



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:49 AM UTC

PDB ID : 6NUO / pdb_00006nuo
Title : Modified tRNA(Pro) bound to Thermus thermophilus 70S (cognate)
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-02-01
Resolution : 3.20 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

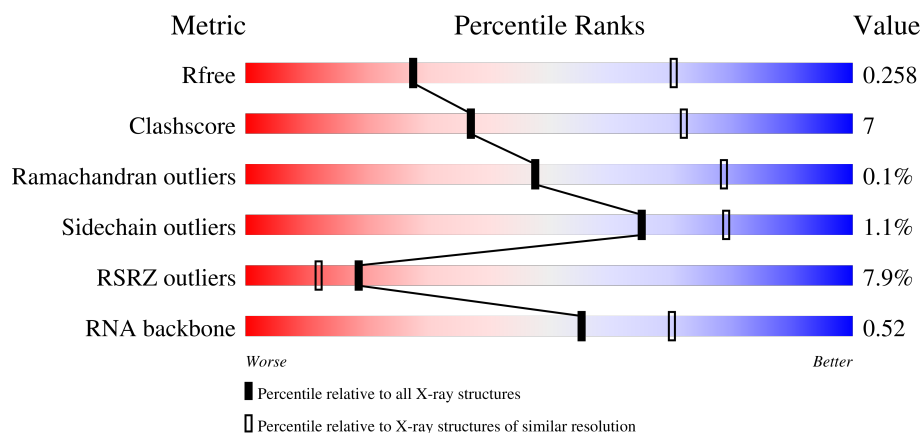
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	1521	5% 52% 39% 8%
1	XA	1521	7% 53% 36% 9%
2	QB	256	% 64% 26% 8%
2	XB	256	7% 62% 28% 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	132	
12	XL	132	
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	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	RF	210	4% 73% 23% .
28	YF	210	3% 73% 22% .
29	RG	182	15% 66% 30% ..
29	YG	182	12% 65% 32% ..
30	RH	180	12% 63% 31% ..
30	YH	180	3% 80% 16% ..
31	RI	148	14% 70% 26% ..
31	YI	148	14% 74% 23% ..
32	RN	140	13% 81% 15% ..
32	YN	140	% 80% 19% .
33	RO	122	% 76% 22% .
33	YO	122	4% 80% 20%
34	RP	150	8% 77% 19% ...
34	YP	150	3% 75% 23% .
35	RQ	141	8% 61% 35% .
35	YQ	141	% 85% 15%
36	RR	118	4% 75% 23% ..
36	YR	118	3% 82% 15% ..
37	RS	112	27% 71% 26% ..
37	YS	112	% 79% 20% .
38	RT	146	5% 64% 25% 6%
38	YT	146	7% 66% 24% 6%
39	RU	118	14% 77% 19% ...
39	YU	118	6% 82% 14% ..
40	RV	101	5% 78% 20% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	YV	101	
41	RW	113	
41	YW	113	
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	R8	65	
53	Y8	65	
54	R9	37	
54	Y9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	RA	3257	-	-	-	X
55	MG	YA	3144	-	-	-	X
55	MG	YA	3406	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	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-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1648	734	295	542	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1648	734	295	542	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	19	Total	C	N	O	P	0	0	0
			418	186	86	127	19			
23	XX	19	Total	C	N	O	P	0	0	0
			418	186	86	127	19			

- Molecule 24 is a RNA chain called 23S rRNA.

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

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
32	YN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
34	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
37	YS	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YX	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
45	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
47	Y2	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

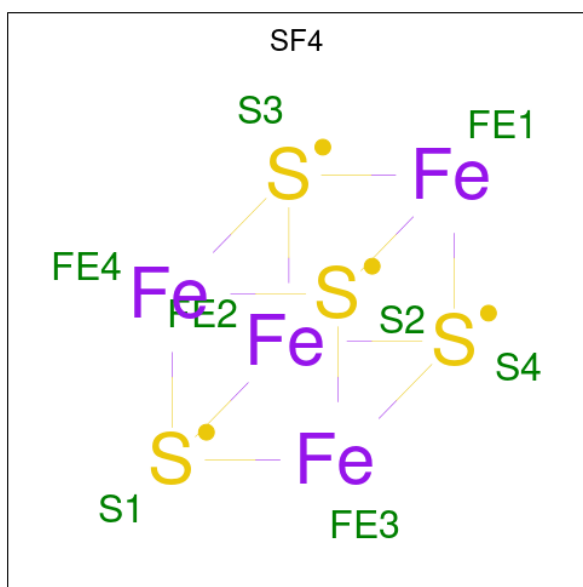
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	64	Total	Mg	0	0
			64	64		
55	QV	1	Total	Mg	0	0
			1	1		
55	RA	444	Total	Mg	0	0
			444	444		
55	RB	7	Total	Mg	0	0
			7	7		
55	RE	5	Total	Mg	0	0
			5	5		
55	RF	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	RQ	1	Total	Mg	0	0
			1	1		
55	RR	1	Total	Mg	0	0
			1	1		
55	RT	1	Total	Mg	0	0
			1	1		
55	RX	1	Total	Mg	0	0
			1	1		
55	R0	2	Total	Mg	0	0
			2	2		
55	R8	2	Total	Mg	0	0
			2	2		
55	XA	78	Total	Mg	0	0
			78	78		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XE	1	Total 1	Mg 1	0	0
55	XM	2	Total 2	Mg 2	0	0
55	XV	1	Total 1	Mg 1	0	0
55	YA	510	Total 510	Mg 510	0	0
55	YB	7	Total 7	Mg 7	0	0
55	YD	2	Total 2	Mg 2	0	0
55	YE	5	Total 5	Mg 5	0	0
55	YP	3	Total 3	Mg 3	0	0
55	YQ	3	Total 3	Mg 3	0	0
55	YR	1	Total 1	Mg 1	0	0
55	Y0	2	Total 2	Mg 2	0	0
55	Y1	2	Total 2	Mg 2	0	0
55	Y3	1	Total 1	Mg 1	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	Y8	1	Total 1	Mg 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

Continued on next page...

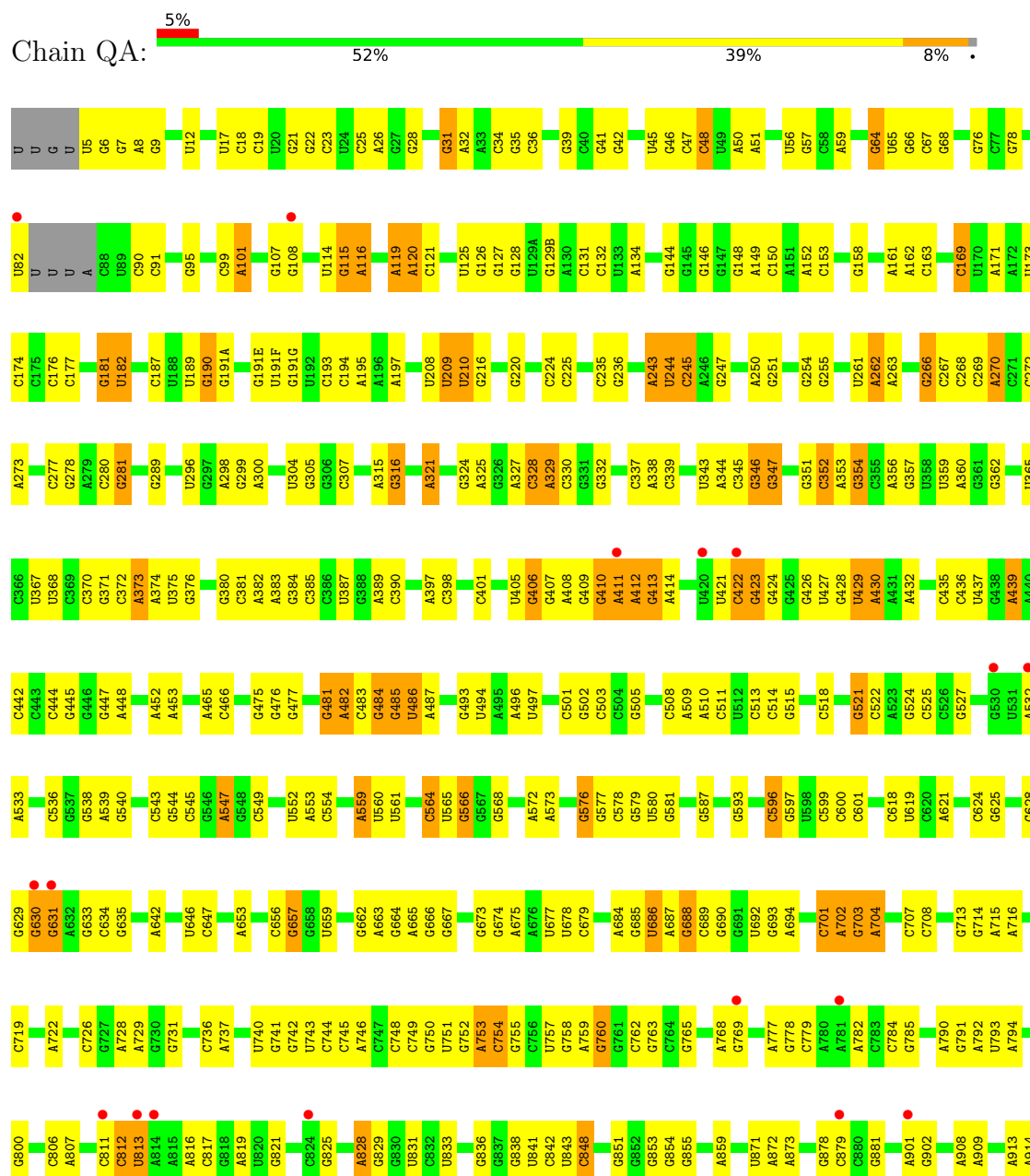
Continued from previous page...

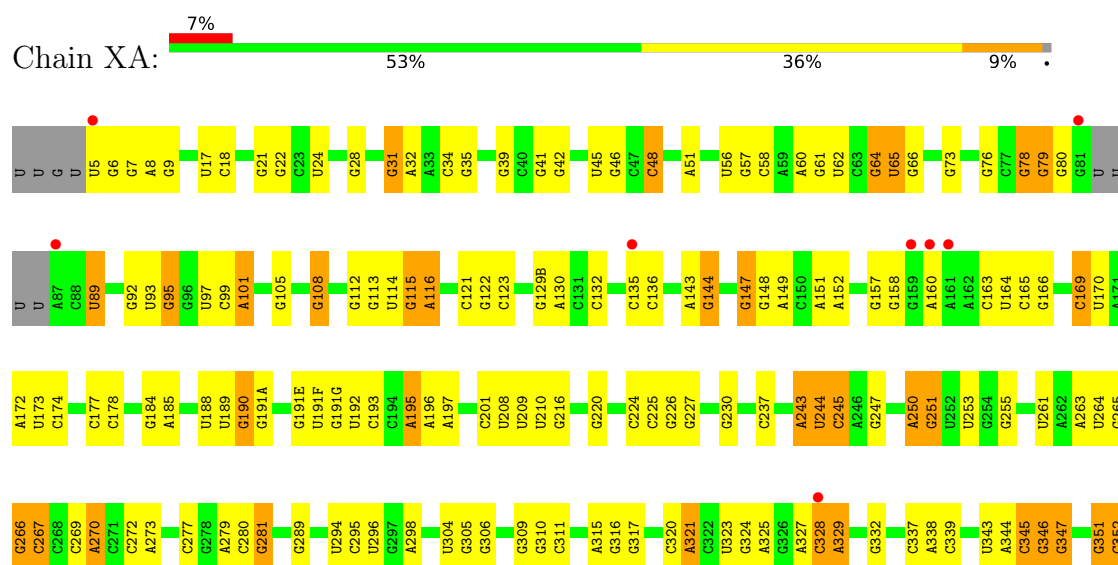
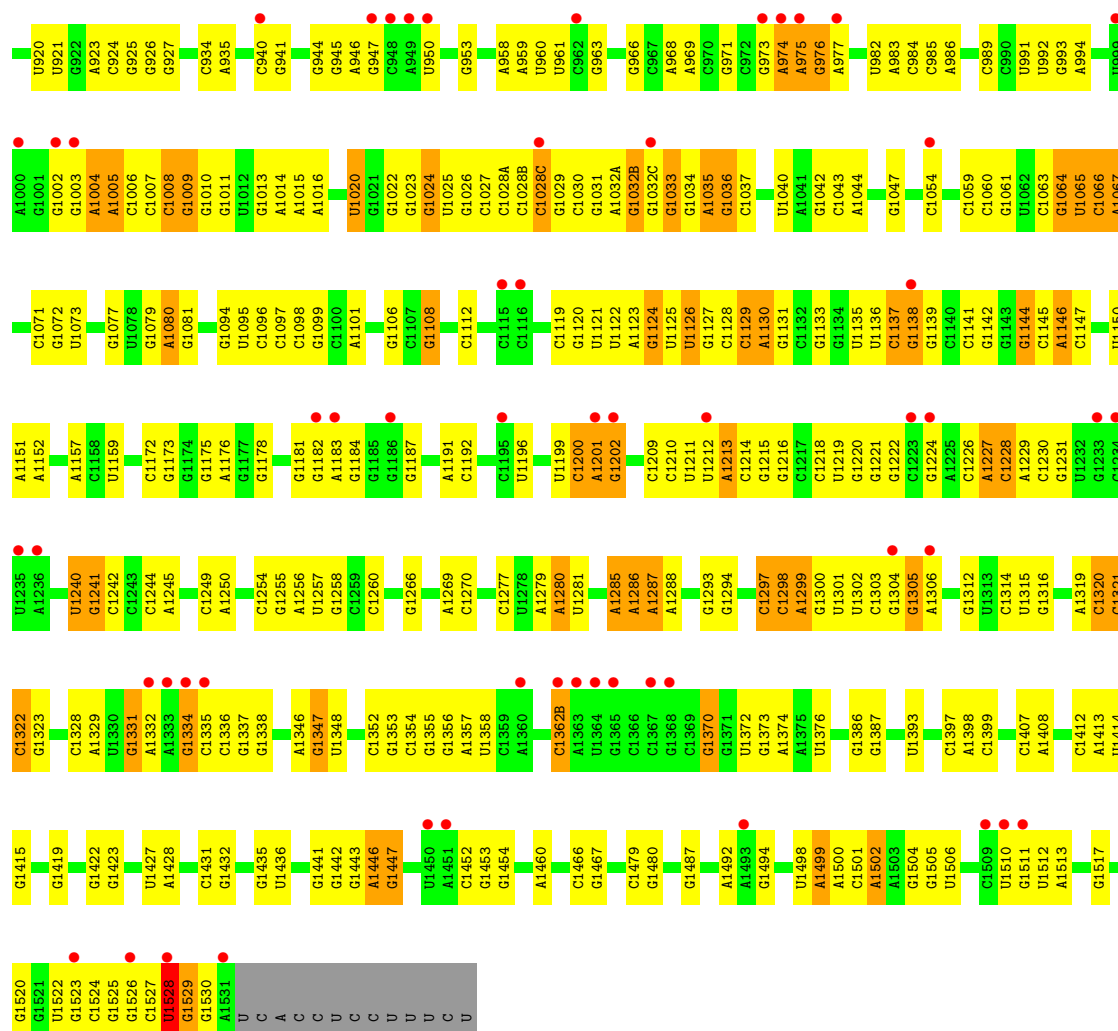
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y6	1	Total 1	Zn 1	0	0
57	Y9	1	Total 1	Zn 1	0	0

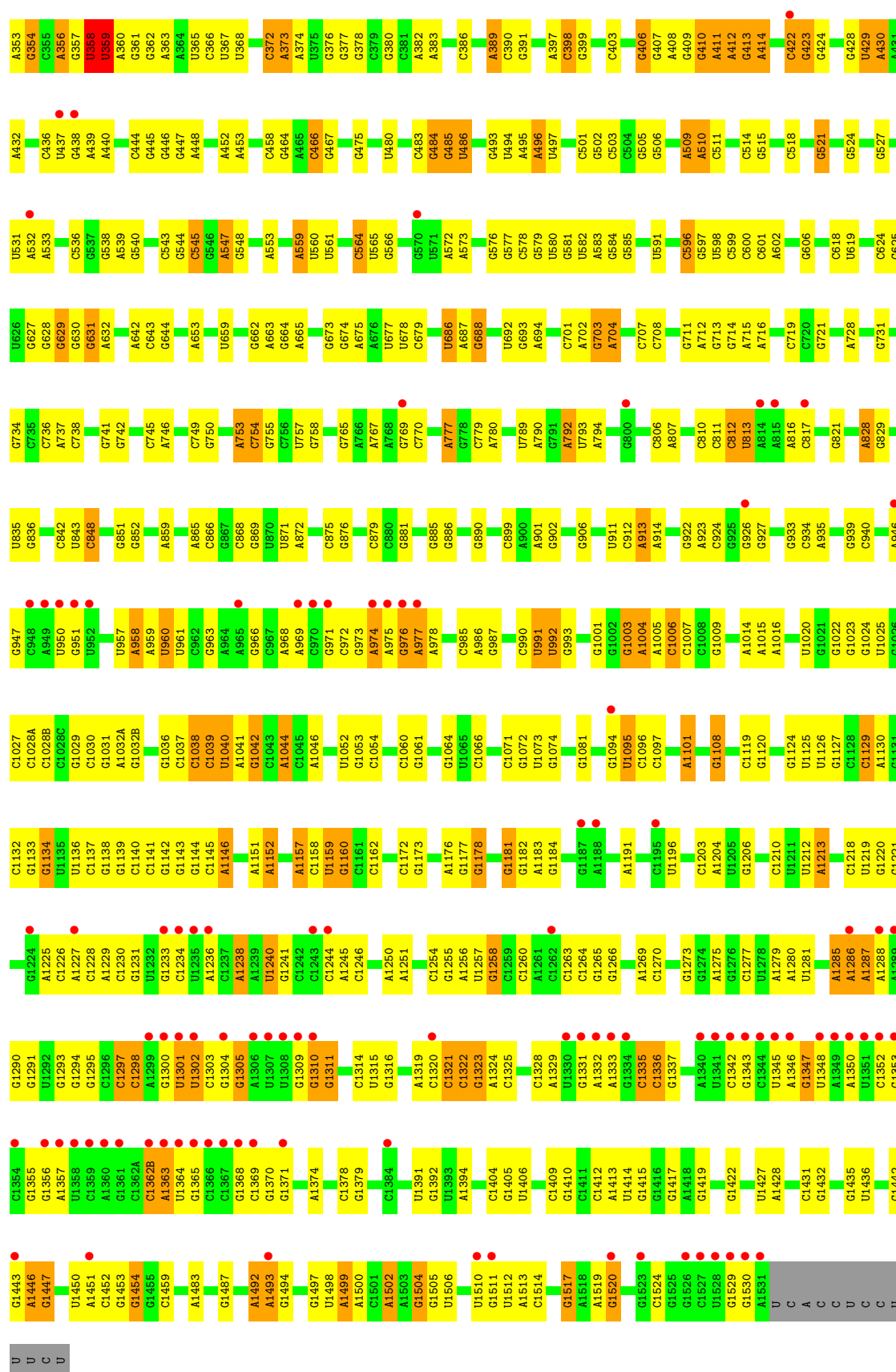
3 Residue-property plots [i](#)

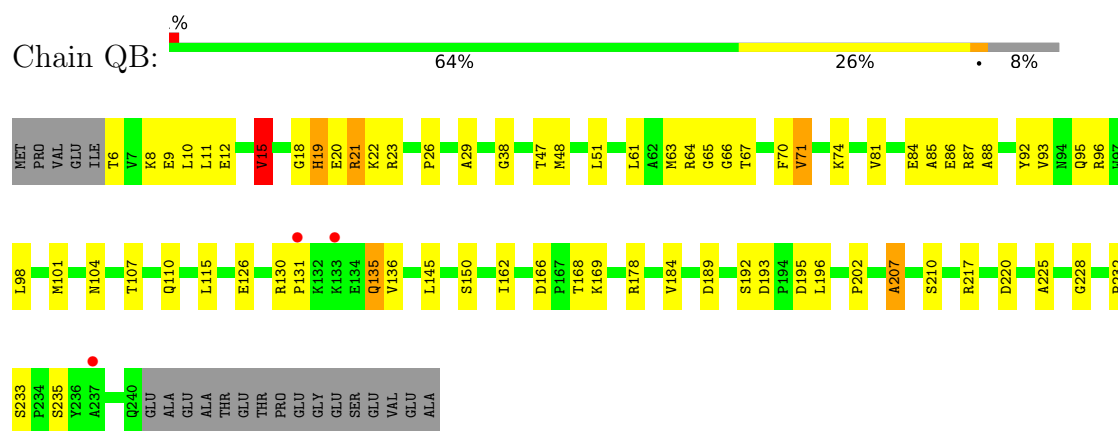
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

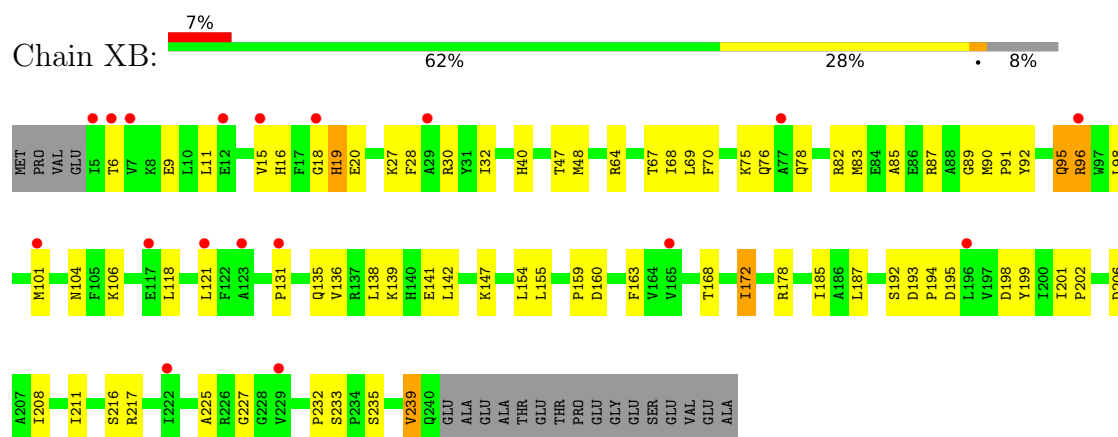




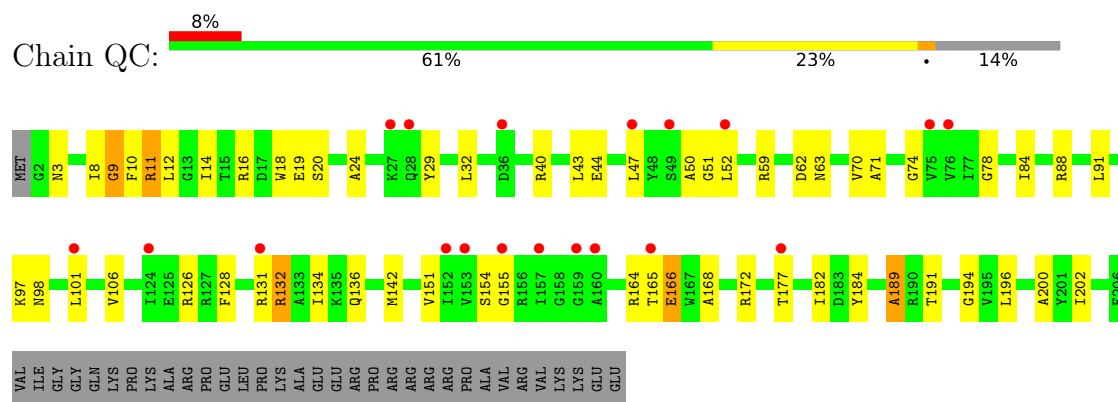




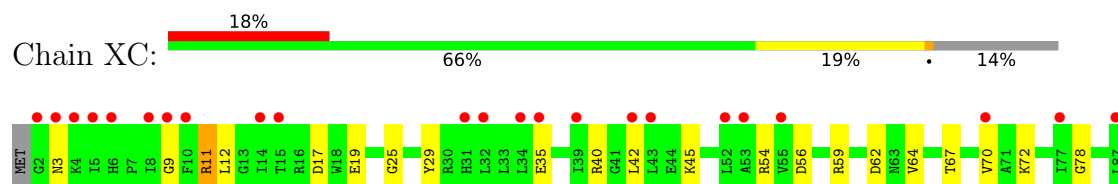
• Molecule 2: 30S ribosomal protein S2

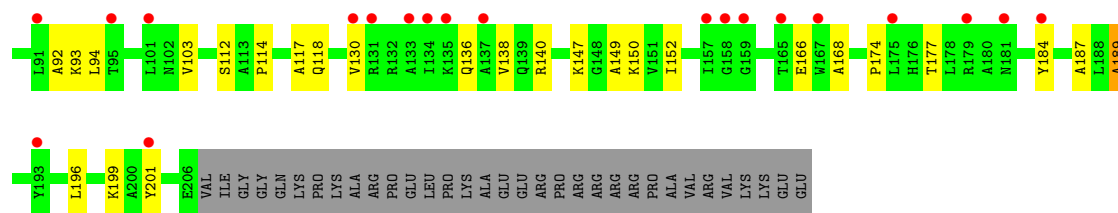


• Molecule 3: 30S ribosomal protein S3

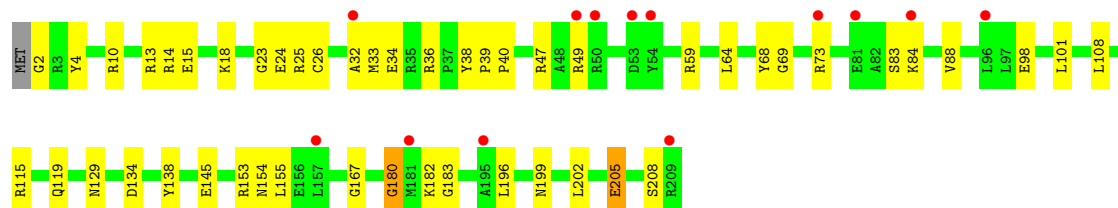
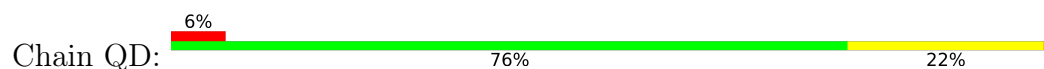


• Molecule 3: 30S ribosomal protein S3

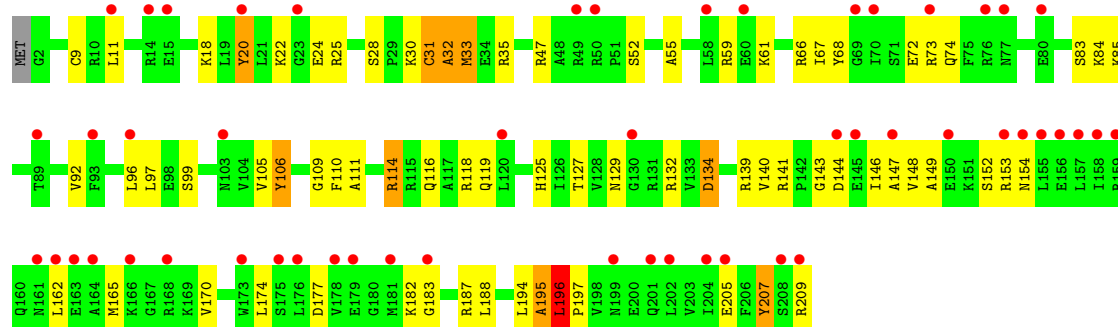




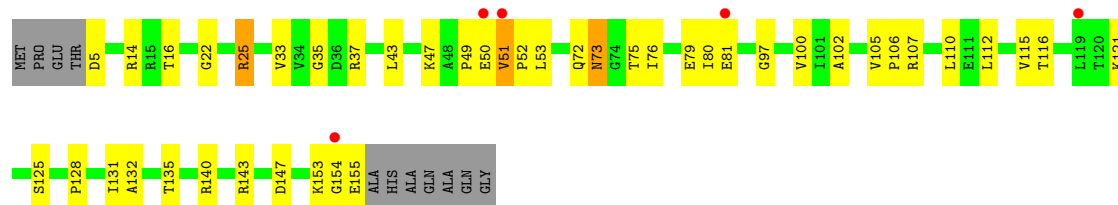
• Molecule 4: 30S ribosomal protein S4



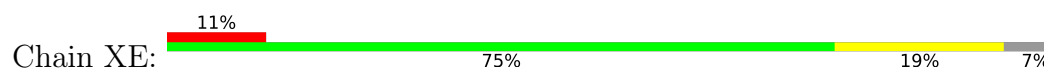
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

