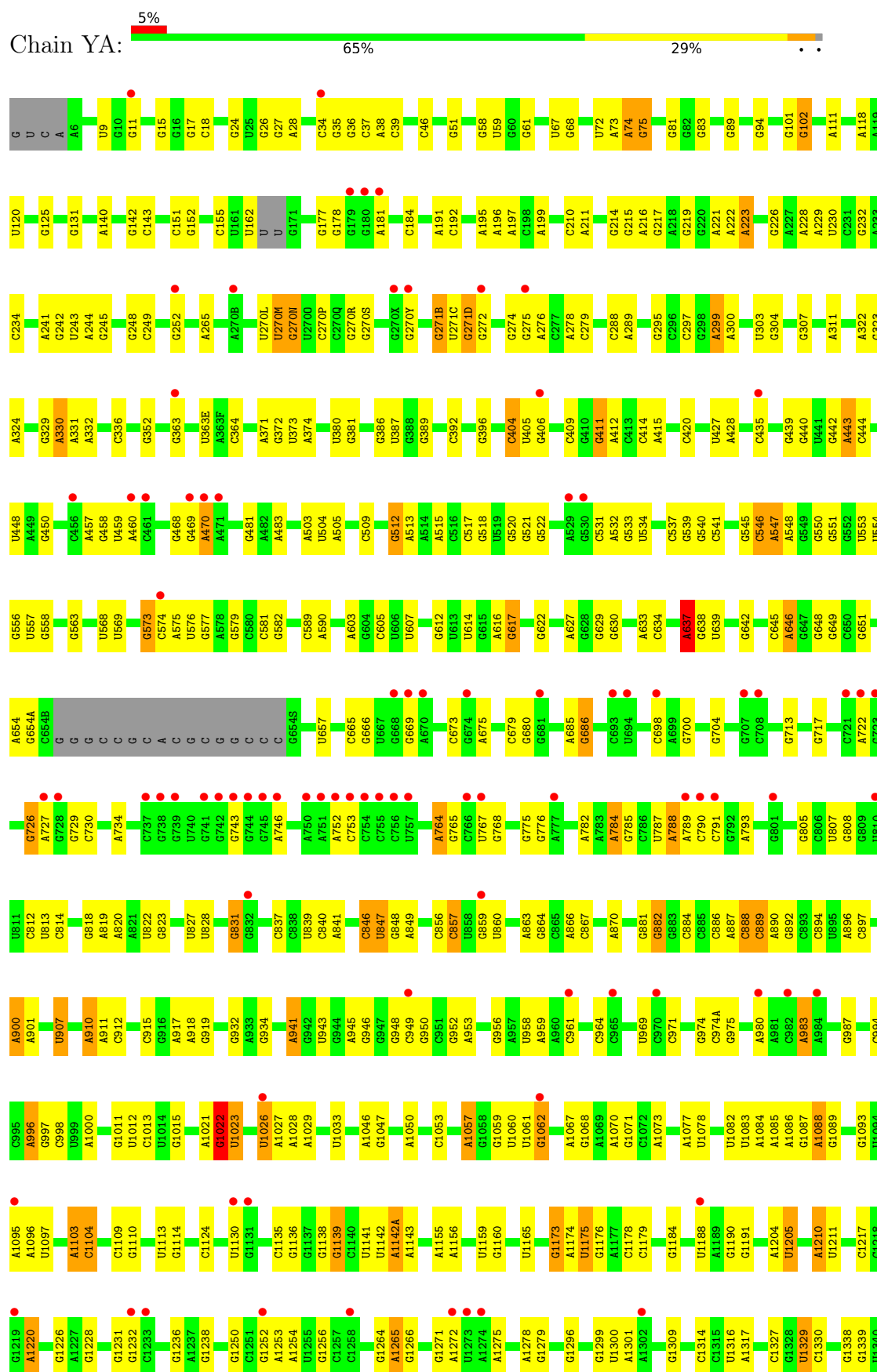


- Molecule 34: 23S rRNA

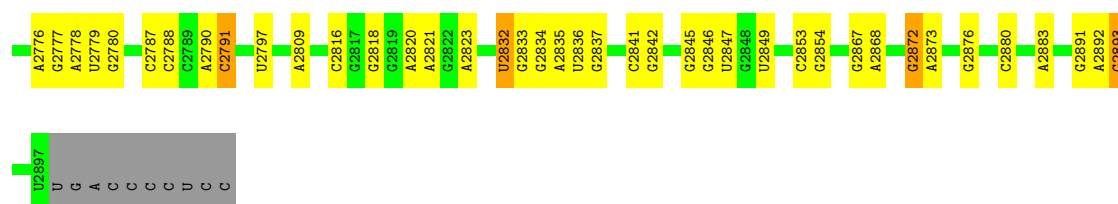




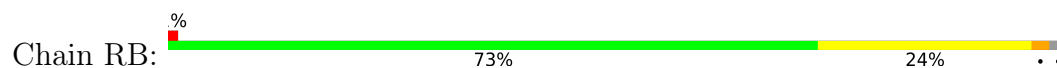




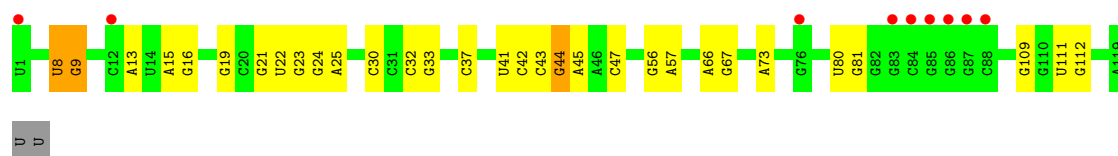
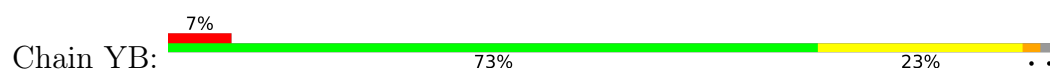
G2673	A2564	G2444	G2334	G2040	G1813	G1678	A1566	A1444A	U1341
C2680	A2565	G2445	A2335	U2041	G1816	A1689	A1567	C1445	A1349
U2682	G2567	G2447	G2133	A2042	G1817	A1689	G1568	A1449	A1353
U2688	C2571	A2448	A2134	U2047	U1819	C1694	A1569	G1449A	A1354
U2689	A2572	A2449	A2135	G2048	G1824	G1695	A1570	U1454	A1359
C2690	G2573	C2451	C2136	A2051	A1825	A1698	A1572	G1455	
C2691	G2574	C2452	C2140	G2052	U1963		U1578	A1460	A1365
C2692	G2575	A2453	G2141	G2056	G1827	G1725	G1578	A1461	
A2693	G2576	A2454	C2145	C2055	G1828		C1585	G1368	G1368
	A2577	G2455	G2147	G2056	A1829	A1729	A1586	C1370	G1370
U2696	G2578	G2354	G2148	A2059	G1830	U1730	G1591	U1372	U1372
G2697	G2579	C2355	G2149	A2060	G1831	A1731		G1478	G1478
G2699	U2580	G2358	U2150	A2061	G1835	C1732	C1598	G1479	G1479
	U2581	G2365	U2151	A2062	C1836	G1733	C1599	G1480	A1378
U2702	U2585		G2152	C2063			C1600	U1482	A1379
	C2586		G2153		A1847	G1743	C1607	G1483	
G2707	A2590	A2266	G2154	G2069	A1853	A1749	A1608	G1487	A1384
G2708	C2591	A2267	G2155	G2070			A1609		G1385
G2709	G2592	A2269	G2156	A2071	G1858	G1754	A1610		A1392
A2710	A2497	C2385	G2157	G2072	A1859	C1755	A1611	G1491	A1393
A2711	C2498	A2273	A2158	C2073	U1864	G1756	A1616	G1492	U1394
U2712	G2499	A2274	G2159	U2074	U1869		C1617	C1493	A1395
A2712A	U2500	C2275	C2164	U2075	A1870	G1762	A1618	U1496	U1396
A2713	C2501	G2278	G2165	G2080	G1871	G1763		U1497	
C2706	G2502	A2279	C2166	C2081	A1872	G1764	G1626		C1399
U2726	A2504	C2283	U2167	A2082	G1878		G1627	G1400	G1400
	G2505		G2168	U2086		G1769	A1507	U1406	
C2610	U2506	A2287	A2169	G2087	C1882		A1508	C1407	
U2611	C2403	A2288	A2173	U2093	A1884	A1773	C1509	C1408	
C2612	G2404	A2289	C2174	G2096	G1903	C1774	A1510	C1409	
G2508	U2406	A2290	C2175	U2096	G1906	U1775	A1511	G1410	
	G2407	U2291	C2179		G1888	U1779	G1522	C1411	
U2615	G2513	C2292	U2180	U2099	A1889	A1780		G1416	
U2618	C2514	C2293	G2181	G2100		C1782	A1528	G1417	
C2515	G2516		G2182	C2107	G1906	A1783	A1529	G1418	
C2517	A2518	G2304	C2183		G1906	A1784		U1419	
		A2306	G2185	C2111	A1913		C1533	U1420	
C2521	C2521	G2307	C2186	G2115	C1914	A1787	G1534	G1421	
G2529	G2529	G2308	G2186	G2116	A1918		U1535	G1422	
A2531	A2531	A2309		G2117	A1919	G1791	A1536	G1423	
	G2530	A2310	U2189	A2117	C1920	G1792	C1537	G1424	
U2546	G2428	U2312	G2190	A2118			G1538	G1425	
U2547	G2429	C2313	G2191	U2119	A1927	G1799	G1539	G1426	
	A2430	G2314	G2192	G2120	A1928	C1800	G1540	A1427	
C2646	A2434	G2315	G2193	G2121	G1929	C1801	A1543	C1428	
U2647	A2435	G2316	G2194	G2122	A1930		A1544	A1429	
	U2438	A2320	A2198	U2123	C1904	A1664	A1545	U1431	
U2554	U2439	G2325	G2210	G2124		G1667		A1434	
C2558	C2440		G2211	G2125	G1807		A1558	G1441	
C2559	C2441	A2328	A2212	A2126	U1908	G1674	G1559	G1442	
C2560	C2442	G2329	U2213	G2127	A1812	A1677	A1562		
A2561	C2443		G2215						



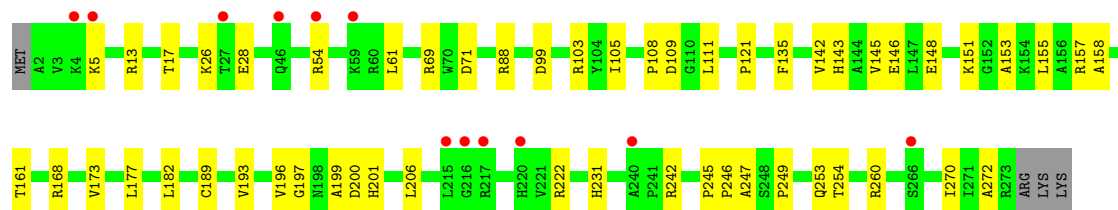
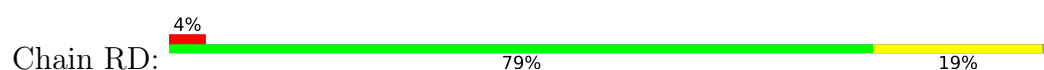
- Molecule 35: 5S rRNA



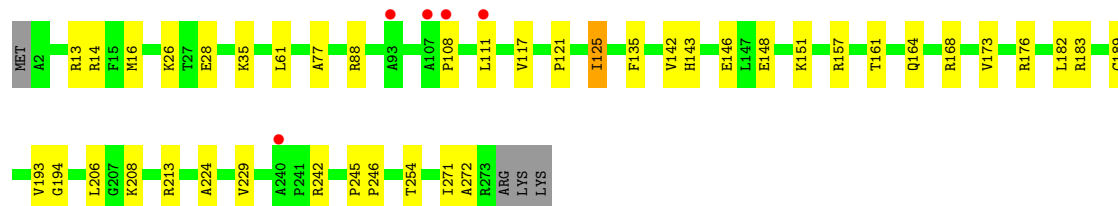
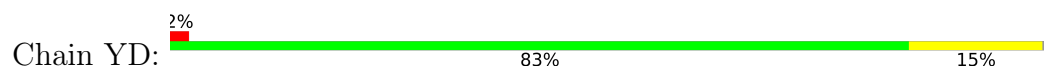
- Molecule 35: 5S rRNA



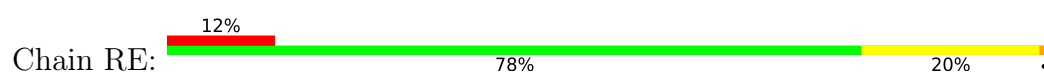
- Molecule 36: 50S ribosomal protein L2

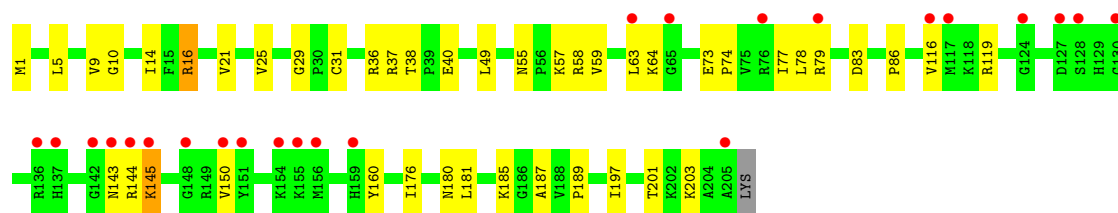


- Molecule 36: 50S ribosomal protein L2

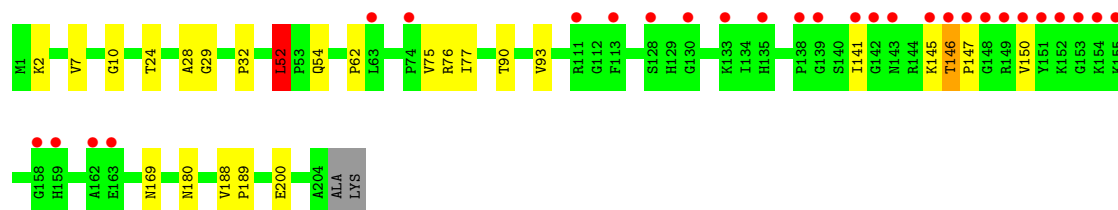
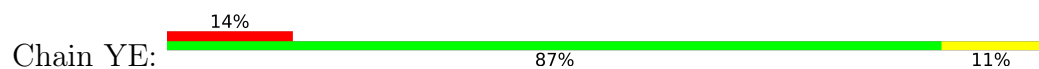


- Molecule 37: 50S ribosomal protein L3

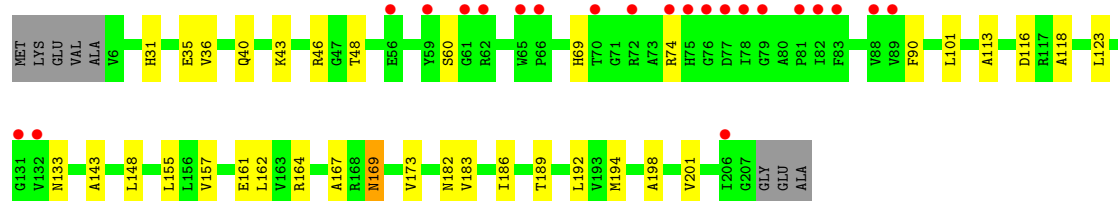
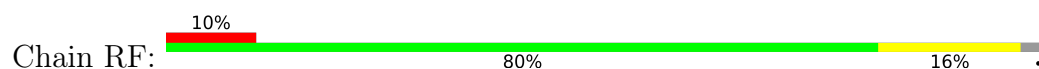




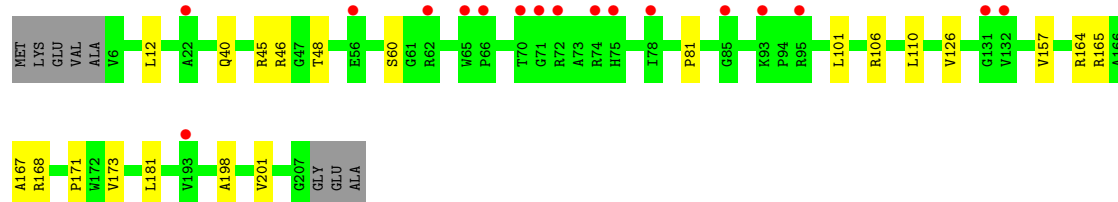
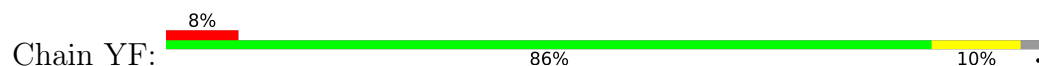
• Molecule 37: 50S ribosomal protein L3



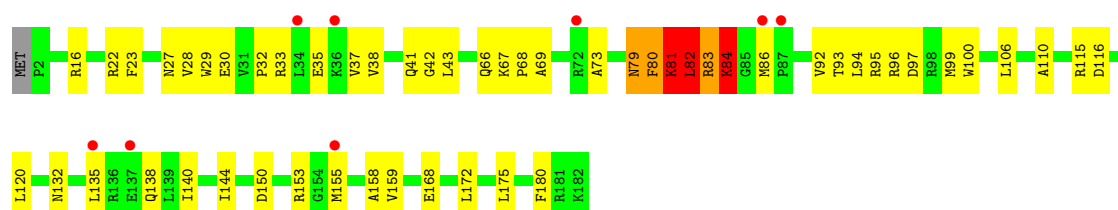
• Molecule 38: 50S ribosomal protein L4



• Molecule 38: 50S ribosomal protein L4

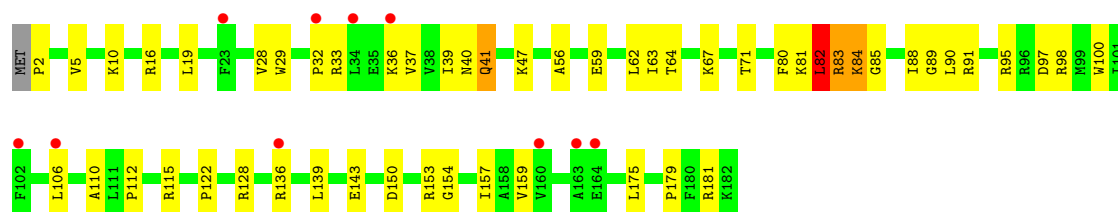


• Molecule 39: 50S ribosomal protein L5



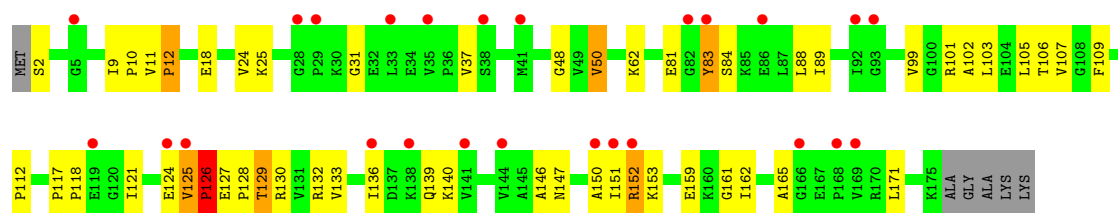
- Molecule 39: 50S ribosomal protein L5

Chain YG:  5% 70% 27% ..



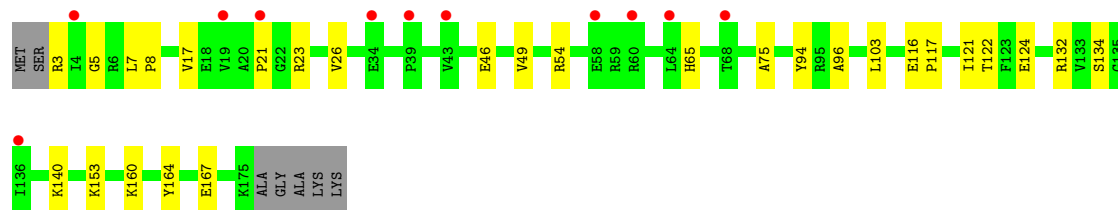
- Molecule 40: 50S ribosomal protein L6

Chain RH:  14% 67% 26% ..



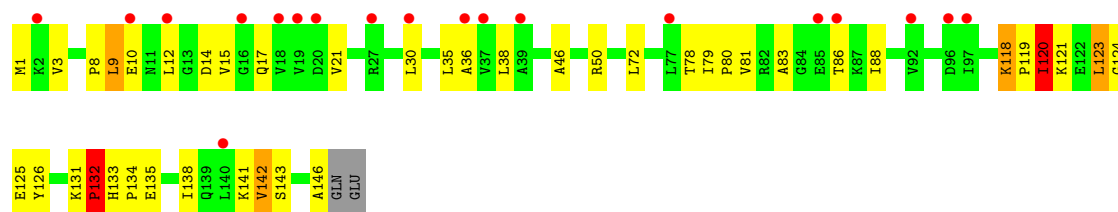
- Molecule 40: 50S ribosomal protein L6

Chain YH:  6% 81% 16% .



- Molecule 41: 50S ribosomal protein L9

Chain RI:  13% 70% 24% ..

