



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 06:25 PM EDT

PDB ID : 6OF6 / pdb_00006of6
Title : Crystal structure of tRNA^{Ala}(GGC) bound to cognate 70S A-site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-03-28
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

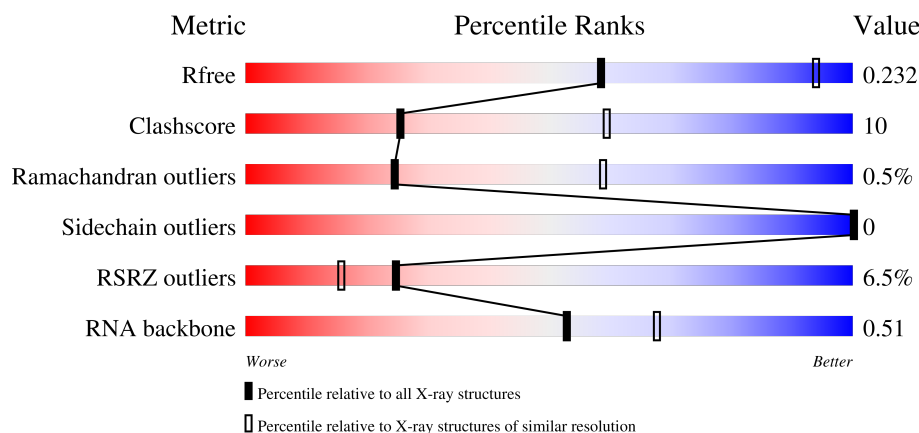
1 Overall quality at a glance

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	1522	2% 51% 39% 8%
1	XA	1522	2% 52% 38% 8%
2	QB	256	10% 73% 19% 7%
2	XB	256	8% 65% 27% 7%

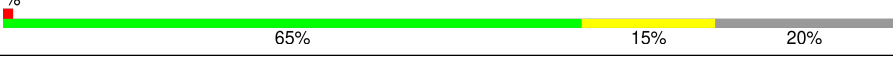
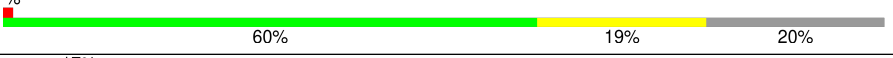
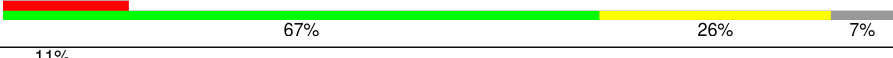
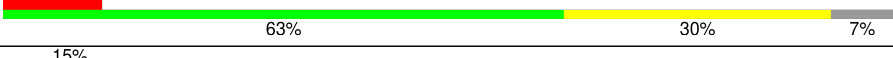
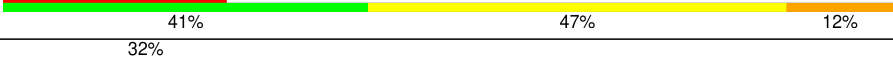
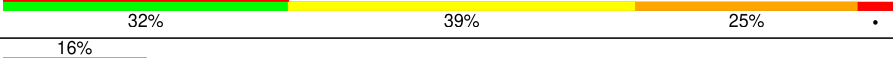
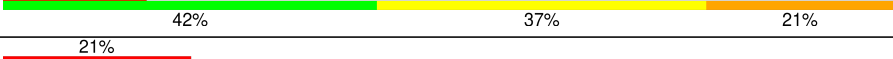
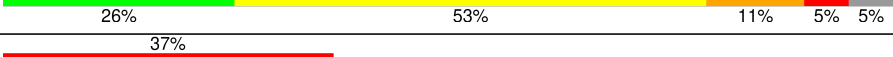
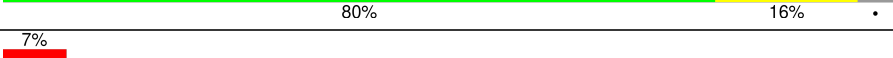
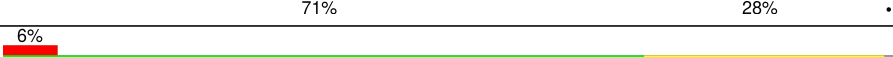
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QW	76	
23	XW	76	
24	QX	19	
24	XX	19	
25	QY	76	
25	XY	76	
26	R0	85	
26	Y0	85	
27	R1	98	
27	Y1	98	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	R2	72	
28	Y2	72	
29	R3	60	
29	Y3	60	
30	R4	71	
30	Y4	71	
31	R5	60	
31	Y5	60	
32	R6	54	
32	Y6	54	
33	R7	49	
33	Y7	49	
34	R8	65	
34	Y8	65	
35	R9	37	
35	Y9	37	
36	RA	2915	
36	YA	2915	
37	RB	122	
37	YB	122	
38	RD	276	
38	YD	276	
39	RE	206	
39	YE	206	
40	RF	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	YF	210	
41	RG	182	
41	YG	182	
42	RH	180	
42	YH	180	
43	RI	148	
43	YI	148	
44	RN	140	
44	YN	140	
45	RO	122	
45	YO	122	
46	RP	150	
46	YP	150	
47	RQ	141	
47	YQ	141	
48	RR	118	
48	YR	118	
49	RS	112	
49	YS	112	
50	RT	146	
50	YT	146	
51	RU	118	
51	YU	118	
52	RV	101	
52	YV	101	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	RW	113	
53	YW	113	
54	RX	96	
54	YX	96	
55	RY	110	
55	YY	110	
56	RZ	206	
56	YZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1610	-	-	-	X
57	MG	QA	1612	-	-	-	X
57	MG	QA	1617	-	-	-	X
57	MG	QA	1618	-	-	-	X
57	MG	QA	1619	-	-	-	X
57	MG	QA	1636	-	-	-	X
57	MG	QA	1638	-	-	-	X
57	MG	QA	1644	-	-	-	X
57	MG	QA	1647	-	-	-	X
57	MG	QA	1649	-	-	-	X
57	MG	QA	1654	-	-	-	X
57	MG	QA	1662	-	-	-	X
57	MG	QA	1688	-	-	-	X
57	MG	QA	1706	-	-	-	X
57	MG	QA	1725	-	-	-	X
57	MG	QV	103	-	-	-	X
57	MG	RA	3010	-	-	-	X
57	MG	RA	3098	-	-	-	X
57	MG	RA	3115	-	-	-	X
57	MG	RA	3125	-	-	-	X
57	MG	RA	3196	-	-	-	X
57	MG	RA	3205	-	-	-	X
57	MG	RA	3225	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3250	-	-	-	X
57	MG	RA	3269	-	-	-	X
57	MG	RA	3277	-	-	-	X
57	MG	RA	3302	-	-	-	X
57	MG	RA	3307	-	-	-	X
57	MG	RA	3319	-	-	-	X
57	MG	RA	3323	-	-	-	X
57	MG	RA	3361	-	-	-	X
57	MG	RA	3366	-	-	-	X
57	MG	XA	1614	-	-	-	X
57	MG	XA	1618	-	-	-	X
57	MG	XA	1682	-	-	-	X
57	MG	XA	1689	-	-	-	X
57	MG	XA	1692	-	-	-	X
57	MG	XA	1694	-	-	-	X
57	MG	XA	1710	-	-	-	X
57	MG	XA	1711	-	-	-	X
57	MG	XM	201	-	-	-	X
57	MG	XV	103	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3105	-	-	-	X
57	MG	YA	3141	-	-	-	X
57	MG	YA	3162	-	-	-	X
57	MG	YA	3166	-	-	-	X
57	MG	YA	3172	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3203	-	-	-	X
57	MG	YA	3231	-	-	-	X
57	MG	YA	3241	-	-	-	X
57	MG	YA	3248	-	-	-	X
57	MG	YA	3281	-	-	-	X
57	MG	YA	3289	-	-	-	X
57	MG	YA	3305	-	-	-	X
57	MG	YA	3312	-	-	-	X
57	MG	YA	3323	-	-	-	X
57	MG	YA	3332	-	-	-	X
57	MG	YA	3339	-	-	-	X
57	MG	YA	3342	-	-	-	X
57	MG	YA	3346	-	-	-	X
57	MG	YA	3350	-	-	-	X
57	MG	YA	3356	-	-	-	X
57	MG	YA	3362	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3368	-	-	-	X
57	MG	YA	3382	-	-	-	X
57	MG	YA	3413	-	-	-	X
57	MG	YA	3437	-	-	-	X
57	MG	YA	3444	-	-	-	X
57	MG	YB	201	-	-	-	X
57	MG	YQ	202	-	-	-	X
57	MG	YX	101	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 298675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

- Molecule 14 is a protein called 30S ribosomal protein S14 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	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called E-site tRNAAla(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total	C	N	O	P	0	0	0
			1627	725	296	530	76			
23	XW	76	Total	C	N	O	P	0	0	0
			1627	725	296	530	76			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	19	Total	C	N	O	P	0	0	0
			416	186	85	126	19			
24	XX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			

- Molecule 25 is a RNA chain called A-site tRNAAla(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	QY	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			
25	XY	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			

- Molecule 26 is a protein called 50S ribosomal protein L27.

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

Continued on next page...

Continued from previous page...

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

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L31.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

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

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a RNA chain called 23S rRNA.

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

- Molecule 37 is a RNA chain called 5S rRNA.

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

- Molecule 38 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
38	YD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 39 is a protein called 50S ribosomal protein L3.

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

- Molecule 40 is a protein called 50S ribosomal protein L4.

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

- Molecule 41 is a protein called 50S ribosomal protein L5.

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

- Molecule 42 is a protein called 50S ribosomal protein L6.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L9.

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

- Molecule 44 is a protein called 50S ribosomal protein L13.

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

- Molecule 45 is a protein called 50S ribosomal protein L14.

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

- Molecule 46 is a protein called 50S ribosomal protein L15.

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

- Molecule 47 is a protein called 50S ribosomal protein L16.

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

- Molecule 48 is a protein called 50S ribosomal protein L17.

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

- Molecule 49 is a protein called 50S ribosomal protein L18.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L20.

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

- Molecule 52 is a protein called 50S ribosomal protein L21.

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

- Molecule 53 is a protein called 50S ribosomal protein L22.

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

- Molecule 54 is a protein called 50S ribosomal protein L23.

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

- Molecule 55 is a protein called 50S ribosomal protein L24.

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

- Molecule 56 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	124	Total	Mg	0	0
			124	124		
57	QD	1	Total	Mg	0	0
			1	1		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QK	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QL	1	Total 1	Mg 1	0	0
57	QM	1	Total 1	Mg 1	0	0
57	QV	6	Total 6	Mg 6	0	0
57	QX	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R1	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	R9	1	Total 1	Mg 1	0	0
57	RA	378	Total 378	Mg 378	0	0
57	RB	4	Total 4	Mg 4	0	0
57	RD	2	Total 2	Mg 2	0	0
57	RE	8	Total 8	Mg 8	0	0
57	RF	2	Total 2	Mg 2	0	0
57	RG	1	Total 1	Mg 1	0	0
57	RI	1	Total 1	Mg 1	0	0
57	RP	3	Total 3	Mg 3	0	0
57	RR	2	Total 2	Mg 2	0	0
57	RT	2	Total 2	Mg 2	0	0
57	XA	123	Total 123	Mg 123	0	0
57	XB	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

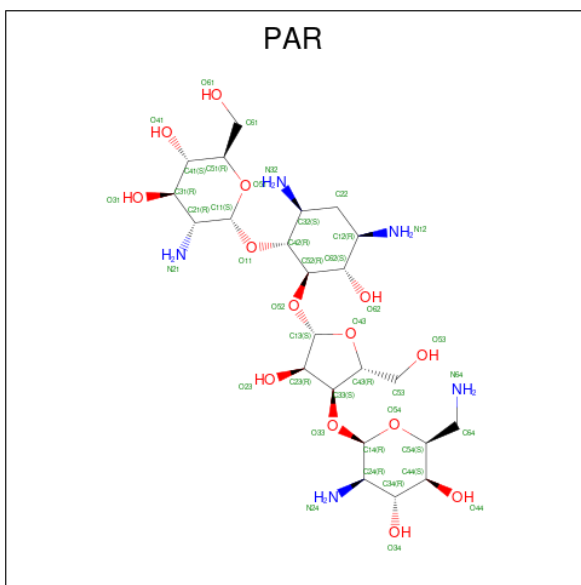
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XD	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	XK	1	Total 1	Mg 1	0	0
57	XL	2	Total 2	Mg 2	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	7	Total 7	Mg 7	0	0
57	XX	1	Total 1	Mg 1	0	0
57	Y0	3	Total 3	Mg 3	0	0
57	Y2	3	Total 3	Mg 3	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	Y4	2	Total 2	Mg 2	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	Y8	3	Total 3	Mg 3	0	0
57	YA	457	Total 457	Mg 457	0	0
57	YB	8	Total 8	Mg 8	0	0
57	YD	4	Total 4	Mg 4	0	0
57	YE	6	Total 6	Mg 6	0	0
57	YF	5	Total 5	Mg 5	0	0
57	YG	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