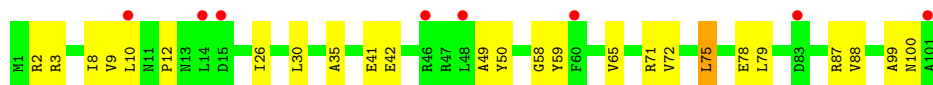
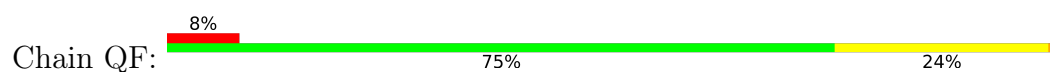


• Molecule 5: 30S ribosomal protein S5

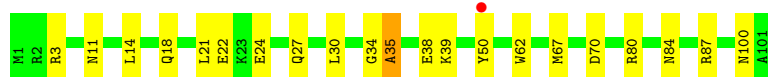
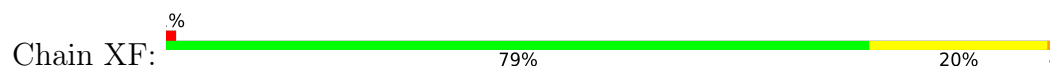




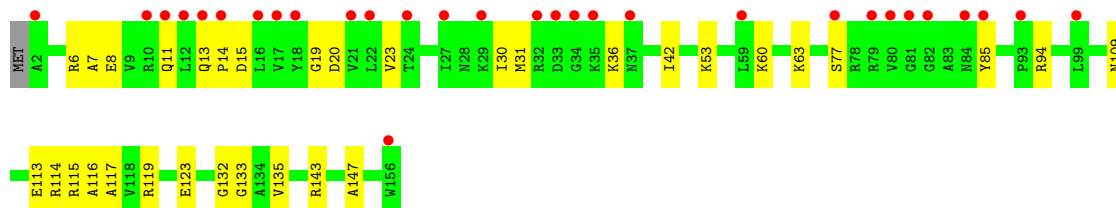
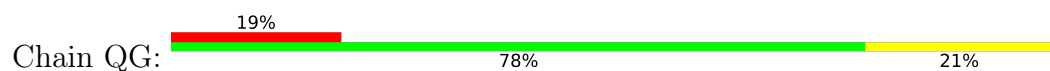
- Molecule 6: 30S ribosomal protein S6



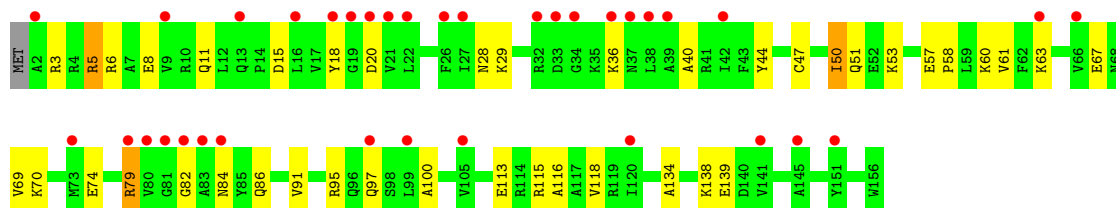
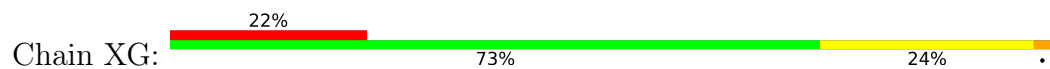
- Molecule 6: 30S ribosomal protein S6



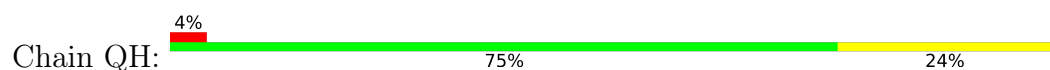
- Molecule 7: 30S ribosomal protein S7

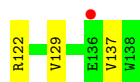


- Molecule 7: 30S ribosomal protein S7

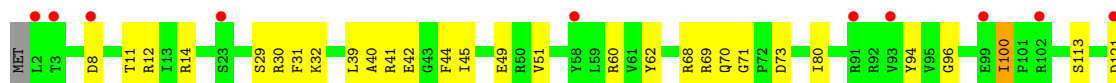
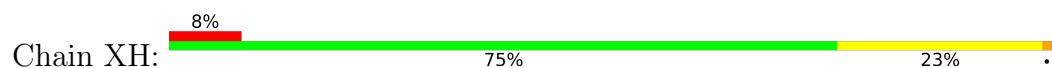


- Molecule 8: 30S ribosomal protein S8

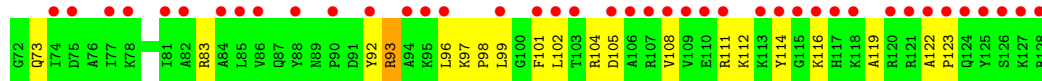




- Molecule 8: 30S ribosomal protein S8



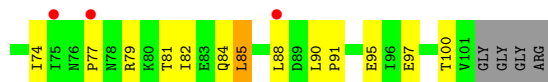
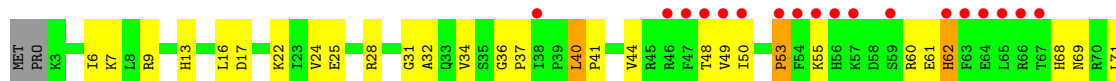
- Molecule 9: 30S ribosomal protein S9



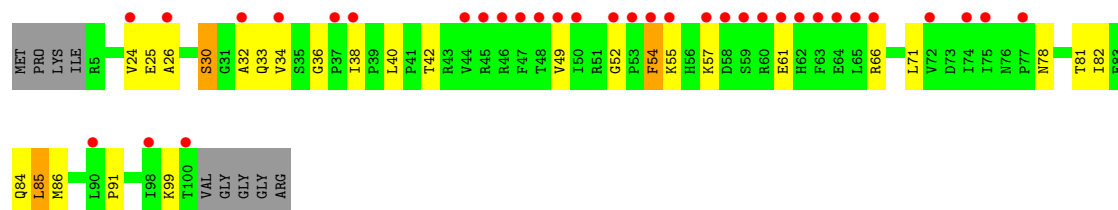
- Molecule 9: 30S ribosomal protein S9



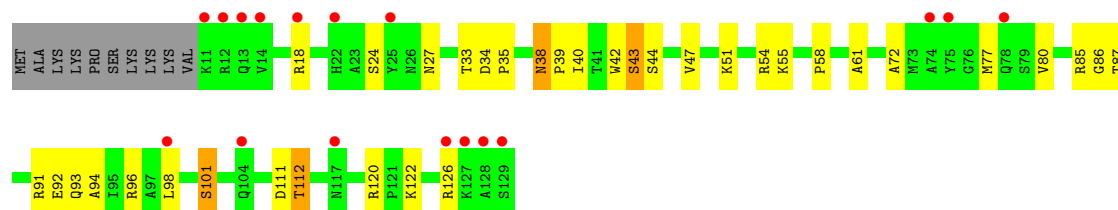
- Molecule 10: 30S ribosomal protein S10



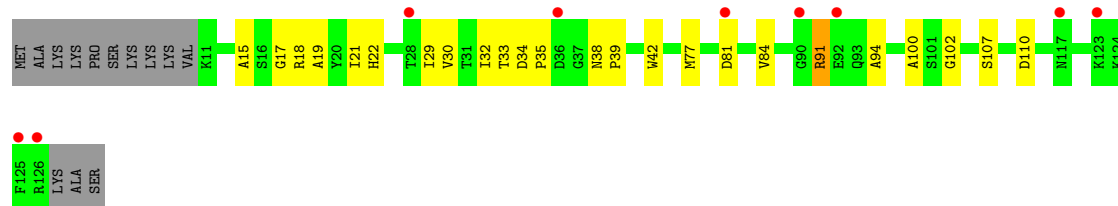
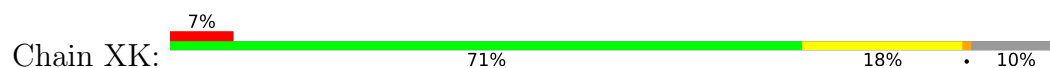
- Molecule 10: 30S ribosomal protein S10



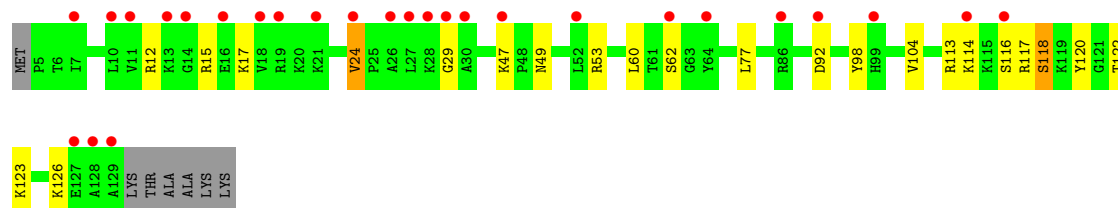
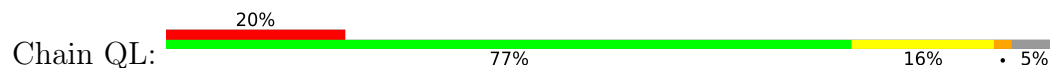
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

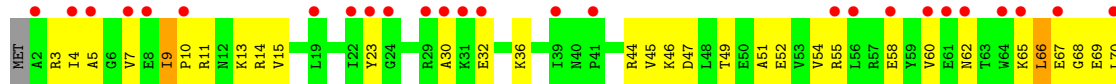
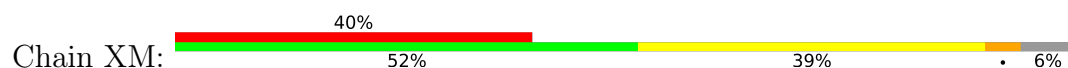




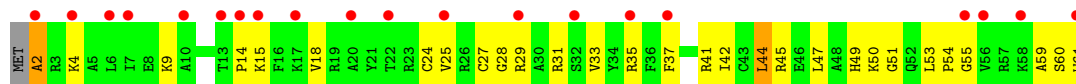
- Molecule 13: 30S ribosomal protein S13



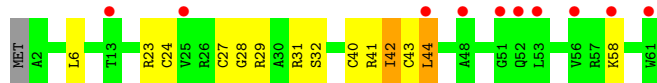
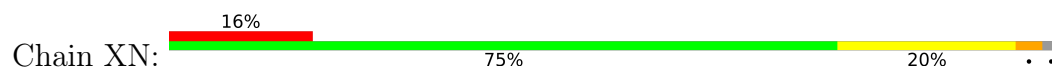
- Molecule 13: 30S ribosomal protein S13



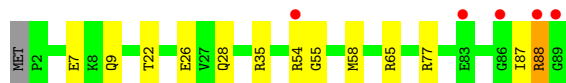
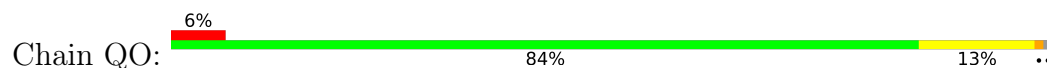
- Molecule 14: 30S ribosomal protein S14 type Z



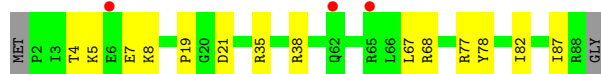
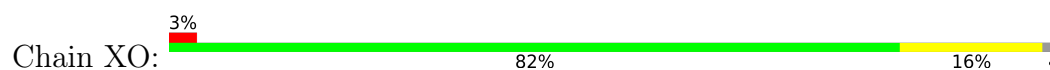
- Molecule 14: 30S ribosomal protein S14 type Z



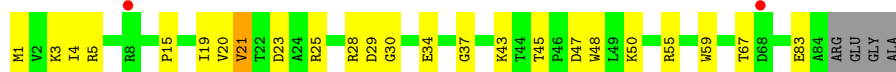
- Molecule 15: 30S ribosomal protein S15



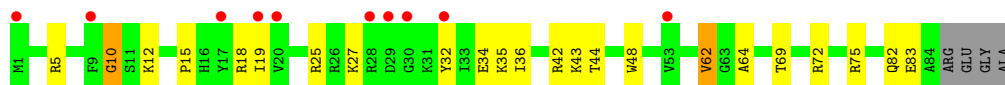
- Molecule 15: 30S ribosomal protein S15



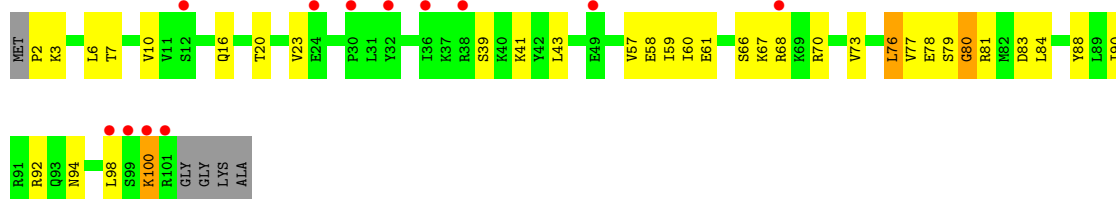
- Molecule 16: 30S ribosomal protein S16



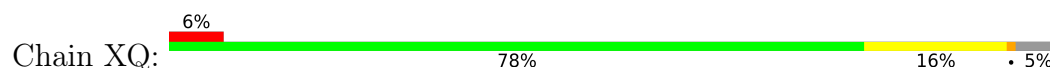
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

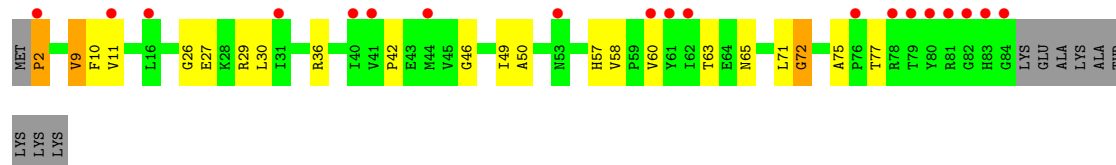


- Molecule 18: 30S ribosomal protein S18

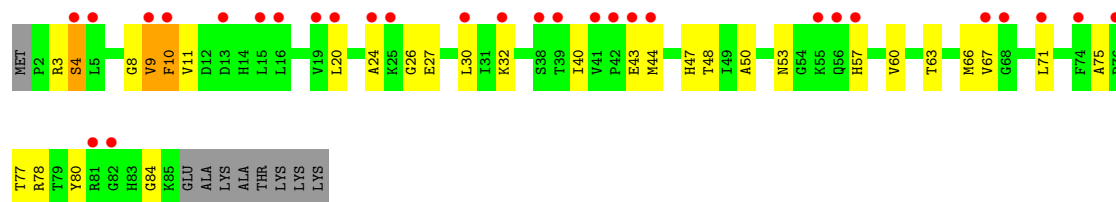




- Molecule 19: 30S ribosomal protein S19



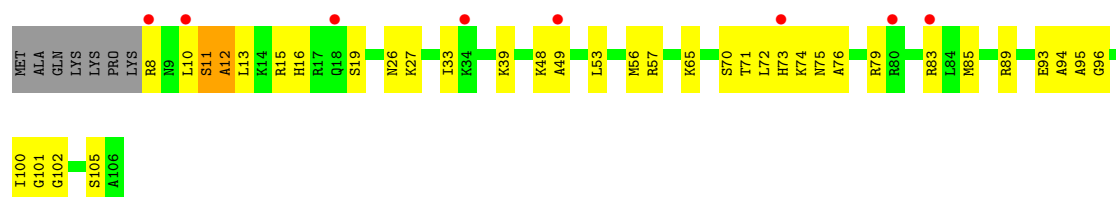
- Molecule 19: 30S ribosomal protein S19



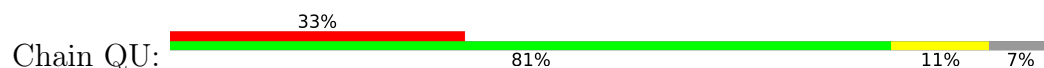
- Molecule 20: 30S ribosomal protein S20

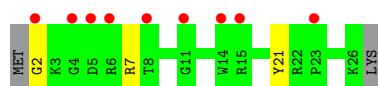


- Molecule 20: 30S ribosomal protein S20

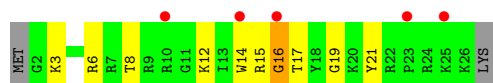


- Molecule 21: 30S ribosomal protein Thx

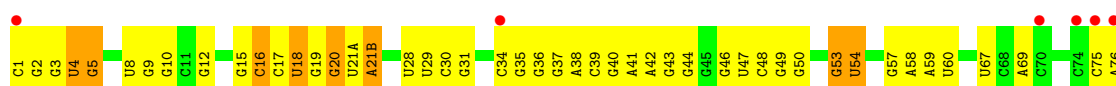




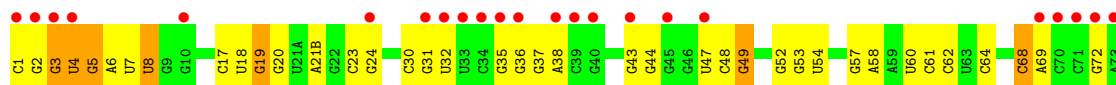
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: P-site tRNA-Pro



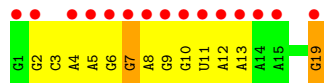
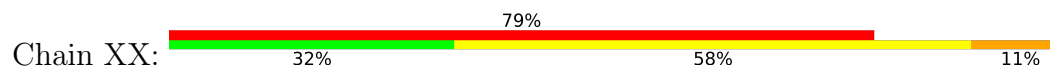
- Molecule 22: P-site tRNA-Pro



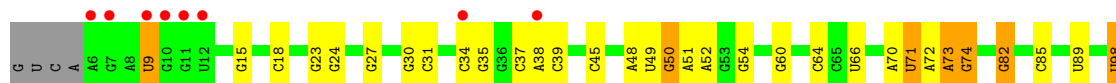
- Molecule 23: mRNA

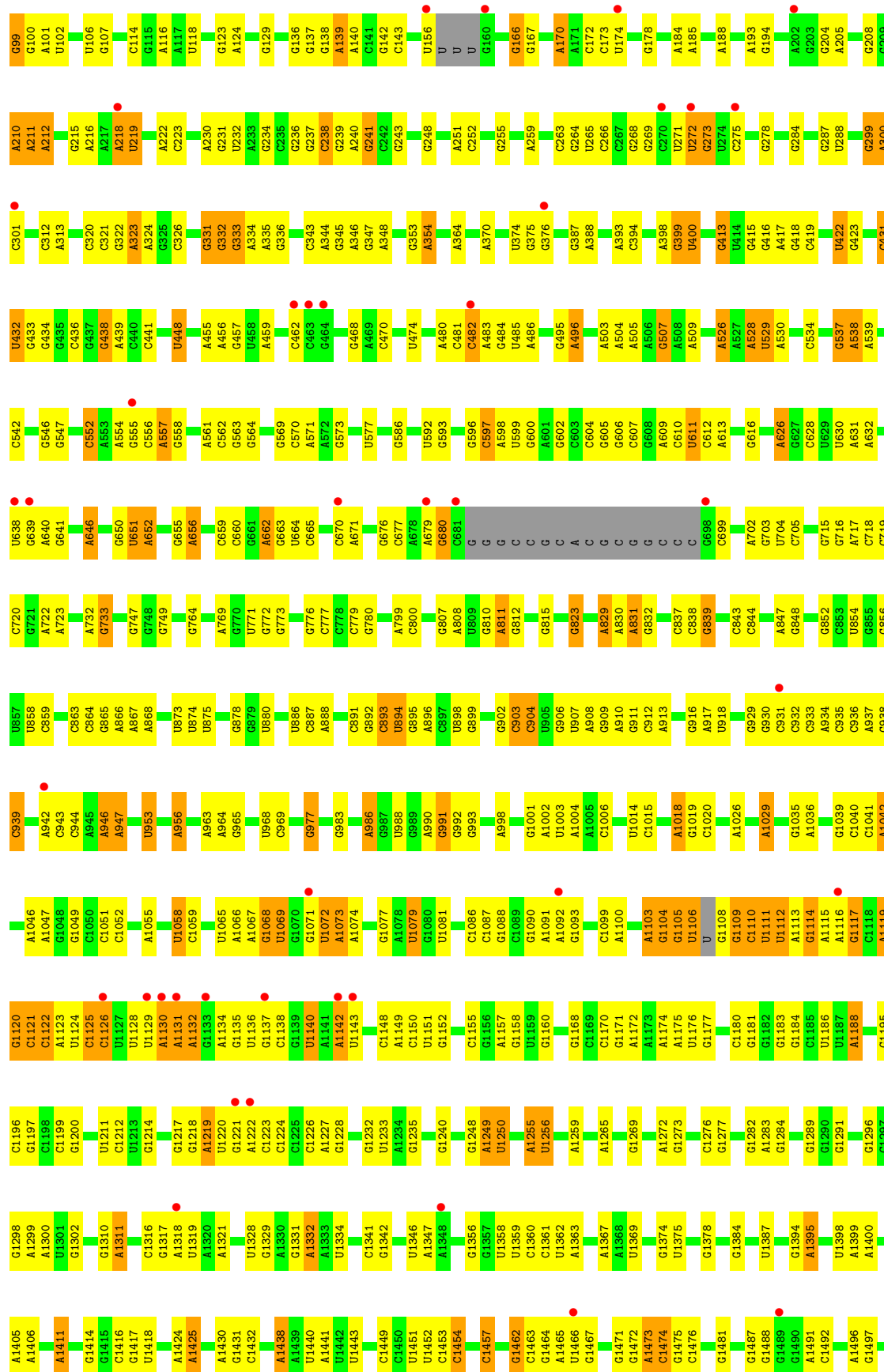


- Molecule 23: mRNA



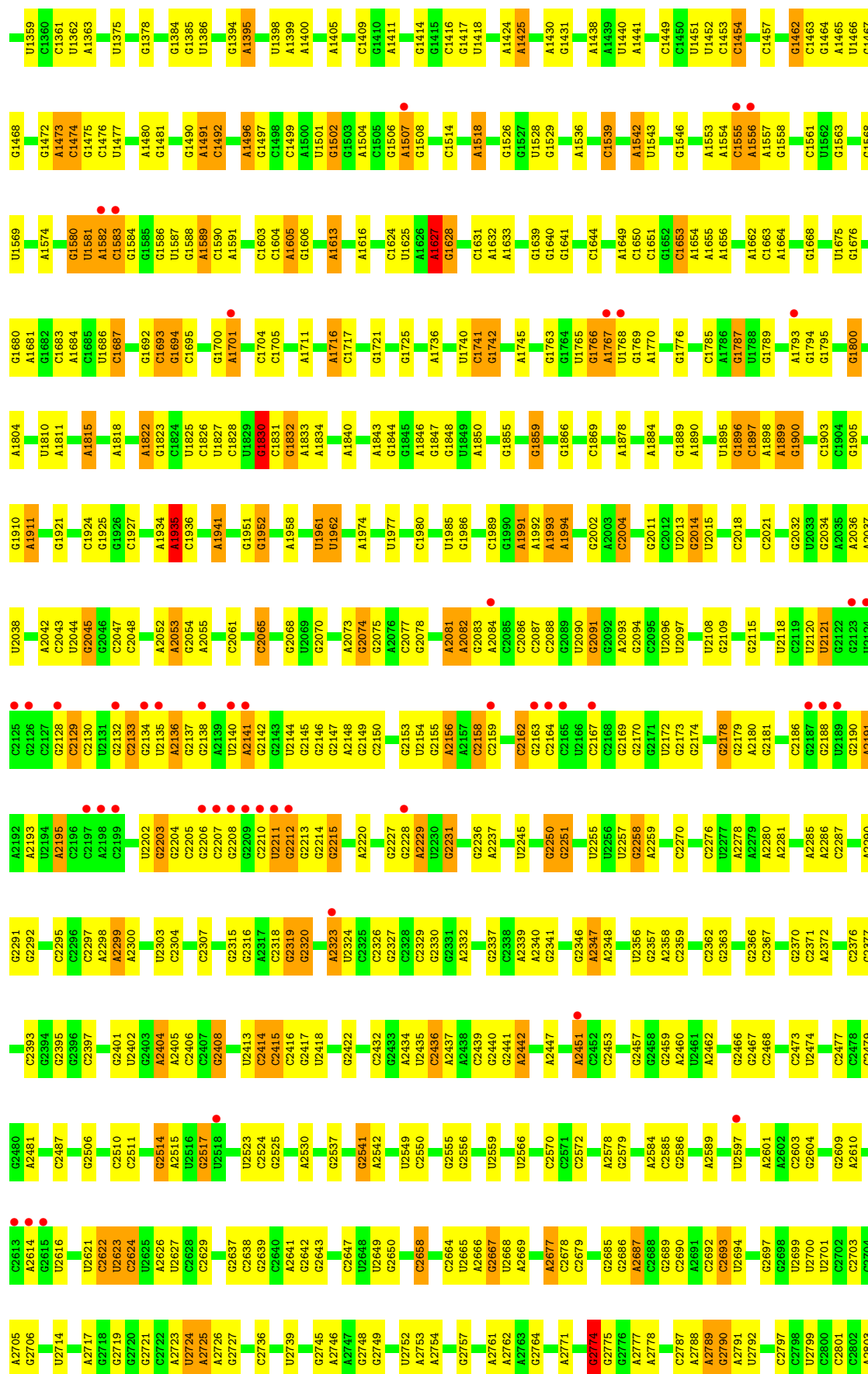
- Molecule 24: 23S rRNA

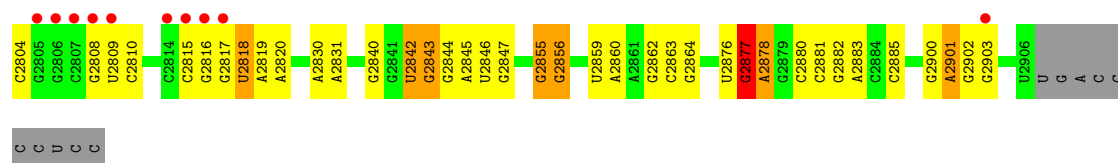




A2771	U2540	G2346	U2257	G2115	G2024	U1895	G1794	G1668	C1583	U1501
G2774	G2541	A2947	G2258	U2118	A2027	G1896	G1795	G1668	G1584	G1502
G2775	A2542	A2348	A2259	C2183	C2028	C1897	G1800	G1674	G1585	C1505
A2778	U2549	G2355	G2262	U2121	G2032	A1898	G1801	G1675	G1586	G1506
G2790	C2550	G2356	C2270	G2122	U2033	A1899	G1802	G1676	U1587	A1507
A2791	C2552	G2357	C2276	U2124	G2034	G1900	G1803	A1679	G1588	G1508
U2792	A2554	A2358	U2277	G2125	A2035	C1904	A1804	A1683	C1590	C1514
G2793	G2555	C2359	A2278	G2126	A2035	G1910	G1807	A1684	A1591	A1518
C2798	G2556	C2362	A2281	C2129	A2041	A1911	G1810	C1683	C1592	A1524
U2795	U2559	G2366	C2287	U2130	U2044	A1912	A1811	G1692	C1594	G1525
C2800	U2566	C2367	C2287	U2131	U2044	A1921	C1812	C1693	C1604	G1526
C2801	C2693	C2376	A2290	C2132	G2045	G1922	C1813	G1694	A1605	G1527
A2802	A2460	G2377	G2291	C2133	G2046	A1923	A1814	C1695	G1606	U1528
C2804	G2466	G2377	G2292	U2135	C2047	A1924	A1815	G1698	U1529	G1530
G2805	G2467	G2382	C2293	A2136	G2049	G1925	A1822	A1699	G1531	G1539
U2806	C2473	G2383	G2294	G2137	U2050	G1928	U1827	A1700	A1612	A1540
C2807	C2474	G2383	C2295	U2138	G2051	G1929	U1828	A1701	A1613	U1543
G2808	U2474	A2389	C2296	A2139	A2052	C1930	C1829	C1707	A1615	C1544
U2809	G2474	A2390	C2297	U2140	A2053	G1935	A1830	C1707	A1616	C1545
C2702	G2480	A2390	C2297	G2141	G2054	A1935	C1831	A1712	A1617	G1546
A2811	A2481	G2395	A2299	G2142	A2055	A1935	C1831	A1712	A1618	
C2812	G2482	G2396	A2300	G2143	U2056	A1935	G1832	G1713	U1625	
G2813	C2486	C2397	A2300	U2144	G2059	A1950	A1843	G1714	A1626	U1549
U2707	C2486	C2398	U2303	G2145	G2060	G1951	G1844	A1715	C1544	C1560
C2815	C2487	U2399	C2304	G2146	C2065	U1961	G1845	G1721	C1634	A1553
G2816	C2492	A2400	U2308	U2149	C2075	U1977	A1850	A1736	C1635	A1554
C2817	G2493	G2401	U2312	C2150	A2076	U1977	A1851	G1744	U1636	C1555
U2818	G2498	A2405	G2315	G2153	G2071	C1980	A1852	A1745	A1556	A1566
A2601	G2501	A2406	G2316	U2154	C2072	C1984	G1846	G1768	A1567	
A2614	G2506	C2407	A2317	G2155	A2073	U1985	U1849	G1769	C1558	
G2619	G2514	G2408	C2318	A2156	G2074	C1985	A1850	A1770	G1559	
U2621	A2515	G2409	G2319	C2157	G2075	C1985	A1851	G1771	U1560	
C2622	G2516	C2415	A2321	C2158	A2076	U1985	A1852	A1642	C1561	
U2623	U2517	U2418	A2322	C2161	A2081	C1989	A1852	A1643		
C2624	U2518	G2419	A2323	G2162	C2082	G1990	G1862	C1644	G1565	
U2625	U2518	U2420	G2324	G2163	A2084	A1991	C1863	U1648	U1566	
A2626	C2524	G2421	C2325	C2165	C2085	A1992	G1864	C1649	G1567	
C2628	G2525	A2424	G2326	C2166	U2090	A1993	G1865	A1649	G1568	
G2629	G2526	G2425	C2327	U2167	G2091	A1994	G1866	C1650	U1569	
U2630	C2527	G2426	C2328	C2168	G2094	C2002	C1868		G1570	
A2530	G2528	G2427	G2329	G2169	C2095	A2003	G1878	C1775	G1571	
U2531	A2530	C2428	A2332	G2170	U2096	C2004	A1879	G1776	G1572	
C2532	U2531	U2431	G2337	U2171	U2097	U2013	A1880	G1781	G1573	
G2533	C2532	U2431	C2338	G2172	U2098	G2014	G1881	C1782	A1574	
G2537	G2537	A2434	A2339	G2173	U2099	U2015	A1884	C1783	G1575	
C2538	U2538	U2435	A2340	G2174	U2099	U2016	A1885		G1576	
G2539	C2539	G2436	G2341	G2175	U2108	C2017	A1885	G1787	G1580	
U2648	U2648	C2436	G2341	G2176	G2109	U2017	C1663	A1793	U1581	
U2653	G2653	A2437	G2341	A2180	U2109	C2018	A1664		A1582	