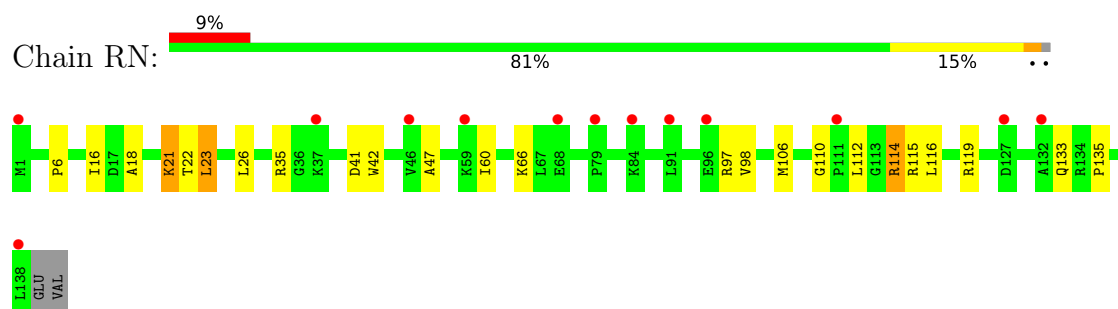


- Molecule 41: 50S ribosomal protein L9

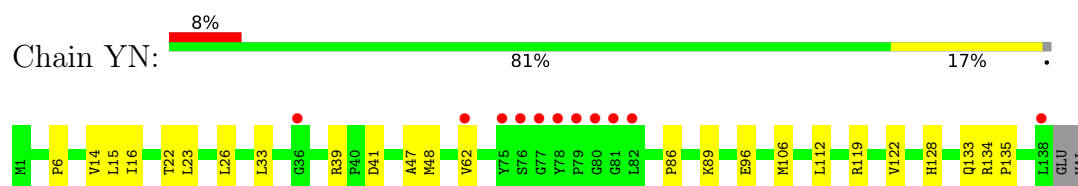
Chain YI:  2% 78% 14% 5% ..



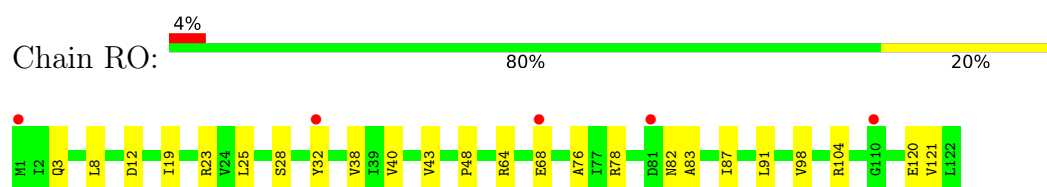
- Molecule 42: 50S ribosomal protein L13



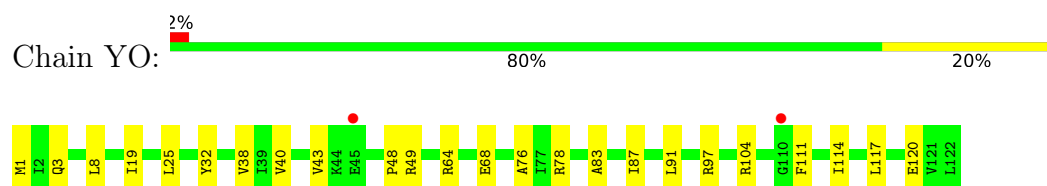
- Molecule 42: 50S ribosomal protein L13



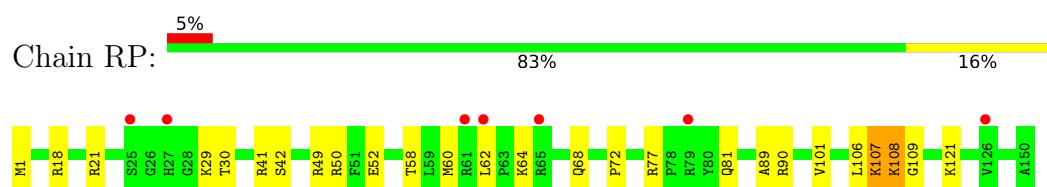
- Molecule 43: 50S ribosomal protein L14



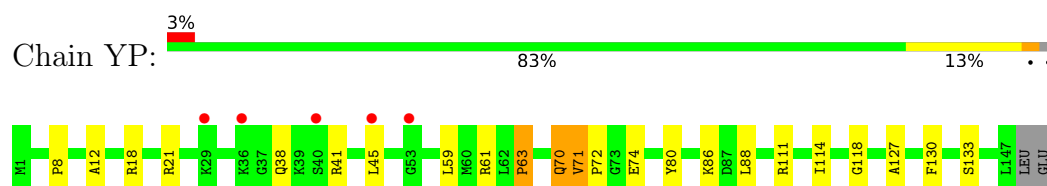
- Molecule 43: 50S ribosomal protein L14



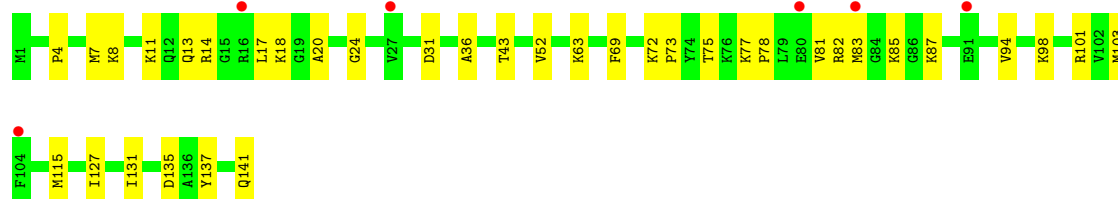
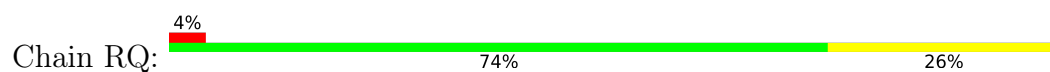
- Molecule 44: 50S ribosomal protein L15



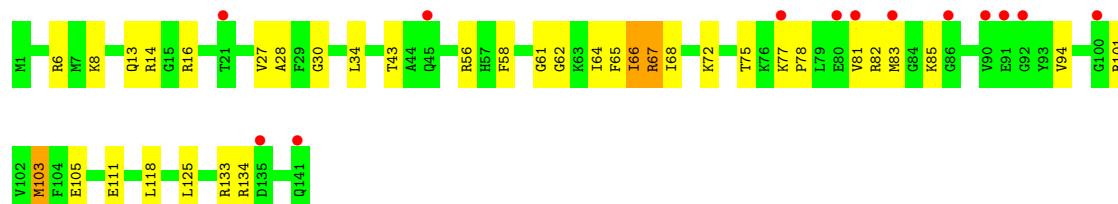
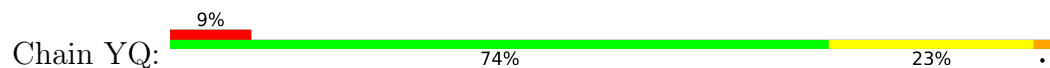
- Molecule 44: 50S ribosomal protein L15



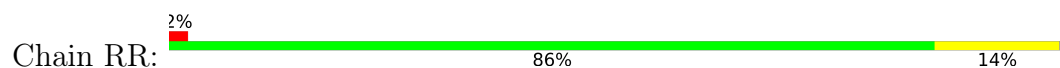
- Molecule 45: 50S ribosomal protein L16



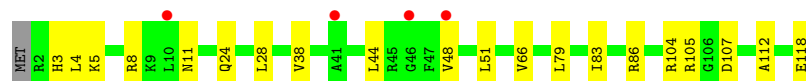
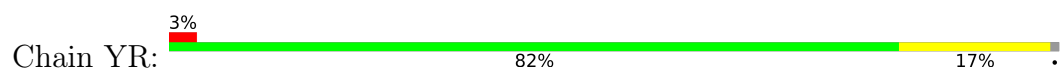
- Molecule 45: 50S ribosomal protein L16



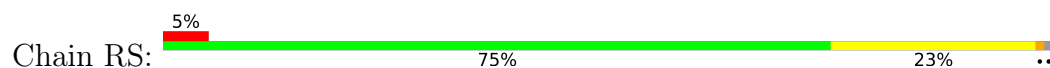
- Molecule 46: 50S ribosomal protein L17



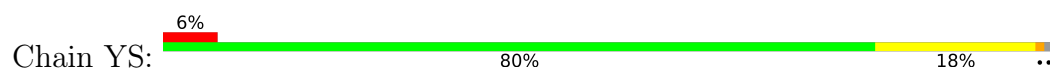
- Molecule 46: 50S ribosomal protein L17



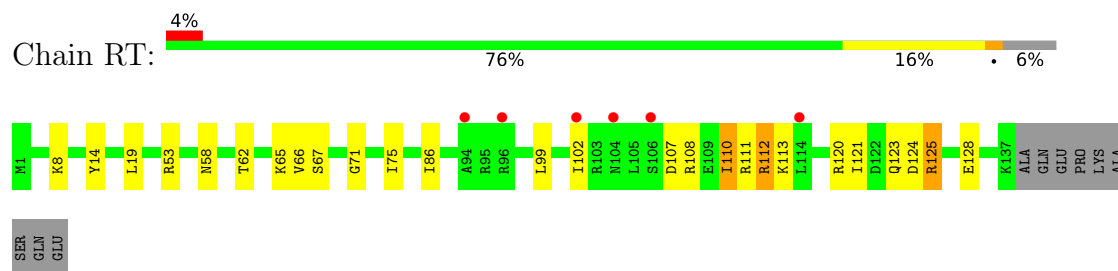
- Molecule 47: 50S ribosomal protein L18



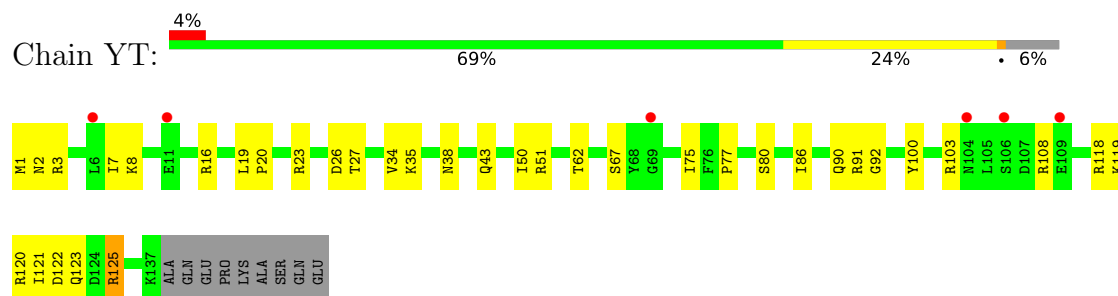
- Molecule 47: 50S ribosomal protein L18



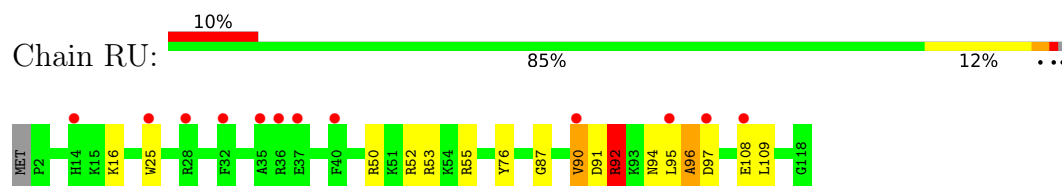
● Molecule 48: 50S ribosomal protein L19



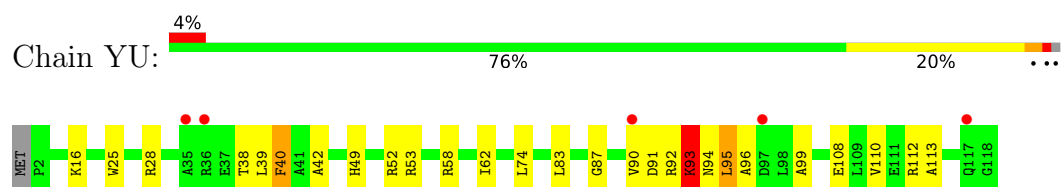
● Molecule 48: 50S ribosomal protein L19



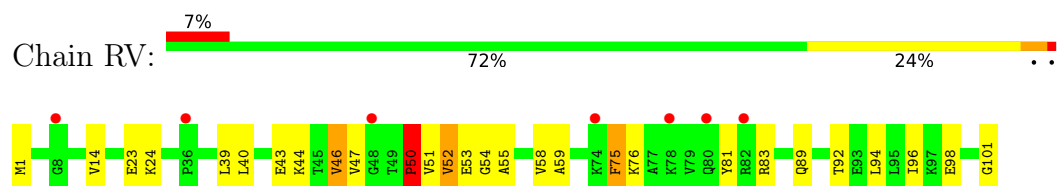
● Molecule 49: 50S ribosomal protein L20



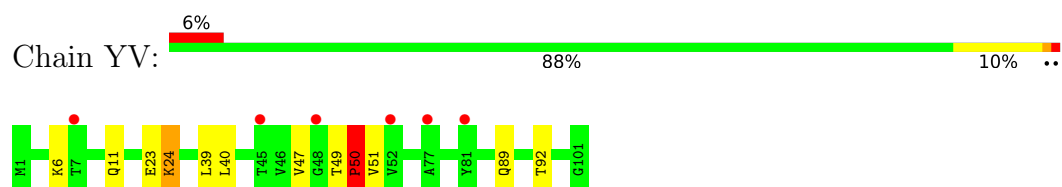
● Molecule 49: 50S ribosomal protein L20



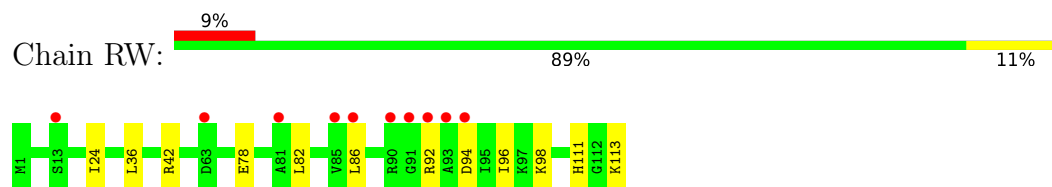
● Molecule 50: 50S ribosomal protein L21



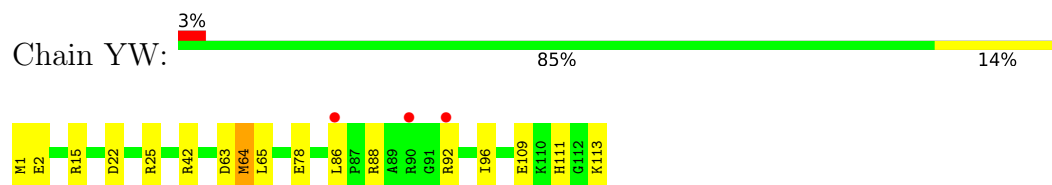
● Molecule 50: 50S ribosomal protein L21



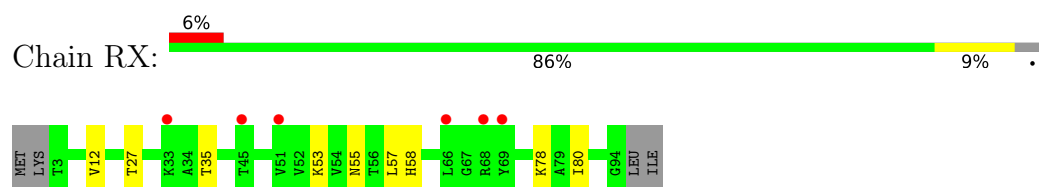
• Molecule 51: 50S ribosomal protein L22



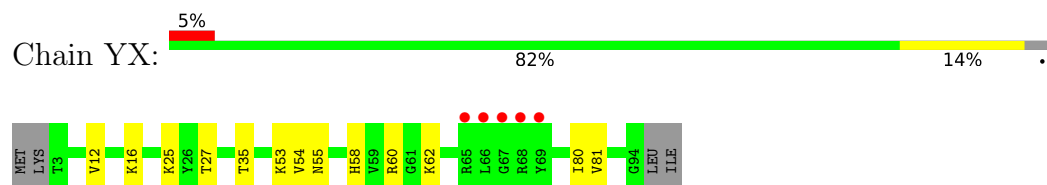
• Molecule 51: 50S ribosomal protein L22



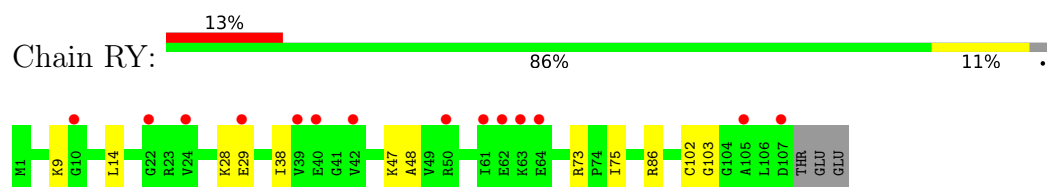
• Molecule 52: 50S ribosomal protein L23



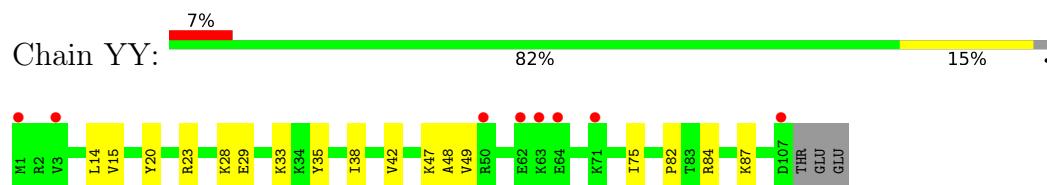
• Molecule 52: 50S ribosomal protein L23



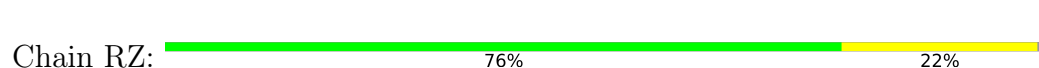
• Molecule 53: 50S ribosomal protein L24

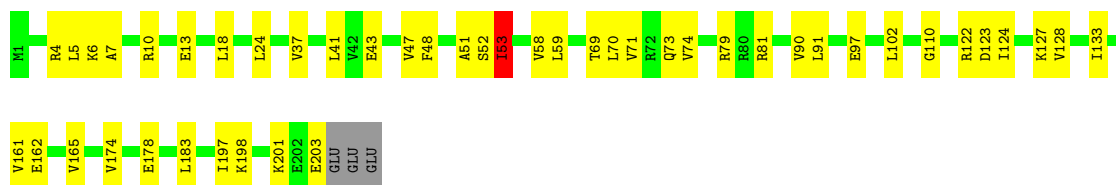


• Molecule 53: 50S ribosomal protein L24

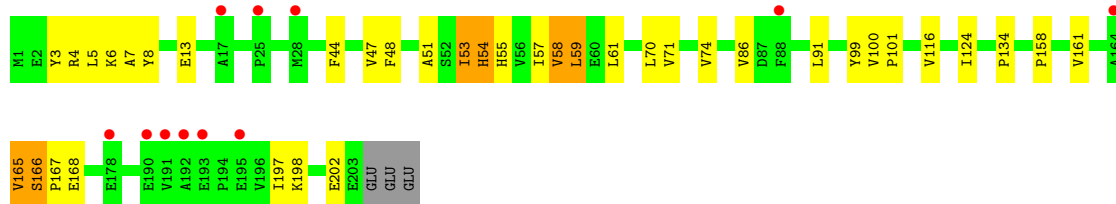
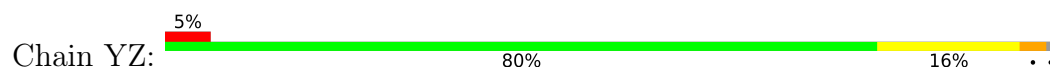


• Molecule 54: 50S ribosomal protein L25

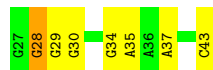




- Molecule 54: 50S ribosomal protein L25



- Molecule 55: A-site ASL^Phe



- Molecule 56: CC-puro



- Molecule 56: CC-puro



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.56Å 447.23Å 618.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	174.01 – 3.64 174.01 – 3.64	Depositor EDS
% Data completeness (in resolution range)	95.7 (174.01-3.64) 95.7 (174.01-3.64)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.278 0.232 , 0.278	Depositor DCC
R_{free} test set	32021 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	105.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 127.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	292577	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: MNU, SF4, MG, ZN, T6A, 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	0.18	0/36098	0.39	11/56341 (0.0%)
1	XA	0.18	0/36346	0.39	8/56725 (0.0%)
2	QB	0.26	0/1942	0.58	2/2619 (0.1%)
2	XB	0.23	0/1950	0.57	4/2630 (0.2%)
3	QC	0.23	0/1629	0.50	0/2195
3	XC	0.24	0/1629	0.54	0/2195
4	QD	0.19	0/1733	0.48	0/2318
4	XD	0.26	0/1733	0.56	0/2318
5	QE	0.20	0/1171	0.49	0/1576
5	XE	0.20	0/1171	0.50	0/1576
6	QF	0.18	0/856	0.44	0/1154
6	XF	0.18	0/856	0.44	0/1154
7	QG	0.20	0/1276	0.48	0/1709
7	XG	0.23	0/1276	0.55	0/1709
8	QH	0.17	0/1128	0.45	0/1517
8	XH	0.18	0/1128	0.46	0/1517
9	QI	0.52	3/1029 (0.3%)	0.72	0/1379
9	XI	0.27	0/1017	0.61	0/1365
10	QJ	0.21	0/814	0.53	0/1095
10	XJ	0.21	0/790	0.55	0/1063
11	QK	0.16	0/900	0.41	0/1213
11	XK	0.18	0/879	0.42	0/1187
12	QL	0.28	0/991	0.55	0/1327
12	XL	0.30	0/972	0.59	0/1301
13	QM	0.28	0/965	0.62	0/1292
13	XM	0.25	0/956	0.71	2/1281 (0.2%)
14	QN	0.27	0/501	0.63	0/664
14	XN	0.25	0/501	0.67	0/664
15	QO	0.19	0/745	0.45	0/992
15	XO	0.18	0/740	0.43	0/987
16	QP	0.18	0/721	0.47	0/970
16	XP	0.18	0/721	0.51	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.16	0/847	0.43	0/1131
17	XQ	0.19	0/847	0.45	0/1131
18	QR	0.20	0/579	0.52	0/768
18	XR	0.19	0/579	0.48	0/768
19	QS	0.21	0/680	0.54	0/915
19	XS	0.21	0/689	0.57	0/926
20	QT	0.24	0/765	0.59	0/1007
20	XT	0.25	0/765	0.60	0/1007
21	QU	0.18	0/221	0.42	0/288
21	XU	0.16	0/221	0.42	0/288
22	QV	0.26	0/1706	0.47	1/2652 (0.0%)
22	XV	0.23	0/1706	0.48	2/2652 (0.1%)
23	QX	0.26	0/72	0.56	0/110
23	XX	0.18	0/560	0.42	0/872
24	R0	0.18	0/611	0.45	0/814
24	Y0	0.17	0/607	0.41	0/809
25	R1	0.21	0/770	0.56	0/1022
25	Y1	0.20	0/736	0.51	0/978
26	R2	0.21	0/583	0.53	0/771
26	Y2	0.25	0/577	0.55	0/764
27	R3	0.19	0/474	0.49	0/635
27	Y3	0.44	0/474	0.71	0/635
28	R4	0.27	0/578	0.68	0/776
28	Y4	0.22	0/578	0.65	0/776
29	R5	0.18	0/473	0.45	0/639
29	Y5	0.17	0/473	0.45	0/639
30	R6	0.17	0/460	0.50	0/613
30	Y6	0.15	0/460	0.41	0/613
31	R7	0.17	0/417	0.47	0/550
31	Y7	0.18	0/426	0.47	0/561
32	R8	0.55	0/525	0.95	1/691 (0.1%)
32	Y8	0.19	0/525	0.45	0/691
33	R9	0.15	0/310	0.41	0/407
33	Y9	0.15	0/310	0.41	0/407
34	RA	0.19	0/69498	0.40	7/108491 (0.0%)
34	YA	0.19	0/69543	0.40	11/108563 (0.0%)
35	RB	0.19	0/2878	0.37	0/4490
35	YB	0.20	0/2878	0.38	0/4490
36	RD	0.25	0/2165	0.53	1/2919 (0.0%)
36	YD	0.24	0/2165	0.50	0/2919
37	RE	0.35	0/1601	0.73	2/2160 (0.1%)
37	YE	0.27	0/1596	0.56	0/2153
38	RF	0.23	0/1620	0.59	0/2194