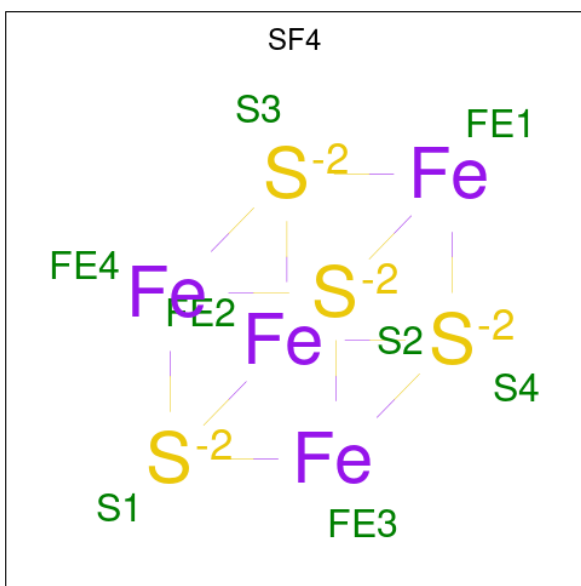
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YH	5	Total 5	Mg 5	0	0
57	YI	1	Total 1	Mg 1	0	0
57	YN	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	7	Total 7	Mg 7	0	0
57	YQ	4	Total 4	Mg 4	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YT	2	Total 2	Mg 2	0	0
57	YU	1	Total 1	Mg 1	0	0
57	YV	1	Total 1	Mg 1	0	0
57	YW	1	Total 1	Mg 1	0	0
57	YX	2	Total 2	Mg 2	0	0
57	YY	5	Total 5	Mg 5	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

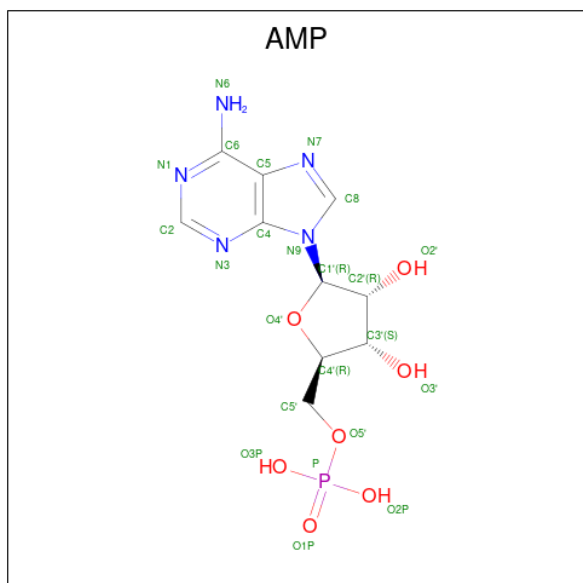


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	QD	1	Total 8	Fe 4	S 4	0	0
59	XD	1	Total 8	Fe 4	S 4	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	QN	1	Total	Zn	0	0
			1	1		
60	XN	1	Total	Zn	0	0
			1	1		

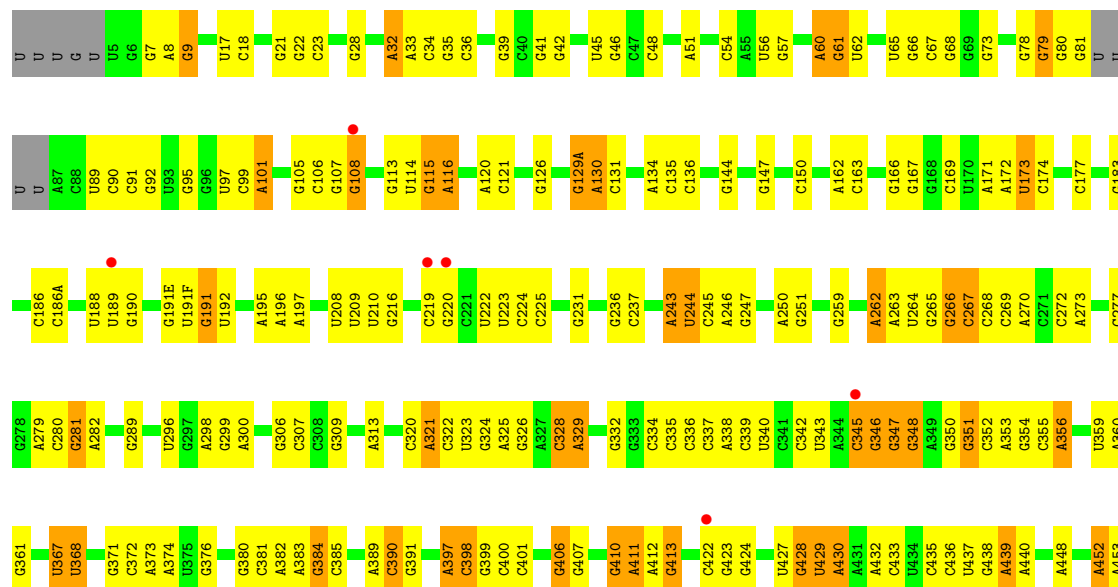
- Molecule 61 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).

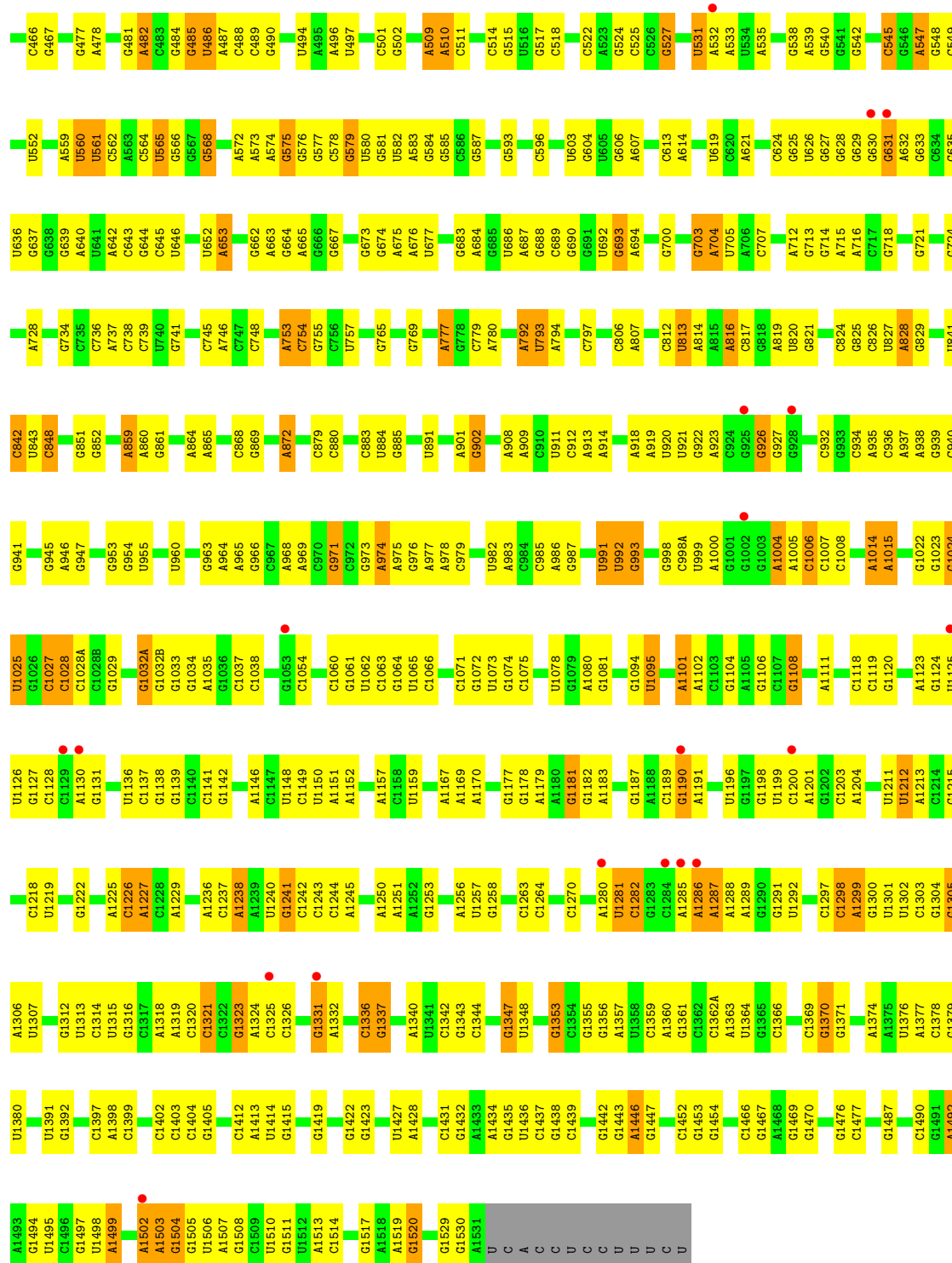


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	QY	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

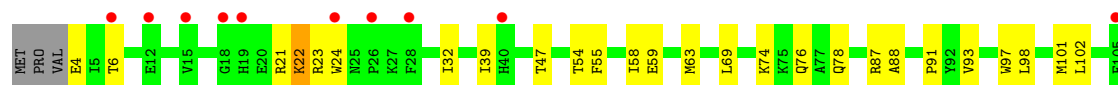
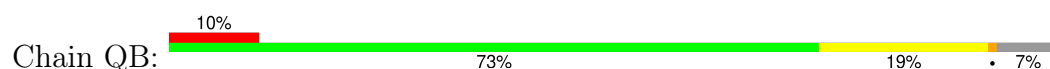
- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	QA	1	Total	O	0	0
			1	1		
62	QX	1	Total	O	0	0
			1	1		





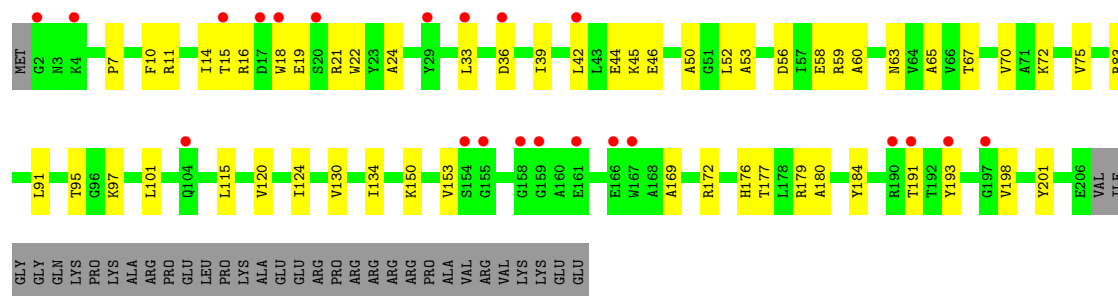
• Molecule 2: 30S ribosomal protein S2



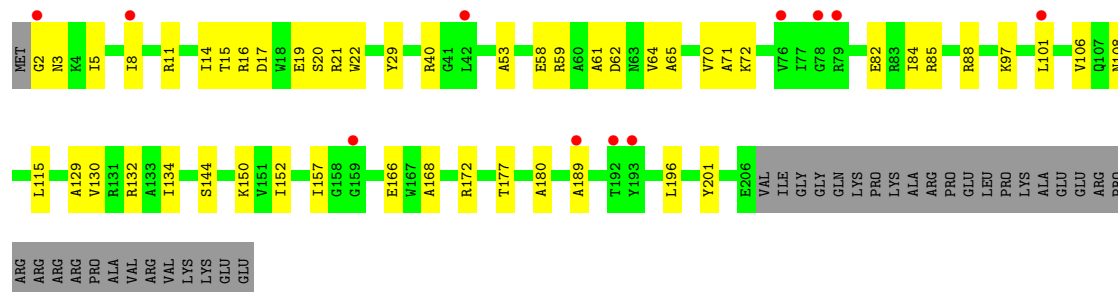
- Molecule 2: 30S ribosomal protein S2



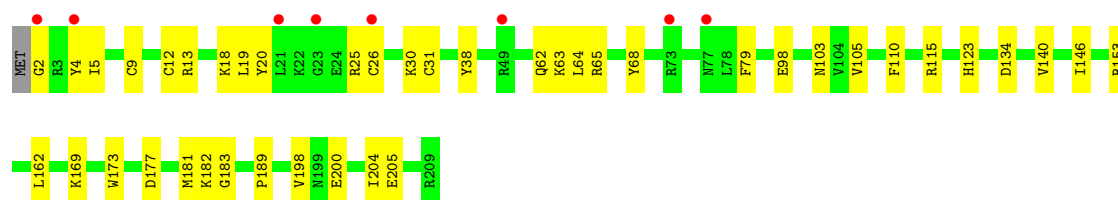
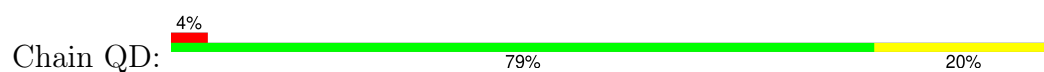
- Molecule 3: 30S ribosomal protein S3



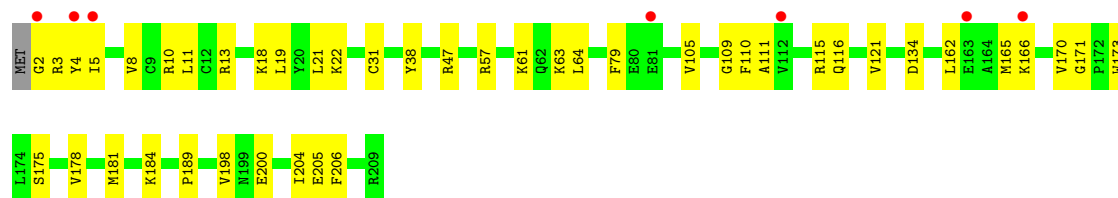
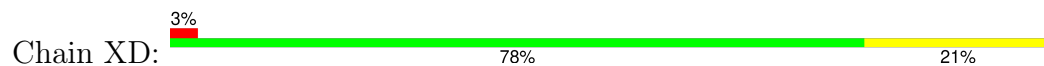
- Molecule 3: 30S ribosomal protein S3