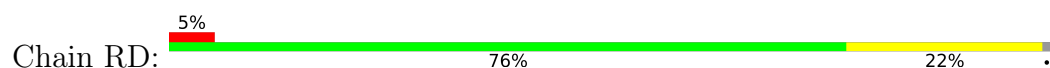
• Molecule 25: 5S rRNA



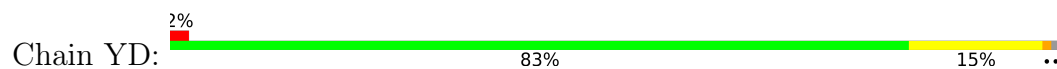
• Molecule 25: 5S rRNA



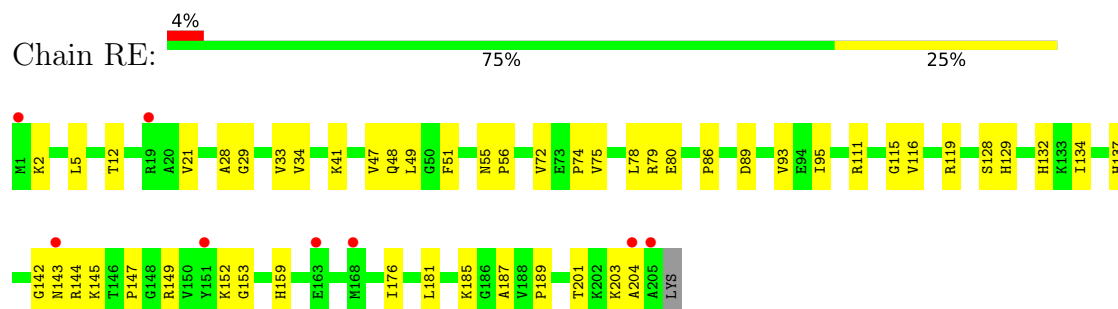
• Molecule 26: 50S ribosomal protein L2



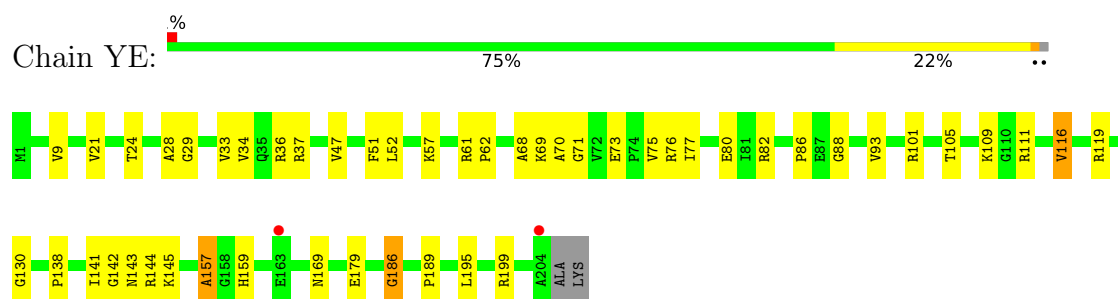
• Molecule 26: 50S ribosomal protein L2



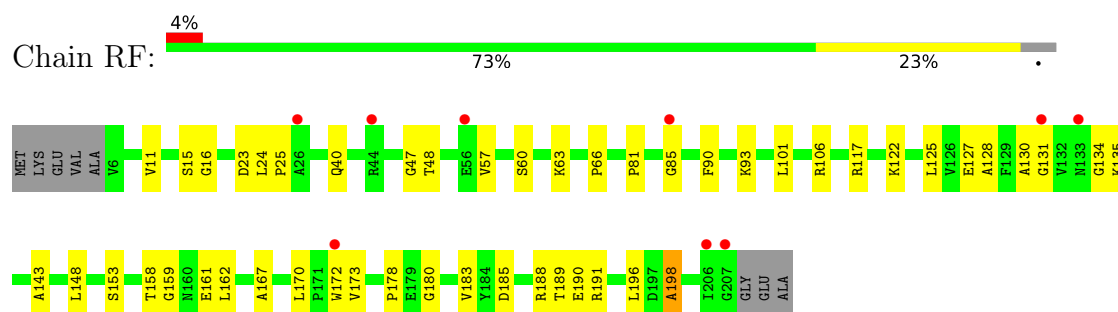
- Molecule 27: 50S ribosomal protein L3



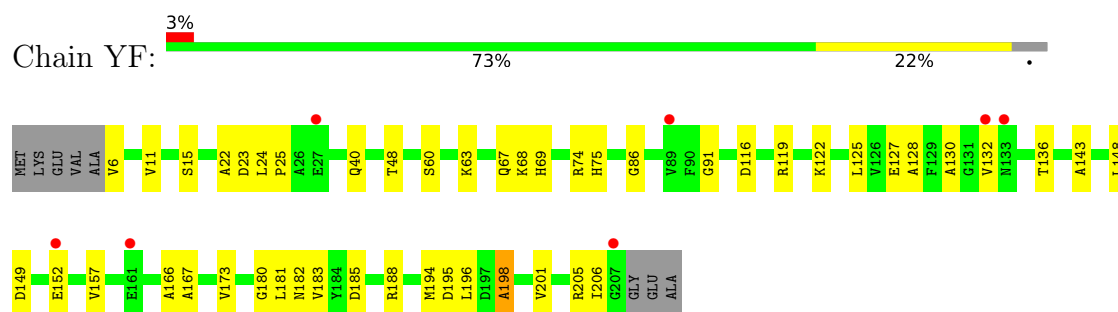
- Molecule 27: 50S ribosomal protein L3



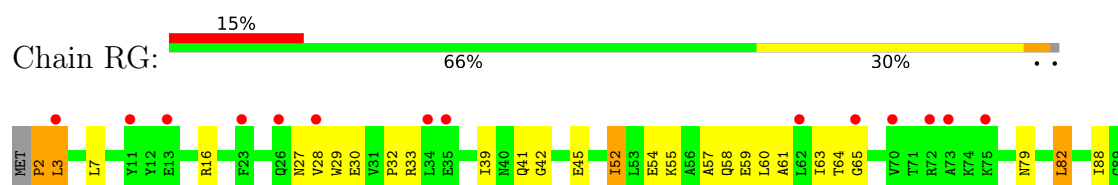
- Molecule 28: 50S ribosomal protein L4

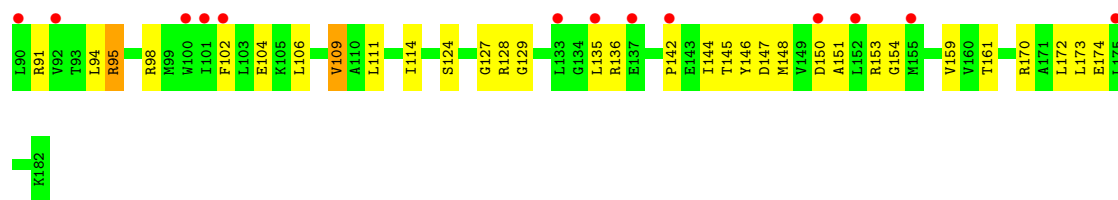


- Molecule 28: 50S ribosomal protein L4

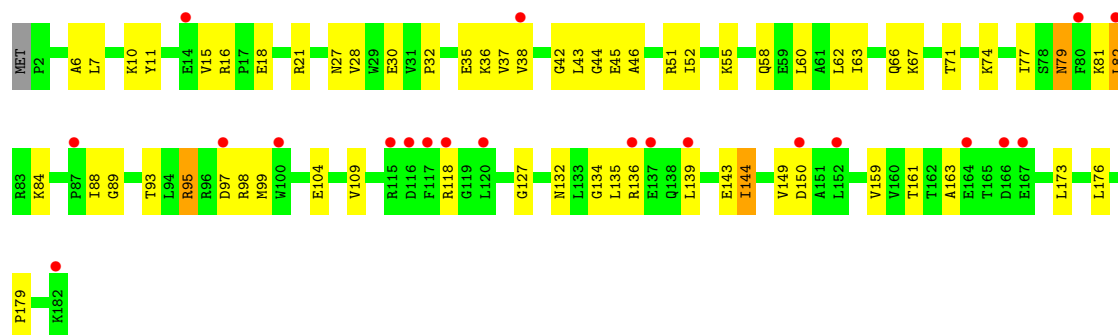


- Molecule 29: 50S ribosomal protein L5

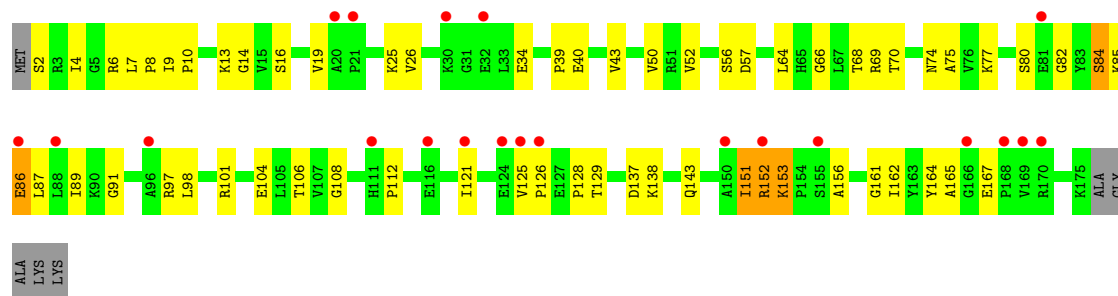




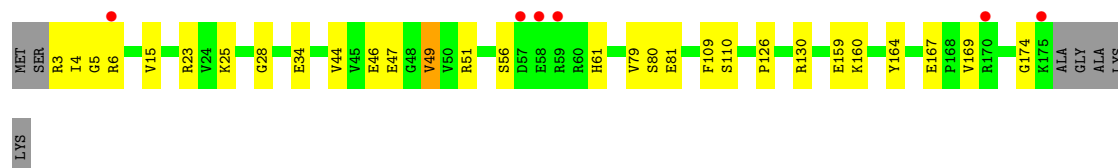
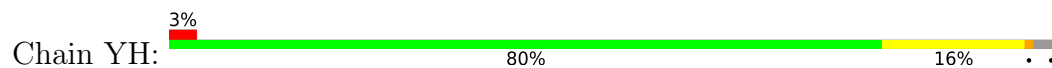
- Molecule 29: 50S ribosomal protein L5



- Molecule 30: 50S ribosomal protein L6

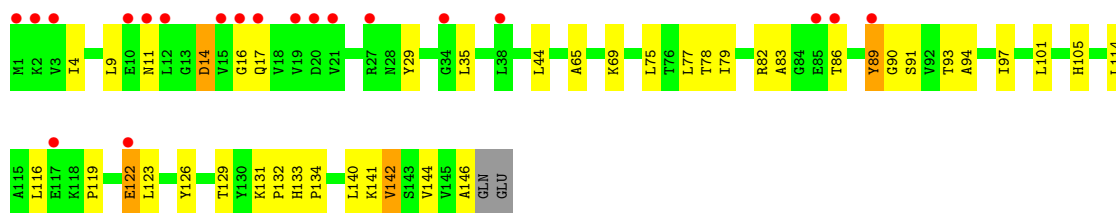


- Molecule 30: 50S ribosomal protein L6

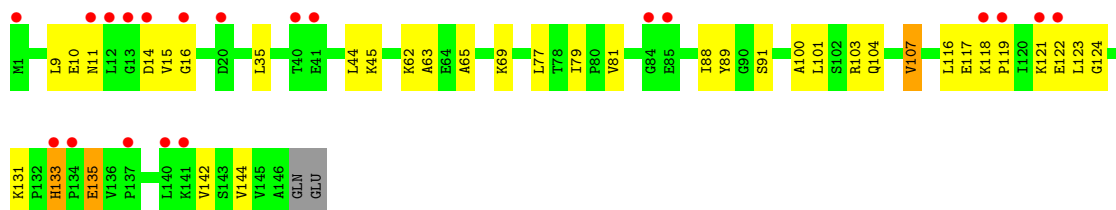
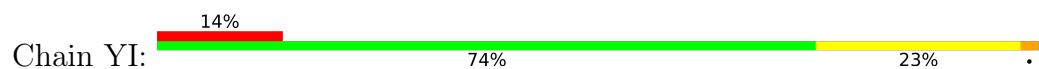


- Molecule 31: 50S ribosomal protein L9

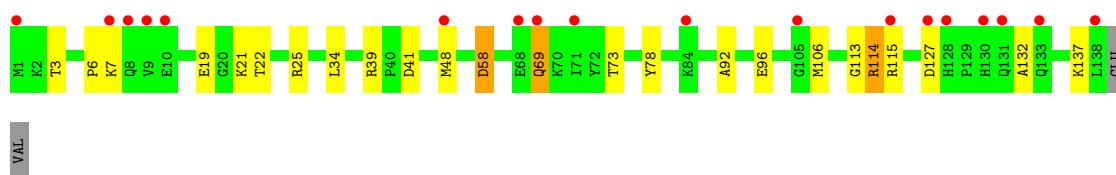
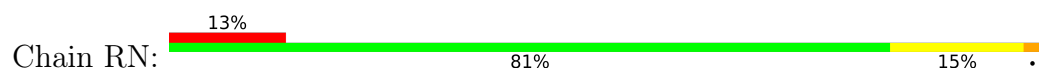




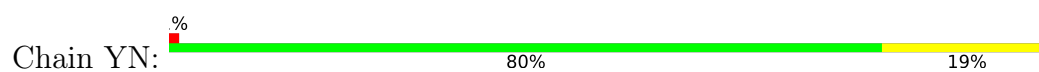
• Molecule 31: 50S ribosomal protein L9



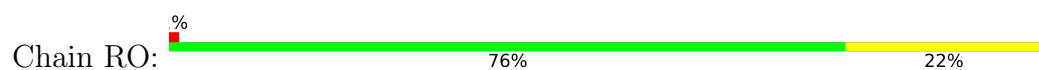
• Molecule 32: 50S ribosomal protein L13



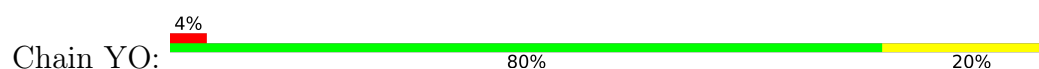
• Molecule 32: 50S ribosomal protein L13



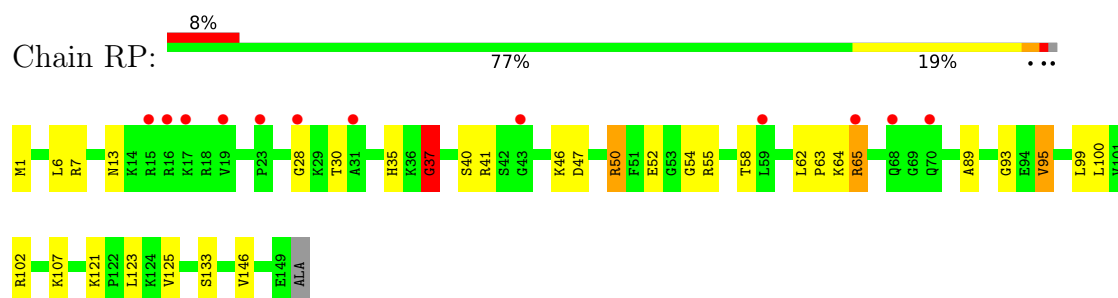
• Molecule 33: 50S ribosomal protein L14



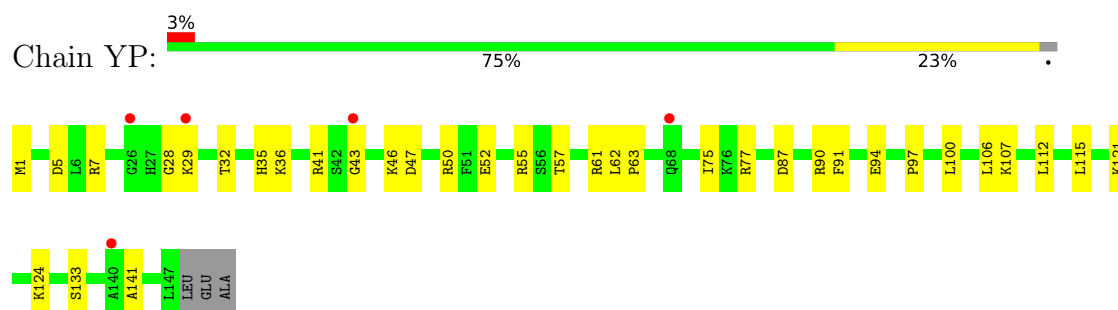
• Molecule 33: 50S ribosomal protein L14



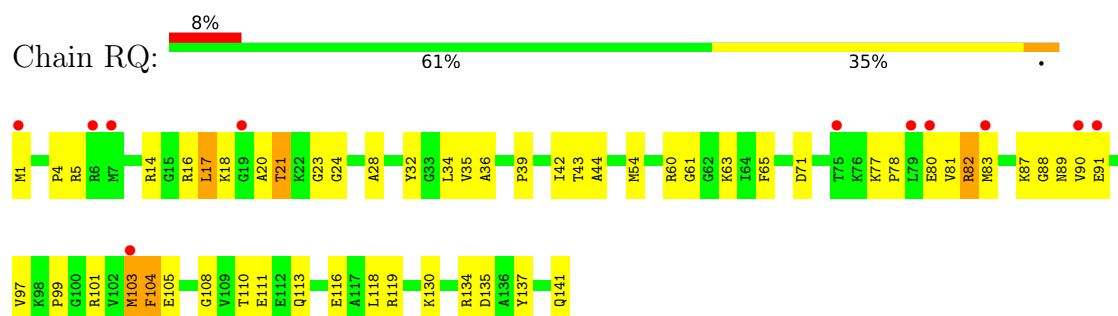
- Molecule 34: 50S ribosomal protein L15



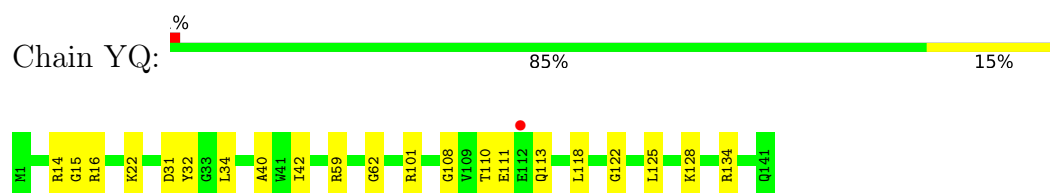
- Molecule 34: 50S ribosomal protein L15



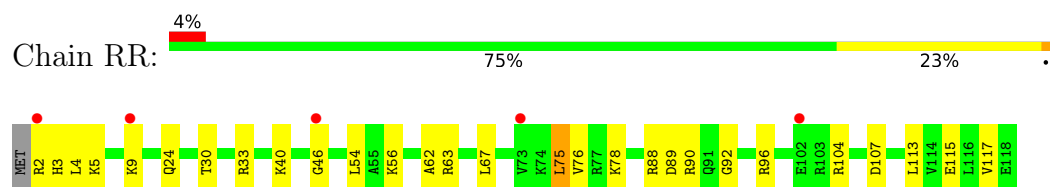
- Molecule 35: 50S ribosomal protein L16



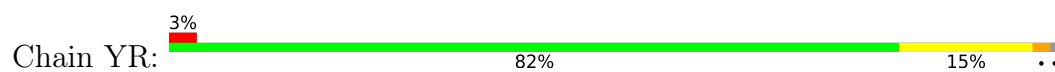
- Molecule 35: 50S ribosomal protein L16



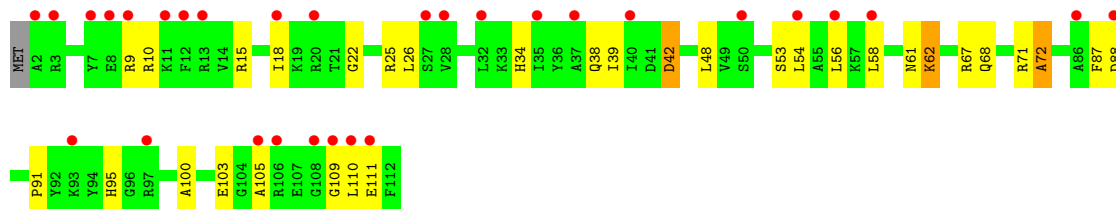
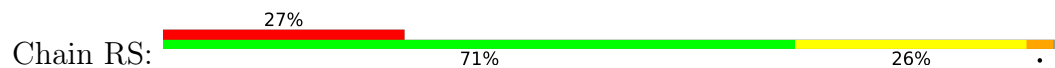
- Molecule 36: 50S ribosomal protein L17



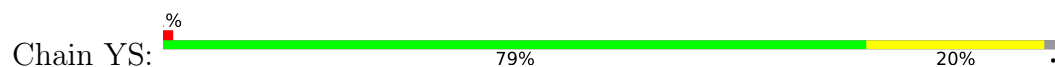
- Molecule 36: 50S ribosomal protein L17



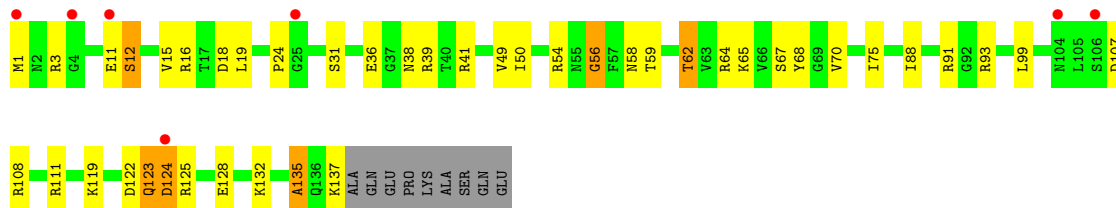
- Molecule 37: 50S ribosomal protein L18



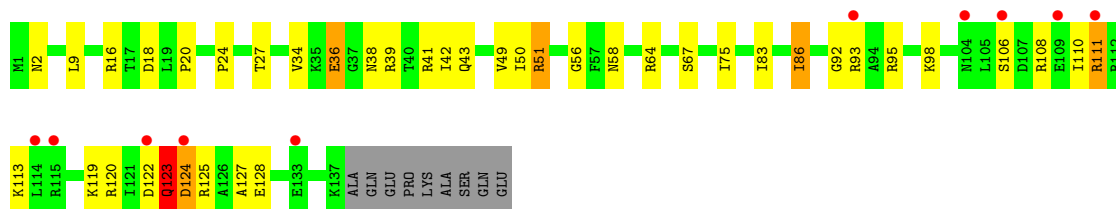
- Molecule 37: 50S ribosomal protein L18



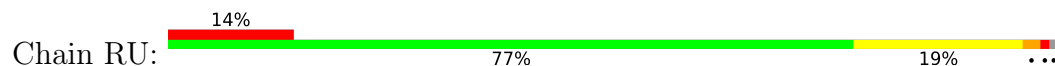
- Molecule 38: 50S ribosomal protein L19

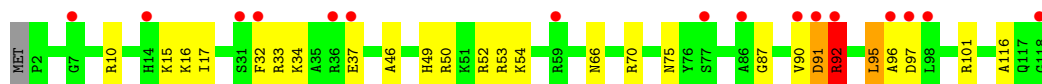


- Molecule 38: 50S ribosomal protein L19

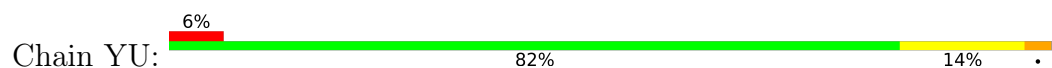


- Molecule 39: 50S ribosomal protein L20

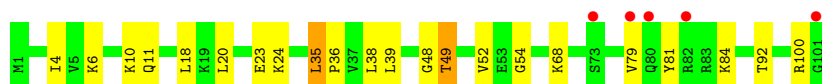
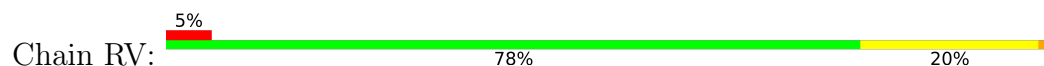




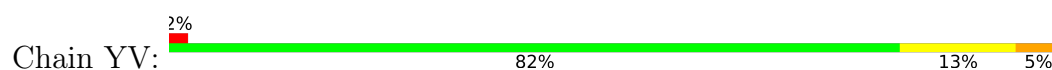
- Molecule 39: 50S ribosomal protein L20



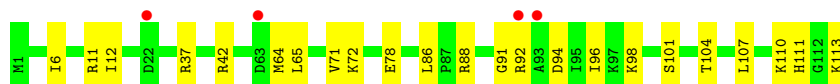
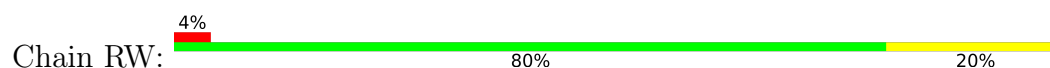
- Molecule 40: 50S ribosomal protein L21



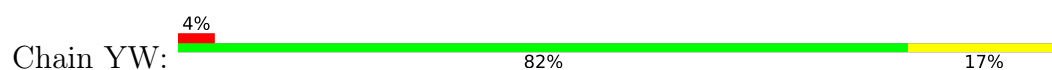
- Molecule 40: 50S ribosomal protein L21



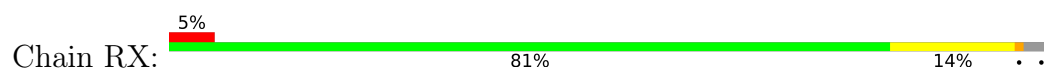
- Molecule 41: 50S ribosomal protein L22



- Molecule 41: 50S ribosomal protein L22

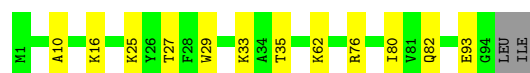


- Molecule 42: 50S ribosomal protein L23



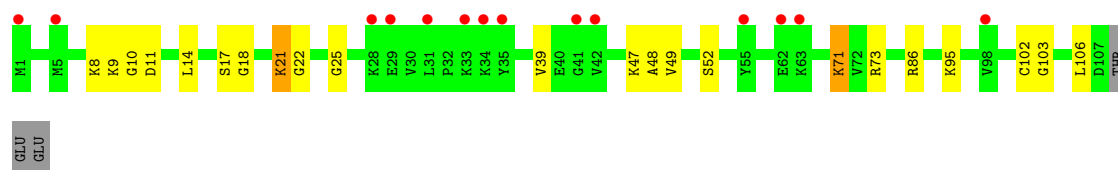
- Molecule 42: 50S ribosomal protein L23

Chain YX:  85% 12% .