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YF	0.22	0/1620	0.56	0/2194
39	RG	0.30	0/1499	0.66	2/2016 (0.1%)
39	YG	0.33	0/1499	0.64	0/2016
40	RH	0.42	0/1362	0.81	5/1841 (0.3%)
40	YH	0.18	0/1356	0.45	0/1833
41	RI	0.45	0/1151	0.81	3/1558 (0.2%)
41	YI	0.54	1/1151 (0.1%)	0.95	2/1558 (0.1%)
42	RN	0.27	0/1131	0.58	0/1525
42	YN	0.20	0/1131	0.52	0/1525
43	RO	0.18	0/943	0.44	0/1269
43	YO	0.17	0/943	0.43	0/1269
44	RP	0.29	0/1162	0.70	0/1544
44	YP	0.26	0/1139	0.59	0/1514
45	RQ	0.28	0/1143	0.63	0/1527
45	YQ	0.32	0/1143	0.65	0/1527
46	RR	0.21	0/974	0.60	0/1302
46	YR	0.22	0/974	0.59	0/1302
47	RS	0.31	0/892	0.76	2/1187 (0.2%)
47	YS	0.30	0/892	0.69	0/1187
48	RT	0.29	0/1155	0.63	1/1542 (0.1%)
48	YT	0.26	0/1155	0.59	0/1542
49	RU	0.28	0/982	0.68	5/1306 (0.4%)
49	YU	0.33	0/982	0.76	4/1306 (0.3%)
50	RV	0.35	0/790	0.76	3/1057 (0.3%)
50	YV	0.33	0/790	0.76	3/1057 (0.3%)
51	RW	0.20	0/911	0.52	0/1220
51	YW	0.25	0/911	0.57	0/1220
52	RX	0.18	0/739	0.48	0/993
52	YX	0.18	0/739	0.48	0/993
53	RY	0.17	0/831	0.43	0/1108
53	YY	0.17	0/831	0.44	0/1108
54	RZ	0.27	0/1634	0.65	2/2216 (0.1%)
54	YZ	0.32	0/1634	0.60	0/2216
55	XY	0.16	0/405	0.37	0/630
56	Z6	0.25	0/40	0.37	0/60
56	Z8	0.23	0/40	0.38	0/60
All	All	0.21	4/316386 (0.0%)	0.45	84/473016 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
27	Y3	0	1
37	YE	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	YI	133	HIS	C-N	13.24	1.50	1.33
9	QI	10	ARG	CA-CB	7.23	1.66	1.53
9	QI	10	ARG	CZ-NH1	6.47	1.41	1.32
9	QI	10	ARG	NE-CZ	5.20	1.38	1.33

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	YI	133	HIS	CA-C-N	17.93	138.27	120.52
41	YI	133	HIS	C-N-CA	17.93	138.27	120.52
22	XV	53	G	OP1-P-O3'	-11.34	73.97	108.00
49	YU	40	PHE	N-CA-CB	7.19	122.11	110.40
49	RU	96	ALA	N-CA-C	-6.80	103.89	111.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	Y3	34	GLU	Mainchain
37	YE	146	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	255	0
1	XA	32471	0	16395	254	0
2	QB	1907	0	1958	21	0
2	XB	1915	0	1969	20	0
3	QC	1605	0	1668	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	XC	1605	0	1668	21	0
4	QD	1703	0	1767	20	0
4	XD	1703	0	1767	48	0
5	QE	1155	0	1213	13	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	6	0
6	XF	843	0	857	9	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	13	0
8	QH	1108	0	1165	13	0
8	XH	1108	0	1165	12	0
9	QI	1010	0	1037	31	0
9	XI	998	0	1024	16	0
10	QJ	801	0	849	15	0
10	XJ	777	0	816	14	0
11	QK	885	0	904	16	0
11	XK	864	0	881	16	0
12	QL	975	0	1062	20	0
12	XL	956	0	1046	25	0
13	QM	955	0	1021	31	0
13	XM	946	0	1008	14	0
14	QN	492	0	531	8	0
14	XN	492	0	529	8	0
15	QO	734	0	771	4	0
15	XO	729	0	768	6	0
16	QP	705	0	725	8	0
16	XP	705	0	725	8	0
17	QQ	834	0	904	10	0
17	XQ	834	0	904	9	0
18	QR	574	0	644	6	0
18	XR	574	0	644	11	0
19	QS	665	0	686	13	0
19	XS	674	0	699	11	0
20	QT	763	0	861	11	0
20	XT	763	0	861	9	0
21	QU	217	0	234	1	0
21	XU	217	0	234	5	0
22	QV	1584	0	808	13	0
22	XV	1584	0	808	13	0
23	QX	65	0	33	1	0
23	XX	499	0	249	6	0
24	R0	603	0	620	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y0	599	0	617	11	0
25	R1	763	0	848	12	0
25	Y1	729	0	802	11	0
26	R2	581	0	629	8	0
26	Y2	575	0	624	7	0
27	R3	469	0	518	4	0
27	Y3	469	0	518	22	0
28	R4	565	0	557	6	0
28	Y4	565	0	559	7	0
29	R5	459	0	478	4	0
29	Y5	459	0	477	6	0
30	R6	453	0	477	5	0
30	Y6	453	0	476	6	0
31	R7	409	0	454	4	0
31	Y7	418	0	467	3	0
32	R8	517	0	582	50	0
32	Y8	517	0	582	10	0
33	R9	307	0	337	5	0
33	Y9	307	0	336	8	0
34	RA	62051	0	31279	384	0
34	YA	62091	0	31298	433	0
35	RB	2573	0	1306	16	0
35	YB	2573	0	1306	11	0
36	RD	2115	0	2195	43	0
36	YD	2115	0	2195	37	0
37	RE	1568	0	1634	29	0
37	YE	1563	0	1629	21	0
38	RF	1585	0	1632	23	0
38	YF	1585	0	1632	16	0
39	RG	1474	0	1535	51	0
39	YG	1474	0	1535	45	0
40	RH	1336	0	1418	48	0
40	YH	1330	0	1413	16	0
41	RI	1136	0	1223	32	0
41	YI	1136	0	1223	55	0
42	RN	1104	0	1180	30	0
42	YN	1104	0	1180	13	0
43	RO	933	0	996	17	0
43	YO	933	0	996	19	0
44	RP	1145	0	1228	41	0
44	YP	1122	0	1204	22	0
45	RQ	1122	0	1179	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	YQ	1122	0	1179	31	0
46	RR	960	0	1021	11	0
46	YR	960	0	1021	11	0
47	RS	882	0	943	20	0
47	YS	882	0	943	18	0
48	RT	1141	0	1202	29	0
48	YT	1141	0	1202	32	0
49	RU	964	0	1022	27	0
49	YU	964	0	1022	50	0
50	RV	779	0	852	32	0
50	YV	779	0	852	16	0
51	RW	900	0	964	9	0
51	YW	900	0	964	24	0
52	RX	725	0	778	6	0
52	YX	725	0	778	10	0
53	RY	818	0	910	8	0
53	YY	818	0	911	12	0
54	RZ	1601	0	1630	32	0
54	YZ	1601	0	1630	30	0
55	XY	362	0	186	4	0
56	Z6	74	0	51	0	0
56	Z8	74	0	51	2	0
57	QA	73	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QJ	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R1	1	0	0	0	0
57	R3	1	0	0	0	0
57	RA	483	0	0	0	0
57	RB	7	0	0	0	0
57	RE	4	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	3	0	0	0	0
57	RQ	3	0	0	0	0
57	RR	1	0	0	0	0
57	RT	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	73	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XE	1	0	0	0	0
57	XK	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XQ	1	0	0	0	0
57	XS	1	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y7	1	0	0	0	0
57	Y8	1	0	0	0	0
57	YA	538	0	0	0	0
57	YB	13	0	0	0	0
57	YD	3	0	0	0	0
57	YE	4	0	0	0	0
57	YN	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	3	0	0	0	0
57	YR	2	0	0	0	0
57	YX	2	0	0	0	0
57	YY	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	RY	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y5	1	0	0	0	0
59	Y6	1	0	0	0	0
59	Y9	1	0	0	0	0
59	YY	1	0	0	0	0
All	All	292577	0	198284	2634	0

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 6.

The worst 5 of 2634 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)
51:YW:1:MET:HG3	51:YW:64:MET:CE	1.51	1.41
50:YV:40:LEU:CD2	50:YV:47:VAL:HG12	1.52	1.40
4:XD:19:LEU:CD2	4:XD:197:PRO:HG3	1.59	1.33
1:QA:1189:C:H5"	3:QC:5:ILE:CD1	1.56	1.33
41:YI:61:ARG:HB2	41:YI:133:HIS:CE1	1.73	1.23

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	233/256 (91%)	210 (90%)	22 (9%)	1 (0%)	30	59
2	XB	234/256 (91%)	211 (90%)	22 (9%)	1 (0%)	30	59
3	QC	203/239 (85%)	195 (96%)	8 (4%)	0	100	100
3	XC	203/239 (85%)	191 (94%)	10 (5%)	2 (1%)	12	41
4	QD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
4	XD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	41
5	QE	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	85 (90%)	9 (10%)	0	100	100
11	QK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
11	XK	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
12	QL	123/131 (94%)	115 (94%)	7 (6%)	1 (1%)	16	45
12	XL	120/131 (92%)	109 (91%)	11 (9%)	0	100	100
13	QM	118/126 (94%)	103 (87%)	13 (11%)	2 (2%)	7	31
13	XM	117/126 (93%)	102 (87%)	14 (12%)	1 (1%)	14	43
14	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	31
14	XN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	31
15	QO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	XO	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
19	XS	82/93 (88%)	72 (88%)	10 (12%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	10 (10%)	1 (1%)	12	41
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
24	R0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
24	Y0	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
25	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
25	Y1	91/98 (93%)	81 (89%)	10 (11%)	0	100	100
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R4	67/71 (94%)	56 (84%)	11 (16%)	0	100	100
28	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	33
29	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	R6	51/54 (94%)	51 (100%)	0	0	100	100
30	Y6	51/54 (94%)	51 (100%)	0	0	100	100
31	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
31	Y7	46/49 (94%)	46 (100%)	0	0	100	100
32	R8	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	1	10
32	Y8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	R9	35/37 (95%)	35 (100%)	0	0	100	100
33	Y9	35/37 (95%)	35 (100%)	0	0	100	100
36	RD	270/276 (98%)	254 (94%)	15 (6%)	1 (0%)	30	59
36	YD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
37	RE	203/206 (98%)	170 (84%)	33 (16%)	0	100	100
37	YE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	12	41
38	RF	200/210 (95%)	185 (92%)	15 (8%)	0	100	100
38	YF	200/210 (95%)	183 (92%)	17 (8%)	0	100	100
39	RG	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	7	31
39	YG	179/182 (98%)	160 (89%)	18 (10%)	1 (1%)	21	51
40	RH	172/180 (96%)	152 (88%)	17 (10%)	3 (2%)	7	31
40	YH	171/180 (95%)	164 (96%)	7 (4%)	0	100	100
41	RI	144/148 (97%)	127 (88%)	14 (10%)	3 (2%)	5	27
41	YI	144/148 (97%)	127 (88%)	12 (8%)	5 (4%)	3	20
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	48
42	YN	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	18	48
43	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
43	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
44	RP	148/150 (99%)	126 (85%)	20 (14%)	2 (1%)	9	34
44	YP	145/150 (97%)	137 (94%)	7 (5%)	1 (1%)	18	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	RQ	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	18	48
45	YQ	139/141 (99%)	122 (88%)	15 (11%)	2 (1%)	9	34
46	RR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
46	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	43
47	RS	109/112 (97%)	90 (83%)	17 (16%)	2 (2%)	6	30
47	YS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
48	RT	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
48	YT	135/146 (92%)	124 (92%)	11 (8%)	0	100	100
49	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	43
49	YU	115/118 (98%)	105 (91%)	8 (7%)	2 (2%)	7	31
50	RV	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	6	28
50	YV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	12	41
51	RW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
51	YW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	14	43
52	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
52	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
53	RY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
53	YY	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
54	RZ	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	24	55
54	YZ	201/206 (98%)	186 (92%)	12 (6%)	3 (2%)	8	33
All	All	11484/12126 (95%)	10639 (93%)	787 (7%)	58 (0%)	24	55

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	R8	62	LEU
40	RH	12	PRO
41	RI	132	PRO
44	RP	108	LYS
50	RV	46	VAL

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	203/220 (92%)	200 (98%)	3 (2%)	57	66
2	XB	204/220 (93%)	204 (100%)	0	100	100
3	QC	159/188 (85%)	158 (99%)	1 (1%)	78	77
3	XC	159/188 (85%)	158 (99%)	1 (1%)	78	77
4	QD	180/181 (99%)	179 (99%)	1 (1%)	78	77
4	XD	180/181 (99%)	179 (99%)	1 (1%)	78	77
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	125 (99%)	1 (1%)	73	74
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	74
9	QI	98/99 (99%)	94 (96%)	4 (4%)	27	50
9	XI	97/99 (98%)	96 (99%)	1 (1%)	68	72
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	63	70
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/108 (96%)	103 (99%)	1 (1%)	68	72
12	XL	103/108 (95%)	102 (99%)	1 (1%)	68	72
13	QM	96/101 (95%)	95 (99%)	1 (1%)	68	72
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	48	63
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	R0	61/67 (91%)	61 (100%)	0	100	100
24	Y0	61/67 (91%)	61 (100%)	0	100	100
25	R1	82/83 (99%)	82 (100%)	0	100	100
25	Y1	78/83 (94%)	78 (100%)	0	100	100
26	R2	64/67 (96%)	64 (100%)	0	100	100
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	55	65
27	R3	51/52 (98%)	51 (100%)	0	100	100
27	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	13
28	R4	62/63 (98%)	62 (100%)	0	100	100
28	Y4	62/63 (98%)	61 (98%)	1 (2%)	55	65
29	R5	51/52 (98%)	51 (100%)	0	100	100
29	Y5	51/52 (98%)	51 (100%)	0	100	100
30	R6	51/52 (98%)	51 (100%)	0	100	100
30	Y6	51/52 (98%)	51 (100%)	0	100	100
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	45 (83%)	9 (17%)	2	12
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	34 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	RD	214/218 (98%)	214 (100%)	0	100	100
36	YD	214/218 (98%)	213 (100%)	1 (0%)	81	78
37	RE	165/166 (99%)	162 (98%)	3 (2%)	51	64
37	YE	165/166 (99%)	163 (99%)	2 (1%)	63	70
38	RF	161/166 (97%)	160 (99%)	1 (1%)	78	77
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	149 (96%)	6 (4%)	28	51
39	YG	155/156 (99%)	151 (97%)	4 (3%)	40	58
40	RH	145/148 (98%)	137 (94%)	8 (6%)	19	44
40	YH	144/148 (97%)	144 (100%)	0	100	100
41	RI	122/124 (98%)	114 (93%)	8 (7%)	15	40
41	YI	122/124 (98%)	116 (95%)	6 (5%)	22	46
42	RN	117/119 (98%)	114 (97%)	3 (3%)	40	58
42	YN	117/119 (98%)	117 (100%)	0	100	100
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	100 (100%)	0	100	100
44	RP	116/116 (100%)	114 (98%)	2 (2%)	53	65
44	YP	114/116 (98%)	112 (98%)	2 (2%)	51	64
45	RQ	111/111 (100%)	110 (99%)	1 (1%)	70	73
45	YQ	111/111 (100%)	108 (97%)	3 (3%)	39	57
46	RR	100/101 (99%)	100 (100%)	0	100	100
46	YR	100/101 (99%)	100 (100%)	0	100	100
47	RS	87/88 (99%)	87 (100%)	0	100	100
47	YS	87/88 (99%)	86 (99%)	1 (1%)	65	71
48	RT	120/127 (94%)	117 (98%)	3 (2%)	42	59
48	YT	120/127 (94%)	119 (99%)	1 (1%)	73	74
49	RU	93/94 (99%)	92 (99%)	1 (1%)	65	71
49	YU	93/94 (99%)	91 (98%)	2 (2%)	45	61
50	RV	82/82 (100%)	80 (98%)	2 (2%)	43	60
50	YV	82/82 (100%)	79 (96%)	3 (4%)	30	52
51	RW	92/92 (100%)	92 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	YW	92/92 (100%)	90 (98%)	2 (2%)	45	61
52	RX	74/78 (95%)	74 (100%)	0	100	100
52	YX	74/78 (95%)	74 (100%)	0	100	100
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	88 (100%)	0	100	100
54	RZ	174/179 (97%)	170 (98%)	4 (2%)	44	61
54	YZ	174/179 (97%)	169 (97%)	5 (3%)	37	56
All	All	9706/10064 (96%)	9594 (99%)	112 (1%)	63	70

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	RV	50	PRO
54	YZ	59	LEU
27	Y3	2	PRO
54	YZ	58	VAL
48	YT	125	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
20	XT	75	ASN
48	YT	90	GLN
28	Y4	46	GLN
40	YH	65	HIS
37	RE	143	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	266 (17%)	30 (2%)
1	XA	1509/1522 (99%)	295 (19%)	25 (1%)
22	QV	72/76 (94%)	17 (23%)	0
22	XV	72/76 (94%)	17 (23%)	0
23	QX	2/23 (8%)	0	0
23	XX	22/23 (95%)	4 (18%)	2 (9%)
34	RA	2877/2915 (98%)	550 (19%)	37 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	YA	2880/2915 (98%)	513 (17%)	37 (1%)
35	RB	119/122 (97%)	16 (13%)	1 (0%)
35	YB	119/122 (97%)	18 (15%)	1 (0%)
55	XY	16/17 (94%)	3 (18%)	0
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9188/9339 (98%)	1699 (18%)	133 (1%)

5 of 1699 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	31	G
1	QA	32	A
1	QA	39	G

5 of 133 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	YA	1204	A
34	YA	1558	A
34	YA	2832	U
34	RA	1065	U
34	RA	1057	A

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

6 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	$\# Z > 2$
22	MNU	XV	34	23,22	21,24,25	1.28	3 (14%)	27,34,37	1.82	8 (29%)
22	T6A	QV	37	22	31,34,35	1.40	4 (12%)	43,49,52	2.06	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	T6A	XV	37	22	31,34,35	1.38	3 (9%)	43,49,52	2.03	10 (23%)
56	PPU	Z8	76	34,56	37,40,41	1.28	4 (10%)	47,57,60	2.10	14 (29%)
56	PPU	Z6	76	34,56	37,40,41	1.27	5 (13%)	47,57,60	2.06	15 (31%)
22	MNU	QV	34	23,22	21,24,25	1.26	3 (14%)	27,34,37	1.63	7 (25%)

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
22	MNU	XV	34	23,22	-	0/10/28/29	0/2/2/2
22	T6A	QV	37	22	-	16/23/41/42	0/3/3/3
22	T6A	XV	37	22	-	17/23/41/42	0/3/3/3
56	PPU	Z8	76	34,56	-	4/25/43/44	0/4/4/4
56	PPU	Z6	76	34,56	-	4/25/43/44	0/4/4/4
22	MNU	QV	34	23,22	-	1/10/28/29	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	C5-C4	5.00	1.48	1.39
56	Z6	76	PPU	C5-C4	4.91	1.47	1.39
22	QV	37	T6A	C5-C4	4.78	1.47	1.39
22	XV	37	T6A	C5-C4	4.64	1.47	1.39
22	XV	34	MNU	C2-N1	3.19	1.43	1.38