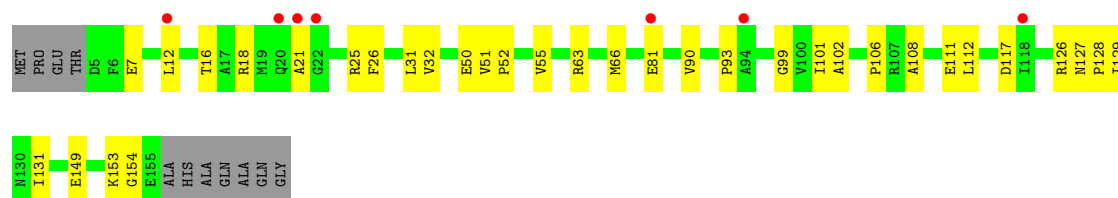
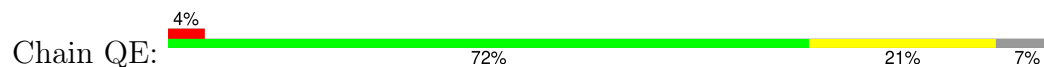
- Molecule 4: 30S ribosomal protein S4



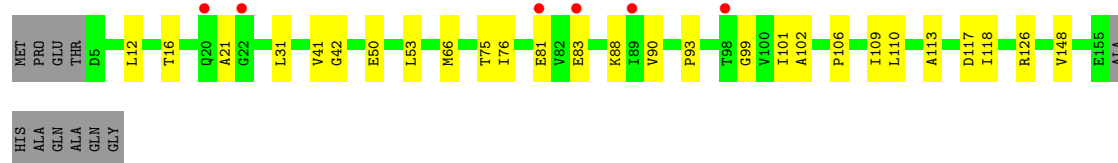
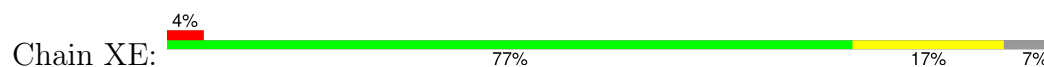
- Molecule 4: 30S ribosomal protein S4



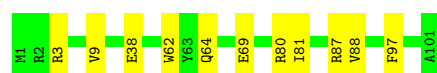
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S6

Chain XF:  69% 31%



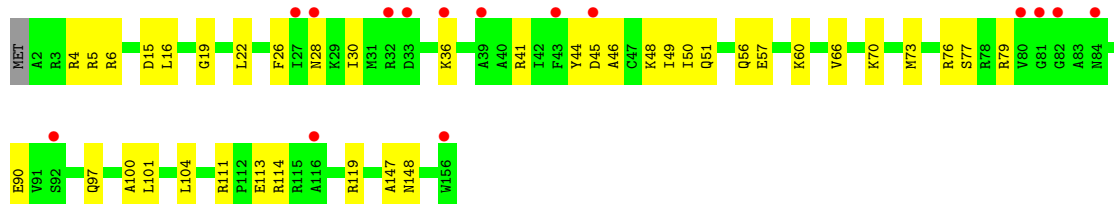
- Molecule 7: 30S ribosomal protein S7

Chain QG:  4% 86% 13%



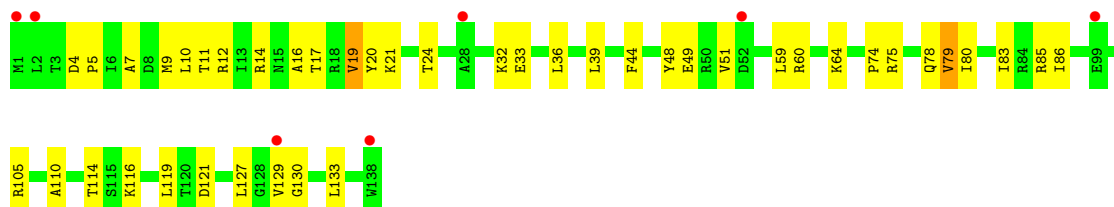
- Molecule 7: 30S ribosomal protein S7

Chain XG:  10% 74% 25%



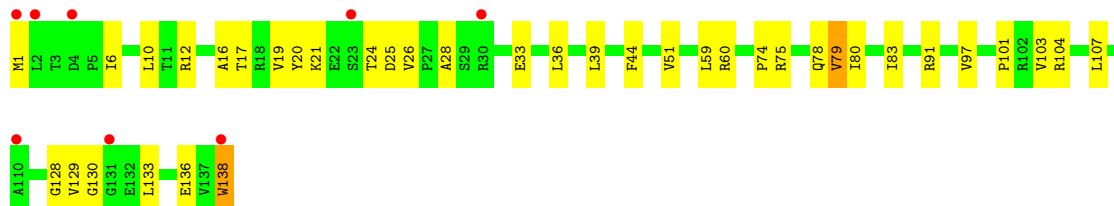
- Molecule 8: 30S ribosomal protein S8

Chain QH:  5% 69% 30%



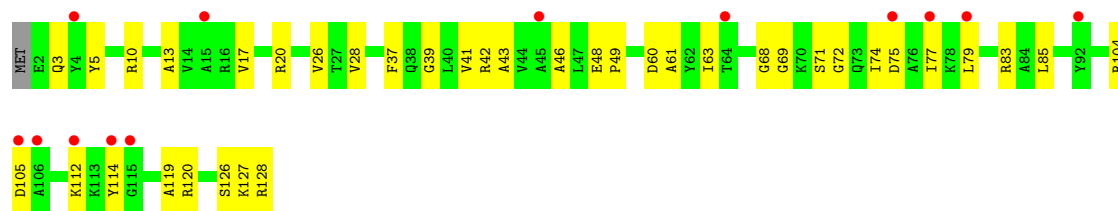
- Molecule 8: 30S ribosomal protein S8

Chain XH:  6% 72% 26%

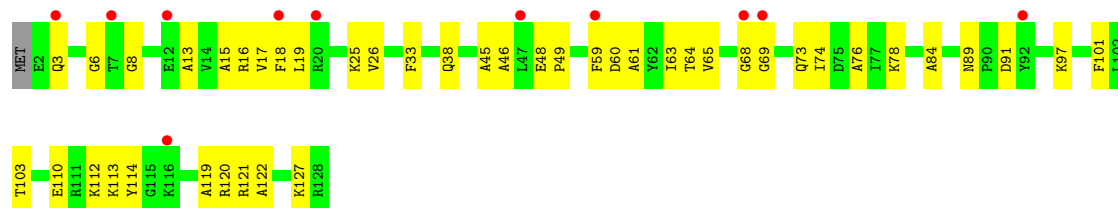


- Molecule 9: 30S ribosomal protein S9

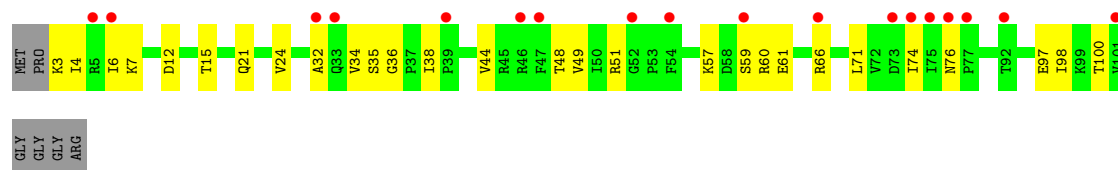
Chain QI:  10% 70% 30%



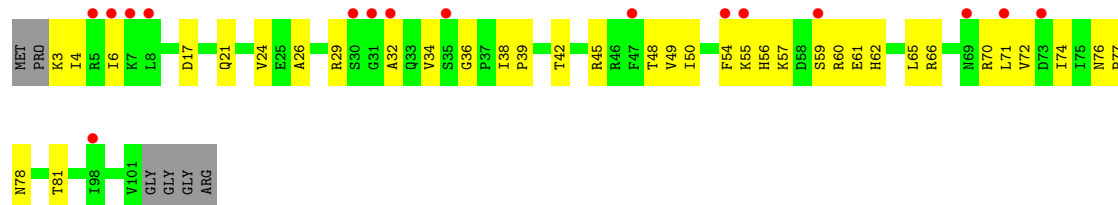
• Molecule 9: 30S ribosomal protein S9



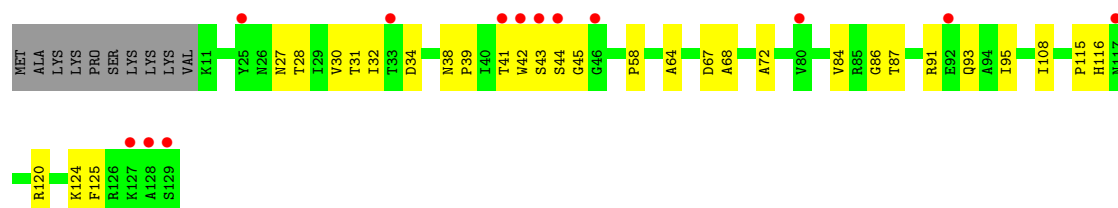
• Molecule 10: 30S ribosomal protein S10



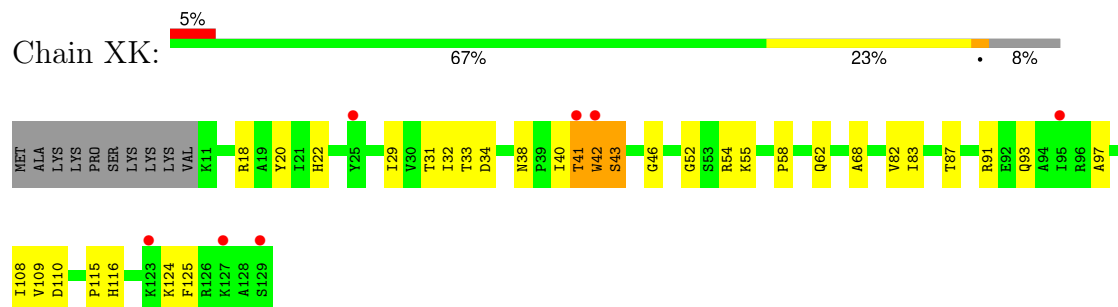
• Molecule 10: 30S ribosomal protein S10



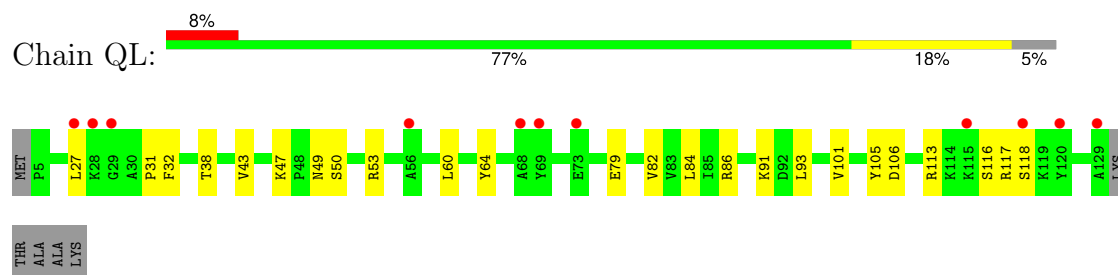
• Molecule 11: 30S ribosomal protein S11



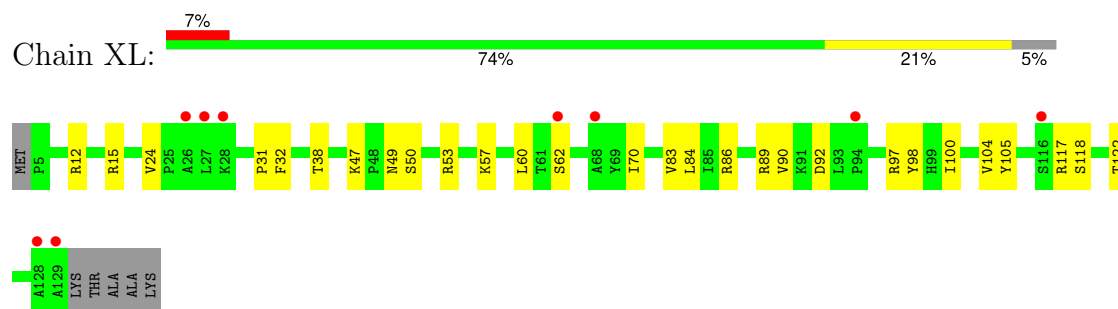
- Molecule 11: 30S ribosomal protein S11