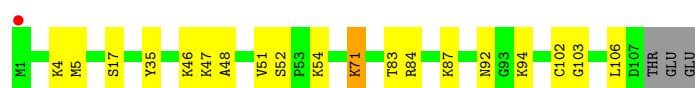
- Molecule 43: 50S ribosomal protein L24

Chain RY:  13% 77% 18% . .



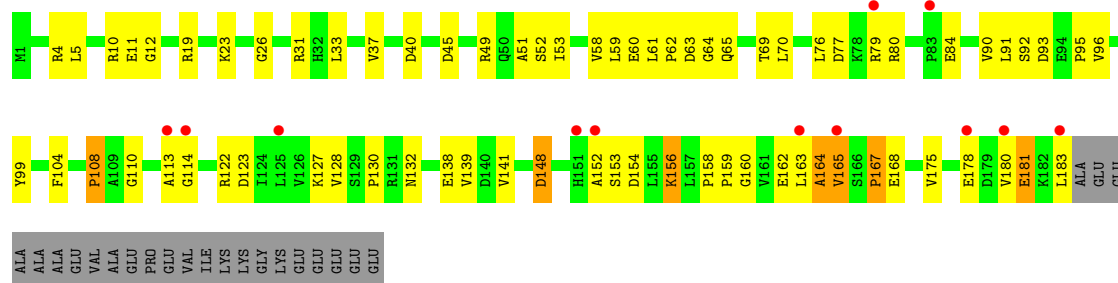
- Molecule 43: 50S ribosomal protein L24

Chain YY:  80% 16% . .



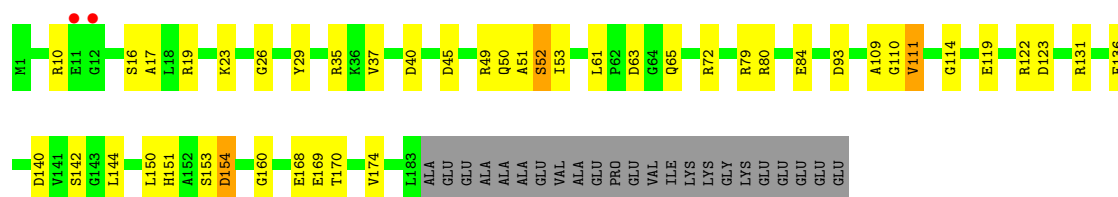
- Molecule 44: 50S ribosomal protein L25

Chain RZ:  6% 54% 32% . 11%



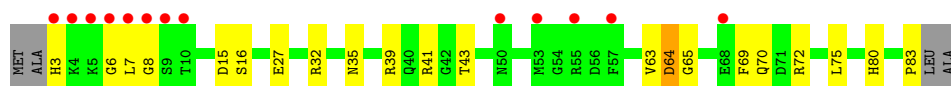
- Molecule 44: 50S ribosomal protein L25

Chain YZ:  67% 20% . 11%

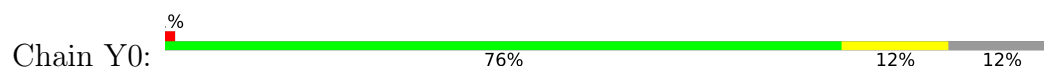


- Molecule 45: 50S ribosomal protein L27

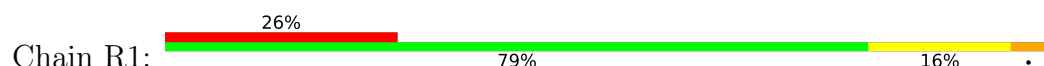
Chain R0:  15% 71% 24% . 5%



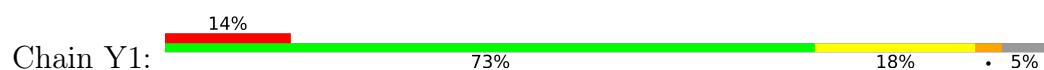
- Molecule 45: 50S ribosomal protein L27



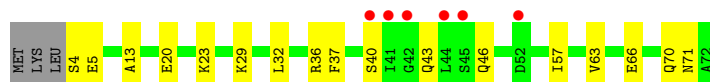
- Molecule 46: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L28



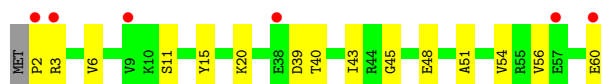
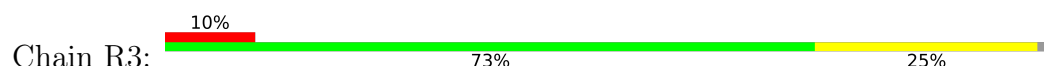
- Molecule 47: 50S ribosomal protein L29



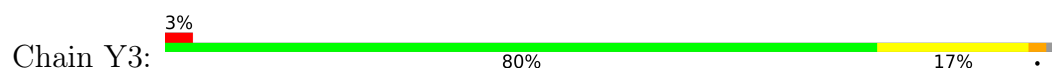
- Molecule 47: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L30



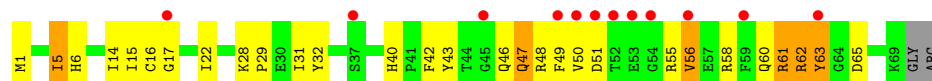
- Molecule 48: 50S ribosomal protein L30



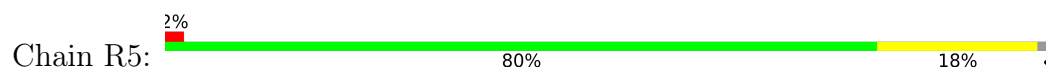
- Molecule 49: 50S ribosomal protein L31



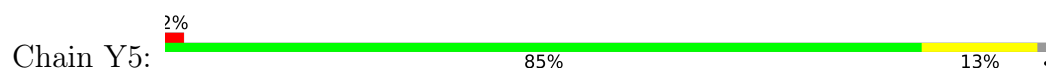
- Molecule 49: 50S ribosomal protein L31



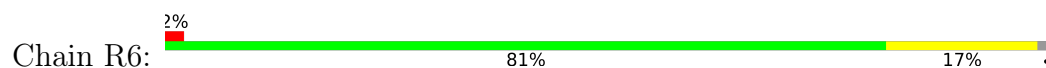
- Molecule 50: 50S ribosomal protein L32



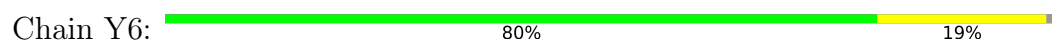
- Molecule 50: 50S ribosomal protein L32



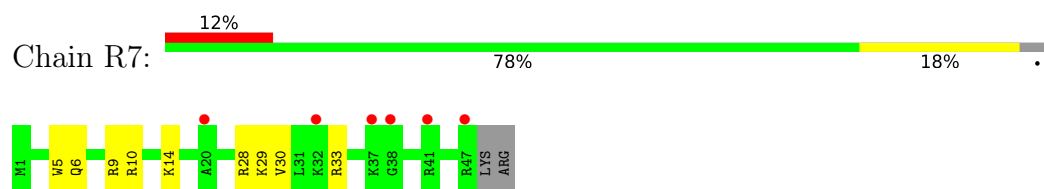
- Molecule 51: 50S ribosomal protein L33



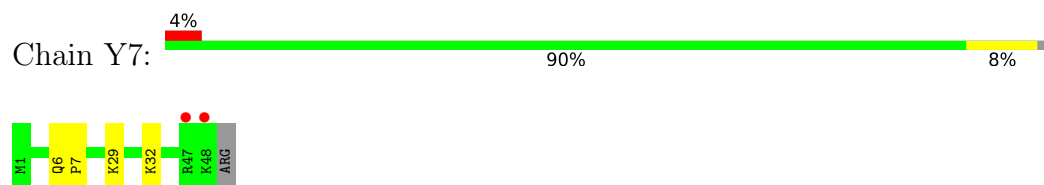
- Molecule 51: 50S ribosomal protein L33



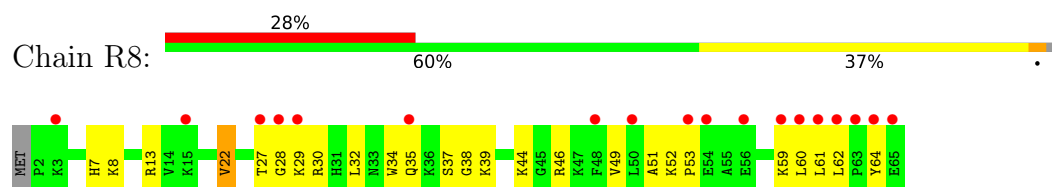
• Molecule 52: 50S ribosomal protein L34



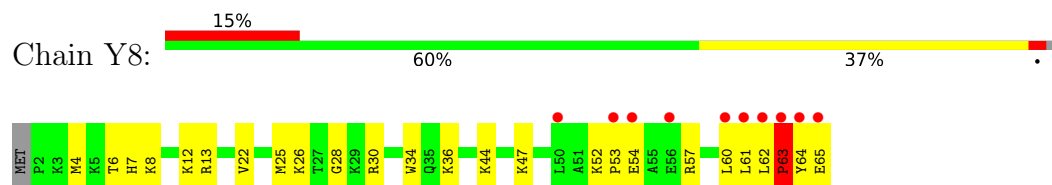
• Molecule 52: 50S ribosomal protein L34



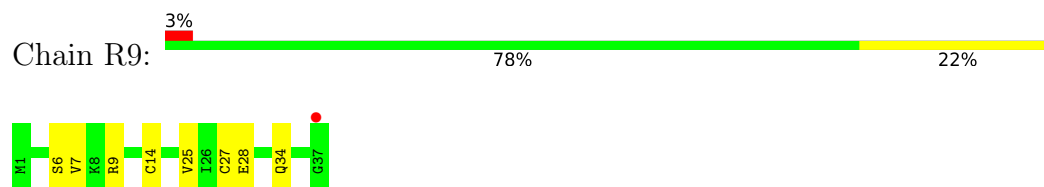
• Molecule 53: 50S ribosomal protein L35



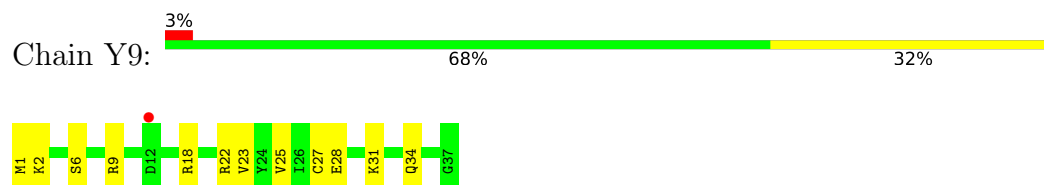
• Molecule 53: 50S ribosomal protein L35



• Molecule 54: 50S ribosomal protein L36



• Molecule 54: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.17Å 451.47Å 620.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.46 – 3.20 152.46 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (152.46-3.20) 99.2 (152.46-3.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.224 , 0.256 0.227 , 0.258	Depositor DCC
R_{free} test set	44319 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	71.2	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 87.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	291964	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, SF4, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	QA	0.37	1/36098 (0.0%)	0.38	3/56341 (0.0%)
1	XA	0.37	1/36101 (0.0%)	0.38	8/56346 (0.0%)
2	QB	0.39	0/1942	0.74	5/2619 (0.2%)
2	XB	0.39	0/1950	0.63	0/2630
3	QC	0.34	0/1629	0.63	0/2195
3	XC	0.33	0/1629	0.58	0/2195
4	QD	0.46	0/1733	0.66	0/2318
4	XD	0.52	0/1733	0.81	5/2318 (0.2%)
5	QE	0.45	0/1171	0.67	1/1576 (0.1%)
5	XE	0.49	0/1171	0.59	0/1576
6	QF	0.40	0/856	0.57	0/1154
6	XF	0.48	0/856	0.54	0/1154
7	QG	0.31	0/1276	0.57	0/1709
7	XG	0.31	0/1276	0.58	0/1709
8	QH	0.48	0/1128	0.63	0/1517
8	XH	0.50	0/1128	0.59	0/1517
9	QI	0.31	0/1029	0.70	0/1379
9	XI	0.33	0/1017	0.67	0/1365
10	QJ	0.32	0/814	0.62	0/1095
10	XJ	0.31	0/790	0.58	0/1063
11	QK	0.47	0/900	0.62	0/1213
11	XK	0.49	0/879	0.54	0/1187
12	QL	0.58	0/991	0.62	0/1327
12	XL	0.55	0/972	0.70	1/1301 (0.1%)
13	QM	0.33	0/965	0.74	0/1292
13	XM	0.32	0/956	0.71	0/1281
14	QN	0.38	0/501	0.76	0/664
14	XN	0.37	0/501	0.69	0/664
15	QO	0.45	0/745	0.61	0/992
15	XO	0.53	0/740	0.50	0/987
16	QP	0.53	0/721	0.59	0/970
16	XP	0.43	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.50	0/847	0.57	0/1131
17	XQ	0.49	0/847	0.55	0/1131
18	QR	0.46	0/579	0.63	0/768
18	XR	0.52	0/579	0.60	0/768
19	QS	0.32	0/680	0.72	0/915
19	XS	0.32	0/689	0.67	0/926
20	QT	0.46	0/765	0.64	0/1007
20	XT	0.41	0/765	0.60	0/1007
21	QU	0.35	0/221	0.63	0/288
21	XU	0.31	0/221	0.61	0/288
22	QV	0.26	0/1814	0.38	0/2825
22	XV	0.25	0/1814	0.36	0/2825
23	QX	0.18	0/470	0.34	0/733
23	XX	0.20	0/470	0.35	0/733
24	RA	0.50	4/69498 (0.0%)	0.40	4/108491 (0.0%)
24	YA	0.60	0/69543	0.42	13/108563 (0.0%)
25	RB	0.35	0/2878	0.36	0/4490
25	YB	0.70	5/2878 (0.2%)	1.03	16/4490 (0.4%)
26	RD	0.75	1/2185 (0.0%)	0.62	0/2944
26	YD	0.91	1/2185 (0.0%)	0.78	2/2944 (0.1%)
27	RE	0.69	0/1601	0.66	2/2160 (0.1%)
27	YE	0.82	0/1596	0.71	0/2153
28	RF	0.63	0/1620	0.62	0/2194
28	YF	0.79	0/1620	0.66	0/2194
29	RG	0.40	0/1499	0.71	0/2016
29	YG	0.49	0/1499	0.68	0/2016
30	RH	0.43	0/1362	0.68	0/1841
30	YH	0.70	0/1356	0.60	0/1833
31	RI	0.44	0/1151	0.75	2/1558 (0.1%)
31	YI	0.50	0/1151	0.75	0/1558
32	RN	0.59	0/1131	0.65	2/1525 (0.1%)
32	YN	0.81	0/1148	0.68	0/1547
33	RO	0.69	0/943	0.60	0/1269
33	YO	0.81	1/943 (0.1%)	0.63	0/1269
34	RP	0.63	0/1156	0.68	1/1537 (0.1%)
34	YP	0.79	0/1139	0.72	0/1514
35	RQ	0.56	0/1143	0.68	0/1527
35	YQ	0.77	0/1143	0.59	0/1527
36	RR	0.71	0/974	0.65	0/1302
36	YR	0.82	0/974	0.73	0/1302
37	RS	0.45	0/892	0.71	0/1187
37	YS	0.65	0/887	0.60	0/1180
38	RT	0.59	0/1155	0.71	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.66	0/1155	0.72	0/1542
39	RU	0.66	0/982	0.67	2/1306 (0.2%)
39	YU	0.90	0/982	0.66	0/1306
40	RV	0.54	0/790	0.58	0/1057
40	YV	0.80	0/790	0.65	0/1057
41	RW	0.68	0/911	0.62	2/1220 (0.2%)
41	YW	0.86	0/911	0.63	0/1220
42	RX	0.62	0/739	0.63	0/993
42	YX	0.78	0/756	0.57	0/1014
43	RY	0.54	0/831	0.58	0/1108
43	YY	0.69	0/831	0.58	0/1108
44	RZ	0.43	0/1493	0.76	0/2026
44	YZ	0.59	0/1493	0.60	0/2026
45	R0	0.58	0/652	0.58	0/867
45	Y0	0.78	0/607	0.62	0/809
46	R1	0.67	0/770	0.66	0/1022
46	Y1	0.75	0/736	0.67	0/978
47	R2	0.50	0/583	0.55	0/771
47	Y2	0.70	0/560	0.61	0/741
48	R3	0.63	1/474 (0.2%)	0.60	0/635
48	Y3	0.76	0/474	0.71	1/635 (0.2%)
49	R4	0.32	0/578	0.75	0/776
49	Y4	0.36	0/578	0.82	5/776 (0.6%)
50	R5	0.72	0/473	0.64	0/639
50	Y5	0.87	0/473	0.68	0/639
51	R6	0.56	0/460	0.61	0/613
51	Y6	0.71	0/460	0.60	0/613
52	R7	0.77	0/417	0.62	0/550
52	Y7	0.94	0/426	0.66	0/561
53	R8	0.72	0/525	0.78	0/691
53	Y8	0.84	0/525	0.85	0/691
54	R9	0.55	0/310	0.53	0/407
54	Y9	0.78	0/310	0.54	0/407
All	All	0.53	15/315985 (0.0%)	0.49	75/472446 (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
1	XA	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	22
2	XB	0	15
3	QC	0	15
3	XC	0	9
4	QD	0	12
4	XD	0	15
5	QE	0	7
5	XE	0	6
6	QF	0	5
6	XF	0	3
7	QG	0	9
7	XG	0	10
8	QH	0	3
8	XH	0	5
9	QI	0	15
9	XI	0	16
10	QJ	0	12
10	XJ	0	8
11	QK	0	5
11	XK	0	4
12	QL	0	8
12	XL	0	11
13	QM	0	13
13	XM	0	18
14	QN	0	6
14	XN	0	2
15	QO	0	1
15	XO	0	2
16	QP	0	5
16	XP	0	10
17	QQ	0	3
17	XQ	0	1
18	QR	0	5
18	XR	0	6
19	QS	0	13
19	XS	0	14
20	QT	0	10
20	XT	0	12
21	XU	0	4
24	YA	0	2
26	RD	0	13
26	YD	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
27	RE	0	7
27	YE	0	10
28	RF	0	12
28	YF	0	15
29	RG	0	17
29	YG	0	20
30	RH	0	23
30	YH	0	1
31	RI	0	17
31	YI	0	21
32	RN	0	10
32	YN	0	7
33	RO	0	2
33	YO	0	1
34	RP	0	8
34	YP	0	5
35	RQ	0	18
35	YQ	0	6
36	RR	0	4
36	YR	0	5
37	RS	0	11
37	YS	0	1
38	RT	0	15
38	YT	0	11
39	RU	0	5
39	YU	0	5
40	RV	0	6
40	YV	0	7
41	RW	0	5
41	YW	0	5
42	RX	0	2
42	YX	0	1
43	RY	0	7
43	YY	0	5
44	RZ	0	38
44	YZ	0	10
45	R0	0	2
45	Y0	0	1
46	R1	0	10
46	Y1	0	7
47	R2	0	5
47	Y2	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
48	R3	0	1
48	Y3	0	2
49	R4	0	15
49	Y4	0	11
50	R5	0	1
52	R7	0	1
53	R8	0	11
53	Y8	0	6
All	All	0	781

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	YD	264	LYS	C-N	15.58	1.51	1.34
25	YB	112	G	N9-C4	12.28	1.62	1.38
25	YB	114	G	N9-C4	11.30	1.60	1.38
24	RA	1649	A	C5'-C4'	11.02	1.67	1.51
25	YB	112	G	N9-C8	-9.65	1.18	1.37

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YB	114	G	N7-C8-N9	-24.75	38.86	113.10
25	YB	112	G	N7-C8-N9	-24.37	39.98	113.10
25	YB	114	G	C4-C5-N7	-23.53	40.20	110.80
25	YB	112	G	C4-C5-N7	-23.11	41.46	110.80
25	YB	112	G	C8-N9-C4	-17.30	54.49	106.40

There are no chirality outliers.

5 of 781 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	18	GLY	Peptide
2	QB	19	HIS	Peptide
2	QB	21	ARG	Peptide
2	QB	38	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	453	0
1	XA	32249	0	16278	463	3
2	QB	1907	0	1958	35	0
2	XB	1915	0	1969	38	0
3	QC	1605	0	1668	31	0
3	XC	1605	0	1668	21	0
4	QD	1703	0	1766	28	0
4	XD	1703	0	1764	37	0
5	QE	1155	0	1213	28	0
5	XE	1155	0	1213	14	0
6	QF	843	0	857	13	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	16	0
7	XG	1257	0	1296	22	0
8	QH	1108	0	1165	20	0
8	XH	1108	0	1165	22	0
9	QI	1010	0	1037	19	0
9	XI	998	0	1024	29	0
10	QJ	801	0	849	23	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	27	0
11	XK	864	0	881	13	0
12	QL	975	0	1062	14	0
12	XL	956	0	1046	23	0
13	QM	955	0	1021	21	0
13	XM	946	0	1008	25	0
14	QN	492	0	529	19	0
14	XN	492	0	529	11	0
15	QO	734	0	771	11	0
15	XO	729	0	768	8	0
16	QP	705	0	725	15	0
16	XP	705	0	725	13	0
17	QQ	834	0	904	24	0
17	XQ	834	0	904	16	0
18	QR	574	0	644	7	0
18	XR	574	0	644	8	0
19	QS	665	0	686	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	11	0
20	QT	763	0	861	15	0
20	XT	763	0	861	23	0
21	QU	217	0	234	4	0
21	XU	217	0	234	4	0
22	QV	1648	0	834	27	0
22	XV	1648	0	834	23	0
23	QX	418	0	209	7	0
23	XX	418	0	209	7	0
24	RA	62051	0	31279	621	3
24	YA	62091	0	31292	533	0
25	RB	2573	0	1306	21	0
25	YB	2573	0	1304	41	0
26	RD	2135	0	2221	37	0
26	YD	2135	0	2221	32	0
27	RE	1568	0	1634	29	0
27	YE	1563	0	1628	29	0
28	RF	1585	0	1632	24	0
28	YF	1585	0	1632	23	0
29	RG	1474	0	1535	36	0
29	YG	1474	0	1535	30	0
30	RH	1336	0	1418	27	0
30	YH	1330	0	1413	19	0
31	RI	1136	0	1223	13	2
31	YI	1136	0	1223	12	0
32	RN	1104	0	1180	10	0
32	YN	1121	0	1195	15	0
33	RO	933	0	996	25	0
33	YO	933	0	996	18	0
34	RP	1139	0	1223	26	0
34	YP	1122	0	1206	26	0
35	RQ	1122	0	1179	29	0
35	YQ	1122	0	1179	10	0
36	RR	960	0	1021	18	0
36	YR	960	0	1021	11	0
37	RS	882	0	943	17	0
37	YS	877	0	938	15	0
38	RT	1141	0	1202	23	0
38	YT	1141	0	1202	27	0
39	RU	964	0	1022	26	0
39	YU	964	0	1021	19	0
40	RV	779	0	852	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YV	779	0	852	12	0
41	RW	900	0	964	11	0
41	YW	900	0	964	11	0
42	RX	725	0	778	8	0
42	YX	742	0	803	8	0
43	RY	818	0	909	12	0
43	YY	818	0	909	14	0
44	RZ	1461	0	1493	26	0
44	YZ	1461	0	1493	22	0
45	R0	643	0	667	12	0
45	Y0	599	0	617	7	0
46	R1	763	0	848	9	0
46	Y1	729	0	801	10	0
47	R2	581	0	629	7	0
47	Y2	558	0	610	5	2
48	R3	469	0	518	7	0
48	Y3	469	0	518	8	0
49	R4	565	0	558	9	0
49	Y4	565	0	557	13	0
50	R5	459	0	476	9	0
50	Y5	459	0	476	9	0
51	R6	453	0	473	8	0
51	Y6	453	0	473	10	0
52	R7	409	0	454	7	0
52	Y7	418	0	467	3	0
53	R8	517	0	582	13	0
53	Y8	517	0	582	14	0
54	R9	307	0	335	6	0
54	Y9	307	0	335	8	0
55	QA	64	0	0	0	0
55	QV	1	0	0	0	0
55	R0	2	0	0	0	0
55	R8	2	0	0	0	0
55	RA	444	0	0	0	0
55	RB	7	0	0	0	0
55	RE	5	0	0	0	0
55	RF	1	0	0	0	0
55	RN	1	0	0	0	0
55	RQ	1	0	0	0	0
55	RR	1	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	XA	78	0	0	0	0
55	XE	1	0	0	0	0
55	XM	2	0	0	0	0
55	XV	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	2	0	0	0	0
55	Y3	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	510	0	0	0	0
55	YB	7	0	0	0	0
55	YD	2	0	0	0	0
55	YE	5	0	0	0	0
55	YP	3	0	0	0	0
55	YQ	3	0	0	0	0
55	YR	1	0	0	0	0
56	QD	8	0	0	0	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
All	All	291964	0	197875	3337	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3337 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)
24:RA:1712:A:C2'	24:RA:1713:G:H5'	1.74	1.18
43:YY:92:ASN:ND2	43:YY:94:LYS:HG2	1.60	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:1405:A:N6	24:YA:1418:U:H3	1.48	1.10
24:RA:2818:U:C2	24:RA:2901:A:N6	2.27	1.02
24:RA:2226:C:H1'	24:RA:2232:G:N2	1.74	1.01

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.00	0.20
24:RA:331:G:OP2	47:Y2:17:SER:CA[3_555]	2.01	0.19
24:RA:331:G:OP2	47:Y2:17:SER:CB[3_555]	2.10	0.10
31:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	2.10	0.10
24:RA:2158:C:O2'	1:XA:1042:G:O2'[4_555]	2.13	0.07