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	T6A	C5-C4-N3	-6.75	117.42	126.72
22	QV	37	T6A	C5-C4-N3	-6.63	117.59	126.72
22	XV	37	T6A	N3-C4-N9	5.76	136.96	127.17
22	QV	37	T6A	N3-C4-N9	5.62	136.72	127.17
56	Z8	76	PPU	C5-C4-N3	-5.58	119.03	126.72

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	QV	34	MNU	C5-C7-N8-C9
22	QV	37	T6A	O4'-C1'-N9-C8
22	QV	37	T6A	O4'-C1'-N9-C4
22	QV	37	T6A	C5-C6-N6-C10
22	QV	37	T6A	O10-C10-N6-C6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	QV	37	T6A	1	0
22	XV	37	T6A	1	0
56	Z8	76	PPU	2	0
22	QV	34	MNU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1253 ligands modelled in this entry, 1251 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	QD	301	4	0,12,12	-	-	-		
58	SF4	XD	301	-	0,12,12	-	-	-		

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
58	SF4	QD	301	4	-	-	0/6/5/5
58	SF4	XD	301	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.33	51 (3%)	48	28	78, 129, 224, 338	0
1	XA	1511/1522 (99%)	0.38	57 (3%)	44	26	74, 126, 218, 321	0
2	QB	235/256 (91%)	0.16	3 (1%)	75	49	133, 173, 225, 251	0
2	XB	236/256 (92%)	0.37	5 (2%)	63	38	107, 157, 207, 237	0
3	QC	205/239 (85%)	0.12	3 (1%)	72	45	113, 165, 211, 257	0
3	XC	205/239 (85%)	0.39	7 (3%)	48	28	104, 144, 192, 229	0
4	QD	208/209 (99%)	0.36	7 (3%)	48	28	97, 130, 176, 204	0
4	XD	208/209 (99%)	0.48	11 (5%)	32	20	81, 121, 169, 223	0
5	QE	151/162 (93%)	-0.10	0	100	100	85, 128, 164, 214	0
5	XE	151/162 (93%)	0.20	1 (0%)	84	62	74, 114, 151, 196	0
6	QF	101/101 (100%)	0.28	3 (2%)	52	31	100, 129, 164, 175	0
6	XF	101/101 (100%)	0.14	0	100	100	108, 136, 171, 205	0
7	QG	155/156 (99%)	0.68	14 (9%)	15	11	121, 159, 205, 242	0
7	XG	155/156 (99%)	0.68	15 (9%)	13	11	111, 153, 200, 226	0
8	QH	137/138 (99%)	0.43	5 (3%)	46	27	100, 135, 176, 221	0
8	XH	137/138 (99%)	0.40	4 (2%)	53	31	98, 128, 163, 171	0
9	QI	127/128 (99%)	1.40	26 (20%)	2	3	128, 168, 217, 239	0
9	XI	126/128 (98%)	0.88	20 (15%)	5	5	117, 160, 211, 241	0
10	QJ	99/105 (94%)	0.48	6 (6%)	27	17	136, 177, 221, 261	0
10	XJ	96/105 (91%)	0.64	8 (8%)	17	12	128, 163, 208, 231	0
11	QK	119/129 (92%)	0.80	11 (9%)	14	11	105, 136, 187, 207	0
11	XK	116/129 (89%)	0.55	4 (3%)	48	28	84, 125, 171, 211	0
12	QL	125/131 (95%)	0.64	7 (5%)	30	19	84, 112, 156, 230	0
12	XL	122/131 (93%)	0.67	12 (9%)	13	11	75, 103, 136, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	1.00	19 (15%) 5 5	121, 178, 222, 280	0
13	XM	119/126 (94%)	0.80	13 (10%) 10 10	104, 155, 213, 233	0
14	QN	60/61 (98%)	0.42	2 (3%) 49 29	133, 170, 205, 236	0
14	XN	60/61 (98%)	1.08	6 (10%) 12 11	108, 140, 186, 197	0
15	QO	88/89 (98%)	0.27	3 (3%) 48 28	95, 129, 172, 202	0
15	XO	87/89 (97%)	-0.03	0 100 100	78, 111, 152, 167	0
16	QP	84/88 (95%)	0.44	1 (1%) 76 50	80, 111, 155, 183	0
16	XP	84/88 (95%)	0.42	2 (2%) 59 35	100, 136, 184, 221	0
17	QQ	100/105 (95%)	0.43	4 (4%) 42 25	86, 115, 152, 165	0
17	XQ	100/105 (95%)	0.55	8 (8%) 18 13	85, 126, 161, 185	0
18	QR	70/88 (79%)	0.38	1 (1%) 73 47	101, 134, 187, 244	0
18	XR	70/88 (79%)	0.18	0 100 100	100, 129, 178, 194	0
19	QS	83/93 (89%)	0.45	2 (2%) 59 35	131, 177, 220, 247	0
19	XS	84/93 (90%)	0.30	1 (1%) 76 50	124, 160, 210, 218	0
20	QT	99/106 (93%)	0.49	5 (5%) 33 21	84, 111, 178, 222	0
20	XT	99/106 (93%)	0.75	9 (9%) 15 11	112, 146, 194, 225	0
21	QU	25/27 (92%)	1.19	4 (16%) 5 5	129, 172, 201, 214	0
21	XU	25/27 (92%)	0.77	3 (12%) 9 8	125, 158, 197, 211	0
22	QV	72/76 (94%)	1.02	7 (9%) 13 11	130, 238, 297, 362	0
22	XV	72/76 (94%)	0.85	7 (9%) 13 11	109, 220, 253, 332	0
23	QX	3/23 (13%)	0.64	0 100 100	104, 104, 106, 132	0
23	XX	23/23 (100%)	1.34	6 (26%) 1 2	107, 195, 248, 277	0
24	R0	76/85 (89%)	0.27	1 (1%) 75 49	83, 111, 144, 173	0
24	Y0	75/85 (88%)	0.57	1 (1%) 75 49	75, 102, 139, 175	0
25	R1	97/98 (98%)	0.95	8 (8%) 17 12	66, 104, 162, 225	0
25	Y1	93/98 (94%)	0.86	6 (6%) 25 16	63, 90, 146, 181	0
26	R2	69/72 (95%)	0.50	2 (2%) 53 31	97, 128, 171, 236	0
26	Y2	68/72 (94%)	0.40	2 (2%) 53 31	71, 93, 136, 184	0
27	R3	59/60 (98%)	0.30	0 100 100	85, 117, 153, 229	0
27	Y3	59/60 (98%)	0.71	3 (5%) 33 21	82, 107, 145, 180	0
28	R4	69/71 (97%)	0.25	1 (1%) 73 47	139, 181, 227, 245	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y4	69/71 (97%)	0.51	3 (4%) 40 23	126, 183, 242, 277	0
29	R5	59/60 (98%)	0.47	4 (6%) 23 16	59, 88, 161, 188	0
29	Y5	59/60 (98%)	0.15	1 (1%) 69 42	58, 106, 195, 205	0
30	R6	53/54 (98%)	0.98	8 (15%) 5 6	154, 213, 254, 262	0
30	Y6	53/54 (98%)	0.73	5 (9%) 14 11	177, 210, 240, 259	0
31	R7	47/49 (95%)	0.55	2 (4%) 40 23	54, 75, 104, 138	0
31	Y7	48/49 (97%)	0.19	2 (4%) 40 24	54, 66, 100, 130	0
32	R8	64/65 (98%)	0.76	3 (4%) 36 22	76, 98, 145, 196	0
32	Y8	64/65 (98%)	0.87	4 (6%) 26 17	72, 89, 128, 153	0
33	R9	37/37 (100%)	1.51	9 (24%) 2 2	176, 195, 233, 256	0
33	Y9	37/37 (100%)	1.13	2 (5%) 31 19	145, 193, 249, 254	0
34	RA	2881/2915 (98%)	0.56	157 (5%) 31 19	59, 98, 232, 354	0
34	YA	2883/2915 (98%)	0.53	156 (5%) 31 19	55, 92, 228, 366	0
35	RB	120/122 (98%)	0.21	1 (0%) 82 60	109, 165, 211, 244	0
35	YB	120/122 (98%)	0.74	9 (7%) 20 14	110, 148, 185, 223	0
36	RD	272/276 (98%)	0.55	12 (4%) 39 23	56, 83, 116, 157	0
36	YD	272/276 (98%)	0.22	5 (1%) 67 41	45, 76, 110, 138	0
37	RE	205/206 (99%)	0.71	24 (11%) 9 9	56, 93, 153, 199	0
37	YE	204/206 (99%)	0.86	28 (13%) 6 7	54, 97, 150, 205	0
38	RF	202/210 (96%)	0.71	22 (10%) 10 10	62, 108, 161, 212	0
38	YF	202/210 (96%)	0.61	17 (8%) 17 12	51, 93, 146, 179	0
39	RG	181/182 (99%)	0.59	8 (4%) 39 23	124, 173, 220, 288	0
39	YG	181/182 (99%)	0.65	10 (5%) 30 19	116, 151, 197, 223	0
40	RH	174/180 (96%)	1.00	25 (14%) 6 6	100, 167, 226, 292	0
40	YH	173/180 (96%)	0.56	11 (6%) 25 17	82, 114, 156, 185	0
41	RI	146/148 (98%)	0.79	19 (13%) 7 7	93, 138, 193, 228	0
41	YI	146/148 (98%)	0.39	3 (2%) 63 38	82, 134, 178, 225	0
42	RN	138/140 (98%)	0.88	13 (9%) 14 11	69, 110, 164, 196	0
42	YN	138/140 (98%)	0.72	11 (7%) 18 13	66, 112, 167, 208	0
43	RO	122/122 (100%)	0.12	5 (4%) 41 24	52, 86, 117, 138	0
43	YO	122/122 (100%)	0.37	2 (1%) 70 44	55, 89, 118, 155	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RP	150/150 (100%)	0.60	7 (4%) 36 22	62, 114, 164, 237	0
44	YP	147/150 (98%)	0.40	5 (3%) 48 28	53, 97, 141, 166	0
45	RQ	141/141 (100%)	0.46	6 (4%) 40 23	72, 112, 158, 208	0
45	YQ	141/141 (100%)	0.66	13 (9%) 14 11	68, 102, 148, 216	0
46	RR	117/118 (99%)	0.19	2 (1%) 69 42	56, 86, 120, 208	0
46	YR	117/118 (99%)	0.41	4 (3%) 48 28	61, 92, 125, 170	0
47	RS	111/112 (99%)	0.54	6 (5%) 31 19	119, 154, 214, 254	0
47	YS	111/112 (99%)	0.75	7 (6%) 26 17	107, 144, 196, 226	0
48	RT	137/146 (93%)	0.31	6 (4%) 39 23	64, 95, 158, 188	0
48	YT	137/146 (93%)	0.56	6 (4%) 39 23	54, 104, 172, 232	0
49	RU	117/118 (99%)	0.80	12 (10%) 12 11	66, 101, 160, 193	0
49	YU	117/118 (99%)	0.57	5 (4%) 40 23	56, 110, 164, 242	0
50	RV	101/101 (100%)	0.44	7 (6%) 23 15	83, 122, 167, 271	0
50	YV	101/101 (100%)	0.52	6 (5%) 28 18	71, 120, 174, 217	0
51	RW	113/113 (100%)	0.57	10 (8%) 15 12	60, 84, 134, 233	0
51	YW	113/113 (100%)	0.31	3 (2%) 56 33	58, 85, 138, 204	0
52	RX	92/96 (95%)	0.57	6 (6%) 25 16	69, 102, 145, 159	0
52	YX	92/96 (95%)	0.43	5 (5%) 31 19	58, 80, 111, 181	0
53	RY	107/110 (97%)	1.10	14 (13%) 7 7	91, 125, 168, 188	0
53	YY	107/110 (97%)	0.86	8 (7%) 20 14	75, 107, 152, 174	0
54	RZ	203/206 (98%)	0.20	0 100 100	114, 153, 202, 282	0
54	YZ	203/206 (98%)	0.47	11 (5%) 31 19	108, 142, 192, 226	0
55	XY	17/17 (100%)	0.45	0 100 100	141, 155, 229, 295	0
56	Z6	2/3 (66%)	0.07	0 100 100	136, 136, 136, 146	0
56	Z8	2/3 (66%)	0.78	0 100 100	129, 129, 129, 136	0
All	All	20886/21465 (97%)	0.51	1137 (5%) 31 19	45, 118, 209, 366	0