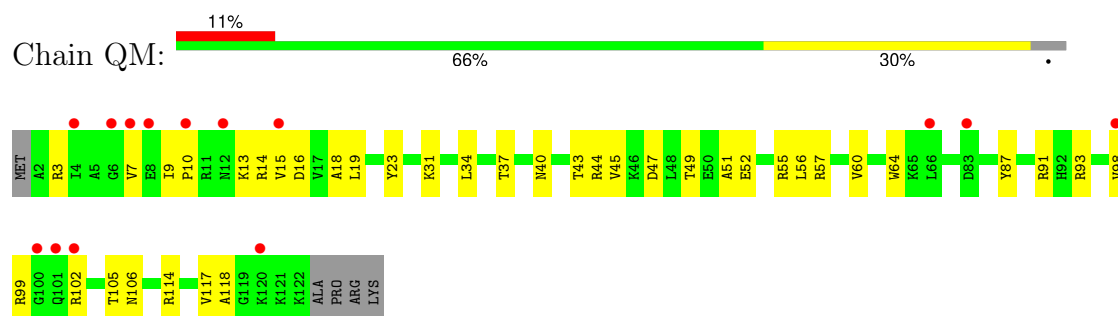
- Molecule 12: 30S ribosomal protein S12



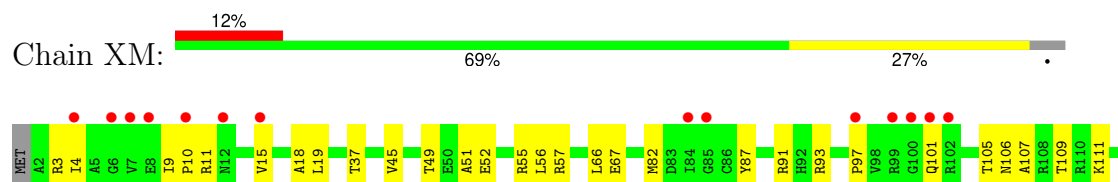
- Molecule 12: 30S ribosomal protein S12

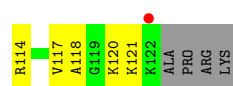


- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

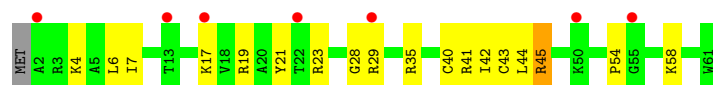




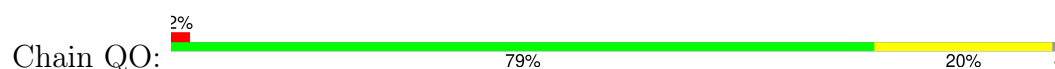
- Molecule 14: 30S ribosomal protein S14 type Z



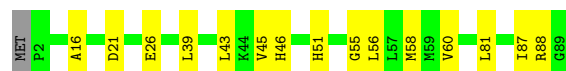
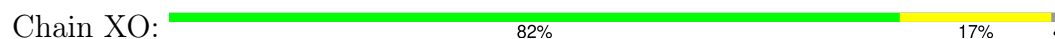
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



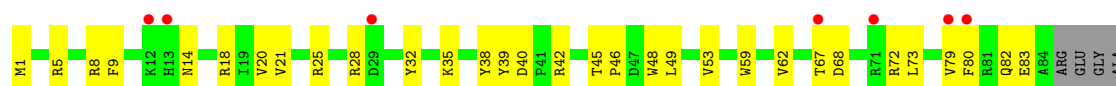
- Molecule 15: 30S ribosomal protein S15



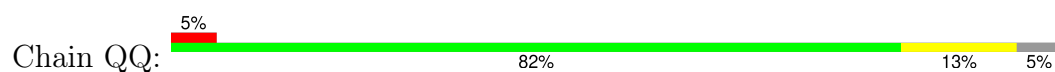
- Molecule 16: 30S ribosomal protein S16



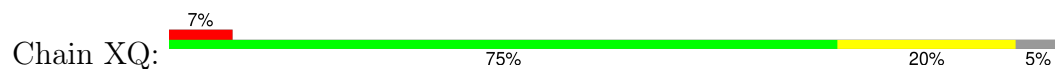
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



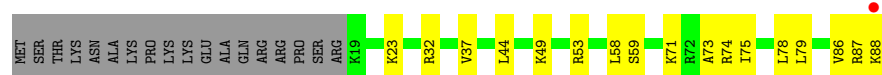
- Molecule 17: 30S ribosomal protein S17



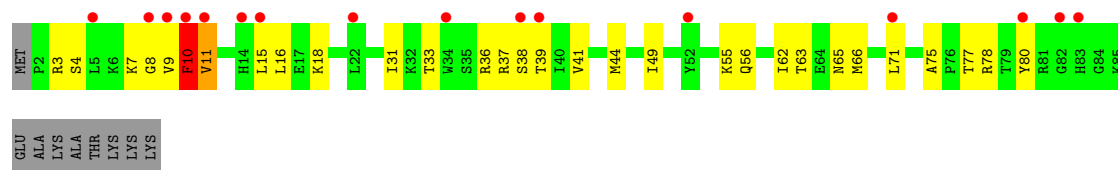
- Molecule 18: 30S ribosomal protein S18



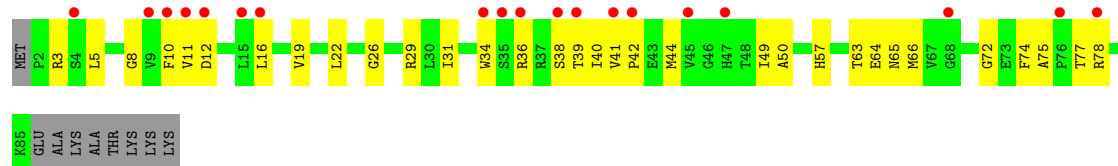
- Molecule 18: 30S ribosomal protein S18



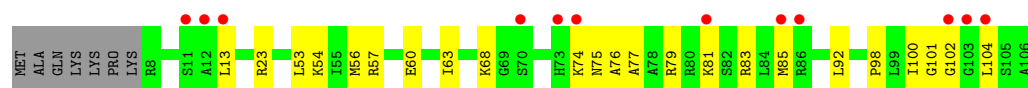
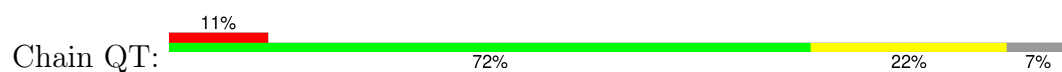
- Molecule 19: 30S ribosomal protein S19



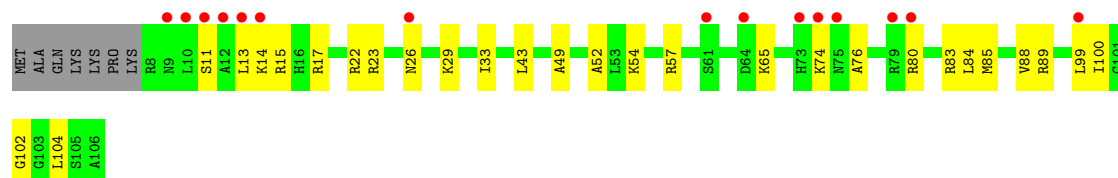
- Molecule 19: 30S ribosomal protein S19



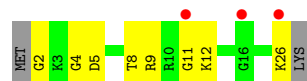
- Molecule 20: 30S ribosomal protein S20



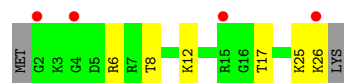
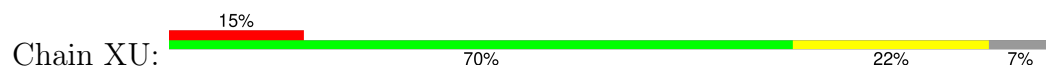
- Molecule 20: 30S ribosomal protein S20



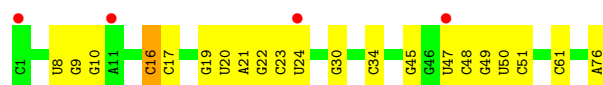
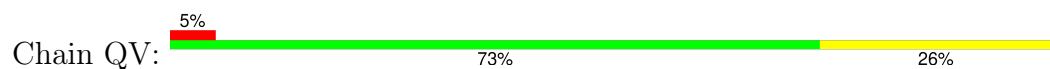
- Molecule 21: 30S ribosomal protein Thx



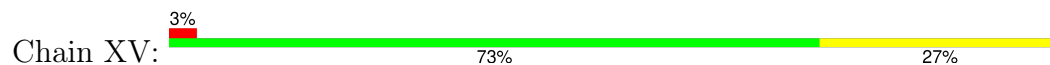
- Molecule 21: 30S ribosomal protein Thx



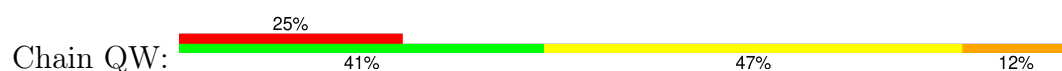
- Molecule 22: P-site tRNA^{fMet}

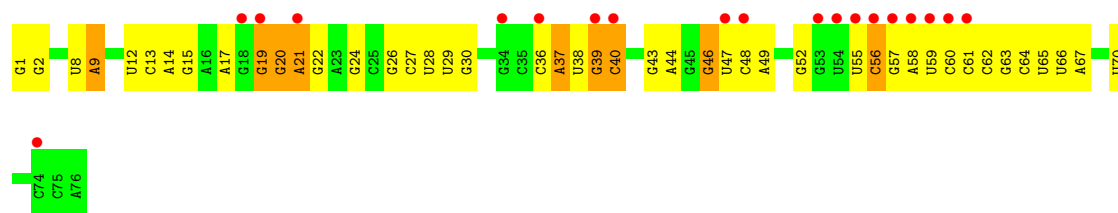


- Molecule 22: P-site tRNA^{fMet}

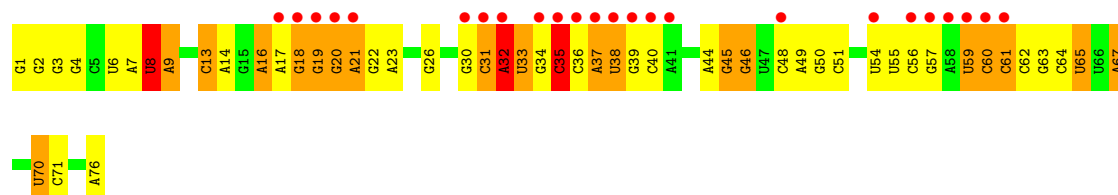


- Molecule 23: E-site tRNA^{Ala}(GGC)

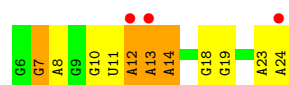




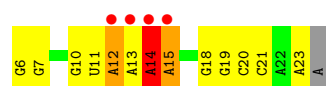
- Molecule 23: E-site tRNAAla(GGC)



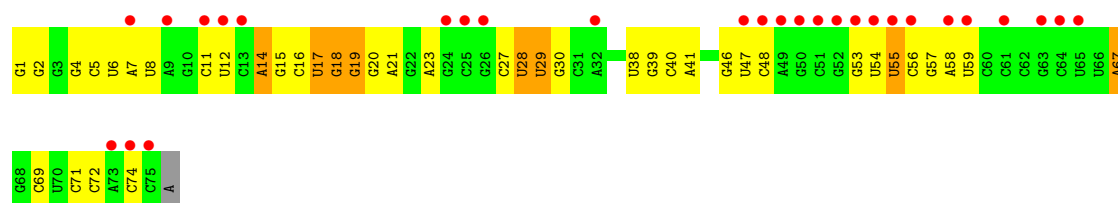
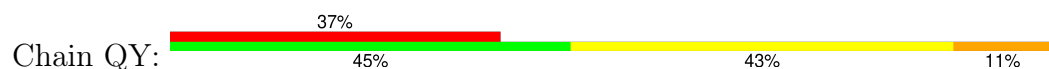
- Molecule 24: mRNA



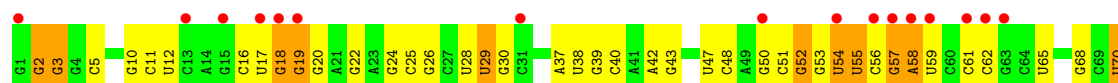
- Molecule 24: mRNA



- Molecule 25: A-site tRNAAla(GGC)

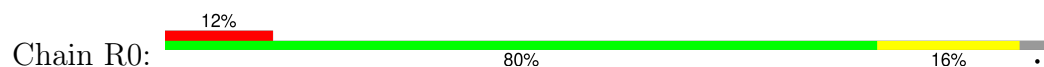


- Molecule 25: A-site tRNAAla(GGC)





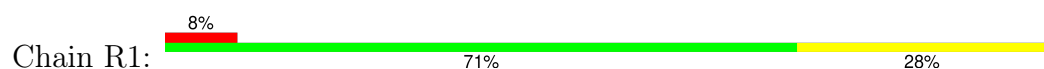
- Molecule 26: 50S ribosomal protein L27



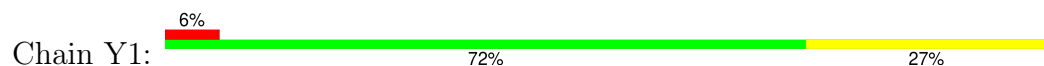
- Molecule 26: 50S ribosomal protein L27



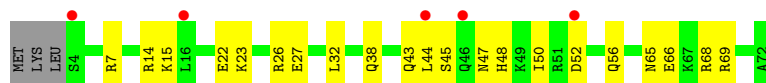
- Molecule 27: 50S ribosomal protein L28



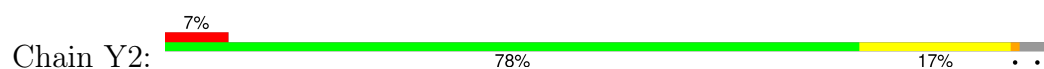
- Molecule 27: 50S ribosomal protein L28