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%)	205 (88%)	28 (12%)	0	100	100
2	XB	234/256 (91%)	207 (88%)	27 (12%)	0	100	100
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
4	XD	206/209 (99%)	191 (93%)	12 (6%)	3 (2%)	8	37
5	QE	149/162 (92%)	140 (94%)	9 (6%)	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%)	97 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	124/128 (97%)	107 (86%)	17 (14%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	88 (94%)	6 (6%)	0	100	100
11	QK	117/129 (91%)	101 (86%)	16 (14%)	0	100	100
11	XK	114/129 (88%)	102 (90%)	12 (10%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	13 (11%)	0	100	100
12	XL	120/132 (91%)	100 (83%)	20 (17%)	0	100	100
13	QM	118/126 (94%)	102 (86%)	16 (14%)	0	100	100
13	XM	117/126 (93%)	99 (85%)	17 (14%)	1 (1%)	14	47
14	QN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
14	XN	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
17	QQ	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	63 (93%)	5 (7%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	11 (13%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	272/276 (99%)	259 (95%)	13 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	YD	272/276 (99%)	253 (93%)	19 (7%)	0	100	100
27	RE	203/206 (98%)	187 (92%)	16 (8%)	0	100	100
27	YE	202/206 (98%)	189 (94%)	13 (6%)	0	100	100
28	RF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
28	YF	200/210 (95%)	185 (92%)	15 (8%)	0	100	100
29	RG	179/182 (98%)	155 (87%)	24 (13%)	0	100	100
29	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	21	56
30	RH	172/180 (96%)	142 (83%)	29 (17%)	1 (1%)	21	56
30	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
31	RI	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
31	YI	144/148 (97%)	120 (83%)	24 (17%)	0	100	100
32	RN	136/140 (97%)	119 (88%)	17 (12%)	0	100	100
32	YN	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
33	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
34	RP	147/150 (98%)	142 (97%)	5 (3%)	0	100	100
34	YP	145/150 (97%)	138 (95%)	6 (4%)	1 (1%)	18	52
35	RQ	139/141 (99%)	116 (84%)	22 (16%)	1 (1%)	18	52
35	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
36	RR	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	47
36	YR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
37	RS	109/112 (97%)	89 (82%)	20 (18%)	0	100	100
37	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
38	RT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	8	37
38	YT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	8	37
39	RU	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
39	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	47
40	RV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	YV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
41	RW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
41	YW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
42	YX	92/96 (96%)	90 (98%)	2 (2%)	0	100	100
43	RY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
43	YY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
44	RZ	181/206 (88%)	143 (79%)	38 (21%)	0	100	100
44	YZ	181/206 (88%)	176 (97%)	4 (2%)	1 (1%)	21	56
45	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
45	Y0	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	84 (92%)	7 (8%)	0	100	100
47	R2	67/72 (93%)	65 (97%)	2 (3%)	0	100	100
47	Y2	64/72 (89%)	61 (95%)	3 (5%)	0	100	100
48	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	54 (81%)	13 (19%)	0	100	100
49	Y4	67/71 (94%)	55 (82%)	12 (18%)	0	100	100
50	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	R8	62/65 (95%)	49 (79%)	13 (21%)	0	100	100
53	Y8	62/65 (95%)	53 (86%)	8 (13%)	1 (2%)	7	36
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11453/12128 (94%)	10502 (92%)	935 (8%)	16 (0%)	48	79

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	RR	4	LEU
4	XD	31	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	YZ	52	SER
38	RT	123	GLN
38	RT	124	ASP

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%)	203 (100%)	0	100	100
2	XB	204/220 (93%)	201 (98%)	3 (2%)	57	76
3	QC	159/188 (85%)	158 (99%)	1 (1%)	78	84
3	XC	159/188 (85%)	156 (98%)	3 (2%)	50	73
4	QD	180/181 (99%)	178 (99%)	2 (1%)	65	79
4	XD	180/181 (99%)	170 (94%)	10 (6%)	19	52
5	QE	116/123 (94%)	114 (98%)	2 (2%)	53	75
5	XE	116/123 (94%)	115 (99%)	1 (1%)	70	81
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	79
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	125 (99%)	1 (1%)	73	82
7	XG	126/127 (99%)	124 (98%)	2 (2%)	55	75
8	QH	118/119 (99%)	116 (98%)	2 (2%)	53	75
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	82
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	86 (97%)	3 (3%)	32	64
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	89 (99%)	1 (1%)	65	79
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	93 (97%)	3 (3%)	35	66
13	XM	95/101 (94%)	94 (99%)	1 (1%)	65	79
14	QN	49/50 (98%)	47 (96%)	2 (4%)	27	60
14	XN	49/50 (98%)	48 (98%)	1 (2%)	48	72
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%)	71 (99%)	1 (1%)	59	77
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	65	79
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	65	79
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	60 (98%)	1 (2%)	55	75
19	QS	72/80 (90%)	71 (99%)	1 (1%)	59	77
19	XS	73/80 (91%)	72 (99%)	1 (1%)	59	77
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%)	19 (95%)	1 (5%)	22	55
26	RD	216/218 (99%)	216 (100%)	0	100	100
26	YD	216/218 (99%)	213 (99%)	3 (1%)	59	77
27	RE	165/166 (99%)	161 (98%)	4 (2%)	43	70
27	YE	165/166 (99%)	158 (96%)	7 (4%)	26	60
28	RF	161/166 (97%)	160 (99%)	1 (1%)	78	84
28	YF	161/166 (97%)	160 (99%)	1 (1%)	78	84
29	RG	155/156 (99%)	155 (100%)	0	100	100
29	YG	155/156 (99%)	154 (99%)	1 (1%)	78	84
30	RH	145/148 (98%)	144 (99%)	1 (1%)	76	83
30	YH	144/148 (97%)	140 (97%)	4 (3%)	38	68
31	RI	122/124 (98%)	120 (98%)	2 (2%)	55	75
31	YI	122/124 (98%)	121 (99%)	1 (1%)	73	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	RN	117/119 (98%)	113 (97%)	4 (3%)	32	64
32	YN	119/119 (100%)	119 (100%)	0	100	100
33	RO	100/100 (100%)	99 (99%)	1 (1%)	68	80
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	115 (99%)	1 (1%)	70	81
34	YP	114/116 (98%)	114 (100%)	0	100	100
35	RQ	111/111 (100%)	110 (99%)	1 (1%)	70	81
35	YQ	111/111 (100%)	110 (99%)	1 (1%)	70	81
36	RR	100/101 (99%)	99 (99%)	1 (1%)	68	80
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	87 (100%)	0	100	100
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	118 (98%)	2 (2%)	53	75
38	YT	120/127 (94%)	116 (97%)	4 (3%)	33	65
39	RU	93/94 (99%)	92 (99%)	1 (1%)	65	79
39	YU	93/94 (99%)	91 (98%)	2 (2%)	45	71
40	RV	82/82 (100%)	80 (98%)	2 (2%)	43	70
40	YV	82/82 (100%)	79 (96%)	3 (4%)	30	63
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	92 (100%)	0	100	100
42	RX	74/78 (95%)	73 (99%)	1 (1%)	59	77
42	YX	76/78 (97%)	75 (99%)	1 (1%)	61	78
43	RY	88/91 (97%)	87 (99%)	1 (1%)	65	79
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	162/179 (90%)	160 (99%)	2 (1%)	63	79
44	YZ	162/179 (90%)	160 (99%)	2 (1%)	63	79
45	R0	65/67 (97%)	63 (97%)	2 (3%)	35	66
45	Y0	61/67 (91%)	61 (100%)	0	100	100
46	R1	82/83 (99%)	82 (100%)	0	100	100
46	Y1	78/83 (94%)	77 (99%)	1 (1%)	61	78
47	R2	64/67 (96%)	64 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Y2	62/67 (92%)	62 (100%)	0	100	100
48	R3	51/52 (98%)	51 (100%)	0	100	100
48	Y3	51/52 (98%)	51 (100%)	0	100	100
49	R4	62/63 (98%)	62 (100%)	0	100	100
49	Y4	62/63 (98%)	61 (98%)	1 (2%)	55	75
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	51 (100%)	0	100	100
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	53 (98%)	1 (2%)	50	73
53	Y8	54/55 (98%)	54 (100%)	0	100	100
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9692/10066 (96%)	9585 (99%)	107 (1%)	65	79

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	XD	20	TYR
17	XQ	57	VAL
40	YV	72	VAL
4	XD	31	CYS
5	XE	51	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
27	YE	121	ASN
44	YZ	34	ASN
28	YF	40	GLN
35	YQ	113	GLN
31	RI	43	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1521 (98%)	289 (19%)	39 (2%)
1	XA	1499/1521 (98%)	271 (18%)	33 (2%)
22	QV	76/77 (98%)	22 (28%)	1 (1%)
22	XV	76/77 (98%)	18 (23%)	1 (1%)
23	QX	18/19 (94%)	7 (38%)	1 (5%)
23	XX	18/19 (94%)	6 (33%)	0
24	RA	2877/2915 (98%)	591 (20%)	37 (1%)
24	YA	2880/2915 (98%)	552 (19%)	43 (1%)
25	RB	119/122 (97%)	18 (15%)	1 (0%)
25	YB	119/122 (97%)	21 (17%)	1 (0%)
All	All	9181/9308 (98%)	1795 (19%)	157 (1%)

5 of 1795 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 157 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	YA	210	A
24	YA	1700	G
24	YA	302	A
24	YA	1068	G
24	YA	2622	C

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

2 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	1MG	XV	37	22	23,26,27	1.19	3 (13%)	33,39,42	1.76	5 (15%)
22	1MG	QV	37	22	23,26,27	1.20	3 (13%)	33,39,42	1.73	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	XV	37	22	-	0/7/25/26	0/3/3/3
22	1MG	QV	37	22	-	0/7/25/26	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	37	1MG	C5-C4	3.23	1.47	1.38
22	XV	37	1MG	C5-C4	3.19	1.47	1.38
22	XV	37	1MG	C2-N1	2.47	1.41	1.37
22	QV	37	1MG	C2-N1	2.40	1.41	1.37
22	QV	37	1MG	C5-N7	-2.17	1.34	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	1MG	C5-C4-N3	-5.24	120.05	128.39
22	QV	37	1MG	C5-C4-N3	-5.17	120.16	128.39
22	XV	37	1MG	C2-N3-C4	4.35	121.76	111.98
22	QV	37	1MG	C2-N3-C4	4.28	121.61	111.98
22	QV	37	1MG	N9-C4-N3	3.90	133.76	125.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1166 ligands modelled in this entry, 1164 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	$\# Z > 2$
56	SF4	XD	301	4	0,12,12	-	-	-		
56	SF4	QD	301	4	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
56	SF4	XD	301	4	-	-	0/6/5/5
56	SF4	QD	301	4	-	-	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	1500/1521 (98%)	0.41	73 (4%) 35 22	58, 110, 240, 377	0
1	XA	1500/1521 (98%)	0.52	108 (7%) 21 14	54, 120, 257, 365	0
2	QB	235/256 (91%)	0.53	3 (1%) 75 55	109, 150, 192, 239	0
2	XB	236/256 (92%)	0.91	18 (7%) 20 13	104, 136, 180, 227	0
3	QC	205/239 (85%)	0.88	19 (9%) 14 9	123, 163, 203, 242	0
3	XC	205/239 (85%)	1.43	43 (20%) 2 2	119, 158, 198, 242	0
4	QD	208/209 (99%)	0.81	13 (6%) 26 17	84, 112, 140, 171	0
4	XD	208/209 (99%)	1.47	52 (25%) 2 2	92, 131, 170, 193	0
5	QE	151/162 (93%)	0.47	5 (3%) 49 30	86, 112, 152, 179	0
5	XE	151/162 (93%)	1.06	18 (11%) 9 6	78, 108, 140, 162	0
6	QF	101/101 (100%)	0.96	8 (7%) 18 12	96, 122, 156, 173	0
6	XF	101/101 (100%)	0.46	1 (0%) 79 63	76, 108, 135, 189	0
7	QG	155/156 (99%)	1.26	30 (19%) 3 2	130, 162, 199, 225	0
7	XG	155/156 (99%)	1.34	35 (22%) 2 2	122, 164, 201, 247	0
8	QH	137/138 (99%)	0.63	5 (3%) 46 28	87, 116, 138, 168	0
8	XH	137/138 (99%)	0.79	11 (8%) 18 12	83, 111, 148, 165	0
9	QI	127/128 (99%)	2.54	71 (55%) 0 0	129, 174, 219, 232	0
9	XI	126/128 (98%)	1.59	35 (27%) 1 1	132, 172, 203, 231	0
10	QJ	99/105 (94%)	1.12	21 (21%) 2 2	140, 178, 215, 240	0
10	XJ	96/105 (91%)	1.97	34 (35%) 1 1	144, 175, 211, 235	0
11	QK	119/129 (92%)	1.32	17 (14%) 6 5	91, 119, 158, 189	0
11	XK	116/129 (89%)	0.91	9 (7%) 19 12	64, 105, 149, 188	0
12	QL	125/132 (94%)	1.23	27 (21%) 2 2	64, 90, 133, 187	0
12	XL	122/132 (92%)	0.98	24 (19%) 3 2	60, 96, 126, 169	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%)	1.19	23 (19%) 3 2	129, 167, 203, 227	0
13	XM	119/126 (94%)	2.11	50 (42%) 0 1	137, 187, 227, 247	0
14	QN	60/61 (98%)	1.72	20 (33%) 1 1	139, 171, 209, 233	0
14	XN	60/61 (98%)	1.16	10 (16%) 4 3	132, 158, 190, 212	0
15	QO	88/89 (98%)	0.63	5 (5%) 29 19	67, 107, 144, 154	0
15	XO	87/89 (97%)	0.65	3 (3%) 48 30	62, 95, 139, 158	0
16	QP	84/88 (95%)	0.76	2 (2%) 59 40	80, 100, 140, 184	0
16	XP	84/88 (95%)	0.92	10 (11%) 9 6	93, 127, 165, 189	0
17	QQ	100/105 (95%)	0.98	12 (12%) 9 6	73, 99, 142, 155	0
17	XQ	100/105 (95%)	0.56	6 (6%) 27 17	68, 104, 134, 149	0
18	QR	70/88 (79%)	0.87	6 (8%) 16 11	95, 126, 152, 179	0
18	XR	70/88 (79%)	0.42	2 (2%) 53 35	73, 111, 152, 172	0
19	QS	83/93 (89%)	1.43	19 (22%) 2 2	153, 182, 217, 240	0
19	XS	84/93 (90%)	1.67	29 (34%) 1 1	160, 195, 230, 246	0
20	QT	99/106 (93%)	1.08	10 (10%) 12 8	67, 99, 143, 165	0
20	XT	99/106 (93%)	0.88	8 (8%) 18 11	76, 115, 152, 193	0
21	QU	25/27 (92%)	1.86	9 (36%) 1 1	124, 153, 183, 204	0
21	XU	25/27 (92%)	1.40	5 (20%) 3 2	108, 168, 192, 212	0
22	QV	76/77 (98%)	0.78	6 (7%) 18 12	151, 202, 240, 251	0
22	XV	76/77 (98%)	1.91	26 (34%) 1 1	225, 332, 347, 358	0
23	QX	19/19 (100%)	1.58	4 (21%) 2 2	116, 227, 311, 319	0
23	XX	19/19 (100%)	2.81	15 (78%) 0 0	131, 254, 297, 308	0
24	RA	2881/2915 (98%)	0.21	116 (4%) 42 26	40, 73, 215, 458	0
24	YA	2883/2915 (98%)	0.09	94 (3%) 49 30	28, 53, 212, 402	0
25	RB	120/122 (98%)	0.35	1 (0%) 82 67	82, 126, 171, 195	0
25	YB	120/122 (98%)	0.18	5 (4%) 40 25	49, 77, 109, 224	0
26	RD	274/276 (99%)	0.71	15 (5%) 30 19	42, 67, 101, 139	0
26	YD	274/276 (99%)	0.29	5 (1%) 67 48	35, 53, 81, 126	0
27	RE	205/206 (99%)	0.44	8 (3%) 43 27	37, 72, 114, 177	0
27	YE	204/206 (99%)	0.21	2 (0%) 79 63	25, 55, 91, 111	0
28	RF	202/210 (96%)	0.54	9 (4%) 38 24	46, 86, 135, 169	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YF	202/210 (96%)	0.45	7 (3%) 47 29	29, 59, 134, 186	0
29	RG	181/182 (99%)	1.18	27 (14%) 5 4	112, 145, 188, 220	0
29	YG	181/182 (99%)	0.99	21 (11%) 9 7	73, 123, 172, 219	0
30	RH	174/180 (96%)	1.03	21 (12%) 8 6	90, 131, 176, 222	0
30	YH	173/180 (96%)	0.25	6 (3%) 47 29	48, 69, 97, 118	0
31	RI	146/148 (98%)	0.97	20 (13%) 6 5	72, 114, 150, 159	0
31	YI	146/148 (98%)	0.85	20 (13%) 6 5	65, 103, 139, 169	0
32	RN	138/140 (98%)	1.10	18 (13%) 7 6	50, 82, 129, 147	0
32	YN	140/140 (100%)	0.50	2 (1%) 73 54	33, 55, 91, 128	0
33	RO	122/122 (100%)	0.17	1 (0%) 82 67	47, 72, 99, 124	0
33	YO	122/122 (100%)	0.40	5 (4%) 41 25	38, 58, 90, 107	0
34	RP	149/150 (99%)	0.76	12 (8%) 18 11	50, 86, 131, 150	0
34	YP	147/150 (98%)	0.43	5 (3%) 48 30	30, 64, 105, 133	0
35	RQ	141/141 (100%)	0.85	11 (7%) 19 12	59, 91, 132, 189	0
35	YQ	141/141 (100%)	0.06	1 (0%) 84 69	39, 59, 88, 136	0
36	RR	117/118 (99%)	0.47	5 (4%) 40 24	53, 68, 100, 156	0
36	YR	117/118 (99%)	0.32	3 (2%) 57 37	39, 52, 83, 154	0
37	RS	111/112 (99%)	1.44	30 (27%) 1 1	98, 126, 166, 186	0
37	YS	110/112 (98%)	0.21	1 (0%) 81 64	52, 72, 103, 117	0
38	RT	137/146 (93%)	0.62	7 (5%) 33 21	50, 83, 143, 196	0
38	YT	137/146 (93%)	0.60	10 (7%) 21 13	47, 68, 125, 170	0
39	RU	117/118 (99%)	0.97	16 (13%) 6 5	47, 81, 131, 174	0
39	YU	117/118 (99%)	0.61	7 (5%) 27 17	29, 45, 88, 151	0
40	RV	101/101 (100%)	0.49	5 (4%) 34 22	57, 94, 123, 167	0
40	YV	101/101 (100%)	0.16	2 (1%) 65 45	28, 55, 89, 133	0
41	RW	113/113 (100%)	0.43	4 (3%) 47 29	46, 65, 114, 204	0
41	YW	113/113 (100%)	0.23	4 (3%) 47 29	29, 48, 82, 192	0
42	RX	92/96 (95%)	0.40	5 (5%) 31 20	52, 77, 114, 122	0
42	YX	94/96 (97%)	-0.03	0 100 100	34, 53, 83, 123	0
43	RY	107/110 (97%)	0.99	14 (13%) 7 6	64, 97, 130, 148	0
43	YY	107/110 (97%)	0.33	1 (0%) 81 64	45, 67, 97, 143	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RZ	183/206 (88%)	0.60	12 (6%) 24 15	98, 131, 173, 201	0
44	YZ	183/206 (88%)	0.20	2 (1%) 78 61	47, 84, 116, 174	0
45	R0	81/85 (95%)	1.00	13 (16%) 5 3	68, 90, 149, 208	0
45	Y0	75/85 (88%)	0.27	1 (1%) 75 55	42, 59, 85, 98	0
46	R1	97/98 (98%)	1.40	25 (25%) 1 2	49, 75, 139, 212	0
46	Y1	93/98 (94%)	0.87	14 (15%) 5 4	41, 65, 121, 135	0
47	R2	69/72 (95%)	0.65	6 (8%) 16 11	67, 93, 143, 158	0
47	Y2	66/72 (91%)	0.48	6 (9%) 15 9	41, 65, 105, 142	0
48	R3	59/60 (98%)	0.86	6 (10%) 12 8	56, 86, 144, 197	0
48	Y3	59/60 (98%)	0.20	2 (3%) 48 30	37, 53, 87, 140	0
49	R4	69/71 (97%)	1.01	8 (11%) 9 7	134, 176, 219, 247	0
49	Y4	69/71 (97%)	1.22	12 (17%) 4 3	102, 153, 229, 258	0
50	R5	59/60 (98%)	0.23	1 (1%) 69 49	43, 66, 105, 144	0
50	Y5	59/60 (98%)	0.26	1 (1%) 69 49	25, 53, 90, 114	0
51	R6	53/54 (98%)	0.36	1 (1%) 66 46	74, 83, 108, 119	0
51	Y6	53/54 (98%)	-0.05	0 100 100	49, 64, 85, 99	0
52	R7	47/49 (95%)	0.66	6 (12%) 7 6	48, 62, 85, 129	0
52	Y7	48/49 (97%)	0.33	2 (4%) 40 25	31, 45, 78, 108	0
53	R8	64/65 (98%)	1.48	18 (28%) 1 1	59, 77, 115, 163	0
53	Y8	64/65 (98%)	1.06	10 (15%) 5 4	37, 55, 92, 254	0
54	R9	37/37 (100%)	0.66	1 (2%) 56 36	76, 91, 120, 147	0
54	Y9	37/37 (100%)	0.18	1 (2%) 56 36	37, 57, 80, 99	0
All	All	20843/21436 (97%)	0.57	1654 (7%) 18 12	25, 91, 206, 458	0

The worst 5 of 1654 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	128	ALA	14.3
11	QK	129	SER	13.6
9	QI	110	GLU	10.7
12	QL	28	LYS	10.2
13	XM	97	PRO	9.4