The worst 5 of 1137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	QI	116	LYS	8.7
37	RE	130	GLY	8.4
53	RY	62	GLU	8.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	YE	153	GLY	7.5
22	XV	1	G	7.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	T6A	QV	37	32/33	0.73	0.15	155,169,201,204	0
22	T6A	XV	37	32/33	0.88	0.18	105,112,148,175	0
22	MNU	QV	34	23/24	0.89	0.10	128,129,139,148	0
56	PPU	Z8	76	37/38	0.90	0.16	88,94,130,143	0
22	MNU	XV	34	23/24	0.92	0.13	103,106,117,124	0
56	PPU	Z6	76	37/38	0.93	0.14	88,101,129,133	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	YA	3398	1/1	0.05	0.16	82,82,82,82	0
57	MG	RB	201	1/1	0.32	0.15	87,87,87,87	0
57	MG	YB	210	1/1	0.45	0.10	82,82,82,82	0
57	MG	RA	3267	1/1	0.46	0.32	76,76,76,76	0
57	MG	RA	3446	1/1	0.51	0.08	65,65,65,65	0
57	MG	YA	3448	1/1	0.51	0.17	91,91,91,91	0
57	MG	RA	3259	1/1	0.51	0.13	73,73,73,73	0
57	MG	YA	3287	1/1	0.53	0.26	92,92,92,92	0
57	MG	YA	3496	1/1	0.55	0.16	72,72,72,72	0
57	MG	RY	201	1/1	0.56	0.12	104,104,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3428	1/1	0.56	0.37	46,46,46,46	0
57	MG	YB	213	1/1	0.57	0.26	57,57,57,57	0
57	MG	RA	3355	1/1	0.59	0.20	75,75,75,75	0
57	MG	RA	3208	1/1	0.60	0.20	78,78,78,78	0
57	MG	RA	3295	1/1	0.61	0.10	64,64,64,64	0
57	MG	RA	3451	1/1	0.61	0.12	68,68,68,68	0
57	MG	YA	3310	1/1	0.62	0.16	62,62,62,62	0
57	MG	RA	3362	1/1	0.63	0.15	68,68,68,68	0
57	MG	YB	207	1/1	0.63	0.14	107,107,107,107	0
57	MG	QA	1655	1/1	0.63	0.28	98,98,98,98	0
57	MG	YA	3466	1/1	0.63	0.22	73,73,73,73	0
57	MG	RA	3139	1/1	0.64	0.15	38,38,38,38	0
57	MG	RA	3186	1/1	0.65	0.14	90,90,90,90	0
57	MG	QA	1672	1/1	0.65	0.30	76,76,76,76	0
57	MG	RA	3321	1/1	0.65	0.13	53,53,53,53	0
57	MG	RA	3449	1/1	0.65	0.26	100,100,100,100	0
57	MG	YA	3336	1/1	0.65	0.23	79,79,79,79	0
57	MG	QA	1661	1/1	0.65	0.20	113,113,113,113	0
57	MG	RA	3405	1/1	0.66	0.25	82,82,82,82	0
57	MG	RA	3414	1/1	0.66	0.08	39,39,39,39	0
57	MG	YA	3525	1/1	0.66	0.32	46,46,46,46	0
57	MG	YA	3225	1/1	0.66	0.12	64,64,64,64	0
57	MG	YA	3409	1/1	0.66	0.18	74,74,74,74	0
57	MG	RA	3171	1/1	0.66	0.12	70,70,70,70	0
57	MG	YA	3410	1/1	0.67	0.08	60,60,60,60	0
57	MG	RA	3400	1/1	0.67	0.25	69,69,69,69	0
57	MG	YA	3453	1/1	0.67	0.10	51,51,51,51	0
57	MG	YB	206	1/1	0.68	0.27	75,75,75,75	0
57	MG	RA	3369	1/1	0.68	0.30	91,91,91,91	0
57	MG	YA	3499	1/1	0.68	0.10	77,77,77,77	0
57	MG	RA	3404	1/1	0.68	0.25	85,85,85,85	0
57	MG	RA	3195	1/1	0.69	0.30	95,95,95,95	0
57	MG	RA	3277	1/1	0.69	0.21	81,81,81,81	0
57	MG	YB	208	1/1	0.69	0.11	76,76,76,76	0
57	MG	RA	3444	1/1	0.69	0.20	57,57,57,57	0
57	MG	YA	3528	1/1	0.69	0.10	51,51,51,51	0
57	MG	RA	3353	1/1	0.70	0.10	67,67,67,67	0
57	MG	RA	3395	1/1	0.70	0.18	77,77,77,77	0
57	MG	YA	3426	1/1	0.70	0.19	62,62,62,62	0
57	MG	YA	3375	1/1	0.70	0.21	67,67,67,67	0
57	MG	RA	3422	1/1	0.70	0.09	57,57,57,57	0
57	MG	YA	3298	1/1	0.71	0.32	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RQ	203	1/1	0.71	0.19	83,83,83,83	0
57	MG	YA	3405	1/1	0.72	0.13	61,61,61,61	0
57	MG	RA	3383	1/1	0.72	0.33	71,71,71,71	0
57	MG	YA	3349	1/1	0.72	0.21	86,86,86,86	0
57	MG	RA	3418	1/1	0.72	0.10	59,59,59,59	0
57	MG	YA	3508	1/1	0.72	0.14	102,102,102,102	0
57	MG	YA	3270	1/1	0.72	0.29	75,75,75,75	0
57	MG	YO	201	1/1	0.72	0.18	70,70,70,70	0
57	MG	RA	3322	1/1	0.73	0.09	59,59,59,59	0
57	MG	YA	3436	1/1	0.73	0.15	75,75,75,75	0
57	MG	RA	3084	1/1	0.73	0.21	38,38,38,38	0
57	MG	YA	3400	1/1	0.73	0.07	68,68,68,68	0
57	MG	RA	3425	1/1	0.74	0.10	73,73,73,73	0
57	MG	XA	1612	1/1	0.74	0.14	73,73,73,73	0
57	MG	YA	3345	1/1	0.74	0.12	38,38,38,38	0
57	MG	YA	3195	1/1	0.74	0.15	46,46,46,46	0
57	MG	RA	3427	1/1	0.74	0.23	81,81,81,81	0
57	MG	YA	3382	1/1	0.74	0.07	97,97,97,97	0
57	MG	RA	3310	1/1	0.74	0.09	71,71,71,71	0
57	MG	RA	3437	1/1	0.74	0.19	69,69,69,69	0
57	MG	YD	302	1/1	0.74	0.39	102,102,102,102	0
57	MG	RA	3360	1/1	0.74	0.10	38,38,38,38	0
57	MG	YA	3160	1/1	0.75	0.25	80,80,80,80	0
57	MG	YA	3290	1/1	0.75	0.15	97,97,97,97	0
57	MG	RA	3430	1/1	0.75	0.21	67,67,67,67	0
57	MG	YE	304	1/1	0.75	0.12	114,114,114,114	0
57	MG	YA	3305	1/1	0.75	0.39	81,81,81,81	0
57	MG	RA	3190	1/1	0.76	0.21	55,55,55,55	0
57	MG	RA	3317	1/1	0.76	0.23	48,48,48,48	0
57	MG	XM	201	1/1	0.76	0.11	97,97,97,97	0
57	MG	RA	3124	1/1	0.76	0.23	68,68,68,68	0
57	MG	YA	3424	1/1	0.76	0.23	65,65,65,65	0
57	MG	RA	3111	1/1	0.76	0.11	54,54,54,54	0
57	MG	YA	3203	1/1	0.76	0.26	38,38,38,38	0
57	MG	RA	3228	1/1	0.76	0.13	38,38,38,38	0
57	MG	RA	3298	1/1	0.76	0.07	62,62,62,62	0
57	MG	YA	3463	1/1	0.76	0.07	72,72,72,72	0
57	MG	YA	3273	1/1	0.76	0.10	45,45,45,45	0
57	MG	RA	3306	1/1	0.76	0.10	58,58,58,58	0
57	MG	YB	204	1/1	0.77	0.27	38,38,38,38	0
57	MG	XA	1669	1/1	0.77	0.14	83,83,83,83	0
57	MG	YA	3362	1/1	0.77	0.07	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3209	1/1	0.77	0.07	38,38,38,38	0
57	MG	RA	3385	1/1	0.77	0.07	67,67,67,67	0
57	MG	YA	3046	1/1	0.77	0.38	61,61,61,61	0
57	MG	YA	3509	1/1	0.77	0.26	63,63,63,63	0
57	MG	RA	3193	1/1	0.77	0.15	59,59,59,59	0
57	MG	YN	201	1/1	0.77	0.09	65,65,65,65	0
57	MG	RA	3368	1/1	0.77	0.16	56,56,56,56	0
57	MG	RA	3246	1/1	0.78	0.15	38,38,38,38	0
57	MG	YA	3311	1/1	0.78	0.07	38,38,38,38	0
57	MG	YA	3322	1/1	0.78	0.10	42,42,42,42	0
57	MG	RA	3343	1/1	0.78	0.09	51,51,51,51	0
57	MG	RA	3392	1/1	0.78	0.14	51,51,51,51	0
57	MG	YA	3456	1/1	0.78	0.16	66,66,66,66	0
57	MG	YA	3188	1/1	0.78	0.12	45,45,45,45	0
57	MG	YA	3190	1/1	0.78	0.10	73,73,73,73	0
57	MG	RA	3256	1/1	0.79	0.09	38,38,38,38	0
57	MG	RB	203	1/1	0.79	0.12	77,77,77,77	0
57	MG	RA	3307	1/1	0.79	0.18	76,76,76,76	0
57	MG	RA	3292	1/1	0.79	0.28	69,69,69,69	0
57	MG	QA	1645	1/1	0.79	0.10	82,82,82,82	0
57	MG	RA	3001	1/1	0.79	0.20	66,66,66,66	0
57	MG	RA	3412	1/1	0.79	0.14	82,82,82,82	0
57	MG	YA	3380	1/1	0.79	0.11	38,38,38,38	0
57	MG	YA	3443	1/1	0.79	0.11	58,58,58,58	0
57	MG	YA	3222	1/1	0.79	0.24	121,121,121,121	0
57	MG	YX	102	1/1	0.79	0.26	95,95,95,95	0
57	MG	RA	3204	1/1	0.80	0.23	77,77,77,77	0
57	MG	RN	201	1/1	0.80	0.39	57,57,57,57	0
57	MG	YA	3216	1/1	0.80	0.09	70,70,70,70	0
57	MG	YA	3367	1/1	0.80	0.11	52,52,52,52	0
57	MG	RA	3152	1/1	0.80	0.17	38,38,38,38	0
57	MG	RA	3406	1/1	0.80	0.09	44,44,44,44	0
57	MG	YA	3242	1/1	0.80	0.09	63,63,63,63	0
57	MG	YA	3512	1/1	0.80	0.10	77,77,77,77	0
57	MG	YA	3396	1/1	0.80	0.12	69,69,69,69	0
57	MG	RA	3302	1/1	0.80	0.14	66,66,66,66	0
57	MG	RA	3227	1/1	0.80	0.14	65,65,65,65	0
57	MG	XA	1673	1/1	0.80	0.10	48,48,48,48	0
57	MG	YA	3408	1/1	0.80	0.11	56,56,56,56	0
57	MG	RA	3268	1/1	0.80	0.10	59,59,59,59	0
57	MG	YA	3012	1/1	0.80	0.16	69,69,69,69	0
57	MG	QF	201	1/1	0.80	0.12	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3450	1/1	0.80	0.07	54,54,54,54	0
57	MG	RA	3424	1/1	0.80	0.10	65,65,65,65	0
57	MG	RA	3455	1/1	0.80	0.10	57,57,57,57	0
57	MG	RA	3149	1/1	0.80	0.18	75,75,75,75	0
57	MG	YA	3342	1/1	0.80	0.07	52,52,52,52	0
57	MG	RA	3314	1/1	0.81	0.17	51,51,51,51	0
57	MG	YA	3460	1/1	0.81	0.14	58,58,58,58	0
57	MG	RA	3242	1/1	0.81	0.26	83,83,83,83	0
57	MG	QA	1649	1/1	0.81	0.11	64,64,64,64	0
57	MG	YA	3479	1/1	0.81	0.20	57,57,57,57	0
57	MG	YA	3483	1/1	0.81	0.09	49,49,49,49	0
57	MG	YA	3501	1/1	0.82	0.28	38,38,38,38	0
57	MG	RA	3286	1/1	0.82	0.21	41,41,41,41	0
57	MG	YA	3355	1/1	0.82	0.15	98,98,98,98	0
57	MG	YA	3433	1/1	0.82	0.21	78,78,78,78	0
57	MG	YA	3201	1/1	0.82	0.56	92,92,92,92	0
57	MG	YA	3441	1/1	0.82	0.08	38,38,38,38	0
57	MG	RA	3461	1/1	0.82	0.37	38,38,38,38	0
57	MG	YA	3301	1/1	0.82	0.23	42,42,42,42	0
57	MG	YA	3304	1/1	0.82	0.17	44,44,44,44	0
57	MG	RA	3162	1/1	0.82	0.12	38,38,38,38	0
57	MG	RA	3083	1/1	0.82	0.29	62,62,62,62	0
57	MG	YB	212	1/1	0.82	0.06	65,65,65,65	0
57	MG	RA	3173	1/1	0.82	0.11	44,44,44,44	0
57	MG	YA	3140	1/1	0.82	0.10	38,38,38,38	0
57	MG	YA	3328	1/1	0.82	0.15	53,53,53,53	0
57	MG	RA	3201	1/1	0.82	0.09	70,70,70,70	0
57	MG	RA	3117	1/1	0.82	0.19	38,38,38,38	0
57	MG	RA	3452	1/1	0.82	0.27	69,69,69,69	0
57	MG	YA	3250	1/1	0.83	0.18	54,54,54,54	0
57	MG	YA	3261	1/1	0.83	0.11	62,62,62,62	0
57	MG	Y0	101	1/1	0.83	0.21	65,65,65,65	0
57	MG	RA	3038	1/1	0.83	0.23	38,38,38,38	0
57	MG	YA	3493	1/1	0.83	0.17	96,96,96,96	0
57	MG	RA	3089	1/1	0.83	0.35	38,38,38,38	0
57	MG	RA	3053	1/1	0.83	0.21	38,38,38,38	0
57	MG	RA	3155	1/1	0.83	0.07	52,52,52,52	0
57	MG	YA	3165	1/1	0.83	0.11	38,38,38,38	0
57	MG	YA	3404	1/1	0.83	0.07	60,60,60,60	0
57	MG	YA	3171	1/1	0.83	0.26	54,54,54,54	0
57	MG	YA	3406	1/1	0.83	0.16	62,62,62,62	0
57	MG	RA	3372	1/1	0.83	0.07	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3535	1/1	0.83	0.15	38,38,38,38	0
57	MG	RA	3156	1/1	0.83	0.15	59,59,59,59	0
57	MG	RA	3061	1/1	0.83	0.23	38,38,38,38	0
57	MG	RA	3122	1/1	0.83	0.18	73,73,73,73	0
57	MG	RA	3211	1/1	0.83	0.18	63,63,63,63	0
57	MG	RA	3431	1/1	0.83	0.15	38,38,38,38	0
57	MG	QA	1656	1/1	0.83	0.16	55,55,55,55	0
57	MG	RA	3351	1/1	0.83	0.24	59,59,59,59	0
57	MG	YA	3346	1/1	0.83	0.32	81,81,81,81	0
57	MG	RA	3179	1/1	0.83	0.08	74,74,74,74	0
57	MG	YA	3354	1/1	0.83	0.06	40,40,40,40	0
57	MG	RA	3239	1/1	0.83	0.15	54,54,54,54	0
57	MG	YA	3356	1/1	0.83	0.11	38,38,38,38	0
59	ZN	R5	101	1/1	0.83	0.29	88,88,88,88	0
57	MG	RA	3396	1/1	0.84	0.14	38,38,38,38	0
57	MG	YA	3248	1/1	0.84	0.07	54,54,54,54	0
57	MG	YA	3170	1/1	0.84	0.11	64,64,64,64	0
57	MG	RA	3079	1/1	0.84	0.10	50,50,50,50	0
57	MG	RA	3384	1/1	0.84	0.06	40,40,40,40	0
57	MG	YA	3007	1/1	0.84	0.15	71,71,71,71	0
57	MG	YA	3514	1/1	0.84	0.40	85,85,85,85	0
57	MG	YA	3353	1/1	0.84	0.06	50,50,50,50	0
57	MG	YA	3284	1/1	0.84	0.10	38,38,38,38	0
57	MG	RA	3254	1/1	0.84	0.11	38,38,38,38	0
57	MG	YA	3020	1/1	0.84	0.13	53,53,53,53	0
57	MG	RA	3081	1/1	0.84	0.26	63,63,63,63	0
57	MG	YA	3444	1/1	0.84	0.26	55,55,55,55	0
57	MG	YA	3053	1/1	0.84	0.24	38,38,38,38	0
57	MG	YA	3211	1/1	0.84	0.07	65,65,65,65	0
57	MG	YA	3069	1/1	0.84	0.14	44,44,44,44	0
57	MG	RA	3070	1/1	0.84	0.13	38,38,38,38	0
57	MG	RA	3483	1/1	0.84	0.16	65,65,65,65	0
57	MG	YA	3397	1/1	0.84	0.20	52,52,52,52	0
57	MG	YA	3314	1/1	0.84	0.21	66,66,66,66	0
57	MG	YA	3320	1/1	0.84	0.14	54,54,54,54	0
57	MG	YQ	201	1/1	0.84	0.20	77,77,77,77	0
57	MG	YA	3486	1/1	0.84	0.08	87,87,87,87	0
57	MG	YA	3239	1/1	0.84	0.19	38,38,38,38	0
59	ZN	Y6	101	1/1	0.84	0.37	106,106,106,106	0
57	MG	YA	3299	1/1	0.85	0.07	43,43,43,43	0
57	MG	YA	3423	1/1	0.85	0.15	73,73,73,73	0
57	MG	YA	3087	1/1	0.85	0.31	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3453	1/1	0.85	0.23	71,71,71,71	0
57	MG	RA	3199	1/1	0.85	0.09	56,56,56,56	0
57	MG	RA	3244	1/1	0.85	0.11	38,38,38,38	0
57	MG	YA	3364	1/1	0.85	0.16	56,56,56,56	0
57	MG	RA	3442	1/1	0.85	0.18	58,58,58,58	0
57	MG	QA	1647	1/1	0.85	0.06	38,38,38,38	0
57	MG	YA	3377	1/1	0.85	0.08	38,38,38,38	0
57	MG	YA	3319	1/1	0.85	0.13	38,38,38,38	0
57	MG	RA	3073	1/1	0.85	0.10	38,38,38,38	0
57	MG	YB	209	1/1	0.85	0.09	51,51,51,51	0
57	MG	YA	3014	1/1	0.85	0.09	69,69,69,69	0
57	MG	RA	3426	1/1	0.85	0.16	91,91,91,91	0
57	MG	YA	3334	1/1	0.85	0.12	64,64,64,64	0
57	MG	YA	3471	1/1	0.85	0.15	47,47,47,47	0
57	MG	YA	3197	1/1	0.85	0.12	38,38,38,38	0
57	MG	RA	3141	1/1	0.85	0.13	57,57,57,57	0
57	MG	RA	3413	1/1	0.85	0.07	45,45,45,45	0
57	MG	YA	3492	1/1	0.85	0.10	52,52,52,52	0
57	MG	RA	3378	1/1	0.85	0.10	73,73,73,73	0
57	MG	YA	3082	1/1	0.85	0.25	38,38,38,38	0
57	MG	YA	3350	1/1	0.85	0.06	54,54,54,54	0
59	ZN	YY	202	1/1	0.85	0.23	93,93,93,93	0
57	MG	RA	3467	1/1	0.86	0.15	51,51,51,51	0
57	MG	RA	3471	1/1	0.86	0.23	38,38,38,38	0
57	MG	YA	3323	1/1	0.86	0.26	38,38,38,38	0
57	MG	RA	3008	1/1	0.86	0.06	38,38,38,38	0
57	MG	YA	3329	1/1	0.86	0.09	38,38,38,38	0
57	MG	RA	3016	1/1	0.86	0.19	38,38,38,38	0
57	MG	RA	3352	1/1	0.86	0.16	55,55,55,55	0
57	MG	RA	3128	1/1	0.86	0.19	38,38,38,38	0
57	MG	RO	201	1/1	0.86	0.22	63,63,63,63	0
57	MG	YA	3202	1/1	0.86	0.12	38,38,38,38	0
57	MG	RP	203	1/1	0.86	0.30	79,79,79,79	0
57	MG	YA	3204	1/1	0.86	0.08	67,67,67,67	0
57	MG	RA	3207	1/1	0.86	0.13	75,75,75,75	0
57	MG	RA	3129	1/1	0.86	0.06	52,52,52,52	0
57	MG	RA	3281	1/1	0.86	0.10	49,49,49,49	0
57	MG	XA	1615	1/1	0.86	0.06	47,47,47,47	0
57	MG	RA	3176	1/1	0.86	0.12	40,40,40,40	0
57	MG	RA	3291	1/1	0.86	0.06	46,46,46,46	0
57	MG	XL	201	1/1	0.86	0.09	42,42,42,42	0
57	MG	RA	3177	1/1	0.86	0.18	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3376	1/1	0.86	0.17	77,77,77,77	0
57	MG	RA	3020	1/1	0.86	0.35	38,38,38,38	0
57	MG	RA	3380	1/1	0.86	0.08	38,38,38,38	0
57	MG	YA	3267	1/1	0.86	0.27	61,61,61,61	0
57	MG	YA	3008	1/1	0.86	0.09	56,56,56,56	0
57	MG	RA	3231	1/1	0.86	0.15	42,42,42,42	0
57	MG	RA	3299	1/1	0.86	0.10	71,71,71,71	0
57	MG	YA	3399	1/1	0.86	0.14	38,38,38,38	0
57	MG	YA	3016	1/1	0.86	0.20	38,38,38,38	0
57	MG	RA	3234	1/1	0.86	0.17	75,75,75,75	0
57	MG	YA	3291	1/1	0.86	0.09	61,61,61,61	0
57	MG	RA	3238	1/1	0.86	0.16	53,53,53,53	0
57	MG	RA	3101	1/1	0.86	0.13	57,57,57,57	0
57	MG	QA	1617	1/1	0.86	0.17	60,60,60,60	0
57	MG	YA	3070	1/1	0.86	0.18	38,38,38,38	0
57	MG	RA	3005	1/1	0.86	0.20	38,38,38,38	0
57	MG	YP	201	1/1	0.86	0.34	72,72,72,72	0
57	MG	RA	3121	1/1	0.86	0.27	38,38,38,38	0
57	MG	RA	3247	1/1	0.86	0.07	38,38,38,38	0
57	MG	RA	3197	1/1	0.86	0.11	51,51,51,51	0
57	MG	YA	3315	1/1	0.86	0.10	38,38,38,38	0
57	MG	RA	3411	1/1	0.86	0.19	71,71,71,71	0
57	MG	YA	3474	1/1	0.87	0.26	38,38,38,38	0
57	MG	YA	3308	1/1	0.87	0.26	66,66,66,66	0
57	MG	RA	3357	1/1	0.87	0.08	57,57,57,57	0
57	MG	YA	3381	1/1	0.87	0.17	39,39,39,39	0
57	MG	RA	3358	1/1	0.87	0.10	74,74,74,74	0
57	MG	RA	3133	1/1	0.87	0.20	38,38,38,38	0
57	MG	RA	3134	1/1	0.87	0.19	38,38,38,38	0
57	MG	YA	3498	1/1	0.87	0.10	45,45,45,45	0
57	MG	RB	205	1/1	0.87	0.21	68,68,68,68	0
57	MG	RE	304	1/1	0.87	0.14	38,38,38,38	0
57	MG	YA	3032	1/1	0.87	0.24	38,38,38,38	0
57	MG	RA	3062	1/1	0.87	0.14	61,61,61,61	0
57	MG	YA	3326	1/1	0.87	0.08	73,73,73,73	0
57	MG	YA	3235	1/1	0.87	0.15	38,38,38,38	0
57	MG	RA	3409	1/1	0.87	0.18	43,43,43,43	0
57	MG	RA	3185	1/1	0.87	0.14	93,93,93,93	0
57	MG	QA	1633	1/1	0.87	0.14	73,73,73,73	0
57	MG	YB	203	1/1	0.87	0.08	107,107,107,107	0
57	MG	YA	3413	1/1	0.87	0.12	56,56,56,56	0
57	MG	RA	3188	1/1	0.87	0.08	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1605	1/1	0.87	0.10	61,61,61,61	0
57	MG	YA	3127	1/1	0.87	0.18	70,70,70,70	0