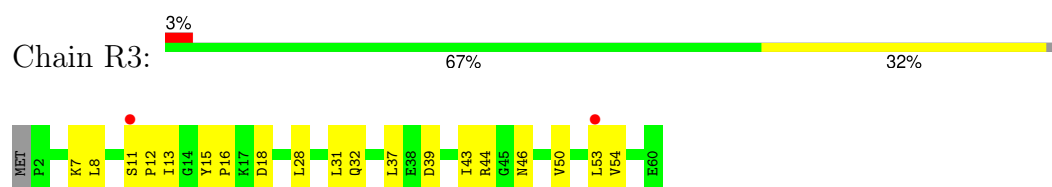
- Molecule 28: 50S ribosomal protein L29



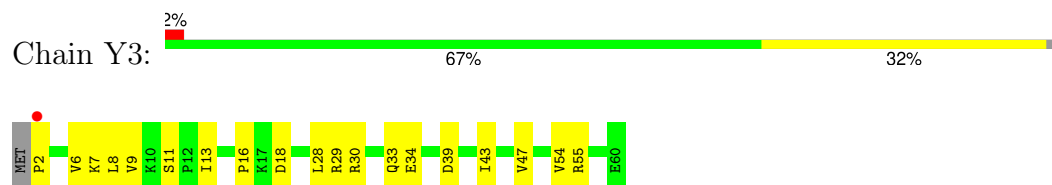
- Molecule 28: 50S ribosomal protein L29



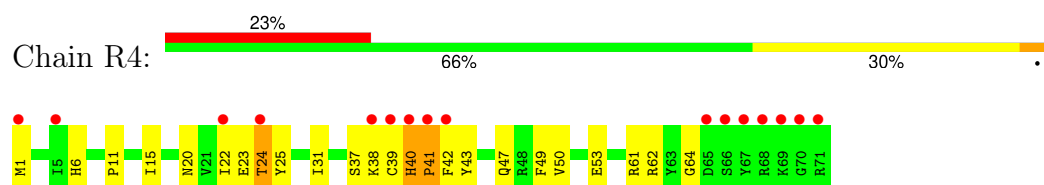
- Molecule 29: 50S ribosomal protein L30



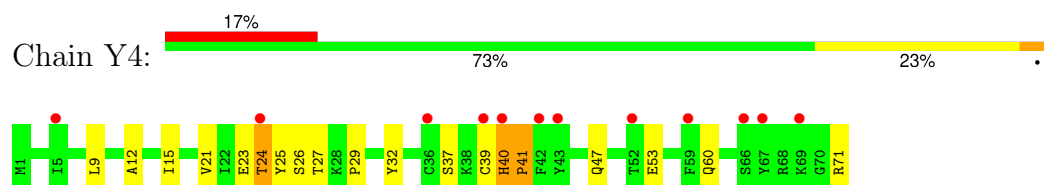
- Molecule 29: 50S ribosomal protein L30



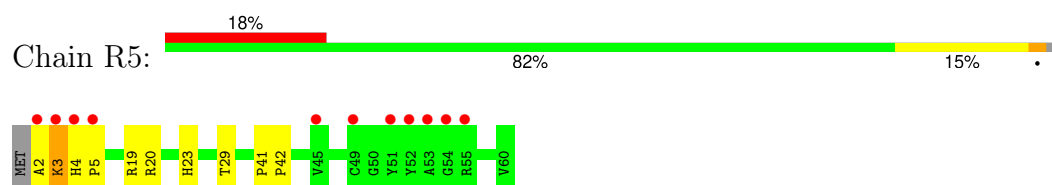
- Molecule 30: 50S ribosomal protein L31



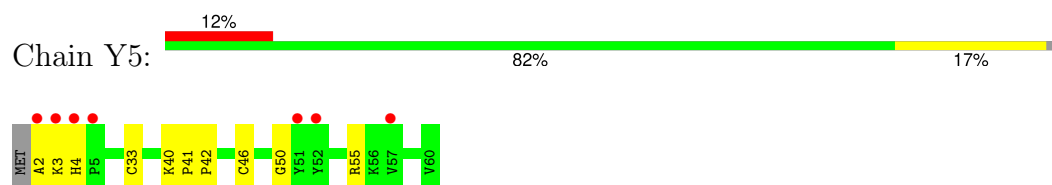
- Molecule 30: 50S ribosomal protein L31



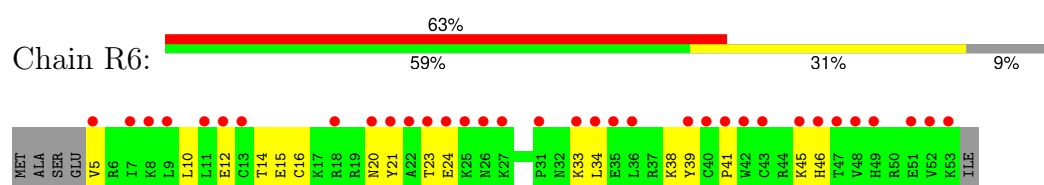
- Molecule 31: 50S ribosomal protein L32



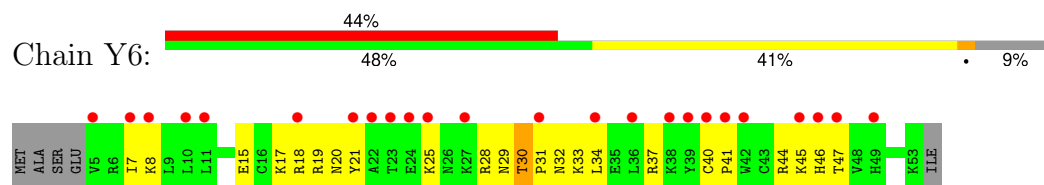
- Molecule 31: 50S ribosomal protein L32



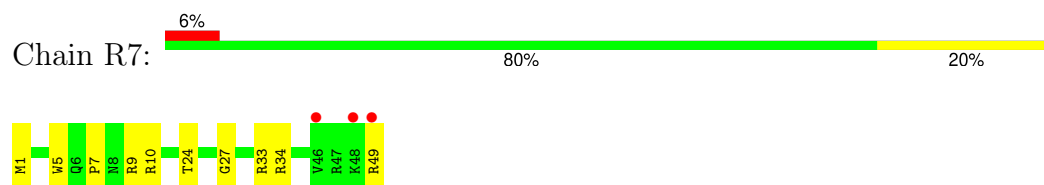
- Molecule 32: 50S ribosomal protein L33



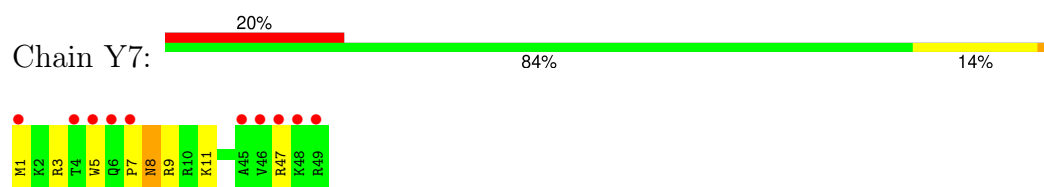
- Molecule 32: 50S ribosomal protein L33



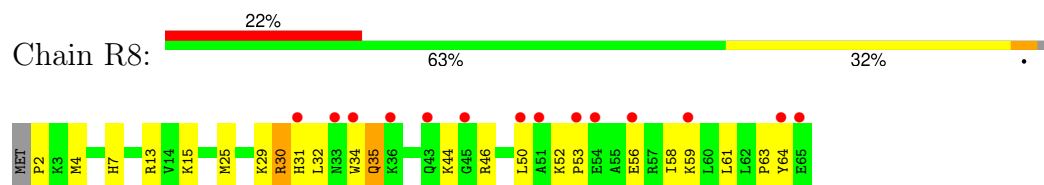
- Molecule 33: 50S ribosomal protein L34



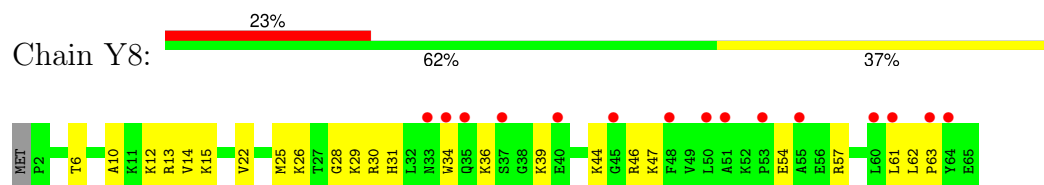
- Molecule 33: 50S ribosomal protein L34



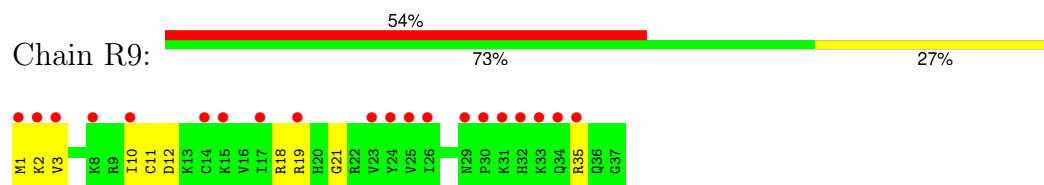
- Molecule 34: 50S ribosomal protein L35



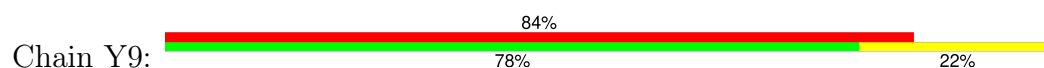
- Molecule 34: 50S ribosomal protein L35