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	1MG	XV	37	24/25	0.53	0.25	287,291,295,297	0
22	1MG	QV	37	24/25	0.69	0.12	165,170,181,185	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
55	MG	RA	3260	1/1	0.38	0.37	128,128,128,128	0
55	MG	YA	3449	1/1	0.43	0.20	85,85,85,85	0
55	MG	RA	3343	1/1	0.51	0.23	83,83,83,83	0
55	MG	RA	3257	1/1	0.52	0.45	93,93,93,93	0
55	MG	YA	3210	1/1	0.54	0.31	57,57,57,57	0
55	MG	XA	1620	1/1	0.55	0.11	85,85,85,85	0
55	MG	RA	3205	1/1	0.56	0.04	8,8,8,8	0
55	MG	YA	3028	1/1	0.56	0.11	10,10,10,10	0
55	MG	XA	1640	1/1	0.58	0.17	66,66,66,66	0
55	MG	RA	3297	1/1	0.58	0.25	79,79,79,79	0
55	MG	XM	202	1/1	0.59	0.14	75,75,75,75	0
55	MG	RA	3412	1/1	0.60	0.18	62,62,62,62	0
55	MG	RB	206	1/1	0.62	0.22	77,77,77,77	0
55	MG	RA	3265	1/1	0.64	0.27	83,83,83,83	0
55	MG	QA	1616	1/1	0.66	0.14	75,75,75,75	0
55	MG	YD	301	1/1	0.66	0.23	72,72,72,72	0
55	MG	YA	3326	1/1	0.67	0.33	62,62,62,62	0
55	MG	YA	3144	1/1	0.67	0.48	63,63,63,63	0
55	MG	YA	3270	1/1	0.67	0.17	66,66,66,66	0
55	MG	RA	3136	1/1	0.68	0.24	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3468	1/1	0.68	0.16	68,68,68,68	0
55	MG	RA	3143	1/1	0.68	0.15	76,76,76,76	0
55	MG	YA	3322	1/1	0.69	0.23	67,67,67,67	0
55	MG	RA	3346	1/1	0.69	0.33	71,71,71,71	0
55	MG	YA	3424	1/1	0.69	0.30	63,63,63,63	0
55	MG	XA	1645	1/1	0.69	0.11	70,70,70,70	0
55	MG	XM	201	1/1	0.69	0.24	77,77,77,77	0
55	MG	RA	3195	1/1	0.69	0.26	76,76,76,76	0
55	MG	XA	1610	1/1	0.70	0.11	67,67,67,67	0
55	MG	RA	3375	1/1	0.70	0.29	72,72,72,72	0
55	MG	RA	3147	1/1	0.70	0.11	64,64,64,64	0
55	MG	YA	3201	1/1	0.70	0.38	80,80,80,80	0
55	MG	RA	3437	1/1	0.70	0.18	32,32,32,32	0
55	MG	RA	3221	1/1	0.70	0.34	63,63,63,63	0
55	MG	RA	3330	1/1	0.71	0.13	70,70,70,70	0
55	MG	RA	3382	1/1	0.71	0.23	59,59,59,59	0
55	MG	RA	3258	1/1	0.71	0.40	69,69,69,69	0
55	MG	QA	1651	1/1	0.71	0.13	58,58,58,58	0
55	MG	YA	3118	1/1	0.71	0.11	42,42,42,42	0
55	MG	QA	1653	1/1	0.72	0.12	58,58,58,58	0
55	MG	YA	3290	1/1	0.72	0.23	65,65,65,65	0
55	MG	RA	3350	1/1	0.72	0.18	81,81,81,81	0
55	MG	YB	202	1/1	0.72	0.10	46,46,46,46	0
55	MG	RA	3318	1/1	0.72	0.20	84,84,84,84	0
55	MG	YA	3180	1/1	0.73	0.24	60,60,60,60	0
55	MG	YA	3379	1/1	0.73	0.16	57,57,57,57	0
55	MG	RA	3272	1/1	0.73	0.12	59,59,59,59	0
55	MG	RA	3171	1/1	0.73	0.15	60,60,60,60	0
55	MG	RA	3233	1/1	0.73	0.20	70,70,70,70	0
55	MG	RA	3175	1/1	0.73	0.20	67,67,67,67	0
55	MG	XA	1653	1/1	0.73	0.10	75,75,75,75	0
55	MG	YA	3353	1/1	0.74	0.21	50,50,50,50	0
55	MG	YA	3378	1/1	0.74	0.14	42,42,42,42	0
55	MG	RA	3170	1/1	0.74	0.16	73,73,73,73	0
55	MG	YA	3275	1/1	0.74	0.32	79,79,79,79	0
55	MG	YA	3429	1/1	0.74	0.14	62,62,62,62	0
55	MG	RA	3045	1/1	0.74	0.37	60,60,60,60	0
55	MG	YA	3301	1/1	0.74	0.16	54,54,54,54	0
55	MG	RA	3365	1/1	0.74	0.27	80,80,80,80	0
55	MG	YA	3234	1/1	0.74	0.15	66,66,66,66	0
55	MG	YA	3406	1/1	0.75	0.49	84,84,84,84	0
55	MG	RA	3396	1/1	0.75	0.18	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3021	1/1	0.75	0.08	9,9,9,9	0
55	MG	QA	1658	1/1	0.75	0.07	92,92,92,92	0
55	MG	RA	3268	1/1	0.75	0.13	52,52,52,52	0
55	MG	QA	1638	1/1	0.75	0.13	85,85,85,85	0
55	MG	QA	1657	1/1	0.75	0.10	44,44,44,44	0
55	MG	YA	3373	1/1	0.76	0.14	52,52,52,52	0
55	MG	RA	3223	1/1	0.76	0.13	44,44,44,44	0
55	MG	YA	3154	1/1	0.76	0.24	49,49,49,49	0
55	MG	RA	3414	1/1	0.76	0.13	71,71,71,71	0
55	MG	QA	1636	1/1	0.76	0.15	62,62,62,62	0
55	MG	XA	1666	1/1	0.76	0.10	74,74,74,74	0
55	MG	XA	1667	1/1	0.76	0.14	76,76,76,76	0
55	MG	YA	3457	1/1	0.76	0.26	87,87,87,87	0
55	MG	YA	3260	1/1	0.76	0.12	67,67,67,67	0
55	MG	YA	3368	1/1	0.76	0.15	57,57,57,57	0
55	MG	YA	3371	1/1	0.76	0.25	51,51,51,51	0
55	MG	RA	3090	1/1	0.77	0.16	40,40,40,40	0
55	MG	RA	3008	1/1	0.77	0.24	58,58,58,58	0
55	MG	RA	3161	1/1	0.77	0.11	43,43,43,43	0
55	MG	RA	3400	1/1	0.77	0.14	63,63,63,63	0
55	MG	RA	3410	1/1	0.77	0.16	80,80,80,80	0
55	MG	YA	3177	1/1	0.77	0.20	59,59,59,59	0
55	MG	YA	3510	1/1	0.77	0.13	29,29,29,29	0
55	MG	RA	3366	1/1	0.77	0.11	47,47,47,47	0
55	MG	YA	3194	1/1	0.77	0.13	46,46,46,46	0
55	MG	RA	3323	1/1	0.78	0.11	65,65,65,65	0
55	MG	RA	3237	1/1	0.78	0.13	52,52,52,52	0
55	MG	RA	3251	1/1	0.78	0.26	61,61,61,61	0
55	MG	YA	3413	1/1	0.78	0.14	42,42,42,42	0
55	MG	YA	3421	1/1	0.78	0.23	69,69,69,69	0
55	MG	QA	1623	1/1	0.78	0.11	50,50,50,50	0
55	MG	RA	3202	1/1	0.78	0.27	66,66,66,66	0
55	MG	YA	3015	1/1	0.78	0.14	48,48,48,48	0
55	MG	RA	3362	1/1	0.78	0.22	74,74,74,74	0
55	MG	YA	3462	1/1	0.78	0.10	46,46,46,46	0
55	MG	RA	3148	1/1	0.78	0.13	36,36,36,36	0
55	MG	YA	3227	1/1	0.78	0.13	57,57,57,57	0
55	MG	YA	3230	1/1	0.78	0.19	51,51,51,51	0
55	MG	YA	3057	1/1	0.78	0.15	19,19,19,19	0
55	MG	RQ	201	1/1	0.79	0.15	58,58,58,58	0
55	MG	RA	3103	1/1	0.79	0.10	52,52,52,52	0
55	MG	YA	3145	1/1	0.79	0.18	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
55	MG	RA	3320	1/1	0.79	0.19	58,58,58,58	0
55	MG	YA	3175	1/1	0.79	0.16	49,49,49,49	0
55	MG	RA	3385	1/1	0.79	0.18	53,53,53,53	0
55	MG	RA	3091	1/1	0.79	0.16	43,43,43,43	0
55	MG	YA	3280	1/1	0.79	0.13	66,66,66,66	0
55	MG	RA	3441	1/1	0.79	0.32	72,72,72,72	0
55	MG	RA	3348	1/1	0.79	0.09	52,52,52,52	0
55	MG	RA	3192	1/1	0.80	0.17	39,39,39,39	0
55	MG	RA	3152	1/1	0.80	0.20	61,61,61,61	0
55	MG	YA	3285	1/1	0.80	0.12	45,45,45,45	0
55	MG	RA	3226	1/1	0.80	0.29	58,58,58,58	0
55	MG	RA	3093	1/1	0.80	0.15	39,39,39,39	0
55	MG	RA	3167	1/1	0.80	0.13	70,70,70,70	0
55	MG	YA	3446	1/1	0.80	0.12	64,64,64,64	0
55	MG	YA	3212	1/1	0.80	0.14	53,53,53,53	0
55	MG	YA	3341	1/1	0.80	0.08	64,64,64,64	0
55	MG	XA	1650	1/1	0.80	0.08	92,92,92,92	0
55	MG	RA	3424	1/1	0.80	0.24	72,72,72,72	0
55	MG	RA	3269	1/1	0.80	0.20	78,78,78,78	0
55	MG	RA	3219	1/1	0.80	0.19	51,51,51,51	0
55	MG	RA	3347	1/1	0.80	0.10	63,63,63,63	0
55	MG	YA	3337	1/1	0.81	0.12	35,35,35,35	0
55	MG	RA	3006	1/1	0.81	0.10	45,45,45,45	0
55	MG	YA	3203	1/1	0.81	0.16	42,42,42,42	0
55	MG	YA	3357	1/1	0.81	0.13	50,50,50,50	0
55	MG	RA	3357	1/1	0.81	0.20	43,43,43,43	0
55	MG	RA	3439	1/1	0.81	0.07	36,36,36,36	0
55	MG	RA	3271	1/1	0.81	0.15	49,49,49,49	0
55	MG	RA	3227	1/1	0.81	0.18	70,70,70,70	0
55	MG	YA	3233	1/1	0.81	0.19	48,48,48,48	0
55	MG	YA	3386	1/1	0.81	0.14	42,42,42,42	0
55	MG	RA	3231	1/1	0.81	0.22	36,36,36,36	0
55	MG	QA	1618	1/1	0.81	0.10	47,47,47,47	0
55	MG	RA	3194	1/1	0.81	0.14	66,66,66,66	0
55	MG	QA	1626	1/1	0.81	0.10	57,57,57,57	0
55	MG	RA	3107	1/1	0.81	0.21	63,63,63,63	0
55	MG	YA	3433	1/1	0.81	0.21	51,51,51,51	0
55	MG	YA	3434	1/1	0.81	0.14	68,68,68,68	0
55	MG	YA	3445	1/1	0.81	0.15	46,46,46,46	0
55	MG	YA	3281	1/1	0.81	0.10	35,35,35,35	0
55	MG	YA	3161	1/1	0.81	0.21	58,58,58,58	0
55	MG	RA	3164	1/1	0.81	0.14	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3061	1/1	0.81	0.23	45,45,45,45	0
55	MG	YA	3316	1/1	0.81	0.25	71,71,71,71	0
55	MG	RA	3141	1/1	0.81	0.10	58,58,58,58	0
55	MG	QA	1632	1/1	0.81	0.19	52,52,52,52	0
55	MG	YA	3327	1/1	0.81	0.12	53,53,53,53	0
55	MG	Y1	101	1/1	0.81	0.22	46,46,46,46	0
55	MG	YA	3289	1/1	0.82	0.12	36,36,36,36	0
55	MG	RA	3196	1/1	0.82	0.35	72,72,72,72	0
55	MG	YA	3058	1/1	0.82	0.20	34,34,34,34	0
55	MG	XA	1663	1/1	0.82	0.12	64,64,64,64	0
55	MG	YA	3220	1/1	0.82	0.11	27,27,27,27	0
55	MG	YA	3133	1/1	0.82	0.14	26,26,26,26	0
55	MG	RA	3298	1/1	0.82	0.18	45,45,45,45	0
55	MG	RA	3300	1/1	0.82	0.09	62,62,62,62	0
55	MG	RA	3301	1/1	0.82	0.15	57,57,57,57	0
55	MG	YA	3239	1/1	0.82	0.37	67,67,67,67	0
55	MG	QA	1615	1/1	0.82	0.11	69,69,69,69	0
55	MG	YA	3359	1/1	0.82	0.14	57,57,57,57	0
55	MG	YA	3363	1/1	0.82	0.09	55,55,55,55	0
55	MG	YA	3002	1/1	0.82	0.06	33,33,33,33	0
55	MG	YA	3492	1/1	0.82	0.23	49,49,49,49	0
55	MG	YA	3009	1/1	0.82	0.22	52,52,52,52	0
55	MG	RA	3430	1/1	0.82	0.17	69,69,69,69	0
55	MG	YB	207	1/1	0.82	0.06	48,48,48,48	0
55	MG	RA	3239	1/1	0.82	0.13	57,57,57,57	0
55	MG	RA	3174	1/1	0.82	0.12	36,36,36,36	0
55	MG	RA	3166	1/1	0.83	0.20	58,58,58,58	0
55	MG	YA	3004	1/1	0.83	0.11	35,35,35,35	0
55	MG	YA	3188	1/1	0.83	0.14	34,34,34,34	0
55	MG	YA	3384	1/1	0.83	0.14	36,36,36,36	0
55	MG	RA	3064	1/1	0.83	0.13	41,41,41,41	0
55	MG	RA	3228	1/1	0.83	0.13	49,49,49,49	0
55	MG	YA	3292	1/1	0.83	0.17	48,48,48,48	0
55	MG	YA	3417	1/1	0.83	0.10	43,43,43,43	0
55	MG	YA	3017	1/1	0.83	0.20	52,52,52,52	0
55	MG	YA	3310	1/1	0.83	0.35	84,84,84,84	0
55	MG	RA	3207	1/1	0.83	0.14	59,59,59,59	0
55	MG	XA	1643	1/1	0.83	0.11	59,59,59,59	0
55	MG	RA	3232	1/1	0.83	0.21	53,53,53,53	0
55	MG	YA	3224	1/1	0.83	0.11	32,32,32,32	0
55	MG	QA	1640	1/1	0.83	0.14	59,59,59,59	0
55	MG	QA	1659	1/1	0.83	0.11	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
55	MG	YA	3345	1/1	0.83	0.27	59,59,59,59	0
55	MG	YA	3350	1/1	0.83	0.18	54,54,54,54	0
55	MG	YA	3352	1/1	0.83	0.08	45,45,45,45	0
55	MG	YA	3476	1/1	0.83	0.09	59,59,59,59	0
55	MG	XA	1654	1/1	0.83	0.19	63,63,63,63	0
55	MG	RA	3436	1/1	0.83	0.28	66,66,66,66	0
55	MG	RA	3372	1/1	0.83	0.20	63,63,63,63	0
55	MG	RA	3117	1/1	0.83	0.08	61,61,61,61	0
55	MG	RA	3245	1/1	0.83	0.24	57,57,57,57	0
55	MG	RA	3273	1/1	0.83	0.20	53,53,53,53	0
55	MG	RA	3247	1/1	0.84	0.17	45,45,45,45	0
55	MG	YA	3283	1/1	0.84	0.16	38,38,38,38	0
55	MG	YA	3181	1/1	0.84	0.14	45,45,45,45	0
55	MG	YA	3183	1/1	0.84	0.15	51,51,51,51	0
55	MG	YA	3398	1/1	0.84	0.21	66,66,66,66	0
55	MG	RA	3307	1/1	0.84	0.19	41,41,41,41	0
55	MG	RA	3316	1/1	0.84	0.18	58,58,58,58	0
55	MG	YA	3034	1/1	0.84	0.16	31,31,31,31	0
55	MG	YA	3306	1/1	0.84	0.29	61,61,61,61	0
55	MG	RA	3392	1/1	0.84	0.13	51,51,51,51	0
55	MG	RA	3156	1/1	0.84	0.18	60,60,60,60	0
55	MG	RA	3442	1/1	0.84	0.12	32,32,32,32	0
55	MG	YA	3120	1/1	0.84	0.16	36,36,36,36	0
55	MG	YA	3435	1/1	0.84	0.09	28,28,28,28	0
55	MG	YA	3440	1/1	0.84	0.18	63,63,63,63	0
55	MG	RA	3319	1/1	0.84	0.10	56,56,56,56	0
55	MG	RA	3287	1/1	0.84	0.10	55,55,55,55	0
55	MG	RA	3253	1/1	0.84	0.17	50,50,50,50	0
55	MG	XA	1613	1/1	0.84	0.12	61,61,61,61	0
55	MG	YA	3159	1/1	0.84	0.17	43,43,43,43	0
55	MG	YA	3238	1/1	0.84	0.26	57,57,57,57	0
55	MG	RA	3413	1/1	0.84	0.21	69,69,69,69	0
55	MG	YA	3246	1/1	0.84	0.20	39,39,39,39	0
55	MG	YA	3254	1/1	0.84	0.20	41,41,41,41	0
55	MG	YA	3166	1/1	0.84	0.12	40,40,40,40	0
55	MG	YA	3170	1/1	0.84	0.19	48,48,48,48	0
55	MG	RA	3177	1/1	0.84	0.10	41,41,41,41	0
55	MG	QA	1648	1/1	0.84	0.12	70,70,70,70	0
55	MG	RA	3280	1/1	0.85	0.20	52,52,52,52	0
55	MG	RA	3082	1/1	0.85	0.17	33,33,33,33	0
55	MG	RA	3250	1/1	0.85	0.18	59,59,59,59	0
55	MG	XA	1670	1/1	0.85	0.10	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3087	1/1	0.85	0.22	35,35,35,35	0
55	MG	YA	3392	1/1	0.85	0.10	27,27,27,27	0
55	MG	RA	3354	1/1	0.85	0.08	62,62,62,62	0
55	MG	RA	3112	1/1	0.85	0.12	36,36,36,36	0
55	MG	RA	3359	1/1	0.85	0.16	66,66,66,66	0
55	MG	RA	3113	1/1	0.85	0.32	42,42,42,42	0
55	MG	RA	3230	1/1	0.85	0.16	48,48,48,48	0
55	MG	RA	3309	1/1	0.85	0.15	57,57,57,57	0
55	MG	RA	3314	1/1	0.85	0.12	46,46,46,46	0
55	MG	RA	3203	1/1	0.85	0.15	62,62,62,62	0
55	MG	YA	3216	1/1	0.85	0.12	30,30,30,30	0
55	MG	RA	3378	1/1	0.85	0.13	49,49,49,49	0
55	MG	YA	3336	1/1	0.85	0.35	65,65,65,65	0
55	MG	YA	3442	1/1	0.85	0.08	59,59,59,59	0
55	MG	XA	1611	1/1	0.85	0.18	56,56,56,56	0
55	MG	RA	3049	1/1	0.85	0.11	46,46,46,46	0
55	MG	YA	3447	1/1	0.85	0.32	104,104,104,104	0
55	MG	YA	3343	1/1	0.85	0.10	45,45,45,45	0
55	MG	YA	3080	1/1	0.85	0.11	37,37,37,37	0
55	MG	YA	3459	1/1	0.85	0.17	49,49,49,49	0
55	MG	QA	1602	1/1	0.85	0.14	30,30,30,30	0
55	MG	YA	3463	1/1	0.85	0.25	70,70,70,70	0
55	MG	RA	3210	1/1	0.85	0.17	32,32,32,32	0
55	MG	RA	3394	1/1	0.85	0.12	45,45,45,45	0
55	MG	QA	1612	1/1	0.85	0.07	44,44,44,44	0
55	MG	XA	1646	1/1	0.85	0.12	57,57,57,57	0
55	MG	YA	3360	1/1	0.85	0.14	53,53,53,53	0
55	MG	RA	3242	1/1	0.85	0.11	30,30,30,30	0
55	MG	RA	3403	1/1	0.85	0.10	55,55,55,55	0
55	MG	YQ	203	1/1	0.85	0.12	55,55,55,55	0
55	MG	Y0	102	1/1	0.85	0.12	42,42,42,42	0
55	MG	RA	3165	1/1	0.85	0.20	55,55,55,55	0
55	MG	RA	3364	1/1	0.86	0.09	56,56,56,56	0
55	MG	YA	3396	1/1	0.86	0.10	42,42,42,42	0
55	MG	RA	3102	1/1	0.86	0.21	44,44,44,44	0
55	MG	YA	3018	1/1	0.86	0.24	49,49,49,49	0
55	MG	RA	3340	1/1	0.86	0.16	39,39,39,39	0
55	MG	RA	3302	1/1	0.86	0.19	53,53,53,53	0
55	MG	YA	3420	1/1	0.86	0.08	48,48,48,48	0
55	MG	RA	3159	1/1	0.86	0.20	69,69,69,69	0
55	MG	YA	3423	1/1	0.86	0.05	46,46,46,46	0
55	MG	RA	3160	1/1	0.86	0.09	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3281	1/1	0.86	0.09	58,58,58,58	0
55	MG	RA	3191	1/1	0.86	0.12	45,45,45,45	0
55	MG	YA	3081	1/1	0.86	0.13	41,41,41,41	0
55	MG	YA	3103	1/1	0.86	0.23	47,47,47,47	0
55	MG	XA	1655	1/1	0.86	0.07	46,46,46,46	0
55	MG	XA	1661	1/1	0.86	0.09	46,46,46,46	0
55	MG	YA	3228	1/1	0.86	0.18	56,56,56,56	0
55	MG	RA	3387	1/1	0.86	0.09	44,44,44,44	0
55	MG	YA	3137	1/1	0.86	0.11	33,33,33,33	0
55	MG	RA	3390	1/1	0.86	0.18	50,50,50,50	0
55	MG	YA	3450	1/1	0.86	0.07	52,52,52,52	0
55	MG	YA	3454	1/1	0.86	0.10	28,28,28,28	0
55	MG	RA	3295	1/1	0.86	0.15	39,39,39,39	0
55	MG	RA	3074	1/1	0.86	0.23	41,41,41,41	0
55	MG	YA	3156	1/1	0.86	0.13	30,30,30,30	0
55	MG	XA	1673	1/1	0.86	0.13	44,44,44,44	0
55	MG	YA	3464	1/1	0.86	0.08	49,49,49,49	0
55	MG	RA	3236	1/1	0.86	0.12	61,61,61,61	0
55	MG	YA	3267	1/1	0.86	0.15	47,47,47,47	0
55	MG	YA	3369	1/1	0.86	0.33	77,77,77,77	0
55	MG	RR	201	1/1	0.86	0.10	22,22,22,22	0
55	MG	RA	3397	1/1	0.86	0.11	56,56,56,56	0
55	MG	YA	3172	1/1	0.86	0.12	20,20,20,20	0
55	MG	RA	3360	1/1	0.86	0.07	40,40,40,40	0
55	MG	YE	304	1/1	0.86	0.13	60,60,60,60	0
55	MG	YA	3381	1/1	0.86	0.15	40,40,40,40	0
55	MG	Y0	101	1/1	0.86	0.12	34,34,34,34	0
55	MG	QA	1643	1/1	0.86	0.17	57,57,57,57	0
55	MG	YA	3178	1/1	0.86	0.17	36,36,36,36	0
55	MG	YA	3320	1/1	0.87	0.13	50,50,50,50	0
55	MG	RA	3438	1/1	0.87	0.13	46,46,46,46	0
55	MG	QA	1647	1/1	0.87	0.11	64,64,64,64	0
55	MG	RA	3218	1/1	0.87	0.36	55,55,55,55	0
55	MG	YA	3150	1/1	0.87	0.15	31,31,31,31	0
55	MG	YA	3151	1/1	0.87	0.15	45,45,45,45	0
55	MG	YA	3430	1/1	0.87	0.19	57,57,57,57	0
55	MG	YA	3152	1/1	0.87	0.07	21,21,21,21	0
55	MG	YA	3010	1/1	0.87	0.20	76,76,76,76	0
55	MG	YA	3011	1/1	0.87	0.15	47,47,47,47	0
55	MG	YA	3439	1/1	0.87	0.20	39,39,39,39	0
55	MG	YA	3347	1/1	0.87	0.08	31,31,31,31	0
55	MG	YA	3012	1/1	0.87	0.20	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3379	1/1	0.87	0.09	46,46,46,46	0
55	MG	RA	3305	1/1	0.87	0.15	54,54,54,54	0
55	MG	YA	3355	1/1	0.87	0.21	45,45,45,45	0
55	MG	RA	3198	1/1	0.87	0.15	42,42,42,42	0
55	MG	RA	3162	1/1	0.87	0.10	44,44,44,44	0
55	MG	RT	201	1/1	0.87	0.07	75,75,75,75	0
55	MG	YA	3456	1/1	0.87	0.14	52,52,52,52	0
55	MG	YA	3269	1/1	0.87	0.14	14,14,14,14	0
55	MG	YA	3458	1/1	0.87	0.12	66,66,66,66	0
55	MG	RA	3158	1/1	0.87	0.12	40,40,40,40	0
55	MG	XA	1665	1/1	0.87	0.12	57,57,57,57	0
55	MG	RA	3031	1/1	0.87	0.22	49,49,49,49	0
55	MG	RA	3393	1/1	0.87	0.16	60,60,60,60	0
55	MG	YA	3466	1/1	0.87	0.15	46,46,46,46	0
55	MG	RA	3133	1/1	0.87	0.13	27,27,27,27	0
55	MG	YA	3471	1/1	0.87	0.21	53,53,53,53	0
55	MG	XA	1622	1/1	0.87	0.08	55,55,55,55	0
55	MG	YA	3489	1/1	0.87	0.07	40,40,40,40	0
55	MG	XA	1631	1/1	0.87	0.10	62,62,62,62	0
55	MG	RA	3256	1/1	0.87	0.14	38,38,38,38	0
55	MG	YA	3128	1/1	0.87	0.20	28,28,28,28	0
55	MG	YA	3206	1/1	0.87	0.09	31,31,31,31	0
55	MG	YA	3132	1/1	0.87	0.18	31,31,31,31	0
55	MG	YA	3309	1/1	0.87	0.17	47,47,47,47	0
55	MG	YQ	201	1/1	0.87	0.16	48,48,48,48	0
55	MG	YA	3001	1/1	0.87	0.29	46,46,46,46	0
55	MG	YA	3408	1/1	0.87	0.16	53,53,53,53	0
55	MG	YA	3411	1/1	0.87	0.10	9,9,9,9	0
55	MG	YA	3213	1/1	0.87	0.12	29,29,29,29	0
55	MG	YA	3149	1/1	0.88	0.15	56,56,56,56	0
55	MG	YA	3333	1/1	0.88	0.17	45,45,45,45	0
55	MG	QA	1622	1/1	0.88	0.19	55,55,55,55	0
55	MG	RA	3313	1/1	0.88	0.15	50,50,50,50	0
55	MG	RA	3381	1/1	0.88	0.16	38,38,38,38	0
55	MG	YA	3432	1/1	0.88	0.18	46,46,46,46	0
55	MG	YA	3342	1/1	0.88	0.18	79,79,79,79	0
55	MG	RA	3423	1/1	0.88	0.22	52,52,52,52	0
55	MG	RA	3292	1/1	0.88	0.13	41,41,41,41	0
55	MG	RA	3243	1/1	0.88	0.12	22,22,22,22	0
55	MG	RA	3131	1/1	0.88	0.20	56,56,56,56	0
55	MG	RA	3075	1/1	0.88	0.11	39,39,39,39	0
55	MG	YA	3168	1/1	0.88	0.21	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
55	MG	YA	3354	1/1	0.88	0.11	27,27,27,27	0
55	MG	QA	1624	1/1	0.88	0.10	80,80,80,80	0
55	MG	YA	3448	1/1	0.88	0.16	54,54,54,54	0
55	MG	YA	3257	1/1	0.88	0.29	54,54,54,54	0
55	MG	RA	3274	1/1	0.88	0.20	35,35,35,35	0
55	MG	YA	3451	1/1	0.88	0.16	59,59,59,59	0
55	MG	RA	3363	1/1	0.88	0.14	57,57,57,57	0
55	MG	YA	3361	1/1	0.88	0.26	63,63,63,63	0
55	MG	RA	3325	1/1	0.88	0.13	42,42,42,42	0
55	MG	RA	3444	1/1	0.88	0.14	45,45,45,45	0
55	MG	YA	3179	1/1	0.88	0.13	30,30,30,30	0
55	MG	YA	3070	1/1	0.88	0.17	27,27,27,27	0
55	MG	RB	202	1/1	0.88	0.08	41,41,41,41	0
55	MG	RA	3263	1/1	0.88	0.21	45,45,45,45	0
55	MG	YA	3184	1/1	0.88	0.14	35,35,35,35	0
55	MG	RE	301	1/1	0.88	0.10	56,56,56,56	0
55	MG	RA	3399	1/1	0.88	0.19	43,43,43,43	0
55	MG	RA	3140	1/1	0.88	0.16	48,48,48,48	0
55	MG	YA	3390	1/1	0.88	0.08	29,29,29,29	0
55	MG	XA	1671	1/1	0.88	0.16	35,35,35,35	0
55	MG	RA	3306	1/1	0.88	0.10	60,60,60,60	0
55	MG	R0	101	1/1	0.88	0.26	58,58,58,58	0
55	MG	YA	3405	1/1	0.88	0.16	31,31,31,31	0
55	MG	R8	101	1/1	0.88	0.16	40,40,40,40	0
55	MG	RA	3405	1/1	0.88	0.12	39,39,39,39	0
55	MG	YA	3319	1/1	0.88	0.19	59,59,59,59	0
55	MG	YA	3412	1/1	0.88	0.09	67,67,67,67	0
55	MG	YA	3214	1/1	0.88	0.07	45,45,45,45	0