57	MG	YA	3132	1/1	0.87	0.07	38,38,38,38	0
57	MG	XA	1611	1/1	0.87	0.12	39,39,39,39	0
57	MG	YA	3351	1/1	0.87	0.24	38,38,38,38	0
57	MG	RA	3144	1/1	0.87	0.12	38,38,38,38	0
57	MG	RA	3221	1/1	0.87	0.09	38,38,38,38	0
57	MG	RA	3421	1/1	0.87	0.07	38,38,38,38	0
57	MG	YA	3449	1/1	0.87	0.09	56,56,56,56	0
57	MG	YA	3451	1/1	0.87	0.06	63,63,63,63	0
57	MG	RA	3131	1/1	0.87	0.14	48,48,48,48	0
57	MG	RA	3194	1/1	0.87	0.14	48,48,48,48	0
57	MG	YQ	202	1/1	0.87	0.11	82,82,82,82	0
57	MG	YR	202	1/1	0.87	0.12	38,38,38,38	0
57	MG	RA	3175	1/1	0.87	0.16	70,70,70,70	0
57	MG	RA	3356	1/1	0.87	0.07	49,49,49,49	0
59	ZN	R9	101	1/1	0.87	0.44	88,88,88,88	0
59	ZN	RY	202	1/1	0.87	0.28	88,88,88,88	0
57	MG	YA	3003	1/1	0.87	0.10	67,67,67,67	0
57	MG	YA	3006	1/1	0.87	0.14	38,38,38,38	0
57	MG	XA	1617	1/1	0.88	0.15	38,38,38,38	0
57	MG	YA	3194	1/1	0.88	0.15	64,64,64,64	0
57	MG	XA	1620	1/1	0.88	0.12	38,38,38,38	0
57	MG	XA	1645	1/1	0.88	0.20	43,43,43,43	0
57	MG	R1	101	1/1	0.88	0.17	38,38,38,38	0
57	MG	RA	3398	1/1	0.88	0.11	38,38,38,38	0
57	MG	RA	3025	1/1	0.88	0.16	38,38,38,38	0
57	MG	RA	3192	1/1	0.88	0.26	38,38,38,38	0
57	MG	XS	101	1/1	0.88	0.05	51,51,51,51	0
57	MG	RA	3078	1/1	0.88	0.19	40,40,40,40	0
57	MG	YA	3214	1/1	0.88	0.06	38,38,38,38	0
57	MG	YA	3352	1/1	0.88	0.17	48,48,48,48	0
57	MG	RA	3035	1/1	0.88	0.22	38,38,38,38	0
57	MG	YA	3485	1/1	0.88	0.15	76,76,76,76	0
57	MG	YA	3219	1/1	0.88	0.07	38,38,38,38	0
57	MG	YA	3488	1/1	0.88	0.15	63,63,63,63	0
57	MG	QA	1670	1/1	0.88	0.16	38,38,38,38	0
57	MG	RA	3044	1/1	0.88	0.13	38,38,38,38	0
57	MG	YA	3357	1/1	0.88	0.10	91,91,91,91	0
57	MG	RA	3454	1/1	0.88	0.20	60,60,60,60	0
57	MG	RA	3046	1/1	0.88	0.25	38,38,38,38	0
57	MG	QA	1671	1/1	0.88	0.07	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3244	1/1	0.88	0.07	38,38,38,38	0
57	MG	RA	3138	1/1	0.88	0.06	38,38,38,38	0
57	MG	RA	3415	1/1	0.88	0.05	63,63,63,63	0
57	MG	RA	3417	1/1	0.88	0.17	38,38,38,38	0
57	MG	YA	3522	1/1	0.88	0.27	38,38,38,38	0
57	MG	YA	3044	1/1	0.88	0.19	38,38,38,38	0
57	MG	RA	3057	1/1	0.88	0.41	38,38,38,38	0
57	MG	YA	3390	1/1	0.88	0.12	74,74,74,74	0
57	MG	YB	202	1/1	0.88	0.18	38,38,38,38	0
57	MG	YA	3395	1/1	0.88	0.13	86,86,86,86	0
57	MG	RA	3255	1/1	0.88	0.24	38,38,38,38	0
57	MG	YA	3060	1/1	0.88	0.24	38,38,38,38	0
57	MG	RA	3376	1/1	0.88	0.17	76,76,76,76	0
57	MG	QA	1601	1/1	0.88	0.11	38,38,38,38	0
57	MG	QA	1668	1/1	0.88	0.10	55,55,55,55	0
57	MG	YA	3083	1/1	0.88	0.10	38,38,38,38	0
57	MG	RA	3260	1/1	0.88	0.11	60,60,60,60	0
57	MG	YA	3102	1/1	0.88	0.18	38,38,38,38	0
57	MG	YD	301	1/1	0.88	0.33	38,38,38,38	0
57	MG	YA	3106	1/1	0.88	0.23	38,38,38,38	0
57	MG	RA	3220	1/1	0.88	0.23	53,53,53,53	0
57	MG	RA	3328	1/1	0.88	0.22	94,94,94,94	0
57	MG	RA	3387	1/1	0.88	0.08	64,64,64,64	0
57	MG	YA	3416	1/1	0.88	0.13	53,53,53,53	0
57	MG	YA	3142	1/1	0.88	0.09	38,38,38,38	0
57	MG	XA	1604	1/1	0.88	0.07	76,76,76,76	0
57	MG	RA	3332	1/1	0.88	0.06	38,38,38,38	0
57	MG	YX	101	1/1	0.88	0.11	81,81,81,81	0
57	MG	YA	3432	1/1	0.88	0.20	56,56,56,56	0
57	MG	YA	3168	1/1	0.88	0.17	44,44,44,44	0
57	MG	RA	3148	1/1	0.88	0.08	45,45,45,45	0
57	MG	YA	3437	1/1	0.88	0.07	68,68,68,68	0
57	MG	RA	3439	1/1	0.88	0.17	52,52,52,52	0
57	MG	RA	3441	1/1	0.88	0.10	64,64,64,64	0
57	MG	YA	3143	1/1	0.89	0.06	42,42,42,42	0
57	MG	RA	3463	1/1	0.89	0.30	87,87,87,87	0
57	MG	RA	3382	1/1	0.89	0.10	38,38,38,38	0
57	MG	YA	3166	1/1	0.89	0.08	38,38,38,38	0
57	MG	YA	3297	1/1	0.89	0.10	50,50,50,50	0
57	MG	YA	3490	1/1	0.89	0.04	39,39,39,39	0
57	MG	RA	3280	1/1	0.89	0.11	42,42,42,42	0
57	MG	RA	3477	1/1	0.89	0.28	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3386	1/1	0.89	0.07	38,38,38,38	0
57	MG	RA	3329	1/1	0.89	0.27	38,38,38,38	0
57	MG	QA	1657	1/1	0.89	0.19	63,63,63,63	0
57	MG	RA	3341	1/1	0.89	0.05	38,38,38,38	0
57	MG	RA	3285	1/1	0.89	0.11	38,38,38,38	0
57	MG	YA	3309	1/1	0.89	0.10	38,38,38,38	0
57	MG	RA	3349	1/1	0.89	0.10	41,41,41,41	0
57	MG	RA	3009	1/1	0.89	0.10	65,65,65,65	0
57	MG	YA	3017	1/1	0.89	0.08	38,38,38,38	0
57	MG	YA	3019	1/1	0.89	0.23	49,49,49,49	0
57	MG	RA	3436	1/1	0.89	0.13	77,77,77,77	0
57	MG	RA	3287	1/1	0.89	0.16	70,70,70,70	0
57	MG	RA	3245	1/1	0.89	0.10	38,38,38,38	0
57	MG	RA	3214	1/1	0.89	0.08	73,73,73,73	0
57	MG	YA	3212	1/1	0.89	0.13	53,53,53,53	0
57	MG	YA	3049	1/1	0.89	0.34	38,38,38,38	0
57	MG	QA	1605	1/1	0.89	0.21	47,47,47,47	0
57	MG	QA	1652	1/1	0.89	0.12	68,68,68,68	0
57	MG	RA	3196	1/1	0.89	0.07	50,50,50,50	0
57	MG	YA	3339	1/1	0.89	0.11	38,38,38,38	0
57	MG	RA	3119	1/1	0.89	0.10	38,38,38,38	0
57	MG	YA	3343	1/1	0.89	0.09	38,38,38,38	0
57	MG	YA	3230	1/1	0.89	0.09	38,38,38,38	0
57	MG	RA	3229	1/1	0.89	0.11	38,38,38,38	0
57	MG	RA	3024	1/1	0.89	0.26	38,38,38,38	0
57	MG	RA	3266	1/1	0.89	0.19	61,61,61,61	0
57	MG	XA	1626	1/1	0.89	0.17	38,38,38,38	0
57	MG	XA	1633	1/1	0.89	0.14	38,38,38,38	0
57	MG	RA	3158	1/1	0.89	0.10	86,86,86,86	0
57	MG	YA	3260	1/1	0.89	0.21	38,38,38,38	0
57	MG	QA	1608	1/1	0.89	0.09	54,54,54,54	0
57	MG	YA	3457	1/1	0.89	0.09	72,72,72,72	0
57	MG	YA	3136	1/1	0.89	0.12	53,53,53,53	0
57	MG	QA	1604	1/1	0.89	0.10	38,38,38,38	0
57	MG	RA	3279	1/1	0.89	0.14	51,51,51,51	0
57	MG	YA	3363	1/1	0.89	0.06	49,49,49,49	0
57	MG	YA	3274	1/1	0.89	0.23	38,38,38,38	0
57	MG	YA	3475	1/1	0.89	0.13	38,38,38,38	0
57	MG	YA	3445	1/1	0.90	0.12	69,69,69,69	0
57	MG	YA	3447	1/1	0.90	0.16	38,38,38,38	0
57	MG	RA	3004	1/1	0.90	0.23	38,38,38,38	0
57	MG	RA	3037	1/1	0.90	0.23	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3450	1/1	0.90	0.23	70,70,70,70	0
57	MG	YA	3196	1/1	0.90	0.12	38,38,38,38	0
57	MG	YA	3330	1/1	0.90	0.10	42,42,42,42	0
57	MG	YA	3454	1/1	0.90	0.07	53,53,53,53	0
57	MG	YA	3455	1/1	0.90	0.06	38,38,38,38	0
57	MG	RA	3174	1/1	0.90	0.13	57,57,57,57	0
57	MG	RA	3249	1/1	0.90	0.10	38,38,38,38	0
57	MG	YA	3338	1/1	0.90	0.14	38,38,38,38	0
57	MG	RA	3468	1/1	0.90	0.13	55,55,55,55	0
57	MG	RA	3305	1/1	0.90	0.12	44,44,44,44	0
57	MG	YA	3013	1/1	0.90	0.10	52,52,52,52	0
57	MG	RA	3363	1/1	0.90	0.09	38,38,38,38	0
57	MG	RA	3419	1/1	0.90	0.15	41,41,41,41	0
57	MG	YA	3476	1/1	0.90	0.11	47,47,47,47	0
57	MG	RA	3367	1/1	0.90	0.27	56,56,56,56	0
57	MG	RB	202	1/1	0.90	0.06	57,57,57,57	0
57	MG	RA	3206	1/1	0.90	0.28	71,71,71,71	0
57	MG	YA	3218	1/1	0.90	0.20	99,99,99,99	0
57	MG	QA	1628	1/1	0.90	0.06	52,52,52,52	0
57	MG	YA	3221	1/1	0.90	0.11	59,59,59,59	0
57	MG	YA	3043	1/1	0.90	0.34	38,38,38,38	0
57	MG	RA	3309	1/1	0.90	0.14	59,59,59,59	0
57	MG	RA	3042	1/1	0.90	0.15	38,38,38,38	0
57	MG	QA	1611	1/1	0.90	0.21	38,38,38,38	0
57	MG	YA	3236	1/1	0.90	0.15	38,38,38,38	0
57	MG	YA	3238	1/1	0.90	0.07	38,38,38,38	0
57	MG	YA	3502	1/1	0.90	0.07	45,45,45,45	0
57	MG	RA	3085	1/1	0.90	0.30	38,38,38,38	0
57	MG	YA	3374	1/1	0.90	0.07	38,38,38,38	0
57	MG	YA	3511	1/1	0.90	0.06	41,41,41,41	0
57	MG	RA	3429	1/1	0.90	0.05	38,38,38,38	0
57	MG	RA	3218	1/1	0.90	0.15	57,57,57,57	0
57	MG	YA	3517	1/1	0.90	0.24	38,38,38,38	0
57	MG	RA	3180	1/1	0.90	0.11	77,77,77,77	0
57	MG	YA	3074	1/1	0.90	0.22	38,38,38,38	0
57	MG	RA	3325	1/1	0.90	0.08	54,54,54,54	0
57	MG	XA	1608	1/1	0.90	0.11	38,38,38,38	0
57	MG	QA	1663	1/1	0.90	0.20	65,65,65,65	0
57	MG	YA	3269	1/1	0.90	0.09	57,57,57,57	0
57	MG	RA	3090	1/1	0.90	0.27	38,38,38,38	0
57	MG	RA	3440	1/1	0.90	0.11	51,51,51,51	0
57	MG	YA	3114	1/1	0.90	0.21	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3096	1/1	0.90	0.15	38,38,38,38	0
57	MG	YA	3129	1/1	0.90	0.31	38,38,38,38	0
57	MG	XA	1619	1/1	0.90	0.17	38,38,38,38	0
57	MG	RA	3049	1/1	0.90	0.23	38,38,38,38	0
57	MG	RA	3010	1/1	0.90	0.15	38,38,38,38	0
57	MG	RA	3346	1/1	0.90	0.18	48,48,48,48	0
57	MG	XA	1641	1/1	0.90	0.15	38,38,38,38	0
57	MG	XA	1643	1/1	0.90	0.09	38,38,38,38	0
57	MG	QH	201	1/1	0.90	0.11	60,60,60,60	0
57	MG	XA	1662	1/1	0.90	0.20	64,64,64,64	0
57	MG	YA	3307	1/1	0.90	0.07	38,38,38,38	0
57	MG	RA	3019	1/1	0.90	0.20	38,38,38,38	0
57	MG	QM	201	1/1	0.90	0.15	54,54,54,54	0
57	MG	QA	1619	1/1	0.90	0.07	61,61,61,61	0
57	MG	YA	3176	1/1	0.90	0.10	76,76,76,76	0
57	MG	YA	3182	1/1	0.90	0.21	38,38,38,38	0
57	MG	YA	3184	1/1	0.90	0.15	38,38,38,38	0
57	MG	RA	3354	1/1	0.90	0.08	38,38,38,38	0
57	MG	YA	3189	1/1	0.90	0.11	41,41,41,41	0
57	MG	QA	1624	1/1	0.90	0.06	50,50,50,50	0
57	MG	YA	3193	1/1	0.90	0.16	38,38,38,38	0
57	MG	RA	3300	1/1	0.91	0.14	38,38,38,38	0
57	MG	RA	3065	1/1	0.91	0.09	38,38,38,38	0
57	MG	RA	3165	1/1	0.91	0.12	38,38,38,38	0
57	MG	Y1	101	1/1	0.91	0.07	38,38,38,38	0
57	MG	YA	3180	1/1	0.91	0.09	38,38,38,38	0
57	MG	YA	3313	1/1	0.91	0.28	67,67,67,67	0
57	MG	RA	3222	1/1	0.91	0.09	38,38,38,38	0
57	MG	YA	3004	1/1	0.91	0.24	38,38,38,38	0
57	MG	YA	3316	1/1	0.91	0.06	38,38,38,38	0
57	MG	QA	1621	1/1	0.91	0.17	38,38,38,38	0
57	MG	RA	3088	1/1	0.91	0.17	38,38,38,38	0
57	MG	YA	3321	1/1	0.91	0.12	68,68,68,68	0
57	MG	RA	3420	1/1	0.91	0.12	45,45,45,45	0
57	MG	YA	3192	1/1	0.91	0.11	72,72,72,72	0
57	MG	RA	3261	1/1	0.91	0.23	49,49,49,49	0
57	MG	RA	3313	1/1	0.91	0.11	59,59,59,59	0
57	MG	RA	3142	1/1	0.91	0.14	45,45,45,45	0
57	MG	RA	3371	1/1	0.91	0.17	56,56,56,56	0
57	MG	RA	3316	1/1	0.91	0.19	70,70,70,70	0
57	MG	RA	3373	1/1	0.91	0.09	47,47,47,47	0
57	MG	YA	3467	1/1	0.91	0.09	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RP	202	1/1	0.91	0.22	51,51,51,51	0
57	MG	YA	3031	1/1	0.91	0.20	38,38,38,38	0
57	MG	YA	3340	1/1	0.91	0.23	41,41,41,41	0
57	MG	RA	3230	1/1	0.91	0.14	45,45,45,45	0
57	MG	YA	3034	1/1	0.91	0.26	38,38,38,38	0
57	MG	QA	1622	1/1	0.91	0.06	38,38,38,38	0
57	MG	RT	201	1/1	0.91	0.18	56,56,56,56	0
57	MG	RA	3275	1/1	0.91	0.13	65,65,65,65	0
57	MG	XA	1601	1/1	0.91	0.08	38,38,38,38	0
57	MG	YA	3217	1/1	0.91	0.12	58,58,58,58	0
57	MG	YA	3051	1/1	0.91	0.20	38,38,38,38	0
57	MG	YA	3052	1/1	0.91	0.26	38,38,38,38	0
57	MG	RA	3323	1/1	0.91	0.16	38,38,38,38	0
57	MG	YA	3497	1/1	0.91	0.09	40,40,40,40	0
57	MG	RA	3146	1/1	0.91	0.22	38,38,38,38	0
57	MG	YA	3061	1/1	0.91	0.23	38,38,38,38	0
57	MG	YA	3226	1/1	0.91	0.05	38,38,38,38	0
57	MG	XA	1607	1/1	0.91	0.21	38,38,38,38	0
57	MG	YA	3503	1/1	0.91	0.26	69,69,69,69	0
57	MG	RA	3236	1/1	0.91	0.04	38,38,38,38	0
57	MG	QA	1613	1/1	0.91	0.09	38,38,38,38	0
57	MG	YA	3080	1/1	0.91	0.17	38,38,38,38	0
57	MG	YA	3371	1/1	0.91	0.21	77,77,77,77	0
57	MG	RA	3093	1/1	0.91	0.16	38,38,38,38	0
57	MG	YA	3241	1/1	0.91	0.20	64,64,64,64	0
57	MG	RA	3338	1/1	0.91	0.07	50,50,50,50	0
57	MG	YA	3524	1/1	0.91	0.40	54,54,54,54	0
57	MG	YA	3086	1/1	0.91	0.26	38,38,38,38	0
57	MG	YA	3378	1/1	0.91	0.07	44,44,44,44	0
57	MG	RA	3151	1/1	0.91	0.07	38,38,38,38	0
57	MG	RA	3443	1/1	0.91	0.10	38,38,38,38	0
57	MG	YA	3251	1/1	0.91	0.05	38,38,38,38	0
57	MG	YA	3257	1/1	0.91	0.12	38,38,38,38	0
57	MG	RA	3094	1/1	0.91	0.14	38,38,38,38	0
57	MG	YA	3113	1/1	0.91	0.21	38,38,38,38	0
57	MG	RA	3040	1/1	0.91	0.24	38,38,38,38	0
57	MG	YA	3116	1/1	0.91	0.13	38,38,38,38	0
57	MG	YA	3120	1/1	0.91	0.27	38,38,38,38	0
57	MG	YA	3125	1/1	0.91	0.24	38,38,38,38	0
57	MG	RA	3347	1/1	0.91	0.11	61,61,61,61	0
57	MG	YA	3403	1/1	0.91	0.10	43,43,43,43	0
57	MG	YA	3277	1/1	0.91	0.27	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1660	1/1	0.91	0.13	44,44,44,44	0
57	MG	QA	1654	1/1	0.91	0.06	83,83,83,83	0
57	MG	RA	3191	1/1	0.91	0.42	38,38,38,38	0
57	MG	XA	1655	1/1	0.91	0.07	53,53,53,53	0
57	MG	RA	3407	1/1	0.91	0.09	60,60,60,60	0
57	MG	XA	1664	1/1	0.91	0.05	79,79,79,79	0
57	MG	YA	3145	1/1	0.91	0.14	60,60,60,60	0
57	MG	YA	3419	1/1	0.91	0.06	38,38,38,38	0
57	MG	YA	3420	1/1	0.91	0.08	38,38,38,38	0
57	MG	YY	201	1/1	0.91	0.14	77,77,77,77	0
57	MG	YA	3421	1/1	0.91	0.18	38,38,38,38	0
59	ZN	R6	101	1/1	0.91	0.41	88,88,88,88	0
57	MG	RA	3296	1/1	0.91	0.11	38,38,38,38	0
57	MG	RA	3250	1/1	0.91	0.04	44,44,44,44	0
57	MG	RA	3253	1/1	0.91	0.21	38,38,38,38	0
57	MG	YA	3306	1/1	0.91	0.13	54,54,54,54	0
57	MG	RA	3147	1/1	0.92	0.18	67,67,67,67	0
57	MG	RA	3445	1/1	0.92	0.10	38,38,38,38	0
57	MG	YA	3018	1/1	0.92	0.15	38,38,38,38	0
57	MG	RA	3318	1/1	0.92	0.14	38,38,38,38	0
57	MG	XA	1606	1/1	0.92	0.13	38,38,38,38	0
57	MG	YA	3022	1/1	0.92	0.22	38,38,38,38	0
57	MG	YA	3025	1/1	0.92	0.09	38,38,38,38	0
57	MG	RA	3109	1/1	0.92	0.12	95,95,95,95	0
57	MG	RA	3205	1/1	0.92	0.10	84,84,84,84	0
57	MG	YA	3033	1/1	0.92	0.34	38,38,38,38	0
57	MG	XA	1610	1/1	0.92	0.09	73,73,73,73	0
57	MG	YA	3040	1/1	0.92	0.09	45,45,45,45	0
57	MG	YA	3042	1/1	0.92	0.20	38,38,38,38	0
57	MG	RA	3087	1/1	0.92	0.18	38,38,38,38	0
57	MG	RA	3150	1/1	0.92	0.07	42,42,42,42	0
57	MG	QA	1603	1/1	0.92	0.17	38,38,38,38	0
57	MG	RA	3210	1/1	0.92	0.07	56,56,56,56	0
57	MG	YA	3464	1/1	0.92	0.07	63,63,63,63	0
57	MG	RA	3331	1/1	0.92	0.23	66,66,66,66	0
57	MG	RA	3460	1/1	0.92	0.24	38,38,38,38	0
57	MG	YA	3215	1/1	0.92	0.36	62,62,62,62	0
57	MG	YA	3473	1/1	0.92	0.05	38,38,38,38	0
57	MG	XA	1621	1/1	0.92	0.23	38,38,38,38	0
57	MG	RA	3135	1/1	0.92	0.27	46,46,46,46	0
57	MG	XA	1629	1/1	0.92	0.23	38,38,38,38	0
57	MG	YA	3478	1/1	0.92	0.07	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3062	1/1	0.92	0.14	38,38,38,38	0
57	MG	RA	3377	1/1	0.92	0.33	38,38,38,38	0
57	MG	RA	3464	1/1	0.92	0.08	38,38,38,38	0
57	MG	YA	3223	1/1	0.92	0.12	38,38,38,38	0
57	MG	YA	3487	1/1	0.92	0.06	47,47,47,47	0
57	MG	RA	3336	1/1	0.92	0.07	64,64,64,64	0
57	MG	XA	1644	1/1	0.92	0.14	38,38,38,38	0
57	MG	YA	3227	1/1	0.92	0.09	38,38,38,38	0
57	MG	RA	3153	1/1	0.92	0.12	53,53,53,53	0
57	MG	RA	3340	1/1	0.92	0.06	64,64,64,64	0
57	MG	XA	1656	1/1	0.92	0.10	53,53,53,53	0
57	MG	YA	3366	1/1	0.92	0.13	68,68,68,68	0
57	MG	XA	1660	1/1	0.92	0.08	61,61,61,61	0
57	MG	YA	3370	1/1	0.92	0.21	48,48,48,48	0
57	MG	YA	3095	1/1	0.92	0.15	38,38,38,38	0
57	MG	YA	3372	1/1	0.92	0.09	51,51,51,51	0
57	MG	YA	3098	1/1	0.92	0.15	38,38,38,38	0
57	MG	YA	3099	1/1	0.92	0.24	38,38,38,38	0
57	MG	YA	3100	1/1	0.92	0.20	38,38,38,38	0
57	MG	YA	3246	1/1	0.92	0.29	66,66,66,66	0
57	MG	RA	3187	1/1	0.92	0.19	38,38,38,38	0
57	MG	YA	3379	1/1	0.92	0.15	57,57,57,57	0
57	MG	YA	3521	1/1	0.92	0.10	38,38,38,38	0
57	MG	XA	1663	1/1	0.92	0.04	38,38,38,38	0
57	MG	RA	3479	1/1	0.92	0.09	69,69,69,69	0
57	MG	RA	3136	1/1	0.92	0.14	38,38,38,38	0
57	MG	XA	1671	1/1	0.92	0.06	71,71,71,71	0
57	MG	YA	3529	1/1	0.92	0.12	38,38,38,38	0
57	MG	YA	3530	1/1	0.92	0.20	50,50,50,50	0