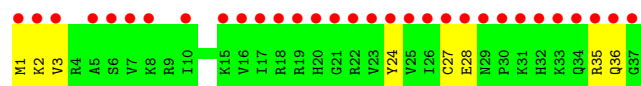


- Molecule 35: 50S ribosomal protein L36

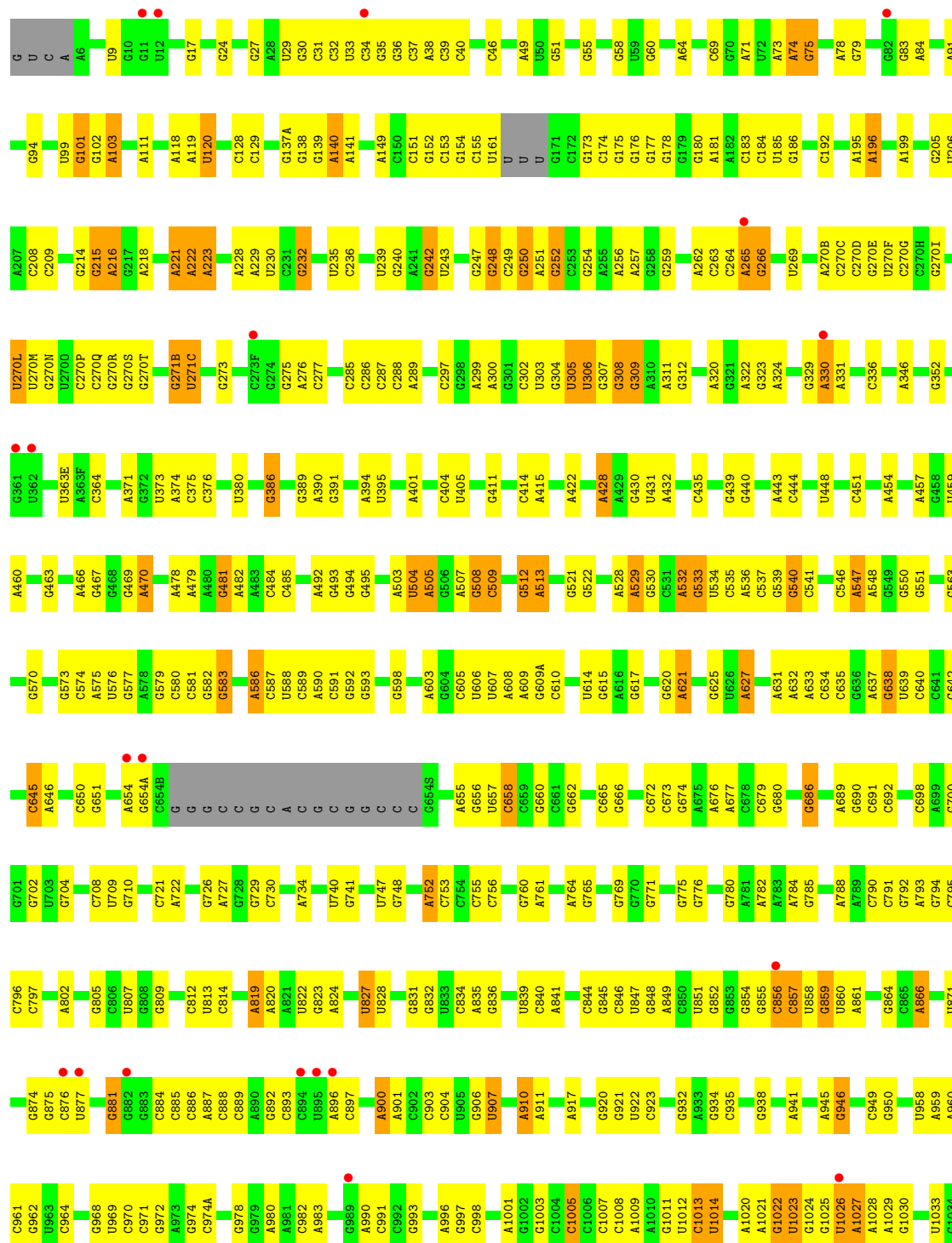


- Molecule 35: 50S ribosomal protein L36

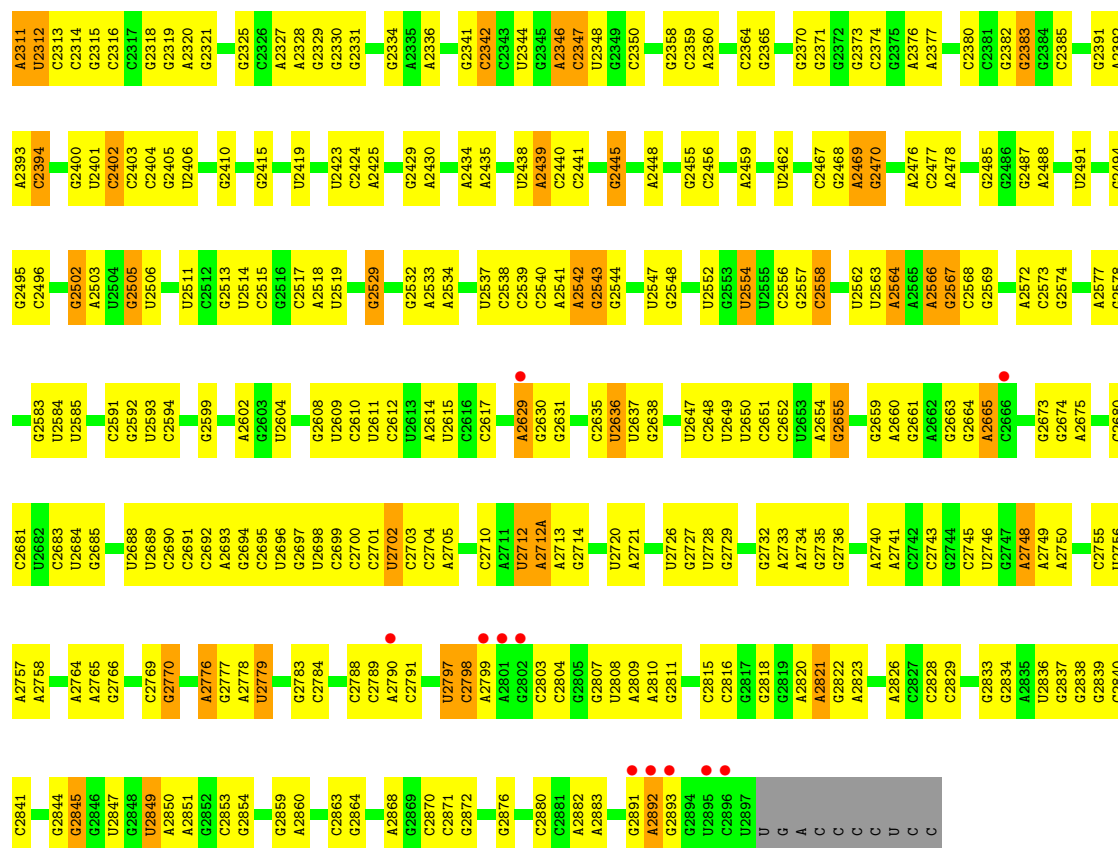




• Molecule 36: 23S rRNA

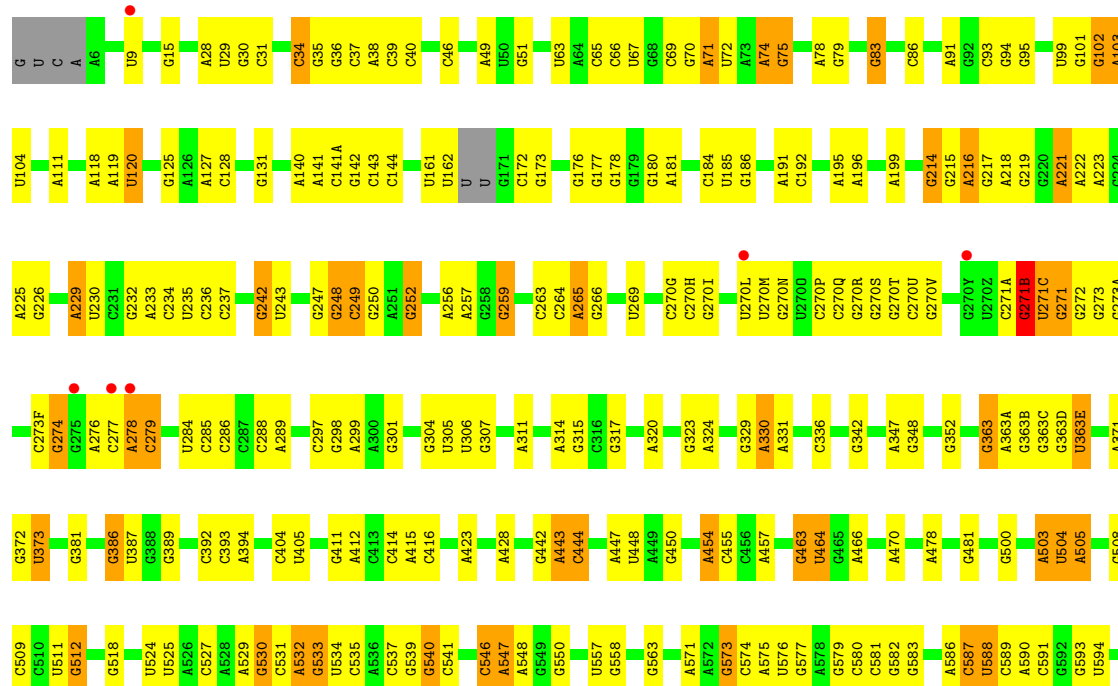


A2198	G2115	U2022	C1797	G1560	G1478	U1396	C1289	G195	G1106	U1035
G2210	G2116	G2023	U1798	C1566	G1479	U1397	C1290	G196	G1107	G1036
G2211	A2117	G2024	C1675	C1565	G1483	C1398	C1291	C1201	C1109	G1042
G2212	U2118	C2025	A1676	A1566	G1487	G1401	C1292	G1202	G1110	G1043
U2213	A2119	C2026	G1677	A1567	G1490	C1402	C1293	G1203	A1111	G1044
G2215	G2126	G2029	A1689	A1568	A1490	C1403	U1300	A1204	G1112	A1045
G2219	G2127	A2030	U1693	A1570	A1494	U1405	A1301	U1205	G1113	A1046
G2224	C2129	G2032	C1694	A1571	C1493	C1404	A1302	G1206	G1114	G1047
A2225	U2130	A2033	G1694	A1572	A1494	U1406	G1303	C1207	G1115	G1048
U2233	G2131	G2037	G1695	C1577	A1495	C1407	G1309	U1210	G1116	C1049
G2234	U2132	G2038	A1698	U1578	U1497	C1408	G1310	U1211	G1117	A1050
A2238	A2134	C2043	U1498	A1586	C1498	C1411	G1311	G1212	G1122	G1051
G2239	U2141	C2044	U1709	A1587	C1499	U1412	U1312	A1220	G1125	A1054
G2240	G2142	A2051	C1710	C1588	G1500	G1413	U1313	G1226	A1129	G1055
G2241	C2142	G2052	G1725	C1589	C1501	G1416	C1314	U1227	U1130	A1057
G2242	C2143	C2055	G1728	G1595	U1503	C1417	G1315	G1228	G1131	G1058
U2244	G2146	G2056	U1729	A1596	C1504	G1418	U1316	C1230	C1135	G1059
G2250	G2147	A2059	U1730	A1597	C1506	A1419	A1321	G1231	G1136	U1060
G2255	U2148	A2060	G1731	C1599	A1507	G1421	A1322	G1232	G1137	G1061
A2268	G2149	G2061	G1732	C1607	C1509	A1427	U1329	G1236	G1138	C1063
G2269	U2150	G2062	U1733	A1608	A1510	C1428	C1330	A1237	G1139	U1065
G2270	C2151	C2063	C1742	A1609	G1511	G1429	C1331	G1238	C1140	U1066
G2271	G2152	A1966	G1743	A1610	G1512	C1430	G1332	G1239	U1141	G1067
U2272	C2153	C2065	C1752	G1615	C1513	C1431	A1336	G1243	U1142	G1068
A2273	A1968	G1968	G1753	A1616	U1514	C1432	U1337	G1248	A1142A	A1069
G2274	U2156	A1969	G1754	C1617	C1515	U1433	G1337	U1249	C1152	G1071
C2275	G2157	A1970	U1755	A1618	U1516	G1435	U1341	G1251	C1153	G1072
G2280	G2165	A1971	G1756	G1622	U1520	G1441	A1348	G1252	G1154	A1073
C2283	U2167	A1972	G1757	A1632	G1521	G1442	A1349	A1253	A1155	G1074
A2287	G2168	G1980	U1758	C1636	G1522	A1444A	A1353	A1254	U1159	G1075
A2288	A2170	A1981	G1762	A1637	A1528	C1445	A1354	U1255	G1160	A1077
U2291	U2171	C1982	G1763	A1638	A1529	C1446	G1355	G1256	G1164	U1078
C2292	A2173	U1991	G1764	C1639	G1534	G1447	G1356	G1264	U1165	C1080
U2296	G2176	G1992	G1769	A1640	U1535	G1448	U1357	G1265	C1166	U1081
A2298	C2177	U1993	A1773	A1641	C1537	A1449	G1358	U1267	G1170	U1082
G2299	G2181	A2001	U1780	C1648	G1539	C1451	A1365	A1268	G1171	U1083
G2300	G2182	G2002	C1781	A1652	G1540	U1453	A1378	A1269	G1173	A1084
G2301	C2183	C2008	C1782	G1651	U1541	G1455	A1379	G1270	U1174	A1085
G2302	G2184	G2009	A1783	G1652	G1542	C1460	G1368	G1271	U1175	G1087
G2303	G2185	U2011	G1786	G1653	A1543	G1461	G1369	A1272	G1176	A1088
G2304	G2186	G1888	C1790	A1654	C1544	G1465	C1370	U1273	A1177	G1089
A2305	U2187	A1889	A1791	C1655	A1545	G1466	G1371	G1278	C1179	U1090
G2306	G2188	A1890	G1792	C1656	A1546	C1467	A1384	A1284	G1186	A1095
G2307	U2189	G1899	C1793	C1657	C1547	A1471	G1385	G1285	U1187	A1096
G2308	G2190	U1794	U1795	G1666	C1550	A1472	A1394	A1287	U1188	U1097
	G2191	U2113	C1902	A1668	A1558	A1472	U1395	G1190	A1189	C1102
	G2192	A2114			G1559		A1395	G1191	G1192	A1103