55	MG	RA	3282	1/1	0.88	0.21	49,49,49,49	0
55	MG	YA	3218	1/1	0.88	0.10	31,31,31,31	0
55	MG	Y1	102	1/1	0.88	0.10	46,46,46,46	0
55	MG	XA	1658	1/1	0.89	0.17	37,37,37,37	0
55	MG	RA	3317	1/1	0.89	0.07	48,48,48,48	0
55	MG	YA	3418	1/1	0.89	0.17	61,61,61,61	0
55	MG	YA	3419	1/1	0.89	0.07	36,36,36,36	0
55	MG	YA	3312	1/1	0.89	0.14	44,44,44,44	0
55	MG	YA	3205	1/1	0.89	0.10	54,54,54,54	0
55	MG	RA	3361	1/1	0.89	0.17	60,60,60,60	0
55	MG	RA	3185	1/1	0.89	0.07	56,56,56,56	0
55	MG	YA	3125	1/1	0.89	0.11	27,27,27,27	0
55	MG	RA	3234	1/1	0.89	0.09	45,45,45,45	0
55	MG	YA	3431	1/1	0.89	0.13	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3217	1/1	0.89	0.08	49,49,49,49	0
55	MG	XA	1669	1/1	0.89	0.19	49,49,49,49	0
55	MG	RA	3404	1/1	0.89	0.14	50,50,50,50	0
55	MG	RA	3149	1/1	0.89	0.07	48,48,48,48	0
55	MG	RA	3151	1/1	0.89	0.12	38,38,38,38	0
55	MG	XA	1603	1/1	0.89	0.14	58,58,58,58	0
55	MG	XA	1606	1/1	0.89	0.07	40,40,40,40	0
55	MG	YA	3443	1/1	0.89	0.17	44,44,44,44	0
55	MG	RA	3327	1/1	0.89	0.08	37,37,37,37	0
55	MG	YA	3231	1/1	0.89	0.12	38,38,38,38	0
55	MG	RA	3373	1/1	0.89	0.16	43,43,43,43	0
55	MG	RA	3138	1/1	0.89	0.14	40,40,40,40	0
55	MG	YA	3237	1/1	0.89	0.27	40,40,40,40	0
55	MG	XA	1615	1/1	0.89	0.07	66,66,66,66	0
55	MG	XA	1619	1/1	0.89	0.14	74,74,74,74	0
55	MG	RA	3417	1/1	0.89	0.16	50,50,50,50	0
55	MG	YA	3253	1/1	0.89	0.15	49,49,49,49	0
55	MG	YA	3164	1/1	0.89	0.07	27,27,27,27	0
55	MG	RA	3335	1/1	0.89	0.09	40,40,40,40	0
55	MG	QA	1656	1/1	0.89	0.10	48,48,48,48	0
55	MG	YA	3461	1/1	0.89	0.11	52,52,52,52	0
55	MG	YA	3261	1/1	0.89	0.12	21,21,21,21	0
55	MG	RA	3004	1/1	0.89	0.15	39,39,39,39	0
55	MG	RA	3246	1/1	0.89	0.20	36,36,36,36	0
55	MG	YA	3465	1/1	0.89	0.15	50,50,50,50	0
55	MG	XA	1644	1/1	0.89	0.10	54,54,54,54	0
55	MG	YA	3374	1/1	0.89	0.12	39,39,39,39	0
55	MG	YA	3469	1/1	0.89	0.08	39,39,39,39	0
55	MG	YA	3375	1/1	0.89	0.18	45,45,45,45	0
55	MG	QA	1637	1/1	0.89	0.08	77,77,77,77	0
55	MG	YA	3030	1/1	0.89	0.16	32,32,32,32	0
55	MG	YA	3490	1/1	0.89	0.18	30,30,30,30	0
55	MG	RA	3146	1/1	0.89	0.10	58,58,58,58	0
55	MG	YA	3504	1/1	0.89	0.17	39,39,39,39	0
55	MG	YA	3505	1/1	0.89	0.09	55,55,55,55	0
55	MG	YA	3509	1/1	0.89	0.14	56,56,56,56	0
55	MG	RA	3275	1/1	0.89	0.20	50,50,50,50	0
55	MG	RA	3111	1/1	0.89	0.17	32,32,32,32	0
55	MG	YA	3061	1/1	0.89	0.15	15,15,15,15	0
55	MG	YA	3066	1/1	0.89	0.14	41,41,41,41	0
55	MG	YA	3291	1/1	0.89	0.15	51,51,51,51	0
55	MG	QA	1628	1/1	0.89	0.17	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
55	MG	YA	3295	1/1	0.89	0.27	64,64,64,64	0
55	MG	YA	3300	1/1	0.89	0.22	57,57,57,57	0
55	MG	RA	3182	1/1	0.89	0.11	22,22,22,22	0
55	MG	YA	3305	1/1	0.89	0.23	55,55,55,55	0
55	MG	YA	3199	1/1	0.89	0.14	34,34,34,34	0
55	MG	YA	3324	1/1	0.90	0.09	38,38,38,38	0
55	MG	RE	305	1/1	0.90	0.12	29,29,29,29	0
55	MG	RA	3303	1/1	0.90	0.11	32,32,32,32	0
55	MG	YA	3425	1/1	0.90	0.13	33,33,33,33	0
55	MG	YA	3331	1/1	0.90	0.06	35,35,35,35	0
55	MG	RA	3333	1/1	0.90	0.21	44,44,44,44	0
55	MG	YA	3334	1/1	0.90	0.20	56,56,56,56	0
55	MG	YA	3335	1/1	0.90	0.22	62,62,62,62	0
55	MG	YA	3050	1/1	0.90	0.13	16,16,16,16	0
55	MG	QA	1664	1/1	0.90	0.21	53,53,53,53	0
55	MG	RA	3276	1/1	0.90	0.26	60,60,60,60	0
55	MG	QV	101	1/1	0.90	0.14	69,69,69,69	0
55	MG	YA	3240	1/1	0.90	0.28	45,45,45,45	0
55	MG	RA	3201	1/1	0.90	0.11	40,40,40,40	0
55	MG	YA	3248	1/1	0.90	0.17	23,23,23,23	0
55	MG	RA	3415	1/1	0.90	0.12	52,52,52,52	0
55	MG	XA	1609	1/1	0.90	0.19	42,42,42,42	0
55	MG	YA	3256	1/1	0.90	0.08	20,20,20,20	0
55	MG	RA	3310	1/1	0.90	0.12	32,32,32,32	0
55	MG	YA	3086	1/1	0.90	0.20	25,25,25,25	0
55	MG	YA	3356	1/1	0.90	0.18	51,51,51,51	0
55	MG	YA	3095	1/1	0.90	0.10	28,28,28,28	0
55	MG	RA	3421	1/1	0.90	0.28	20,20,20,20	0
55	MG	QA	1606	1/1	0.90	0.07	51,51,51,51	0
55	MG	YA	3185	1/1	0.90	0.09	54,54,54,54	0
55	MG	RA	3284	1/1	0.90	0.05	42,42,42,42	0
55	MG	YA	3191	1/1	0.90	0.23	50,50,50,50	0
55	MG	YA	3193	1/1	0.90	0.14	48,48,48,48	0
55	MG	YA	3370	1/1	0.90	0.11	35,35,35,35	0
55	MG	YA	3122	1/1	0.90	0.08	22,22,22,22	0
55	MG	YA	3284	1/1	0.90	0.15	53,53,53,53	0
55	MG	YA	3195	1/1	0.90	0.20	47,47,47,47	0
55	MG	YA	3288	1/1	0.90	0.17	40,40,40,40	0
55	MG	QA	1642	1/1	0.90	0.12	73,73,73,73	0
55	MG	RA	3355	1/1	0.90	0.15	62,62,62,62	0
55	MG	RA	3124	1/1	0.90	0.19	24,24,24,24	0
55	MG	YA	3473	1/1	0.90	0.17	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3003	1/1	0.90	0.11	35,35,35,35	0
55	MG	YA	3485	1/1	0.90	0.13	9,9,9,9	0
55	MG	YA	3135	1/1	0.90	0.12	35,35,35,35	0
55	MG	YA	3299	1/1	0.90	0.15	46,46,46,46	0
55	MG	RA	3066	1/1	0.90	0.09	45,45,45,45	0
55	MG	YA	3394	1/1	0.90	0.07	39,39,39,39	0
55	MG	YA	3395	1/1	0.90	0.12	35,35,35,35	0
55	MG	XA	1635	1/1	0.90	0.06	54,54,54,54	0
55	MG	RA	3270	1/1	0.90	0.17	56,56,56,56	0
55	MG	RA	3072	1/1	0.90	0.19	51,51,51,51	0
55	MG	QA	1604	1/1	0.90	0.09	26,26,26,26	0
55	MG	RA	3137	1/1	0.90	0.11	47,47,47,47	0
55	MG	QA	1644	1/1	0.90	0.08	49,49,49,49	0
55	MG	YA	3313	1/1	0.90	0.15	58,58,58,58	0
55	MG	YA	3222	1/1	0.90	0.18	55,55,55,55	0
55	MG	RA	3401	1/1	0.90	0.11	55,55,55,55	0
55	MG	YA	3155	1/1	0.90	0.13	33,33,33,33	0
55	MG	YA	3321	1/1	0.90	0.10	44,44,44,44	0
55	MG	RA	3328	1/1	0.90	0.10	41,41,41,41	0
55	MG	YA	3153	1/1	0.91	0.11	31,31,31,31	0
55	MG	RA	3084	1/1	0.91	0.18	24,24,24,24	0
55	MG	YA	3215	1/1	0.91	0.08	26,26,26,26	0
55	MG	RA	3285	1/1	0.91	0.13	41,41,41,41	0
55	MG	YA	3367	1/1	0.91	0.10	57,57,57,57	0
55	MG	YA	3041	1/1	0.91	0.28	26,26,26,26	0
55	MG	YA	3219	1/1	0.91	0.06	11,11,11,11	0
55	MG	YA	3158	1/1	0.91	0.08	21,21,21,21	0
55	MG	RA	3062	1/1	0.91	0.13	30,30,30,30	0
55	MG	YA	3160	1/1	0.91	0.18	38,38,38,38	0
55	MG	RA	3180	1/1	0.91	0.23	42,42,42,42	0
55	MG	RA	3114	1/1	0.91	0.11	40,40,40,40	0
55	MG	YA	3376	1/1	0.91	0.12	37,37,37,37	0
55	MG	YA	3165	1/1	0.91	0.21	35,35,35,35	0
55	MG	RA	3409	1/1	0.91	0.17	47,47,47,47	0
55	MG	RA	3296	1/1	0.91	0.36	69,69,69,69	0
55	MG	RA	3184	1/1	0.91	0.13	54,54,54,54	0
55	MG	YA	3171	1/1	0.91	0.22	35,35,35,35	0
55	MG	XA	1604	1/1	0.91	0.08	50,50,50,50	0
55	MG	RA	3368	1/1	0.91	0.13	49,49,49,49	0
55	MG	RA	3267	1/1	0.91	0.22	43,43,43,43	0
55	MG	YA	3092	1/1	0.91	0.06	10,10,10,10	0
55	MG	RA	3010	1/1	0.91	0.13	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3121	1/1	0.91	0.08	38,38,38,38	0
55	MG	YA	3400	1/1	0.91	0.11	51,51,51,51	0
55	MG	YA	3401	1/1	0.91	0.08	39,39,39,39	0
55	MG	YA	3112	1/1	0.91	0.09	11,11,11,11	0
55	MG	YA	3255	1/1	0.91	0.18	45,45,45,45	0
55	MG	YA	3407	1/1	0.91	0.06	43,43,43,43	0
55	MG	QA	1629	1/1	0.91	0.06	59,59,59,59	0
55	MG	YA	3484	1/1	0.91	0.11	24,24,24,24	0
55	MG	YA	3409	1/1	0.91	0.13	18,18,18,18	0
55	MG	YA	3410	1/1	0.91	0.12	44,44,44,44	0
55	MG	RA	3336	1/1	0.91	0.08	36,36,36,36	0
55	MG	QA	1610	1/1	0.91	0.22	41,41,41,41	0
55	MG	YA	3493	1/1	0.91	0.07	31,31,31,31	0
55	MG	QA	1661	1/1	0.91	0.11	40,40,40,40	0
55	MG	RA	3224	1/1	0.91	0.10	26,26,26,26	0
55	MG	RA	3225	1/1	0.91	0.21	35,35,35,35	0
55	MG	RA	3051	1/1	0.91	0.07	25,25,25,25	0
55	MG	RA	3197	1/1	0.91	0.10	41,41,41,41	0
55	MG	YA	3349	1/1	0.91	0.12	25,25,25,25	0
55	MG	XA	1641	1/1	0.91	0.10	62,62,62,62	0
55	MG	YE	302	1/1	0.91	0.09	36,36,36,36	0
55	MG	RA	3353	1/1	0.91	0.14	55,55,55,55	0
55	MG	RA	3312	1/1	0.91	0.17	23,23,23,23	0
55	MG	YA	3428	1/1	0.91	0.07	19,19,19,19	0
55	MG	RA	3076	1/1	0.91	0.19	30,30,30,30	0
55	MG	RA	3255	1/1	0.91	0.17	43,43,43,43	0
55	MG	XA	1647	1/1	0.91	0.06	47,47,47,47	0
55	MG	QA	1652	1/1	0.91	0.10	45,45,45,45	0
55	MG	Y8	101	1/1	0.91	0.29	45,45,45,45	0
55	MG	RA	3293	1/1	0.92	0.09	51,51,51,51	0
55	MG	YA	3328	1/1	0.92	0.18	43,43,43,43	0
55	MG	RA	3018	1/1	0.92	0.14	22,22,22,22	0
55	MG	YA	3422	1/1	0.92	0.25	48,48,48,48	0
55	MG	RA	3426	1/1	0.92	0.06	32,32,32,32	0
55	MG	RA	3429	1/1	0.92	0.17	34,34,34,34	0
55	MG	YA	3236	1/1	0.92	0.11	40,40,40,40	0
55	MG	XA	1636	1/1	0.92	0.07	65,65,65,65	0
55	MG	RA	3209	1/1	0.92	0.16	23,23,23,23	0
55	MG	RA	3349	1/1	0.92	0.09	44,44,44,44	0
55	MG	RA	3054	1/1	0.92	0.10	72,72,72,72	0
55	MG	YA	3243	1/1	0.92	0.19	20,20,20,20	0
55	MG	RA	3254	1/1	0.92	0.25	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3169	1/1	0.92	0.09	39,39,39,39	0
55	MG	RA	3299	1/1	0.92	0.11	53,53,53,53	0
55	MG	RA	3092	1/1	0.92	0.12	40,40,40,40	0
55	MG	RA	3356	1/1	0.92	0.10	47,47,47,47	0
55	MG	YA	3173	1/1	0.92	0.09	26,26,26,26	0
55	MG	RA	3322	1/1	0.92	0.11	43,43,43,43	0
55	MG	YA	3258	1/1	0.92	0.13	10,10,10,10	0
55	MG	YA	3259	1/1	0.92	0.16	33,33,33,33	0
55	MG	RB	201	1/1	0.92	0.18	80,80,80,80	0
55	MG	RA	3060	1/1	0.92	0.14	47,47,47,47	0
55	MG	YA	3076	1/1	0.92	0.09	52,52,52,52	0
55	MG	QA	1627	1/1	0.92	0.10	84,84,84,84	0
55	MG	YA	3362	1/1	0.92	0.18	33,33,33,33	0
55	MG	YA	3452	1/1	0.92	0.13	37,37,37,37	0
55	MG	YA	3453	1/1	0.92	0.08	53,53,53,53	0
55	MG	RA	3037	1/1	0.92	0.15	25,25,25,25	0
55	MG	XA	1660	1/1	0.92	0.07	46,46,46,46	0
55	MG	YA	3276	1/1	0.92	0.19	36,36,36,36	0
55	MG	RE	302	1/1	0.92	0.17	28,28,28,28	0
55	MG	RA	3130	1/1	0.92	0.12	33,33,33,33	0
55	MG	RA	3179	1/1	0.92	0.09	71,71,71,71	0
55	MG	YA	3190	1/1	0.92	0.06	26,26,26,26	0
55	MG	QA	1646	1/1	0.92	0.08	50,50,50,50	0
55	MG	YA	3113	1/1	0.92	0.12	24,24,24,24	0
55	MG	RA	3334	1/1	0.92	0.14	38,38,38,38	0
55	MG	YA	3377	1/1	0.92	0.14	45,45,45,45	0
55	MG	RA	3406	1/1	0.92	0.13	52,52,52,52	0
55	MG	R0	102	1/1	0.92	0.07	33,33,33,33	0
55	MG	RA	3407	1/1	0.92	0.14	62,62,62,62	0
55	MG	RA	3181	1/1	0.92	0.24	31,31,31,31	0
55	MG	YA	3475	1/1	0.92	0.16	53,53,53,53	0
55	MG	YA	3298	1/1	0.92	0.09	24,24,24,24	0
55	MG	YA	3387	1/1	0.92	0.18	45,45,45,45	0
55	MG	YA	3389	1/1	0.92	0.13	33,33,33,33	0
55	MG	XA	1676	1/1	0.92	0.11	48,48,48,48	0
55	MG	XA	1677	1/1	0.92	0.09	54,54,54,54	0
55	MG	XA	1678	1/1	0.92	0.12	56,56,56,56	0
55	MG	YA	3302	1/1	0.92	0.13	48,48,48,48	0
55	MG	YA	3304	1/1	0.92	0.14	30,30,30,30	0
55	MG	QA	1633	1/1	0.92	0.16	53,53,53,53	0
55	MG	YA	3508	1/1	0.92	0.10	36,36,36,36	0
55	MG	RA	3411	1/1	0.92	0.09	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1607	1/1	0.92	0.22	40,40,40,40	0
55	MG	YA	3146	1/1	0.92	0.07	21,21,21,21	0
55	MG	YA	3147	1/1	0.92	0.09	19,19,19,19	0
55	MG	RA	3369	1/1	0.92	0.15	30,30,30,30	0
55	MG	RA	3339	1/1	0.92	0.09	21,21,21,21	0
55	MG	YA	3318	1/1	0.92	0.11	22,22,22,22	0
55	MG	RA	3311	1/1	0.92	0.09	33,33,33,33	0
55	MG	YA	3005	1/1	0.92	0.06	47,47,47,47	0
55	MG	RA	3134	1/1	0.92	0.16	44,44,44,44	0
55	MG	YA	3226	1/1	0.92	0.18	23,23,23,23	0
55	MG	YA	3416	1/1	0.92	0.07	29,29,29,29	0
55	MG	RA	3376	1/1	0.92	0.16	51,51,51,51	0
55	MG	RA	3345	1/1	0.92	0.18	48,48,48,48	0
57	ZN	Y4	101	1/1	0.92	0.07	270,270,270,270	0
55	MG	YA	3308	1/1	0.93	0.06	19,19,19,19	0
55	MG	XA	1642	1/1	0.93	0.10	46,46,46,46	0
55	MG	YA	3084	1/1	0.93	0.19	21,21,21,21	0
55	MG	RA	3321	1/1	0.93	0.06	42,42,42,42	0
55	MG	YA	3414	1/1	0.93	0.20	33,33,33,33	0
55	MG	YA	3090	1/1	0.93	0.06	20,20,20,20	0
55	MG	YA	3315	1/1	0.93	0.28	57,57,57,57	0
55	MG	YA	3091	1/1	0.93	0.19	24,24,24,24	0
55	MG	YA	3317	1/1	0.93	0.08	44,44,44,44	0
55	MG	RA	3241	1/1	0.93	0.05	67,67,67,67	0
55	MG	RA	3027	1/1	0.93	0.12	26,26,26,26	0
55	MG	RA	3428	1/1	0.93	0.06	27,27,27,27	0
55	MG	YA	3111	1/1	0.93	0.08	12,12,12,12	0
55	MG	RA	3168	1/1	0.93	0.16	35,35,35,35	0
55	MG	RA	3326	1/1	0.93	0.25	47,47,47,47	0
55	MG	YA	3426	1/1	0.93	0.14	47,47,47,47	0
55	MG	YA	3427	1/1	0.93	0.07	30,30,30,30	0
55	MG	XA	1652	1/1	0.93	0.07	39,39,39,39	0
55	MG	RA	3432	1/1	0.93	0.09	45,45,45,45	0
55	MG	RA	3433	1/1	0.93	0.21	59,59,59,59	0
55	MG	YA	3329	1/1	0.93	0.20	62,62,62,62	0
55	MG	RA	3104	1/1	0.93	0.08	30,30,30,30	0
55	MG	RA	3291	1/1	0.93	0.20	41,41,41,41	0
55	MG	YA	3130	1/1	0.93	0.12	18,18,18,18	0
55	MG	RA	3106	1/1	0.93	0.07	25,25,25,25	0
55	MG	YA	3438	1/1	0.93	0.11	46,46,46,46	0
55	MG	RA	3028	1/1	0.93	0.19	41,41,41,41	0
55	MG	RA	3294	1/1	0.93	0.18	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
55	MG	YA	3339	1/1	0.93	0.10	36,36,36,36	0
55	MG	RA	3144	1/1	0.93	0.07	39,39,39,39	0
55	MG	RA	3443	1/1	0.93	0.17	52,52,52,52	0
55	MG	RA	3383	1/1	0.93	0.05	44,44,44,44	0
55	MG	RA	3384	1/1	0.93	0.23	50,50,50,50	0
55	MG	RA	3211	1/1	0.93	0.20	14,14,14,14	0
55	MG	YA	3348	1/1	0.93	0.07	29,29,29,29	0
55	MG	RA	3212	1/1	0.93	0.11	42,42,42,42	0
55	MG	RA	3213	1/1	0.93	0.21	45,45,45,45	0
55	MG	RA	3341	1/1	0.93	0.08	45,45,45,45	0
55	MG	RA	3030	1/1	0.93	0.18	24,24,24,24	0
55	MG	RA	3178	1/1	0.93	0.12	51,51,51,51	0
55	MG	YA	3250	1/1	0.93	0.20	18,18,18,18	0
55	MG	YA	3251	1/1	0.93	0.14	20,20,20,20	0
55	MG	RA	3395	1/1	0.93	0.05	71,71,71,71	0
55	MG	RA	3073	1/1	0.93	0.09	37,37,37,37	0
55	MG	QA	1631	1/1	0.93	0.15	51,51,51,51	0
55	MG	RA	3398	1/1	0.93	0.21	47,47,47,47	0
55	MG	QA	1641	1/1	0.93	0.07	68,68,68,68	0
55	MG	RA	3040	1/1	0.93	0.17	27,27,27,27	0
55	MG	RA	3183	1/1	0.93	0.14	82,82,82,82	0
55	MG	YA	3008	1/1	0.93	0.09	34,34,34,34	0
55	MG	YA	3467	1/1	0.93	0.13	29,29,29,29	0
55	MG	RA	3402	1/1	0.93	0.06	58,58,58,58	0
55	MG	YA	3263	1/1	0.93	0.11	42,42,42,42	0
55	MG	RA	3352	1/1	0.93	0.11	50,50,50,50	0
55	MG	YA	3268	1/1	0.93	0.10	23,23,23,23	0
55	MG	RA	3118	1/1	0.93	0.10	28,28,28,28	0
55	MG	RA	3120	1/1	0.93	0.25	45,45,45,45	0
55	MG	YA	3272	1/1	0.93	0.12	31,31,31,31	0
55	MG	YA	3014	1/1	0.93	0.18	24,24,24,24	0
55	MG	YA	3488	1/1	0.93	0.14	46,46,46,46	0
55	MG	RA	3187	1/1	0.93	0.11	38,38,38,38	0
55	MG	QA	1621	1/1	0.93	0.06	48,48,48,48	0
55	MG	XA	1614	1/1	0.93	0.09	21,21,21,21	0
55	MG	QA	1620	1/1	0.93	0.05	67,67,67,67	0
55	MG	YA	3495	1/1	0.93	0.14	24,24,24,24	0
55	MG	YA	3496	1/1	0.93	0.15	30,30,30,30	0
55	MG	YA	3499	1/1	0.93	0.16	23,23,23,23	0
55	MG	XA	1618	1/1	0.93	0.20	44,44,44,44	0
55	MG	RA	3358	1/1	0.93	0.09	34,34,34,34	0
55	MG	RA	3050	1/1	0.93	0.14	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3017	1/1	0.93	0.11	10,10,10,10	0
55	MG	XA	1623	1/1	0.93	0.12	44,44,44,44	0
55	MG	YA	3056	1/1	0.93	0.13	27,27,27,27	0
55	MG	YB	203	1/1	0.93	0.07	45,45,45,45	0
55	MG	YB	204	1/1	0.93	0.12	30,30,30,30	0
55	MG	XA	1626	1/1	0.93	0.08	32,32,32,32	0
55	MG	QA	1649	1/1	0.93	0.19	65,65,65,65	0
55	MG	YA	3397	1/1	0.93	0.15	48,48,48,48	0
55	MG	YA	3187	1/1	0.93	0.14	35,35,35,35	0
55	MG	RA	3019	1/1	0.93	0.13	15,15,15,15	0
55	MG	RA	3022	1/1	0.93	0.06	25,25,25,25	0
55	MG	YA	3404	1/1	0.93	0.14	40,40,40,40	0
55	MG	XA	1638	1/1	0.93	0.11	44,44,44,44	0
55	MG	YA	3074	1/1	0.93	0.14	19,19,19,19	0
55	MG	RA	3026	1/1	0.93	0.13	17,17,17,17	0
55	MG	YA	3078	1/1	0.93	0.15	23,23,23,23	0
55	MG	RA	3240	1/1	0.93	0.12	52,52,52,52	0
55	MG	RA	3029	1/1	0.94	0.26	24,24,24,24	0
55	MG	YA	3031	1/1	0.94	0.18	7,7,7,7	0
55	MG	XA	1630	1/1	0.94	0.09	13,13,13,13	0
55	MG	RA	3422	1/1	0.94	0.13	33,33,33,33	0
55	MG	YA	3044	1/1	0.94	0.15	13,13,13,13	0
55	MG	QA	1613	1/1	0.94	0.10	75,75,75,75	0
55	MG	RA	3100	1/1	0.94	0.20	31,31,31,31	0
55	MG	RA	3374	1/1	0.94	0.13	37,37,37,37	0
55	MG	YA	3297	1/1	0.94	0.18	31,31,31,31	0
55	MG	XA	1639	1/1	0.94	0.17	37,37,37,37	0
55	MG	YA	3059	1/1	0.94	0.08	10,10,10,10	0
55	MG	RA	3063	1/1	0.94	0.12	25,25,25,25	0
55	MG	RA	3331	1/1	0.94	0.14	46,46,46,46	0
55	MG	YA	3415	1/1	0.94	0.06	29,29,29,29	0
55	MG	RA	3377	1/1	0.94	0.17	40,40,40,40	0
55	MG	RA	3173	1/1	0.94	0.09	20,20,20,20	0
55	MG	RA	3011	1/1	0.94	0.12	26,26,26,26	0
55	MG	RA	3380	1/1	0.94	0.14	32,32,32,32	0
55	MG	YA	3307	1/1	0.94	0.18	50,50,50,50	0
55	MG	RA	3248	1/1	0.94	0.15	46,46,46,46	0
55	MG	RA	3015	1/1	0.94	0.18	41,41,41,41	0
55	MG	YA	3082	1/1	0.94	0.18	22,22,22,22	0
55	MG	YA	3311	1/1	0.94	0.07	39,39,39,39	0
55	MG	YA	3197	1/1	0.94	0.14	51,51,51,51	0
55	MG	RA	3337	1/1	0.94	0.07	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3314	1/1	0.94	0.09	39,39,39,39	0
55	MG	RA	3338	1/1	0.94	0.16	30,30,30,30	0
55	MG	RA	3070	1/1	0.94	0.16	31,31,31,31	0
55	MG	YA	3204	1/1	0.94	0.16	29,29,29,29	0
55	MG	RA	3386	1/1	0.94	0.07	46,46,46,46	0
55	MG	RA	3216	1/1	0.94	0.21	32,32,32,32	0
55	MG	YA	3207	1/1	0.94	0.05	23,23,23,23	0
55	MG	XA	1657	1/1	0.94	0.04	48,48,48,48	0
55	MG	YA	3211	1/1	0.94	0.08	33,33,33,33	0
55	MG	YA	3096	1/1	0.94	0.09	11,11,11,11	0
55	MG	YA	3325	1/1	0.94	0.15	62,62,62,62	0
55	MG	YA	3098	1/1	0.94	0.14	31,31,31,31	0
55	MG	RA	3071	1/1	0.94	0.12	13,13,13,13	0
55	MG	YA	3104	1/1	0.94	0.07	20,20,20,20	0
55	MG	YA	3444	1/1	0.94	0.12	37,37,37,37	0
55	MG	YA	3109	1/1	0.94	0.17	13,13,13,13	0
55	MG	XA	1659	1/1	0.94	0.05	42,42,42,42	0
55	MG	RA	3110	1/1	0.94	0.18	45,45,45,45	0
55	MG	RA	3039	1/1	0.94	0.13	16,16,16,16	0
55	MG	RA	3220	1/1	0.94	0.20	46,46,46,46	0
55	MG	XA	1664	1/1	0.94	0.09	41,41,41,41	0
55	MG	YA	3121	1/1	0.94	0.06	32,32,32,32	0
55	MG	QA	1662	1/1	0.94	0.09	29,29,29,29	0
55	MG	YA	3340	1/1	0.94	0.07	45,45,45,45	0
55	MG	YA	3124	1/1	0.94	0.17	27,27,27,27	0
55	MG	RA	3259	1/1	0.94	0.07	29,29,29,29	0
55	MG	QA	1663	1/1	0.94	0.13	76,76,76,76	0
55	MG	YA	3344	1/1	0.94	0.17	38,38,38,38	0
55	MG	YA	3129	1/1	0.94	0.07	5,5,5,5	0
55	MG	YA	3346	1/1	0.94	0.23	53,53,53,53	0
55	MG	XA	1668	1/1	0.94	0.05	41,41,41,41	0
55	MG	RA	3048	1/1	0.94	0.12	8,8,8,8	0
55	MG	RA	3351	1/1	0.94	0.16	42,42,42,42	0
55	MG	YA	3134	1/1	0.94	0.15	31,31,31,31	0
55	MG	YA	3351	1/1	0.94	0.11	36,36,36,36	0
55	MG	QA	1639	1/1	0.94	0.07	48,48,48,48	0
55	MG	RA	3154	1/1	0.94	0.08	16,16,16,16	0
55	MG	YA	3138	1/1	0.94	0.10	22,22,22,22	0
55	MG	YA	3142	1/1	0.94	0.06	29,29,29,29	0