57	MG	YA	3389	1/1	0.92	0.13	53,53,53,53	0
57	MG	RA	3047	1/1	0.92	0.10	38,38,38,38	0
57	MG	YA	3393	1/1	0.92	0.23	77,77,77,77	0
57	MG	XE	201	1/1	0.92	0.07	55,55,55,55	0
57	MG	RA	3157	1/1	0.92	0.05	38,38,38,38	0
57	MG	RA	3223	1/1	0.92	0.16	38,38,38,38	0
57	MG	R0	101	1/1	0.92	0.10	38,38,38,38	0
57	MG	RE	302	1/1	0.92	0.17	48,48,48,48	0
57	MG	YA	3138	1/1	0.92	0.18	38,38,38,38	0
57	MG	YA	3402	1/1	0.92	0.08	59,59,59,59	0
57	MG	RA	3433	1/1	0.92	0.10	64,64,64,64	0
57	MG	Y7	101	1/1	0.92	0.10	56,56,56,56	0
57	MG	Y8	101	1/1	0.92	0.18	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3002	1/1	0.92	0.09	38,38,38,38	0
57	MG	YA	3296	1/1	0.92	0.11	38,38,38,38	0
57	MG	YA	3146	1/1	0.92	0.14	38,38,38,38	0
57	MG	YA	3149	1/1	0.92	0.07	38,38,38,38	0
57	MG	YA	3158	1/1	0.92	0.06	38,38,38,38	0
57	MG	YA	3415	1/1	0.92	0.18	38,38,38,38	0
57	MG	RA	3082	1/1	0.92	0.14	38,38,38,38	0
57	MG	RA	3007	1/1	0.92	0.08	38,38,38,38	0
57	MG	RA	3168	1/1	0.92	0.11	38,38,38,38	0
57	MG	RA	3143	1/1	0.92	0.15	51,51,51,51	0
57	MG	RQ	201	1/1	0.92	0.12	38,38,38,38	0
57	MG	RA	3270	1/1	0.92	0.05	84,84,84,84	0
57	MG	RA	3022	1/1	0.92	0.19	38,38,38,38	0
57	MG	YA	3177	1/1	0.92	0.11	38,38,38,38	0
57	MG	YA	3179	1/1	0.92	0.09	38,38,38,38	0
57	MG	RA	3075	1/1	0.92	0.26	38,38,38,38	0
57	MG	RA	3482	1/1	0.93	0.13	38,38,38,38	0
57	MG	YA	3055	1/1	0.93	0.19	38,38,38,38	0
57	MG	YA	3446	1/1	0.93	0.11	38,38,38,38	0
57	MG	RA	3333	1/1	0.93	0.12	47,47,47,47	0
57	MG	YA	3325	1/1	0.93	0.12	38,38,38,38	0
57	MG	XA	1658	1/1	0.93	0.07	50,50,50,50	0
57	MG	YA	3327	1/1	0.93	0.06	38,38,38,38	0
57	MG	RA	3335	1/1	0.93	0.14	38,38,38,38	0
57	MG	XA	1661	1/1	0.93	0.05	63,63,63,63	0
57	MG	QA	1606	1/1	0.93	0.09	77,77,77,77	0
57	MG	YA	3207	1/1	0.93	0.11	49,49,49,49	0
57	MG	RA	3337	1/1	0.93	0.19	91,91,91,91	0
57	MG	YA	3076	1/1	0.93	0.09	38,38,38,38	0
57	MG	QA	1612	1/1	0.93	0.09	52,52,52,52	0
57	MG	XA	1665	1/1	0.93	0.21	38,38,38,38	0
57	MG	RA	3432	1/1	0.93	0.05	66,66,66,66	0
57	MG	QA	1659	1/1	0.93	0.07	38,38,38,38	0
57	MG	RA	3048	1/1	0.93	0.15	38,38,38,38	0
57	MG	YA	3090	1/1	0.93	0.17	38,38,38,38	0
57	MG	YA	3347	1/1	0.93	0.12	38,38,38,38	0
57	MG	RA	3100	1/1	0.93	0.42	96,96,96,96	0
57	MG	RA	3345	1/1	0.93	0.05	38,38,38,38	0
57	MG	QA	1635	1/1	0.93	0.15	63,63,63,63	0
57	MG	RA	3235	1/1	0.93	0.11	38,38,38,38	0
57	MG	YA	3101	1/1	0.93	0.12	38,38,38,38	0
57	MG	YA	3482	1/1	0.93	0.14	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3348	1/1	0.93	0.12	39,39,39,39	0
57	MG	YA	3103	1/1	0.93	0.13	38,38,38,38	0
57	MG	YA	3228	1/1	0.93	0.15	38,38,38,38	0
57	MG	RR	201	1/1	0.93	0.08	38,38,38,38	0
57	MG	YA	3109	1/1	0.93	0.09	38,38,38,38	0
57	MG	YA	3112	1/1	0.93	0.14	38,38,38,38	0
57	MG	YA	3237	1/1	0.93	0.12	38,38,38,38	0
57	MG	RA	3183	1/1	0.93	0.09	65,65,65,65	0
57	MG	YA	3495	1/1	0.93	0.08	40,40,40,40	0
57	MG	RA	3237	1/1	0.93	0.18	52,52,52,52	0
57	MG	RA	3103	1/1	0.93	0.17	38,38,38,38	0
57	MG	XA	1602	1/1	0.93	0.16	47,47,47,47	0
57	MG	XA	1603	1/1	0.93	0.22	38,38,38,38	0
57	MG	YA	3500	1/1	0.93	0.17	38,38,38,38	0
57	MG	YA	3245	1/1	0.93	0.08	39,39,39,39	0
57	MG	RA	3312	1/1	0.93	0.09	53,53,53,53	0
57	MG	YA	3247	1/1	0.93	0.23	38,38,38,38	0
57	MG	YA	3506	1/1	0.93	0.11	101,101,101,101	0
57	MG	RA	3107	1/1	0.93	0.14	38,38,38,38	0
57	MG	YA	3130	1/1	0.93	0.23	38,38,38,38	0
57	MG	YA	3131	1/1	0.93	0.18	38,38,38,38	0
57	MG	RA	3278	1/1	0.93	0.05	43,43,43,43	0
57	MG	YA	3011	1/1	0.93	0.11	81,81,81,81	0
57	MG	RA	3209	1/1	0.93	0.08	39,39,39,39	0
57	MG	RA	3030	1/1	0.93	0.41	38,38,38,38	0
57	MG	YA	3388	1/1	0.93	0.07	61,61,61,61	0
57	MG	XA	1609	1/1	0.93	0.10	38,38,38,38	0
57	MG	RA	3012	1/1	0.93	0.27	38,38,38,38	0
57	MG	YA	3271	1/1	0.93	0.21	38,38,38,38	0
57	MG	RA	3319	1/1	0.93	0.13	38,38,38,38	0
57	MG	RA	3282	1/1	0.93	0.07	38,38,38,38	0
57	MG	YA	3275	1/1	0.93	0.16	38,38,38,38	0
57	MG	XA	1613	1/1	0.93	0.08	38,38,38,38	0
57	MG	YA	3154	1/1	0.93	0.10	49,49,49,49	0
57	MG	YA	3155	1/1	0.93	0.07	38,38,38,38	0
57	MG	YB	205	1/1	0.93	0.06	38,38,38,38	0
57	MG	RA	3284	1/1	0.93	0.15	38,38,38,38	0
57	MG	YA	3021	1/1	0.93	0.18	43,43,43,43	0
57	MG	RA	3161	1/1	0.93	0.06	38,38,38,38	0
57	MG	RA	3058	1/1	0.93	0.20	38,38,38,38	0
57	MG	YA	3030	1/1	0.93	0.26	38,38,38,38	0
57	MG	QA	1639	1/1	0.93	0.14	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3465	1/1	0.93	0.06	38,38,38,38	0
57	MG	YA	3302	1/1	0.93	0.11	38,38,38,38	0
57	MG	YA	3412	1/1	0.93	0.07	38,38,38,38	0
57	MG	RA	3017	1/1	0.93	0.18	38,38,38,38	0
57	MG	YA	3414	1/1	0.93	0.09	38,38,38,38	0
57	MG	RA	3330	1/1	0.93	0.10	38,38,38,38	0
57	MG	YA	3037	1/1	0.93	0.20	38,38,38,38	0
57	MG	RA	3018	1/1	0.93	0.18	38,38,38,38	0
57	MG	XA	1635	1/1	0.93	0.14	38,38,38,38	0
57	MG	YA	3183	1/1	0.93	0.14	86,86,86,86	0
57	MG	RA	3474	1/1	0.93	0.10	38,38,38,38	0
57	MG	YA	3186	1/1	0.93	0.17	58,58,58,58	0
57	MG	YA	3312	1/1	0.93	0.20	38,38,38,38	0
57	MG	RA	3475	1/1	0.93	0.07	65,65,65,65	0
57	MG	RA	3375	1/1	0.93	0.09	47,47,47,47	0
57	MG	QA	1625	1/1	0.93	0.10	58,58,58,58	0
57	MG	YA	3050	1/1	0.93	0.26	38,38,38,38	0
57	MG	XA	1646	1/1	0.93	0.24	38,38,38,38	0
57	MG	XA	1653	1/1	0.93	0.09	58,58,58,58	0
57	MG	QA	1607	1/1	0.94	0.09	38,38,38,38	0
57	MG	YA	3205	1/1	0.94	0.05	81,81,81,81	0
57	MG	YA	3206	1/1	0.94	0.09	38,38,38,38	0
57	MG	RA	3072	1/1	0.94	0.25	38,38,38,38	0
57	MG	RA	3200	1/1	0.94	0.11	38,38,38,38	0
57	MG	RA	3043	1/1	0.94	0.22	38,38,38,38	0
57	MG	XQ	201	1/1	0.94	0.07	65,65,65,65	0
57	MG	YA	3093	1/1	0.94	0.22	38,38,38,38	0
57	MG	RA	3102	1/1	0.94	0.16	38,38,38,38	0
57	MG	RA	3438	1/1	0.94	0.09	45,45,45,45	0
57	MG	RA	3003	1/1	0.94	0.07	38,38,38,38	0
57	MG	RA	3045	1/1	0.94	0.13	38,38,38,38	0
57	MG	RA	3290	1/1	0.94	0.09	38,38,38,38	0
57	MG	QA	1638	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3459	1/1	0.94	0.23	38,38,38,38	0
57	MG	RA	3145	1/1	0.94	0.05	38,38,38,38	0
57	MG	RA	3388	1/1	0.94	0.07	46,46,46,46	0
57	MG	YA	3224	1/1	0.94	0.13	51,51,51,51	0
57	MG	YA	3107	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3005	1/1	0.94	0.07	58,58,58,58	0
57	MG	YA	3470	1/1	0.94	0.12	42,42,42,42	0
57	MG	RA	3293	1/1	0.94	0.16	42,42,42,42	0
57	MG	RA	3394	1/1	0.94	0.05	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3229	1/1	0.94	0.06	38,38,38,38	0
57	MG	RA	3248	1/1	0.94	0.07	38,38,38,38	0
57	MG	YA	3009	1/1	0.94	0.06	38,38,38,38	0
57	MG	YA	3118	1/1	0.94	0.13	38,38,38,38	0
57	MG	YA	3119	1/1	0.94	0.19	38,38,38,38	0
57	MG	RA	3178	1/1	0.94	0.05	54,54,54,54	0
57	MG	QA	1626	1/1	0.94	0.15	59,59,59,59	0
57	MG	YA	3484	1/1	0.94	0.06	47,47,47,47	0
57	MG	YA	3358	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3126	1/1	0.94	0.11	38,38,38,38	0
57	MG	RA	3251	1/1	0.94	0.05	62,62,62,62	0
57	MG	RA	3401	1/1	0.94	0.15	57,57,57,57	0
57	MG	YA	3015	1/1	0.94	0.08	38,38,38,38	0
57	MG	XA	1614	1/1	0.94	0.08	38,38,38,38	0
57	MG	YA	3368	1/1	0.94	0.11	43,43,43,43	0
57	MG	YA	3369	1/1	0.94	0.14	53,53,53,53	0
57	MG	RA	3402	1/1	0.94	0.09	38,38,38,38	0
57	MG	XA	1616	1/1	0.94	0.05	51,51,51,51	0
57	MG	RA	3115	1/1	0.94	0.09	40,40,40,40	0
57	MG	RA	3181	1/1	0.94	0.09	38,38,38,38	0
57	MG	RA	3116	1/1	0.94	0.22	38,38,38,38	0
57	MG	QA	1640	1/1	0.94	0.05	77,77,77,77	0
57	MG	QA	1623	1/1	0.94	0.10	62,62,62,62	0
57	MG	YA	3027	1/1	0.94	0.19	38,38,38,38	0
57	MG	YA	3505	1/1	0.94	0.05	47,47,47,47	0
57	MG	RA	3410	1/1	0.94	0.15	57,57,57,57	0
57	MG	YA	3507	1/1	0.94	0.07	40,40,40,40	0
57	MG	RA	3308	1/1	0.94	0.09	38,38,38,38	0
57	MG	QA	1630	1/1	0.94	0.22	38,38,38,38	0
57	MG	XA	1638	1/1	0.94	0.05	48,48,48,48	0
57	MG	YA	3384	1/1	0.94	0.05	60,60,60,60	0
57	MG	RA	3470	1/1	0.94	0.11	38,38,38,38	0
57	MG	YA	3515	1/1	0.94	0.18	38,38,38,38	0
57	MG	YA	3163	1/1	0.94	0.09	41,41,41,41	0
57	MG	YA	3520	1/1	0.94	0.18	38,38,38,38	0
57	MG	RA	3031	1/1	0.94	0.20	38,38,38,38	0
57	MG	YA	3278	1/1	0.94	0.11	38,38,38,38	0
57	MG	YA	3523	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3391	1/1	0.94	0.17	38,38,38,38	0
57	MG	YA	3279	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3038	1/1	0.94	0.16	38,38,38,38	0
57	MG	YA	3285	1/1	0.94	0.07	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3262	1/1	0.94	0.12	40,40,40,40	0
57	MG	YA	3288	1/1	0.94	0.04	38,38,38,38	0
57	MG	YA	3537	1/1	0.94	0.13	38,38,38,38	0
57	MG	YB	201	1/1	0.94	0.10	88,88,88,88	0
57	MG	YA	3041	1/1	0.94	0.16	38,38,38,38	0
57	MG	RA	3263	1/1	0.94	0.16	48,48,48,48	0
57	MG	YA	3293	1/1	0.94	0.13	38,38,38,38	0
57	MG	YA	3294	1/1	0.94	0.11	38,38,38,38	0
57	MG	RA	3086	1/1	0.94	0.09	38,38,38,38	0
57	MG	XA	1650	1/1	0.94	0.04	43,43,43,43	0
57	MG	QA	1631	1/1	0.94	0.04	68,68,68,68	0
57	MG	YA	3048	1/1	0.94	0.12	38,38,38,38	0
57	MG	YA	3181	1/1	0.94	0.17	38,38,38,38	0
57	MG	YB	211	1/1	0.94	0.04	72,72,72,72	0
57	MG	XA	1654	1/1	0.94	0.05	45,45,45,45	0
57	MG	RA	3361	1/1	0.94	0.07	56,56,56,56	0
57	MG	RA	3060	1/1	0.94	0.14	38,38,38,38	0
57	MG	QV	101	1/1	0.94	0.07	38,38,38,38	0
57	MG	YE	303	1/1	0.94	0.21	40,40,40,40	0
57	MG	RA	3273	1/1	0.94	0.06	38,38,38,38	0
57	MG	QA	1610	1/1	0.94	0.10	38,38,38,38	0
57	MG	RA	3232	1/1	0.94	0.09	38,38,38,38	0
57	MG	RA	3370	1/1	0.94	0.09	38,38,38,38	0
57	MG	QA	1664	1/1	0.94	0.25	38,38,38,38	0
57	MG	YA	3066	1/1	0.94	0.17	38,38,38,38	0
57	MG	YQ	203	1/1	0.94	0.09	38,38,38,38	0
57	MG	RA	3068	1/1	0.94	0.18	38,38,38,38	0
57	MG	YA	3425	1/1	0.94	0.09	75,75,75,75	0
57	MG	XA	1667	1/1	0.94	0.09	66,66,66,66	0
57	MG	YA	3431	1/1	0.94	0.13	58,58,58,58	0
57	MG	XA	1668	1/1	0.94	0.26	38,38,38,38	0
57	MG	RA	3326	1/1	0.94	0.05	94,94,94,94	0
57	MG	YA	3318	1/1	0.94	0.07	38,38,38,38	0
57	MG	YA	3077	1/1	0.94	0.17	38,38,38,38	0
57	MG	YA	3439	1/1	0.94	0.18	38,38,38,38	0
57	MG	RA	3374	1/1	0.94	0.05	77,77,77,77	0
57	MG	RA	3013	1/1	0.95	0.19	38,38,38,38	0
57	MG	YA	3442	1/1	0.95	0.06	38,38,38,38	0
57	MG	RA	3416	1/1	0.95	0.06	38,38,38,38	0
57	MG	RA	3164	1/1	0.95	0.04	38,38,38,38	0
57	MG	YA	3067	1/1	0.95	0.15	38,38,38,38	0
57	MG	RA	3080	1/1	0.95	0.23	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3365	1/1	0.95	0.09	77,77,77,77	0
57	MG	YA	3073	1/1	0.95	0.09	48,48,48,48	0
57	MG	YA	3198	1/1	0.95	0.04	39,39,39,39	0
57	MG	XA	1666	1/1	0.95	0.04	38,38,38,38	0
57	MG	YA	3075	1/1	0.95	0.05	38,38,38,38	0
57	MG	YA	3324	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3320	1/1	0.95	0.11	56,56,56,56	0
57	MG	RA	3167	1/1	0.95	0.04	38,38,38,38	0
57	MG	YA	3078	1/1	0.95	0.15	38,38,38,38	0
57	MG	RB	206	1/1	0.95	0.04	79,79,79,79	0
57	MG	RB	207	1/1	0.95	0.06	47,47,47,47	0
57	MG	YA	3208	1/1	0.95	0.06	55,55,55,55	0
57	MG	YA	3461	1/1	0.95	0.05	47,47,47,47	0
57	MG	YA	3462	1/1	0.95	0.12	73,73,73,73	0
57	MG	YA	3333	1/1	0.95	0.11	38,38,38,38	0
57	MG	RE	301	1/1	0.95	0.13	38,38,38,38	0
57	MG	YA	3465	1/1	0.95	0.10	54,54,54,54	0
57	MG	YA	3084	1/1	0.95	0.07	38,38,38,38	0
57	MG	RA	3034	1/1	0.95	0.15	38,38,38,38	0
57	MG	YA	3468	1/1	0.95	0.11	38,38,38,38	0
57	MG	XK	201	1/1	0.95	0.05	55,55,55,55	0
57	MG	RA	3140	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3092	1/1	0.95	0.11	38,38,38,38	0
57	MG	RA	3324	1/1	0.95	0.10	38,38,38,38	0
57	MG	RA	3172	1/1	0.95	0.07	43,43,43,43	0
57	MG	YA	3096	1/1	0.95	0.09	38,38,38,38	0
57	MG	YA	3220	1/1	0.95	0.10	38,38,38,38	0
57	MG	RA	3283	1/1	0.95	0.15	38,38,38,38	0
57	MG	YA	3481	1/1	0.95	0.05	65,65,65,65	0
57	MG	RA	3327	1/1	0.95	0.12	38,38,38,38	0
57	MG	RA	3054	1/1	0.95	0.11	38,38,38,38	0
57	MG	RA	3002	1/1	0.95	0.05	38,38,38,38	0
57	MG	RA	3114	1/1	0.95	0.20	58,58,58,58	0
57	MG	YA	3001	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3036	1/1	0.95	0.12	38,38,38,38	0
57	MG	RA	3288	1/1	0.95	0.16	38,38,38,38	0
57	MG	YA	3489	1/1	0.95	0.12	47,47,47,47	0
57	MG	RA	3435	1/1	0.95	0.09	46,46,46,46	0
57	MG	QA	1673	1/1	0.95	0.05	54,54,54,54	0
57	MG	YA	3361	1/1	0.95	0.36	85,85,85,85	0
57	MG	YA	3494	1/1	0.95	0.14	38,38,38,38	0
57	MG	YA	3231	1/1	0.95	0.06	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3232	1/1	0.95	0.07	38,38,38,38	0
57	MG	RA	3334	1/1	0.95	0.21	54,54,54,54	0
57	MG	QA	1642	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3118	1/1	0.95	0.11	38,38,38,38	0
57	MG	RA	3386	1/1	0.95	0.06	38,38,38,38	0
57	MG	RA	3213	1/1	0.95	0.09	73,73,73,73	0
57	MG	RA	3252	1/1	0.95	0.11	38,38,38,38	0
57	MG	RA	3389	1/1	0.95	0.06	38,38,38,38	0
57	MG	RA	3390	1/1	0.95	0.06	38,38,38,38	0
57	MG	QA	1636	1/1	0.95	0.05	38,38,38,38	0
57	MG	RA	3393	1/1	0.95	0.07	41,41,41,41	0
57	MG	RA	3448	1/1	0.95	0.06	84,84,84,84	0
57	MG	RA	3216	1/1	0.95	0.18	38,38,38,38	0
57	MG	RA	3064	1/1	0.95	0.13	38,38,38,38	0
57	MG	YA	3133	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3255	1/1	0.95	0.10	38,38,38,38	0
57	MG	RA	3219	1/1	0.95	0.11	38,38,38,38	0
57	MG	YA	3259	1/1	0.95	0.17	38,38,38,38	0
57	MG	RA	3301	1/1	0.95	0.09	38,38,38,38	0
57	MG	YA	3385	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3139	1/1	0.95	0.18	65,65,65,65	0
57	MG	YA	3263	1/1	0.95	0.04	38,38,38,38	0
57	MG	YA	3264	1/1	0.95	0.24	38,38,38,38	0
57	MG	QA	1665	1/1	0.95	0.04	47,47,47,47	0
57	MG	YA	3527	1/1	0.95	0.11	53,53,53,53	0
57	MG	YA	3023	1/1	0.95	0.22	38,38,38,38	0
57	MG	YA	3392	1/1	0.95	0.05	38,38,38,38	0
57	MG	RA	3021	1/1	0.95	0.14	38,38,38,38	0
57	MG	YA	3144	1/1	0.95	0.06	38,38,38,38	0
57	MG	YA	3536	1/1	0.95	0.06	38,38,38,38	0
57	MG	YA	3272	1/1	0.95	0.17	38,38,38,38	0
57	MG	RA	3127	1/1	0.95	0.15	38,38,38,38	0
57	MG	RA	3458	1/1	0.95	0.22	38,38,38,38	0
57	MG	YA	3147	1/1	0.95	0.10	51,51,51,51	0
57	MG	RA	3403	1/1	0.95	0.17	38,38,38,38	0
57	MG	YA	3401	1/1	0.95	0.22	38,38,38,38	0
57	MG	QA	1632	1/1	0.95	0.11	59,59,59,59	0
57	MG	RA	3462	1/1	0.95	0.08	38,38,38,38	0
57	MG	XA	1636	1/1	0.95	0.09	38,38,38,38	0
57	MG	QA	1616	1/1	0.95	0.12	38,38,38,38	0
57	MG	YA	3161	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3264	1/1	0.95	0.06	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1609	1/1	0.95	0.21	38,38,38,38	0
57	MG	RA	3408	1/1	0.95	0.13	38,38,38,38	0
57	MG	RA	3098	1/1	0.95	0.09	38,38,38,38	0
57	MG	YA	3169	1/1	0.95	0.17	38,38,38,38	0
57	MG	YD	303	1/1	0.95	0.05	38,38,38,38	0
57	MG	RA	3469	1/1	0.95	0.10	66,66,66,66	0
57	MG	XA	1647	1/1	0.95	0.12	42,42,42,42	0
57	MG	YA	3172	1/1	0.95	0.20	86,86,86,86	0
57	MG	YA	3417	1/1	0.95	0.09	44,44,44,44	0