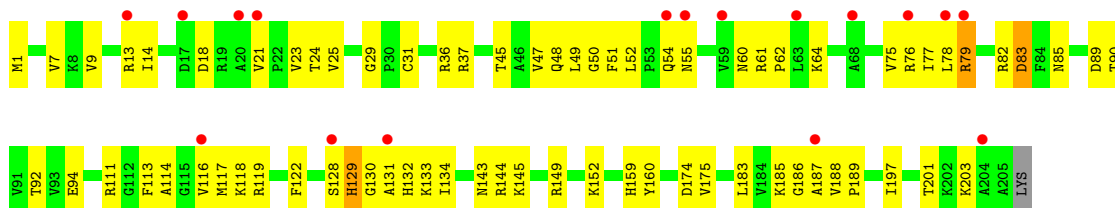


• Molecule 36: 23S rRNA

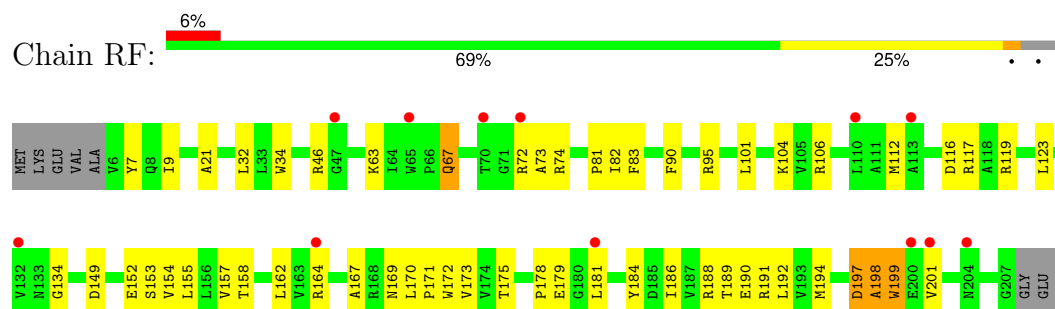
Chain YA: 2% 57% 34% 8%



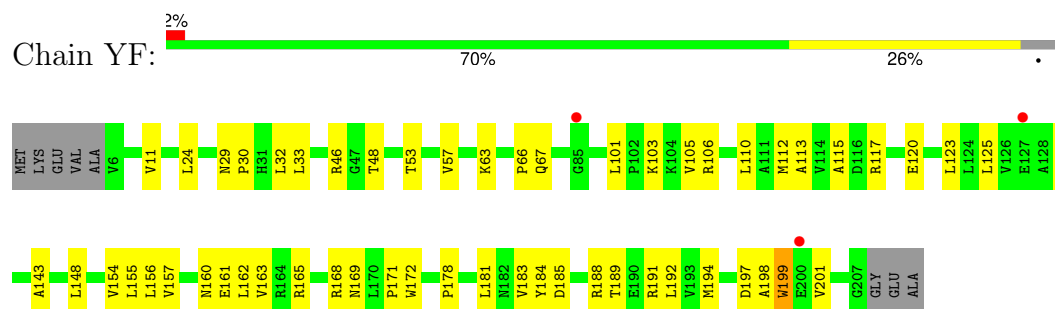




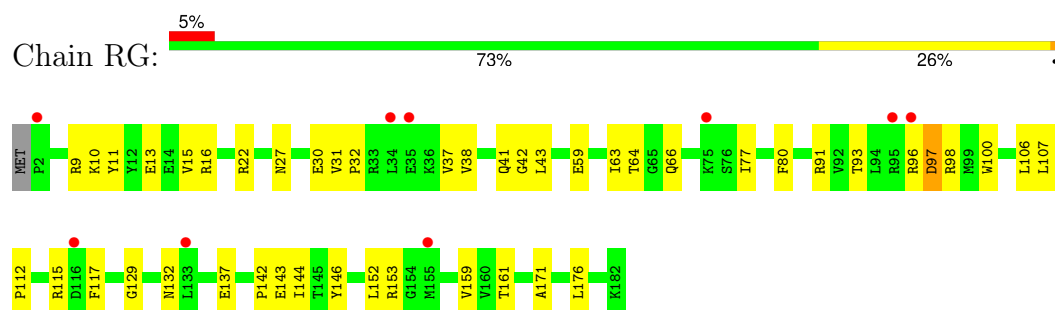
- Molecule 40: 50S ribosomal protein L4



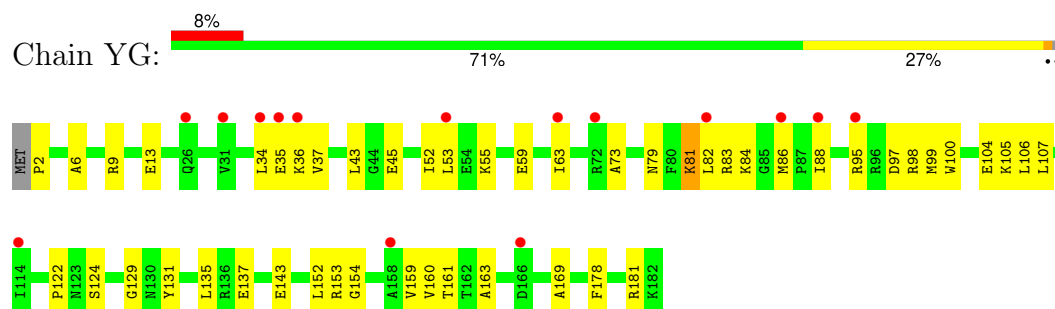
- Molecule 40: 50S ribosomal protein L4



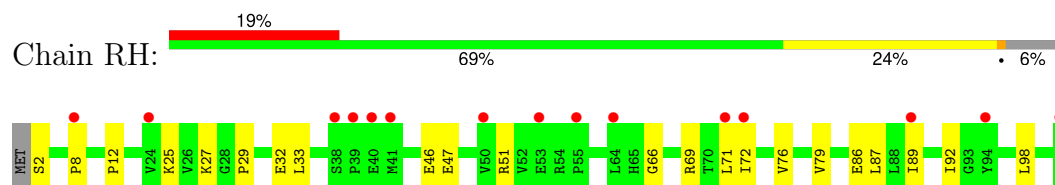
- Molecule 41: 50S ribosomal protein L5

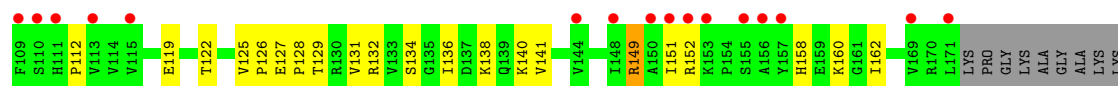


- Molecule 41: 50S ribosomal protein L5



- Molecule 42: 50S ribosomal protein L6

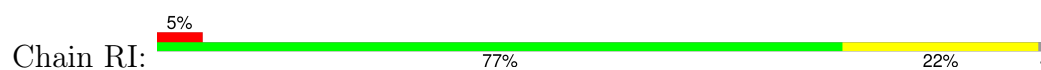




• Molecule 42: 50S ribosomal protein L6



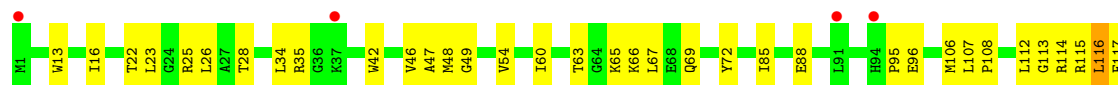
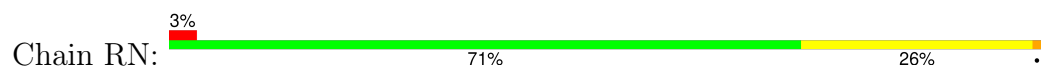
• Molecule 43: 50S ribosomal protein L9



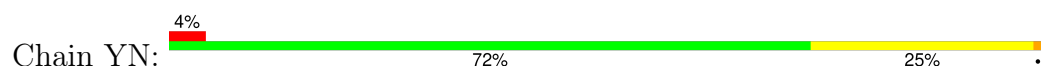
• Molecule 43: 50S ribosomal protein L9

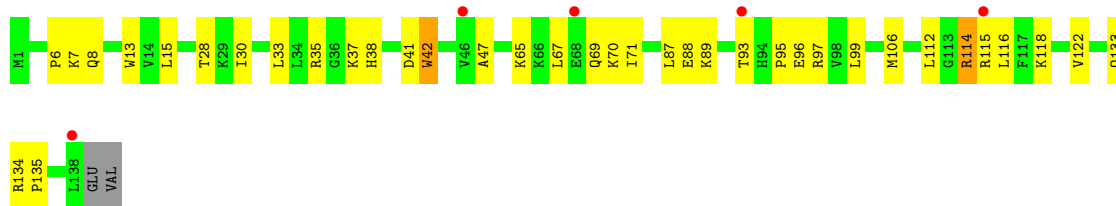


• Molecule 44: 50S ribosomal protein L13

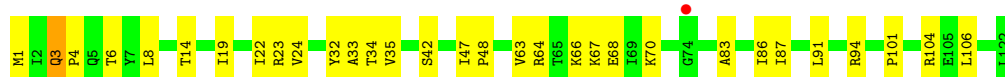
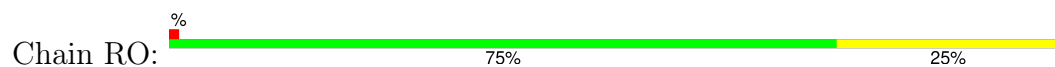


• Molecule 44: 50S ribosomal protein L13

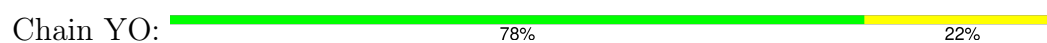




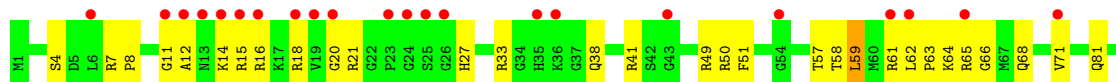
- Molecule 45: 50S ribosomal protein L14



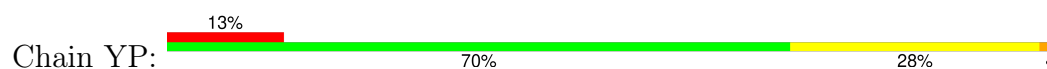
- Molecule 45: 50S ribosomal protein L14



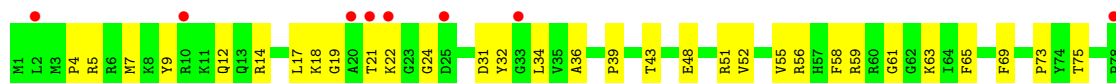
- Molecule 46: 50S ribosomal protein L15



- Molecule 46: 50S ribosomal protein L15

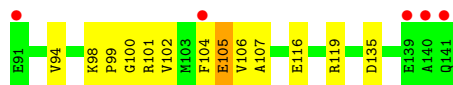


- Molecule 47: 50S ribosomal protein L16

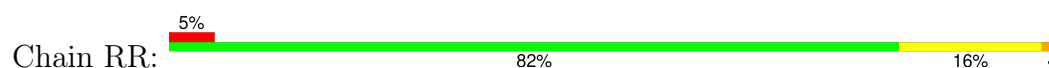




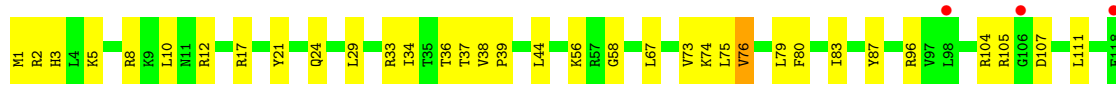
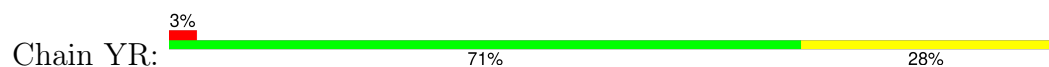
- Molecule 47: 50S ribosomal protein L16



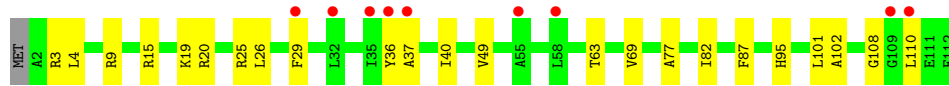
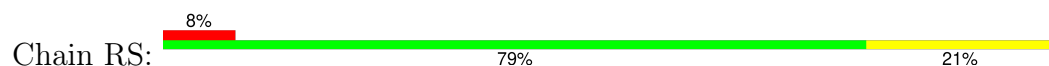
- Molecule 48: 50S ribosomal protein L17



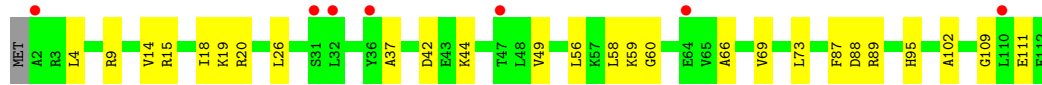
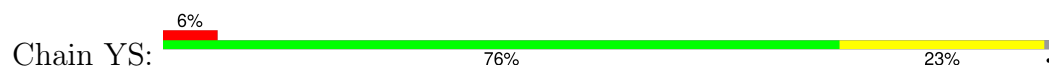
- Molecule 48: 50S ribosomal protein L17



- Molecule 49: 50S ribosomal protein L18



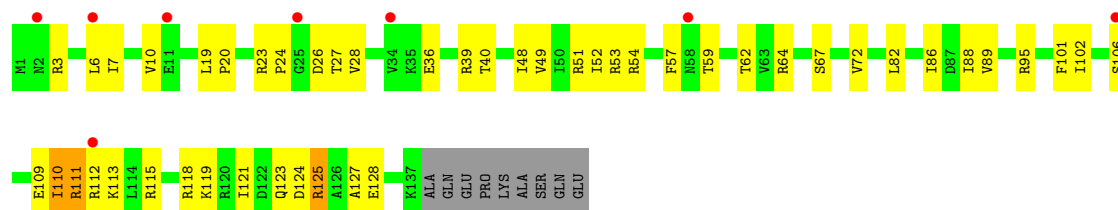
- Molecule 49: 50S ribosomal protein L18



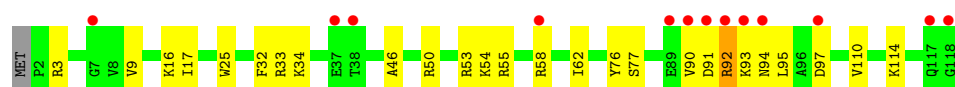
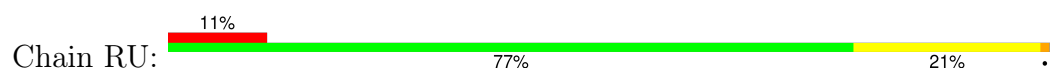
- Molecule 50: 50S ribosomal protein L19



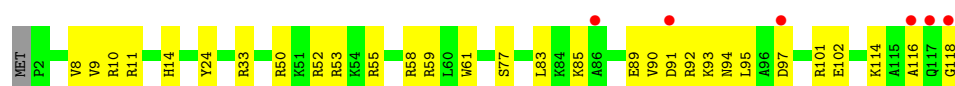
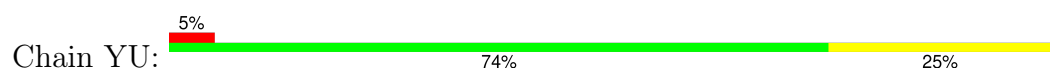
- Molecule 50: 50S ribosomal protein L19