55	MG	RA	3155	1/1	0.94	0.08	27,27,27,27	0
55	MG	YA	3474	1/1	0.94	0.07	37,37,37,37	0
55	MG	YA	3249	1/1	0.94	0.22	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
55	MG	XA	1601	1/1	0.94	0.06	44,44,44,44	0
55	MG	YA	3478	1/1	0.94	0.12	25,25,25,25	0
55	MG	YA	3481	1/1	0.94	0.21	7,7,7,7	0
55	MG	QA	1614	1/1	0.94	0.07	47,47,47,47	0
55	MG	YA	3252	1/1	0.94	0.14	43,43,43,43	0
55	MG	QA	1645	1/1	0.94	0.07	60,60,60,60	0
55	MG	QA	1617	1/1	0.94	0.08	57,57,57,57	0
55	MG	RA	3088	1/1	0.94	0.14	13,13,13,13	0
55	MG	XA	1608	1/1	0.94	0.10	61,61,61,61	0
55	MG	RA	3125	1/1	0.94	0.09	22,22,22,22	0
55	MG	RA	3128	1/1	0.94	0.18	39,39,39,39	0
55	MG	RA	3235	1/1	0.94	0.20	38,38,38,38	0
55	MG	YA	3372	1/1	0.94	0.09	36,36,36,36	0
55	MG	YA	3502	1/1	0.94	0.32	42,42,42,42	0
55	MG	YA	3503	1/1	0.94	0.08	32,32,32,32	0
55	MG	XA	1612	1/1	0.94	0.17	54,54,54,54	0
55	MG	RA	3089	1/1	0.94	0.18	22,22,22,22	0
55	MG	YA	3262	1/1	0.94	0.10	7,7,7,7	0
55	MG	RA	3277	1/1	0.94	0.12	26,26,26,26	0
55	MG	YA	3264	1/1	0.94	0.15	28,28,28,28	0
55	MG	YA	3265	1/1	0.94	0.11	33,33,33,33	0
55	MG	RA	3199	1/1	0.94	0.15	69,69,69,69	0
55	MG	XA	1616	1/1	0.94	0.13	22,22,22,22	0
55	MG	YB	205	1/1	0.94	0.08	12,12,12,12	0
55	MG	RA	3057	1/1	0.94	0.15	31,31,31,31	0
55	MG	YA	3163	1/1	0.94	0.11	44,44,44,44	0
55	MG	QA	1660	1/1	0.94	0.08	59,59,59,59	0
55	MG	YA	3274	1/1	0.94	0.17	38,38,38,38	0
55	MG	RA	3416	1/1	0.94	0.06	35,35,35,35	0
55	MG	RA	3283	1/1	0.94	0.20	42,42,42,42	0
55	MG	YA	3393	1/1	0.94	0.08	48,48,48,48	0
55	MG	YA	3278	1/1	0.94	0.11	17,17,17,17	0
55	MG	RA	3418	1/1	0.94	0.16	17,17,17,17	0
55	MG	YA	3022	1/1	0.94	0.11	18,18,18,18	0
55	MG	Y3	101	1/1	0.94	0.17	25,25,25,25	0
55	MG	YA	3282	1/1	0.94	0.11	36,36,36,36	0
55	MG	XA	1624	1/1	0.94	0.07	23,23,23,23	0
55	MG	YA	3123	1/1	0.95	0.09	7,7,7,7	0
55	MG	RA	3003	1/1	0.95	0.11	24,24,24,24	0
55	MG	YA	3217	1/1	0.95	0.14	28,28,28,28	0
55	MG	YA	3007	1/1	0.95	0.09	45,45,45,45	0
55	MG	XA	1632	1/1	0.95	0.10	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3101	1/1	0.95	0.17	45,45,45,45	0
55	MG	RA	3013	1/1	0.95	0.05	7,7,7,7	0
55	MG	XA	1637	1/1	0.95	0.10	49,49,49,49	0
55	MG	YA	3225	1/1	0.95	0.11	33,33,33,33	0
55	MG	RA	3176	1/1	0.95	0.22	26,26,26,26	0
55	MG	RA	3079	1/1	0.95	0.11	27,27,27,27	0
55	MG	RA	3081	1/1	0.95	0.10	16,16,16,16	0
55	MG	YA	3229	1/1	0.95	0.10	49,49,49,49	0
55	MG	QA	1635	1/1	0.95	0.07	44,44,44,44	0
55	MG	RA	3367	1/1	0.95	0.07	37,37,37,37	0
55	MG	YA	3141	1/1	0.95	0.17	5,5,5,5	0
55	MG	YA	3330	1/1	0.95	0.14	23,23,23,23	0
55	MG	RE	304	1/1	0.95	0.14	28,28,28,28	0
55	MG	YA	3143	1/1	0.95	0.09	18,18,18,18	0
55	MG	RA	3132	1/1	0.95	0.07	40,40,40,40	0
55	MG	YA	3436	1/1	0.95	0.06	25,25,25,25	0
55	MG	YA	3437	1/1	0.95	0.06	37,37,37,37	0
55	MG	YA	3027	1/1	0.95	0.17	7,7,7,7	0
55	MG	RN	201	1/1	0.95	0.27	54,54,54,54	0
55	MG	YA	3029	1/1	0.95	0.08	13,13,13,13	0
55	MG	YA	3241	1/1	0.95	0.10	7,7,7,7	0
55	MG	YA	3242	1/1	0.95	0.09	13,13,13,13	0
55	MG	QA	1605	1/1	0.95	0.05	36,36,36,36	0
55	MG	RA	3408	1/1	0.95	0.18	48,48,48,48	0
55	MG	YA	3032	1/1	0.95	0.17	13,13,13,13	0
55	MG	XA	1649	1/1	0.95	0.04	37,37,37,37	0
55	MG	YA	3035	1/1	0.95	0.20	26,26,26,26	0
55	MG	RA	3370	1/1	0.95	0.08	42,42,42,42	0
55	MG	XA	1651	1/1	0.95	0.05	40,40,40,40	0
55	MG	YA	3047	1/1	0.95	0.16	21,21,21,21	0
55	MG	RX	101	1/1	0.95	0.07	31,31,31,31	0
55	MG	YA	3051	1/1	0.95	0.14	7,7,7,7	0
55	MG	QA	1625	1/1	0.95	0.06	46,46,46,46	0
55	MG	RA	3069	1/1	0.95	0.11	31,31,31,31	0
55	MG	YA	3162	1/1	0.95	0.16	34,34,34,34	0
55	MG	RA	3009	1/1	0.95	0.21	28,28,28,28	0
55	MG	XA	1656	1/1	0.95	0.05	35,35,35,35	0
55	MG	RA	3033	1/1	0.95	0.13	28,28,28,28	0
55	MG	YA	3065	1/1	0.95	0.15	7,7,7,7	0
55	MG	YA	3358	1/1	0.95	0.20	34,34,34,34	0
55	MG	RA	3304	1/1	0.95	0.05	6,6,6,6	0
55	MG	YA	3068	1/1	0.95	0.16	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3069	1/1	0.95	0.11	40,40,40,40	0
55	MG	RA	3186	1/1	0.95	0.14	40,40,40,40	0
55	MG	YA	3071	1/1	0.95	0.11	22,22,22,22	0
55	MG	YA	3364	1/1	0.95	0.05	40,40,40,40	0
55	MG	YA	3072	1/1	0.95	0.13	16,16,16,16	0
55	MG	YA	3472	1/1	0.95	0.22	60,60,60,60	0
55	MG	XA	1605	1/1	0.95	0.13	47,47,47,47	0
55	MG	YA	3271	1/1	0.95	0.16	29,29,29,29	0
55	MG	YA	3176	1/1	0.95	0.10	36,36,36,36	0
55	MG	YA	3273	1/1	0.95	0.07	26,26,26,26	0
55	MG	YA	3075	1/1	0.95	0.16	19,19,19,19	0
55	MG	RA	3244	1/1	0.95	0.31	57,57,57,57	0
55	MG	YA	3482	1/1	0.95	0.14	16,16,16,16	0
55	MG	YA	3483	1/1	0.95	0.13	10,10,10,10	0
55	MG	YA	3077	1/1	0.95	0.22	22,22,22,22	0
55	MG	XA	1662	1/1	0.95	0.05	45,45,45,45	0
55	MG	YA	3486	1/1	0.95	0.10	26,26,26,26	0
55	MG	YA	3487	1/1	0.95	0.14	9,9,9,9	0
55	MG	YA	3279	1/1	0.95	0.14	28,28,28,28	0
55	MG	RA	3139	1/1	0.95	0.06	30,30,30,30	0
55	MG	YA	3182	1/1	0.95	0.05	25,25,25,25	0
55	MG	RA	3308	1/1	0.95	0.10	39,39,39,39	0
55	MG	RA	3020	1/1	0.95	0.07	28,28,28,28	0
55	MG	RA	3116	1/1	0.95	0.06	31,31,31,31	0
55	MG	RA	3279	1/1	0.95	0.06	14,14,14,14	0
55	MG	YA	3498	1/1	0.95	0.12	28,28,28,28	0
55	MG	YA	3286	1/1	0.95	0.08	9,9,9,9	0
55	MG	YA	3501	1/1	0.95	0.05	7,7,7,7	0
55	MG	YA	3089	1/1	0.95	0.17	20,20,20,20	0
55	MG	RA	3222	1/1	0.95	0.15	60,60,60,60	0
55	MG	YA	3391	1/1	0.95	0.14	29,29,29,29	0
55	MG	RA	3059	1/1	0.95	0.07	28,28,28,28	0
55	MG	YA	3506	1/1	0.95	0.10	23,23,23,23	0
55	MG	YA	3507	1/1	0.95	0.23	48,48,48,48	0
55	MG	QA	1601	1/1	0.95	0.07	32,32,32,32	0
55	MG	RA	3315	1/1	0.95	0.11	28,28,28,28	0
55	MG	YA	3293	1/1	0.95	0.12	42,42,42,42	0
55	MG	RA	3388	1/1	0.95	0.05	40,40,40,40	0
55	MG	XA	1674	1/1	0.95	0.04	54,54,54,54	0
55	MG	YA	3198	1/1	0.95	0.18	55,55,55,55	0
55	MG	RA	3252	1/1	0.95	0.24	62,62,62,62	0
55	MG	RA	3169	1/1	0.95	0.06	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3434	1/1	0.95	0.08	25,25,25,25	0
55	MG	RA	3119	1/1	0.95	0.09	44,44,44,44	0
55	MG	YA	3303	1/1	0.95	0.07	30,30,30,30	0
55	MG	YP	202	1/1	0.95	0.10	23,23,23,23	0
55	MG	RA	3286	1/1	0.95	0.17	40,40,40,40	0
55	MG	XV	101	1/1	0.95	0.27	153,153,153,153	0
55	MG	YR	201	1/1	0.95	0.08	16,16,16,16	0
55	MG	YA	3114	1/1	0.95	0.12	17,17,17,17	0
55	MG	YA	3208	1/1	0.95	0.09	23,23,23,23	0
55	MG	YA	3116	1/1	0.95	0.18	29,29,29,29	0
55	MG	RA	3099	1/1	0.95	0.11	60,60,60,60	0
55	MG	XA	1625	1/1	0.95	0.07	30,30,30,30	0
55	MG	Y7	101	1/1	0.95	0.11	51,51,51,51	0
55	MG	RA	3288	1/1	0.95	0.11	34,34,34,34	0
57	ZN	R4	101	1/1	0.95	0.06	250,250,250,250	0
55	MG	RA	3289	1/1	0.95	0.10	32,32,32,32	0
55	MG	YA	3110	1/1	0.96	0.15	35,35,35,35	0
55	MG	YA	3174	1/1	0.96	0.13	38,38,38,38	0
55	MG	RA	3264	1/1	0.96	0.20	41,41,41,41	0
55	MG	YA	3244	1/1	0.96	0.15	7,7,7,7	0
55	MG	YA	3383	1/1	0.96	0.10	11,11,11,11	0
55	MG	RA	3078	1/1	0.96	0.13	29,29,29,29	0
55	MG	YA	3385	1/1	0.96	0.06	15,15,15,15	0
55	MG	YA	3247	1/1	0.96	0.20	20,20,20,20	0
55	MG	RA	3052	1/1	0.96	0.04	1,1,1,1	0
55	MG	YA	3388	1/1	0.96	0.08	24,24,24,24	0
55	MG	XA	1621	1/1	0.96	0.12	25,25,25,25	0
55	MG	YA	3039	1/1	0.96	0.10	7,7,7,7	0
55	MG	RA	3080	1/1	0.96	0.05	12,12,12,12	0
55	MG	YA	3042	1/1	0.96	0.12	15,15,15,15	0
55	MG	RA	3172	1/1	0.96	0.20	49,49,49,49	0
55	MG	YA	3045	1/1	0.96	0.08	17,17,17,17	0
55	MG	YA	3470	1/1	0.96	0.16	47,47,47,47	0
55	MG	RA	3123	1/1	0.96	0.20	21,21,21,21	0
55	MG	RB	204	1/1	0.96	0.11	33,33,33,33	0
55	MG	RA	3053	1/1	0.96	0.10	21,21,21,21	0
55	MG	YA	3126	1/1	0.96	0.10	21,21,21,21	0
55	MG	XA	1629	1/1	0.96	0.06	24,24,24,24	0
55	MG	RA	3206	1/1	0.96	0.05	16,16,16,16	0
55	MG	YA	3403	1/1	0.96	0.17	34,34,34,34	0
55	MG	QA	1608	1/1	0.96	0.09	27,27,27,27	0
55	MG	RA	3208	1/1	0.96	0.10	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1633	1/1	0.96	0.06	42,42,42,42	0
55	MG	YA	3064	1/1	0.96	0.10	15,15,15,15	0
55	MG	XA	1634	1/1	0.96	0.06	90,90,90,90	0
55	MG	YA	3266	1/1	0.96	0.10	22,22,22,22	0
55	MG	YA	3136	1/1	0.96	0.14	10,10,10,10	0
55	MG	RA	3150	1/1	0.96	0.09	40,40,40,40	0
55	MG	RA	3126	1/1	0.96	0.13	37,37,37,37	0
55	MG	YA	3139	1/1	0.96	0.06	23,23,23,23	0
55	MG	RA	3127	1/1	0.96	0.20	17,17,17,17	0
55	MG	RA	3153	1/1	0.96	0.14	43,43,43,43	0
55	MG	YA	3494	1/1	0.96	0.10	24,24,24,24	0
55	MG	RA	3083	1/1	0.96	0.18	21,21,21,21	0
55	MG	RA	3129	1/1	0.96	0.05	24,24,24,24	0
55	MG	YA	3497	1/1	0.96	0.08	21,21,21,21	0
55	MG	RA	3056	1/1	0.96	0.20	15,15,15,15	0
55	MG	RA	3085	1/1	0.96	0.10	14,14,14,14	0
55	MG	YA	3277	1/1	0.96	0.21	33,33,33,33	0
55	MG	RA	3419	1/1	0.96	0.13	23,23,23,23	0
55	MG	R8	102	1/1	0.96	0.06	26,26,26,26	0
55	MG	RA	3109	1/1	0.96	0.09	72,72,72,72	0
55	MG	RA	3001	1/1	0.96	0.10	22,22,22,22	0
55	MG	RA	3047	1/1	0.96	0.10	4,4,4,4	0
55	MG	RA	3023	1/1	0.96	0.13	5,5,5,5	0
55	MG	YA	3083	1/1	0.96	0.10	28,28,28,28	0
55	MG	RA	3188	1/1	0.96	0.12	38,38,38,38	0
55	MG	YA	3013	1/1	0.96	0.04	33,33,33,33	0
55	MG	YA	3157	1/1	0.96	0.05	7,7,7,7	0
55	MG	RA	3391	1/1	0.96	0.17	34,34,34,34	0
55	MG	RA	3163	1/1	0.96	0.06	36,36,36,36	0
55	MG	QA	1607	1/1	0.96	0.07	39,39,39,39	0
55	MG	YB	206	1/1	0.96	0.17	51,51,51,51	0
55	MG	QA	1655	1/1	0.96	0.19	29,29,29,29	0
55	MG	YA	3093	1/1	0.96	0.09	7,7,7,7	0
55	MG	YA	3094	1/1	0.96	0.14	7,7,7,7	0
55	MG	YA	3296	1/1	0.96	0.05	33,33,33,33	0
55	MG	RA	3324	1/1	0.96	0.11	26,26,26,26	0
55	MG	YP	203	1/1	0.96	0.05	4,4,4,4	0
55	MG	YA	3365	1/1	0.96	0.18	58,58,58,58	0
55	MG	YQ	202	1/1	0.96	0.11	36,36,36,36	0
55	MG	YA	3366	1/1	0.96	0.12	30,30,30,30	0
55	MG	RA	3005	1/1	0.96	0.14	24,24,24,24	0
55	MG	YA	3232	1/1	0.96	0.09	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
55	MG	RA	3077	1/1	0.96	0.17	28,28,28,28	0
55	MG	YA	3167	1/1	0.96	0.25	32,32,32,32	0
55	MG	YA	3235	1/1	0.96	0.17	44,44,44,44	0
55	MG	YA	3102	1/1	0.96	0.19	12,12,12,12	0
55	MG	RA	3229	1/1	0.96	0.11	21,21,21,21	0
55	MG	RA	3262	1/1	0.96	0.15	34,34,34,34	0
55	MG	YA	3105	1/1	0.96	0.19	21,21,21,21	0
57	ZN	XN	101	1/1	0.96	0.10	155,155,155,155	0
55	MG	RA	3095	1/1	0.96	0.08	8,8,8,8	0
55	MG	XA	1648	1/1	0.97	0.17	27,27,27,27	0
55	MG	YA	3085	1/1	0.97	0.11	9,9,9,9	0
55	MG	RA	3425	1/1	0.97	0.06	23,23,23,23	0
55	MG	YA	3380	1/1	0.97	0.17	23,23,23,23	0
55	MG	YA	3087	1/1	0.97	0.12	11,11,11,11	0
55	MG	RA	3389	1/1	0.97	0.05	39,39,39,39	0
55	MG	RA	3427	1/1	0.97	0.09	17,17,17,17	0
55	MG	RA	3290	1/1	0.97	0.17	46,46,46,46	0
55	MG	YA	3019	1/1	0.97	0.12	29,29,29,29	0
55	MG	YA	3020	1/1	0.97	0.15	7,7,7,7	0
55	MG	RA	3098	1/1	0.97	0.06	30,30,30,30	0
55	MG	RA	3145	1/1	0.97	0.05	32,32,32,32	0
55	MG	YA	3023	1/1	0.97	0.07	20,20,20,20	0
55	MG	YA	3245	1/1	0.97	0.14	13,13,13,13	0
55	MG	RA	3058	1/1	0.97	0.08	15,15,15,15	0
55	MG	YA	3099	1/1	0.97	0.11	18,18,18,18	0
55	MG	YA	3101	1/1	0.97	0.13	13,13,13,13	0
55	MG	RA	3122	1/1	0.97	0.05	28,28,28,28	0
55	MG	QA	1650	1/1	0.97	0.04	31,31,31,31	0
55	MG	RA	3435	1/1	0.97	0.06	40,40,40,40	0
55	MG	RA	3042	1/1	0.97	0.13	22,22,22,22	0
55	MG	YA	3477	1/1	0.97	0.07	7,7,7,7	0
55	MG	YA	3399	1/1	0.97	0.07	26,26,26,26	0
55	MG	YA	3479	1/1	0.97	0.16	7,7,7,7	0
55	MG	YA	3108	1/1	0.97	0.09	11,11,11,11	0
55	MG	QA	1634	1/1	0.97	0.04	24,24,24,24	0
55	MG	YA	3402	1/1	0.97	0.08	30,30,30,30	0
55	MG	XA	1617	1/1	0.97	0.12	36,36,36,36	0
55	MG	RA	3046	1/1	0.97	0.10	26,26,26,26	0
55	MG	YA	3036	1/1	0.97	0.13	4,4,4,4	0
55	MG	RA	3329	1/1	0.97	0.07	40,40,40,40	0
55	MG	RA	3440	1/1	0.97	0.05	52,52,52,52	0
55	MG	YA	3332	1/1	0.97	0.15	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1611	1/1	0.97	0.06	32,32,32,32	0
55	MG	YA	3491	1/1	0.97	0.19	41,41,41,41	0
55	MG	YA	3043	1/1	0.97	0.14	8,8,8,8	0
55	MG	RA	3007	1/1	0.97	0.05	40,40,40,40	0
55	MG	RA	3332	1/1	0.97	0.17	59,59,59,59	0
55	MG	QA	1603	1/1	0.97	0.06	34,34,34,34	0
55	MG	YA	3338	1/1	0.97	0.20	43,43,43,43	0
55	MG	YA	3192	1/1	0.97	0.14	5,5,5,5	0
55	MG	YA	3048	1/1	0.97	0.10	22,22,22,22	0
55	MG	YA	3049	1/1	0.97	0.10	7,7,7,7	0
55	MG	YA	3500	1/1	0.97	0.04	22,22,22,22	0
55	MG	RA	3108	1/1	0.97	0.07	28,28,28,28	0
55	MG	YA	3196	1/1	0.97	0.08	41,41,41,41	0
55	MG	RA	3068	1/1	0.97	0.12	21,21,21,21	0
55	MG	YA	3127	1/1	0.97	0.11	37,37,37,37	0
55	MG	YA	3052	1/1	0.97	0.12	18,18,18,18	0
55	MG	YA	3053	1/1	0.97	0.09	7,7,7,7	0
55	MG	YA	3202	1/1	0.97	0.04	19,19,19,19	0
55	MG	YA	3054	1/1	0.97	0.04	18,18,18,18	0
55	MG	XA	1627	1/1	0.97	0.09	30,30,30,30	0
55	MG	RA	3157	1/1	0.97	0.05	19,19,19,19	0
55	MG	QA	1654	1/1	0.97	0.30	42,42,42,42	0
55	MG	RB	207	1/1	0.97	0.15	29,29,29,29	0
55	MG	RA	3214	1/1	0.97	0.26	40,40,40,40	0
55	MG	YA	3063	1/1	0.97	0.13	11,11,11,11	0
55	MG	RA	3032	1/1	0.97	0.06	19,19,19,19	0
55	MG	XE	201	1/1	0.97	0.09	71,71,71,71	0
55	MG	YA	3140	1/1	0.97	0.05	21,21,21,21	0
55	MG	YE	301	1/1	0.97	0.08	9,9,9,9	0
55	MG	RA	3002	1/1	0.97	0.04	20,20,20,20	0
55	MG	RA	3135	1/1	0.97	0.09	37,37,37,37	0
55	MG	YE	305	1/1	0.97	0.04	9,9,9,9	0
55	MG	YA	3287	1/1	0.97	0.15	7,7,7,7	0
55	MG	RA	3342	1/1	0.97	0.05	35,35,35,35	0
55	MG	RA	3034	1/1	0.97	0.08	26,26,26,26	0
55	MG	RA	3344	1/1	0.97	0.06	35,35,35,35	0
55	MG	RA	3249	1/1	0.97	0.07	19,19,19,19	0
55	MG	YA	3073	1/1	0.97	0.10	7,7,7,7	0
55	MG	RA	3035	1/1	0.97	0.12	24,24,24,24	0
55	MG	RA	3189	1/1	0.97	0.16	30,30,30,30	0
55	MG	YA	3006	1/1	0.97	0.10	24,24,24,24	0
55	MG	RA	3190	1/1	0.97	0.19	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3115	1/1	0.97	0.12	37,37,37,37	0
55	MG	Y5	102	1/1	0.97	0.09	32,32,32,32	0
55	MG	YA	3079	1/1	0.97	0.16	15,15,15,15	0
55	MG	RA	3055	1/1	0.97	0.20	16,16,16,16	0
56	SF4	XD	301	8/8	0.97	0.06	107,118,132,149	0
55	MG	QA	1630	1/1	0.97	0.07	49,49,49,49	0
55	MG	RA	3025	1/1	0.97	0.10	15,15,15,15	0
55	MG	RA	3096	1/1	0.97	0.05	20,20,20,20	0
55	MG	RA	3014	1/1	0.98	0.09	30,30,30,30	0
55	MG	YA	3223	1/1	0.98	0.03	25,25,25,25	0
55	MG	RA	3067	1/1	0.98	0.14	15,15,15,15	0
55	MG	RA	3215	1/1	0.98	0.12	9,9,9,9	0
55	MG	YA	3067	1/1	0.98	0.07	0,0,0,0	0
55	MG	XA	1602	1/1	0.98	0.05	43,43,43,43	0
55	MG	YA	3106	1/1	0.98	0.11	7,7,7,7	0
55	MG	YA	3107	1/1	0.98	0.24	20,20,20,20	0
55	MG	YA	3186	1/1	0.98	0.03	25,25,25,25	0
55	MG	YA	3148	1/1	0.98	0.07	19,19,19,19	0
55	MG	XA	1628	1/1	0.98	0.05	41,41,41,41	0
55	MG	YA	3455	1/1	0.98	0.25	55,55,55,55	0
55	MG	YA	3189	1/1	0.98	0.10	12,12,12,12	0
55	MG	QA	1609	1/1	0.98	0.07	36,36,36,36	0
55	MG	YA	3033	1/1	0.98	0.05	11,11,11,11	0
55	MG	RA	3420	1/1	0.98	0.12	7,7,7,7	0
55	MG	YA	3460	1/1	0.98	0.04	35,35,35,35	0
55	MG	RA	3142	1/1	0.98	0.07	22,22,22,22	0
55	MG	RA	3043	1/1	0.98	0.08	13,13,13,13	0
55	MG	YB	201	1/1	0.98	0.09	17,17,17,17	0
55	MG	YA	3037	1/1	0.98	0.16	7,7,7,7	0
55	MG	RA	3044	1/1	0.98	0.06	13,13,13,13	0
55	MG	RB	203	1/1	0.98	0.04	63,63,63,63	0
55	MG	YA	3119	1/1	0.98	0.10	6,6,6,6	0
55	MG	RA	3105	1/1	0.98	0.06	11,11,11,11	0
55	MG	RB	205	1/1	0.98	0.21	38,38,38,38	0
55	MG	RA	3238	1/1	0.98	0.05	42,42,42,42	0
55	MG	YD	302	1/1	0.98	0.04	22,22,22,22	0
55	MG	RA	3204	1/1	0.98	0.10	26,26,26,26	0
55	MG	YA	3046	1/1	0.98	0.08	1,1,1,1	0
55	MG	YE	303	1/1	0.98	0.09	7,7,7,7	0
55	MG	RA	3278	1/1	0.98	0.07	27,27,27,27	0
55	MG	RA	3036	1/1	0.98	0.06	17,17,17,17	0
55	MG	YP	201	1/1	0.98	0.05	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3024	1/1	0.98	0.07	29,29,29,29	0
55	MG	YA	3294	1/1	0.98	0.19	38,38,38,38	0
55	MG	RA	3094	1/1	0.98	0.13	31,31,31,31	0
55	MG	YA	3209	1/1	0.98	0.04	30,30,30,30	0
55	MG	RA	3261	1/1	0.98	0.06	43,43,43,43	0
55	MG	YA	3016	1/1	0.98	0.14	23,23,23,23	0
55	MG	YA	3480	1/1	0.98	0.12	7,7,7,7	0
55	MG	RA	3038	1/1	0.98	0.04	13,13,13,13	0
55	MG	RA	3021	1/1	0.98	0.07	8,8,8,8	0
55	MG	RA	3193	1/1	0.98	0.07	30,30,30,30	0
55	MG	RA	3065	1/1	0.98	0.08	19,19,19,19	0
55	MG	XA	1675	1/1	0.98	0.06	20,20,20,20	0
55	MG	RA	3266	1/1	0.98	0.05	54,54,54,54	0
55	MG	YA	3060	1/1	0.98	0.12	7,7,7,7	0
56	SF4	QD	301	8/8	0.98	0.05	67,98,117,173	0
55	MG	RA	3086	1/1	0.98	0.15	20,20,20,20	0
57	ZN	QN	101	1/1	0.98	0.08	175,175,175,175	0
57	ZN	RY	201	1/1	0.98	0.06	112,112,112,112	0
55	MG	YA	3441	1/1	0.98	0.09	53,53,53,53	0
57	ZN	R5	101	1/1	0.98	0.04	124,124,124,124	0
55	MG	YA	3026	1/1	0.98	0.10	12,12,12,12	0
57	ZN	YY	201	1/1	0.98	0.04	72,72,72,72	0
55	MG	YA	3221	1/1	0.98	0.13	36,36,36,36	0
57	ZN	Y5	101	1/1	0.98	0.05	88,88,88,88	0
57	ZN	Y9	101	1/1	0.98	0.06	66,66,66,66	0
55	MG	YA	3117	1/1	0.99	0.03	9,9,9,9	0
55	MG	YA	3323	1/1	0.99	0.09	4,4,4,4	0
55	MG	YA	3062	1/1	0.99	0.05	0,0,0,0	0
55	MG	QA	1619	1/1	0.99	0.10	40,40,40,40	0
55	MG	YA	3088	1/1	0.99	0.12	9,9,9,9	0
55	MG	RA	3097	1/1	0.99	0.05	23,23,23,23	0
55	MG	RA	3016	1/1	0.99	0.11	7,7,7,7	0
55	MG	RE	303	1/1	0.99	0.03	7,7,7,7	0
55	MG	YA	3055	1/1	0.99	0.07	17,17,17,17	0
55	MG	RA	3041	1/1	0.99	0.04	19,19,19,19	0
55	MG	RA	3431	1/1	0.99	0.07	10,10,10,10	0
55	MG	RF	301	1/1	0.99	0.04	34,34,34,34	0
55	MG	YA	3200	1/1	0.99	0.14	27,27,27,27	0
55	MG	XA	1672	1/1	0.99	0.03	32,32,32,32	0
55	MG	YA	3097	1/1	0.99	0.03	7,7,7,7	0
55	MG	RA	3200	1/1	0.99	0.05	25,25,25,25	0
57	ZN	R6	101	1/1	0.99	0.03	71,71,71,71	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	ZN	R9	101	1/1	0.99	0.06	65,65,65,65	0
55	MG	YA	3131	1/1	0.99	0.06	9,9,9,9	0
55	MG	YA	3040	1/1	0.99	0.14	7,7,7,7	0
55	MG	YA	3115	1/1	0.99	0.03	8,8,8,8	0
55	MG	YA	3100	1/1	0.99	0.05	3,3,3,3	0
57	ZN	Y6	101	1/1	0.99	0.03	55,55,55,55	0
55	MG	YA	3382	1/1	0.99	0.07	4,4,4,4	0
55	MG	RA	3012	1/1	1.00	0.06	1,1,1,1	0
55	MG	RA	3371	1/1	1.00	0.03	3,3,3,3	0
55	MG	YA	3024	1/1	1.00	0.05	8,8,8,8	0
55	MG	YA	3025	1/1	1.00	0.11	7,7,7,7	0
55	MG	YA	3038	1/1	1.00	0.03	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.