57	MG	RA	3028	1/1	0.95	0.06	38,38,38,38	0
57	MG	YA	3300	1/1	0.95	0.11	38,38,38,38	0
57	MG	XA	1651	1/1	0.95	0.12	38,38,38,38	0
57	MG	XA	1652	1/1	0.95	0.05	99,99,99,99	0
57	MG	RA	3159	1/1	0.95	0.22	38,38,38,38	0
57	MG	RA	3473	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3315	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3428	1/1	0.95	0.06	64,64,64,64	0
57	MG	RA	3359	1/1	0.95	0.09	38,38,38,38	0
57	MG	YA	3054	1/1	0.95	0.19	38,38,38,38	0
57	MG	RA	3476	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3187	1/1	0.95	0.07	38,38,38,38	0
59	ZN	Y5	101	1/1	0.95	0.22	94,94,94,94	0
57	MG	YA	3056	1/1	0.95	0.11	38,38,38,38	0
57	MG	QA	1641	1/1	0.95	0.07	62,62,62,62	0
57	MG	QA	1634	1/1	0.96	0.10	38,38,38,38	0
57	MG	YA	3373	1/1	0.96	0.07	38,38,38,38	0
57	MG	YA	3472	1/1	0.96	0.07	70,70,70,70	0
57	MG	RA	3233	1/1	0.96	0.15	64,64,64,64	0
57	MG	RQ	202	1/1	0.96	0.10	49,49,49,49	0
57	MG	YA	3108	1/1	0.96	0.13	38,38,38,38	0
57	MG	RA	3271	1/1	0.96	0.10	38,38,38,38	0
57	MG	YA	3477	1/1	0.96	0.15	65,65,65,65	0
57	MG	YA	3199	1/1	0.96	0.23	38,38,38,38	0
57	MG	RA	3272	1/1	0.96	0.09	38,38,38,38	0
57	MG	RA	3163	1/1	0.96	0.06	42,42,42,42	0
57	MG	RA	3108	1/1	0.96	0.10	79,79,79,79	0
57	MG	YA	3115	1/1	0.96	0.07	38,38,38,38	0
57	MG	YA	3039	1/1	0.96	0.27	38,38,38,38	0
57	MG	YA	3117	1/1	0.96	0.14	38,38,38,38	0
57	MG	RA	3023	1/1	0.96	0.06	38,38,38,38	0
57	MG	YA	3387	1/1	0.96	0.04	38,38,38,38	0
57	MG	QA	1620	1/1	0.96	0.06	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3112	1/1	0.96	0.11	38,38,38,38	0
57	MG	YA	3121	1/1	0.96	0.04	38,38,38,38	0
57	MG	YA	3303	1/1	0.96	0.07	38,38,38,38	0
57	MG	YA	3122	1/1	0.96	0.08	38,38,38,38	0
57	MG	RA	3113	1/1	0.96	0.17	38,38,38,38	0
57	MG	RA	3241	1/1	0.96	0.25	38,38,38,38	0
57	MG	YA	3045	1/1	0.96	0.34	38,38,38,38	0
57	MG	YA	3128	1/1	0.96	0.10	44,44,44,44	0
57	MG	R3	101	1/1	0.96	0.06	43,43,43,43	0
57	MG	YA	3047	1/1	0.96	0.05	38,38,38,38	0
57	MG	RA	3027	1/1	0.96	0.16	38,38,38,38	0
57	MG	QA	1618	1/1	0.96	0.07	38,38,38,38	0
57	MG	RA	3029	1/1	0.96	0.15	38,38,38,38	0
57	MG	QA	1650	1/1	0.96	0.07	55,55,55,55	0
57	MG	RA	3466	1/1	0.96	0.14	38,38,38,38	0
57	MG	QA	1651	1/1	0.96	0.04	41,41,41,41	0
57	MG	RA	3120	1/1	0.96	0.08	45,45,45,45	0
57	MG	YA	3407	1/1	0.96	0.17	54,54,54,54	0
57	MG	RA	3032	1/1	0.96	0.12	38,38,38,38	0
57	MG	YA	3510	1/1	0.96	0.04	46,46,46,46	0
57	MG	RA	3077	1/1	0.96	0.17	38,38,38,38	0
57	MG	YA	3059	1/1	0.96	0.09	38,38,38,38	0
57	MG	Y0	102	1/1	0.96	0.23	38,38,38,38	0
57	MG	QA	1602	1/1	0.96	0.16	38,38,38,38	0
57	MG	YA	3516	1/1	0.96	0.30	38,38,38,38	0
57	MG	RA	3125	1/1	0.96	0.20	38,38,38,38	0
57	MG	YA	3518	1/1	0.96	0.23	38,38,38,38	0
57	MG	YA	3519	1/1	0.96	0.32	38,38,38,38	0
57	MG	YA	3233	1/1	0.96	0.05	38,38,38,38	0
57	MG	YA	3234	1/1	0.96	0.06	38,38,38,38	0
57	MG	YA	3063	1/1	0.96	0.08	38,38,38,38	0
57	MG	YA	3418	1/1	0.96	0.13	38,38,38,38	0
57	MG	YA	3064	1/1	0.96	0.18	38,38,38,38	0
57	MG	YA	3065	1/1	0.96	0.19	38,38,38,38	0
57	MG	YA	3526	1/1	0.96	0.15	41,41,41,41	0
57	MG	RA	3294	1/1	0.96	0.10	38,38,38,38	0
57	MG	YA	3331	1/1	0.96	0.06	91,91,91,91	0
57	MG	YA	3332	1/1	0.96	0.06	54,54,54,54	0
57	MG	RA	3184	1/1	0.96	0.09	38,38,38,38	0
57	MG	YA	3531	1/1	0.96	0.07	56,56,56,56	0
57	MG	YA	3240	1/1	0.96	0.07	38,38,38,38	0
57	MG	RA	3126	1/1	0.96	0.10	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3429	1/1	0.96	0.06	45,45,45,45	0
57	MG	YA	3430	1/1	0.96	0.04	41,41,41,41	0
57	MG	RA	3297	1/1	0.96	0.08	38,38,38,38	0
57	MG	RA	3339	1/1	0.96	0.14	38,38,38,38	0
57	MG	XA	1630	1/1	0.96	0.12	38,38,38,38	0
57	MG	YA	3341	1/1	0.96	0.16	38,38,38,38	0
57	MG	YA	3167	1/1	0.96	0.04	38,38,38,38	0
57	MG	QA	1643	1/1	0.96	0.24	38,38,38,38	0
57	MG	YA	3440	1/1	0.96	0.06	38,38,38,38	0
57	MG	YA	3344	1/1	0.96	0.09	38,38,38,38	0
57	MG	RA	3257	1/1	0.96	0.09	38,38,38,38	0
57	MG	RA	3258	1/1	0.96	0.11	38,38,38,38	0
57	MG	RA	3154	1/1	0.96	0.11	38,38,38,38	0
57	MG	YA	3252	1/1	0.96	0.08	38,38,38,38	0
57	MG	YA	3254	1/1	0.96	0.09	38,38,38,38	0
57	MG	YA	3010	1/1	0.96	0.06	90,90,90,90	0
57	MG	YA	3175	1/1	0.96	0.11	38,38,38,38	0
57	MG	YE	301	1/1	0.96	0.15	38,38,38,38	0
57	MG	XA	1639	1/1	0.96	0.12	38,38,38,38	0
57	MG	XA	1640	1/1	0.96	0.04	38,38,38,38	0
57	MG	RA	3055	1/1	0.96	0.11	38,38,38,38	0
57	MG	XA	1642	1/1	0.96	0.06	43,43,43,43	0
57	MG	RA	3226	1/1	0.96	0.14	38,38,38,38	0
57	MG	YA	3266	1/1	0.96	0.14	38,38,38,38	0
57	MG	YA	3359	1/1	0.96	0.06	38,38,38,38	0
57	MG	QA	1644	1/1	0.96	0.06	59,59,59,59	0
57	MG	YR	201	1/1	0.96	0.16	38,38,38,38	0
57	MG	YA	3458	1/1	0.96	0.04	38,38,38,38	0
57	MG	RA	3130	1/1	0.96	0.05	48,48,48,48	0
57	MG	QA	1666	1/1	0.96	0.07	43,43,43,43	0
57	MG	RA	3265	1/1	0.96	0.16	38,38,38,38	0
58	SF4	XD	301	8/8	0.96	0.09	88,97,160,164	0
59	ZN	QN	101	1/1	0.96	0.09	94,94,94,94	0
57	MG	YA	3365	1/1	0.96	0.11	49,49,49,49	0
57	MG	XA	1649	1/1	0.96	0.05	60,60,60,60	0
57	MG	RE	303	1/1	0.96	0.08	38,38,38,38	0
57	MG	RA	3399	1/1	0.96	0.12	38,38,38,38	0
59	ZN	XN	101	1/1	0.96	0.06	134,134,134,134	0
59	ZN	Y4	101	1/1	0.96	0.30	88,88,88,88	0
57	MG	RA	3132	1/1	0.96	0.19	38,38,38,38	0
57	MG	RA	3311	1/1	0.96	0.05	50,50,50,50	0
57	MG	RA	3106	1/1	0.96	0.08	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3026	1/1	0.97	0.14	38,38,38,38	0
57	MG	QA	1627	1/1	0.97	0.09	53,53,53,53	0
57	MG	YA	3281	1/1	0.97	0.18	49,49,49,49	0
57	MG	YA	3029	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3480	1/1	0.97	0.07	44,44,44,44	0
57	MG	RA	3095	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3286	1/1	0.97	0.10	38,38,38,38	0
57	MG	YA	3191	1/1	0.97	0.13	38,38,38,38	0
57	MG	YA	3383	1/1	0.97	0.10	52,52,52,52	0
57	MG	RA	3447	1/1	0.97	0.05	38,38,38,38	0
57	MG	YA	3289	1/1	0.97	0.26	38,38,38,38	0
57	MG	YA	3104	1/1	0.97	0.06	42,42,42,42	0
57	MG	RA	3051	1/1	0.97	0.16	38,38,38,38	0
57	MG	XA	1657	1/1	0.97	0.05	38,38,38,38	0
57	MG	RA	3097	1/1	0.97	0.04	38,38,38,38	0
57	MG	YA	3491	1/1	0.97	0.19	38,38,38,38	0
57	MG	YA	3036	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3111	1/1	0.97	0.14	38,38,38,38	0
57	MG	RA	3074	1/1	0.97	0.12	38,38,38,38	0
57	MG	YA	3200	1/1	0.97	0.04	38,38,38,38	0
57	MG	YA	3394	1/1	0.97	0.05	38,38,38,38	0
57	MG	RA	3212	1/1	0.97	0.04	54,54,54,54	0
57	MG	RA	3099	1/1	0.97	0.06	38,38,38,38	0
57	MG	RA	3052	1/1	0.97	0.05	38,38,38,38	0
57	MG	RA	3182	1/1	0.97	0.14	47,47,47,47	0
57	MG	RA	3289	1/1	0.97	0.18	38,38,38,38	0
57	MG	RA	3457	1/1	0.97	0.16	38,38,38,38	0
57	MG	RA	3026	1/1	0.97	0.15	38,38,38,38	0
57	MG	YA	3504	1/1	0.97	0.08	66,66,66,66	0
57	MG	QA	1615	1/1	0.97	0.04	38,38,38,38	0
57	MG	RA	3039	1/1	0.97	0.12	38,38,38,38	0
57	MG	XA	1670	1/1	0.97	0.10	38,38,38,38	0
57	MG	YA	3123	1/1	0.97	0.05	38,38,38,38	0
57	MG	YA	3213	1/1	0.97	0.04	38,38,38,38	0
57	MG	RA	3104	1/1	0.97	0.04	38,38,38,38	0
57	MG	QA	1648	1/1	0.97	0.04	44,44,44,44	0
57	MG	RA	3041	1/1	0.97	0.15	38,38,38,38	0
57	MG	YA	3513	1/1	0.97	0.09	38,38,38,38	0
57	MG	RA	3225	1/1	0.97	0.28	38,38,38,38	0
57	MG	QA	1637	1/1	0.97	0.06	38,38,38,38	0
57	MG	QA	1629	1/1	0.97	0.05	38,38,38,38	0
57	MG	QA	1614	1/1	0.97	0.05	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3137	1/1	0.97	0.08	38,38,38,38	0
57	MG	RA	3379	1/1	0.97	0.03	38,38,38,38	0
57	MG	YA	3058	1/1	0.97	0.11	38,38,38,38	0
57	MG	YA	3137	1/1	0.97	0.27	38,38,38,38	0
57	MG	RA	3063	1/1	0.97	0.15	38,38,38,38	0
57	MG	XA	1618	1/1	0.97	0.04	38,38,38,38	0
57	MG	RA	3381	1/1	0.97	0.10	38,38,38,38	0
57	MG	YA	3422	1/1	0.97	0.04	55,55,55,55	0
57	MG	YA	3141	1/1	0.97	0.13	50,50,50,50	0
57	MG	RA	3011	1/1	0.97	0.06	38,38,38,38	0
57	MG	RA	3303	1/1	0.97	0.07	38,38,38,38	0
57	MG	RA	3033	1/1	0.97	0.11	38,38,38,38	0
57	MG	XA	1627	1/1	0.97	0.09	38,38,38,38	0
57	MG	XA	1628	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3533	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3534	1/1	0.97	0.12	38,38,38,38	0
57	MG	RA	3342	1/1	0.97	0.18	51,51,51,51	0
57	MG	YA	3148	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3068	1/1	0.97	0.22	38,38,38,38	0
57	MG	YA	3538	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3150	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3434	1/1	0.97	0.27	62,62,62,62	0
57	MG	YA	3153	1/1	0.97	0.05	38,38,38,38	0
57	MG	QA	1667	1/1	0.97	0.04	38,38,38,38	0
57	MG	YA	3438	1/1	0.97	0.13	75,75,75,75	0
57	MG	XA	1632	1/1	0.97	0.08	38,38,38,38	0
57	MG	YA	3157	1/1	0.97	0.07	38,38,38,38	0
57	MG	YA	3071	1/1	0.97	0.22	38,38,38,38	0
57	MG	YA	3072	1/1	0.97	0.08	38,38,38,38	0
57	MG	RA	3481	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3162	1/1	0.97	0.16	38,38,38,38	0
57	MG	RA	3344	1/1	0.97	0.10	38,38,38,38	0
57	MG	YA	3348	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3164	1/1	0.97	0.19	38,38,38,38	0
57	MG	YA	3249	1/1	0.97	0.23	38,38,38,38	0
57	MG	RA	3169	1/1	0.97	0.04	63,63,63,63	0
57	MG	RA	3170	1/1	0.97	0.04	38,38,38,38	0
57	MG	YE	302	1/1	0.97	0.07	38,38,38,38	0
57	MG	RA	3434	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3452	1/1	0.97	0.04	38,38,38,38	0
57	MG	YA	3253	1/1	0.97	0.21	38,38,38,38	0
57	MG	RA	3069	1/1	0.97	0.09	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3079	1/1	0.97	0.09	56,56,56,56	0
57	MG	RB	204	1/1	0.97	0.14	40,40,40,40	0
57	MG	RA	3202	1/1	0.97	0.06	38,38,38,38	0
57	MG	RA	3203	1/1	0.97	0.09	55,55,55,55	0
57	MG	YA	3360	1/1	0.97	0.05	38,38,38,38	0
57	MG	YA	3173	1/1	0.97	0.04	43,43,43,43	0
57	MG	YA	3262	1/1	0.97	0.14	38,38,38,38	0
57	MG	YA	3174	1/1	0.97	0.08	38,38,38,38	0
57	MG	RA	3350	1/1	0.97	0.04	38,38,38,38	0
58	SF4	QD	301	8/8	0.97	0.06	88,107,133,212	0
57	MG	RA	3274	1/1	0.97	0.24	55,55,55,55	0
57	MG	QJ	201	1/1	0.97	0.19	60,60,60,60	0
57	MG	YA	3268	1/1	0.97	0.11	38,38,38,38	0
57	MG	YA	3178	1/1	0.97	0.04	48,48,48,48	0
57	MG	RA	3397	1/1	0.97	0.07	45,45,45,45	0
57	MG	RA	3091	1/1	0.97	0.08	40,40,40,40	0
57	MG	RA	3071	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3094	1/1	0.97	0.10	38,38,38,38	0
57	MG	RA	3243	1/1	0.97	0.24	38,38,38,38	0
57	MG	YA	3024	1/1	0.97	0.09	38,38,38,38	0
59	ZN	Y9	101	1/1	0.97	0.29	90,90,90,90	0
57	MG	RP	201	1/1	0.97	0.11	41,41,41,41	0
57	MG	XA	1672	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3015	1/1	0.98	0.11	38,38,38,38	0
57	MG	XA	1637	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3028	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3166	1/1	0.98	0.07	39,39,39,39	0
57	MG	RA	3006	1/1	0.98	0.17	38,38,38,38	0
57	MG	RA	3456	1/1	0.98	0.04	48,48,48,48	0
57	MG	RA	3364	1/1	0.98	0.07	38,38,38,38	0
57	MG	YA	3335	1/1	0.98	0.05	38,38,38,38	0
57	MG	RA	3304	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3337	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3276	1/1	0.98	0.14	38,38,38,38	0
57	MG	RA	3459	1/1	0.98	0.13	38,38,38,38	0
57	MG	YA	3035	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3366	1/1	0.98	0.10	38,38,38,38	0
57	MG	YA	3532	1/1	0.98	0.05	38,38,38,38	0
57	MG	YA	3280	1/1	0.98	0.10	38,38,38,38	0
57	MG	RA	3092	1/1	0.98	0.12	40,40,40,40	0
57	MG	YA	3469	1/1	0.98	0.06	38,38,38,38	0
57	MG	YA	3282	1/1	0.98	0.18	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3283	1/1	0.98	0.04	38,38,38,38	0
57	MG	RA	3066	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3391	1/1	0.98	0.20	38,38,38,38	0
57	MG	XA	1648	1/1	0.98	0.08	38,38,38,38	0
57	MG	RA	3067	1/1	0.98	0.03	38,38,38,38	0
57	MG	YA	3411	1/1	0.98	0.04	38,38,38,38	0
57	MG	RA	3215	1/1	0.98	0.12	38,38,38,38	0
57	MG	RA	3269	1/1	0.98	0.16	38,38,38,38	0
57	MG	YA	3085	1/1	0.98	0.10	38,38,38,38	0
57	MG	RA	3105	1/1	0.98	0.05	38,38,38,38	0
57	MG	YA	3292	1/1	0.98	0.19	38,38,38,38	0
57	MG	YA	3134	1/1	0.98	0.24	38,38,38,38	0
57	MG	YA	3185	1/1	0.98	0.04	38,38,38,38	0
57	MG	RA	3217	1/1	0.98	0.23	38,38,38,38	0
57	MG	YA	3088	1/1	0.98	0.09	42,42,42,42	0
57	MG	YA	3089	1/1	0.98	0.21	38,38,38,38	0
57	MG	RA	3076	1/1	0.98	0.04	38,38,38,38	0
57	MG	QA	1669	1/1	0.98	0.12	38,38,38,38	0
57	MG	QA	1658	1/1	0.98	0.04	38,38,38,38	0
57	MG	XA	1622	1/1	0.98	0.06	38,38,38,38	0
57	MG	XA	1623	1/1	0.98	0.10	91,91,91,91	0
57	MG	YA	3427	1/1	0.98	0.07	38,38,38,38	0
57	MG	XA	1659	1/1	0.98	0.04	38,38,38,38	0
57	MG	XA	1624	1/1	0.98	0.26	38,38,38,38	0
57	MG	XA	1625	1/1	0.98	0.05	38,38,38,38	0
57	MG	QA	1662	1/1	0.98	0.06	54,54,54,54	0
57	MG	RA	3110	1/1	0.98	0.03	38,38,38,38	0
57	MG	RA	3240	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3123	1/1	0.98	0.09	38,38,38,38	0
57	MG	YA	3435	1/1	0.98	0.03	39,39,39,39	0
57	MG	YA	3151	1/1	0.98	0.13	81,81,81,81	0
57	MG	YA	3152	1/1	0.98	0.04	55,55,55,55	0
57	MG	RA	3224	1/1	0.98	0.21	38,38,38,38	0
57	MG	YA	3105	1/1	0.98	0.05	38,38,38,38	0
57	MG	YA	3256	1/1	0.98	0.25	38,38,38,38	0
57	MG	XA	1631	1/1	0.98	0.04	38,38,38,38	0
59	ZN	R4	101	1/1	0.98	0.22	88,88,88,88	0
57	MG	YA	3317	1/1	0.98	0.11	38,38,38,38	0
57	MG	YA	3258	1/1	0.98	0.23	38,38,38,38	0
57	MG	RA	3478	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3056	1/1	0.98	0.03	43,43,43,43	0
57	MG	YA	3159	1/1	0.98	0.07	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1634	1/1	0.98	0.05	43,43,43,43	0
57	MG	YA	3210	1/1	0.98	0.13	38,38,38,38	0
57	MG	YA	3110	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3265	1/1	0.98	0.12	38,38,38,38	0
57	MG	RA	3480	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3091	1/1	0.99	0.03	38,38,38,38	0
57	MG	YA	3156	1/1	0.99	0.03	38,38,38,38	0
57	MG	QA	1653	1/1	0.99	0.03	58,58,58,58	0
57	MG	QA	1646	1/1	0.99	0.03	58,58,58,58	0
57	MG	YA	3124	1/1	0.99	0.04	38,38,38,38	0
57	MG	RA	3050	1/1	0.99	0.11	38,38,38,38	0
57	MG	YA	3081	1/1	0.99	0.10	38,38,38,38	0
57	MG	YA	3057	1/1	0.99	0.03	38,38,38,38	0
57	MG	YA	3097	1/1	0.99	0.06	38,38,38,38	0
57	MG	RA	3276	1/1	0.99	0.07	54,54,54,54	0
57	MG	RA	3189	1/1	0.99	0.10	38,38,38,38	0
57	MG	YA	3295	1/1	0.99	0.12	38,38,38,38	0
57	MG	RA	3472	1/1	0.99	0.19	38,38,38,38	0
57	MG	RA	3059	1/1	0.99	0.07	38,38,38,38	0
57	MG	RA	3423	1/1	0.99	0.04	38,38,38,38	0
57	MG	RA	3198	1/1	0.99	0.03	46,46,46,46	0
57	MG	YA	3135	1/1	0.99	0.06	38,38,38,38	0
57	MG	YA	3243	1/1	0.99	0.03	38,38,38,38	0
57	MG	RA	3160	1/1	0.99	0.03	38,38,38,38	0
57	MG	RA	3014	1/1	0.99	0.04	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.