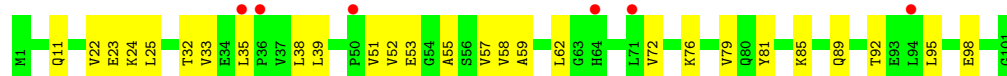
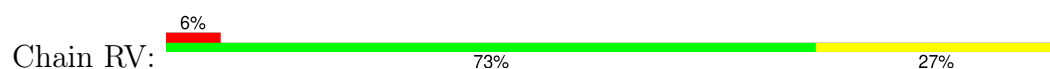
- Molecule 51: 50S ribosomal protein L20



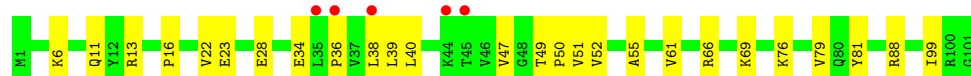
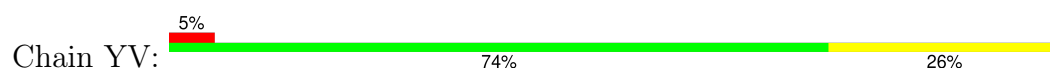
- Molecule 51: 50S ribosomal protein L20



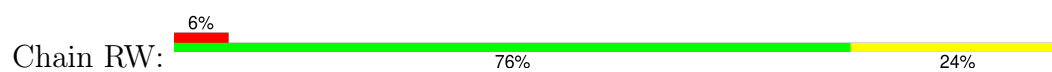
- Molecule 52: 50S ribosomal protein L21



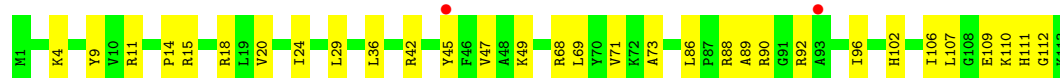
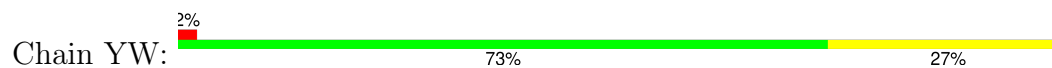
- Molecule 52: 50S ribosomal protein L21



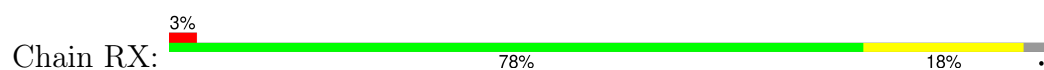
- Molecule 53: 50S ribosomal protein L22



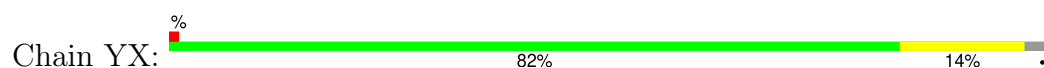
- Molecule 53: 50S ribosomal protein L22



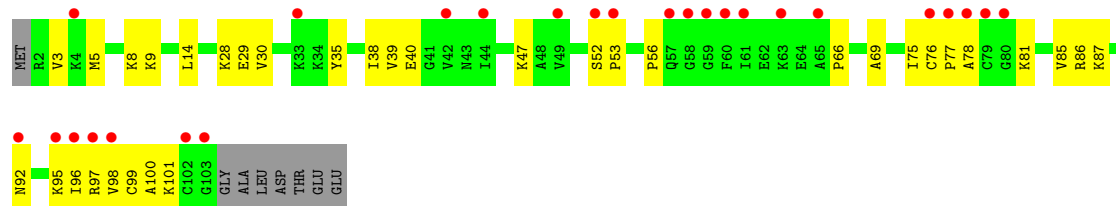
- Molecule 54: 50S ribosomal protein L23



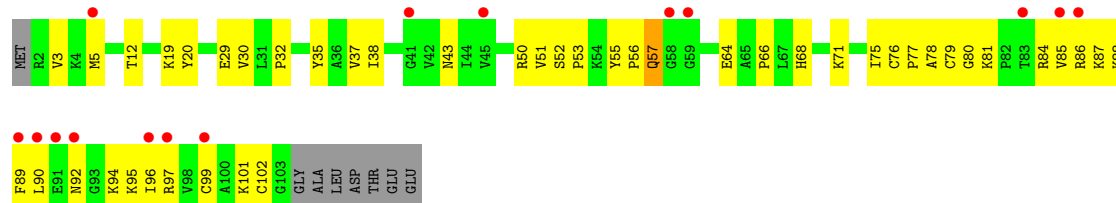
- Molecule 54: 50S ribosomal protein L23



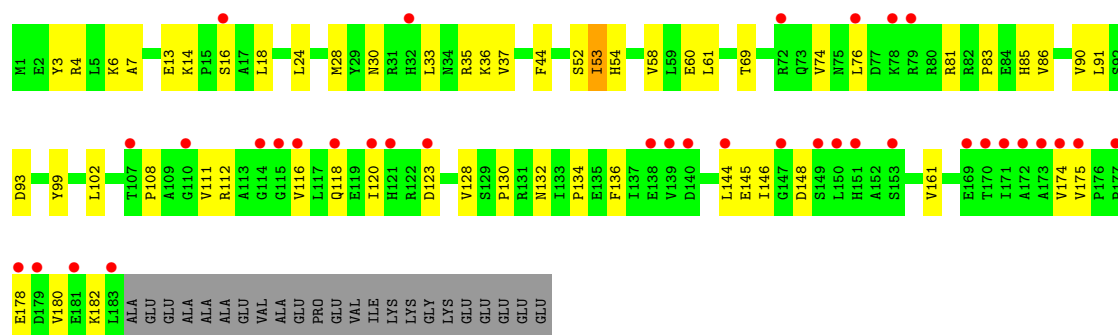
- Molecule 55: 50S ribosomal protein L24



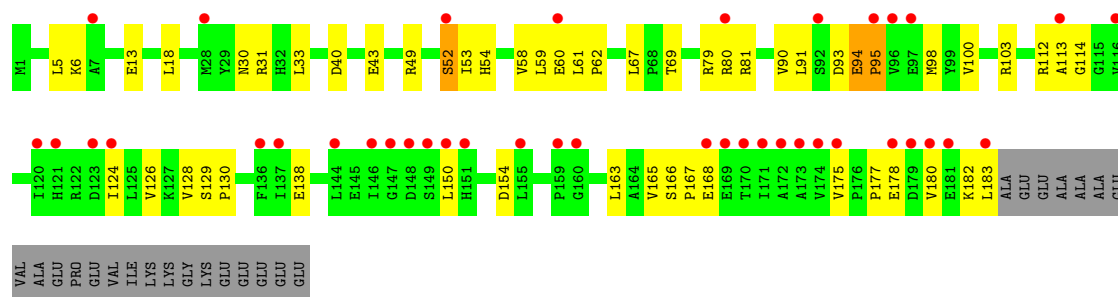
- Molecule 55: 50S ribosomal protein L24



• Molecule 56: 50S ribosomal protein L25



• Molecule 56: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.26Å 452.33Å 626.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.53 – 3.20 44.53 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (44.53-3.20) 91.2 (44.53-3.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.195 , 0.232 0.195 , 0.232	Depositor DCC
R_{free} test set	41783 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	298675	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	QA	0.18	0/36098	0.39	10/56341 (0.0%)
1	XA	0.18	0/36101	0.37	0/56346
2	QB	0.19	0/1959	0.65	0/2642
2	XB	0.21	0/1959	0.65	0/2642
3	QC	0.25	0/1629	0.62	0/2195
3	XC	0.31	1/1629 (0.1%)	0.62	0/2195
4	QD	0.14	0/1704	0.57	0/2284
4	XD	0.40	1/1704 (0.1%)	0.67	3/2284 (0.1%)
5	QE	0.15	0/1171	0.63	1/1576 (0.1%)
5	XE	0.15	0/1171	0.61	0/1576
6	QF	0.12	0/856	0.56	0/1154
6	XF	0.16	0/856	0.61	1/1154 (0.1%)
7	QG	0.18	0/1276	0.56	0/1709
7	XG	0.16	0/1276	0.61	0/1709
8	QH	0.18	0/1136	0.64	2/1527 (0.1%)
8	XH	0.95	8/1136 (0.7%)	1.12	12/1527 (0.8%)
9	QI	0.20	0/1029	0.69	1/1379 (0.1%)
9	XI	0.14	0/1029	0.65	1/1379 (0.1%)
10	QJ	0.13	0/814	0.60	0/1095
10	XJ	0.14	0/814	0.60	0/1095
11	QK	0.29	0/900	0.66	0/1213
11	XK	1.51	12/900 (1.3%)	1.09	8/1213 (0.7%)
12	QL	0.14	0/991	0.69	1/1327 (0.1%)
12	XL	0.17	0/991	0.71	1/1327 (0.1%)
13	QM	0.15	0/974	0.72	1/1303 (0.1%)
13	XM	0.16	0/974	0.73	1/1303 (0.1%)
14	QN	0.22	0/501	0.67	0/664
14	XN	0.29	0/501	0.80	2/664 (0.3%)
15	QO	0.13	0/745	0.60	0/992
15	XO	0.15	0/745	0.57	0/992
16	QP	0.27	0/721	0.64	0/970
16	XP	0.60	1/721 (0.1%)	1.07	2/970 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.12	0/847	0.57	1/1131 (0.1%)
17	XQ	0.13	0/847	0.61	0/1131
18	QR	0.12	0/579	0.61	0/768
18	XR	0.13	0/579	0.60	0/768
19	QS	0.35	0/689	0.75	2/926 (0.2%)
19	XS	0.32	0/689	0.77	2/926 (0.2%)
20	QT	0.12	0/765	0.63	0/1007
20	XT	0.27	0/765	0.75	0/1007
21	QU	0.16	0/221	0.51	0/288
21	XU	0.13	0/221	0.50	0/288
22	QV	0.16	0/1832	0.32	0/2855
22	XV	0.16	0/1832	0.31	0/2855
23	QW	0.12	0/1819	0.31	0/2833
23	XW	0.33	3/1819 (0.2%)	0.64	3/2833 (0.1%)
24	QX	0.14	0/468	0.36	0/729
24	XX	0.18	0/443	0.50	2/690 (0.3%)
25	QY	0.10	0/1791	0.23	0/2791
25	XY	0.13	0/1791	0.27	0/2791
26	R0	0.14	0/657	0.70	1/874 (0.1%)
26	Y0	0.16	0/657	0.66	0/874
27	R1	0.20	0/770	0.65	0/1022
27	Y1	0.18	0/770	0.61	0/1022
28	R2	0.15	0/583	0.66	0/771
28	Y2	0.18	0/583	0.72	1/771 (0.1%)
29	R3	0.12	0/474	0.60	0/635
29	Y3	0.18	0/474	0.63	0/635
30	R4	0.23	0/594	0.82	1/795 (0.1%)
30	Y4	0.18	0/594	0.77	0/795
31	R5	0.20	0/473	0.67	1/639 (0.2%)
31	Y5	0.20	0/473	0.69	0/639
32	R6	0.29	0/431	0.85	0/575
32	Y6	0.27	0/431	0.97	3/575 (0.5%)
33	R7	0.27	0/438	0.65	0/575
33	Y7	0.39	0/438	0.87	2/575 (0.3%)
34	R8	0.46	0/525	0.98	2/691 (0.3%)
34	Y8	0.21	0/525	0.70	0/691
35	R9	0.11	0/310	0.54	0/407
35	Y9	0.11	0/310	0.53	0/407
36	RA	0.22	0/69521	0.41	8/108529 (0.0%)
36	YA	0.24	1/69543 (0.0%)	0.43	11/108563 (0.0%)
37	RB	0.20	0/2878	0.36	0/4490
37	YB	0.20	0/2878	0.39	0/4490
38	RD	0.29	0/2165	0.74	3/2919 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YD	0.24	0/2195	0.64	0/2955
39	RE	0.17	0/1601	0.75	3/2160 (0.1%)
39	YE	0.20	0/1601	0.79	2/2160 (0.1%)
40	RF	1.14	9/1620 (0.6%)	0.83	9/2194 (0.4%)
40	YF	2.10	13/1620 (0.8%)	1.00	13/2194 (0.6%)
41	RG	0.13	0/1499	0.61	0/2016
41	YG	0.16	0/1499	0.71	3/2016 (0.1%)
42	RH	0.13	0/1332	0.65	1/1802 (0.1%)
42	YH	0.21	0/1332	0.78	4/1802 (0.2%)
43	RI	0.15	0/1151	0.70	2/1558 (0.1%)
43	YI	0.18	0/1151	0.74	1/1558 (0.1%)
44	RN	0.27	0/1131	0.78	2/1525 (0.1%)
44	YN	1.67	10/1131 (0.9%)	1.27	15/1525 (1.0%)
45	RO	0.24	0/943	0.64	0/1269
45	YO	0.15	0/943	0.63	0/1269
46	RP	0.19	0/1162	0.77	2/1544 (0.1%)
46	YP	0.23	0/1162	0.84	2/1544 (0.1%)
47	RQ	0.16	0/1143	0.72	0/1527
47	YQ	0.19	0/1143	0.76	1/1527 (0.1%)
48	RR	0.16	0/982	0.74	3/1312 (0.2%)
48	YR	0.19	0/982	0.77	2/1312 (0.2%)
49	RS	0.14	0/892	0.71	0/1187
49	YS	0.17	0/892	0.71	0/1187
50	RT	0.16	0/1155	0.67	2/1542 (0.1%)
50	YT	0.18	0/1155	0.78	6/1542 (0.4%)
51	RU	0.20	0/982	0.73	2/1306 (0.2%)
51	YU	0.17	0/982	0.67	2/1306 (0.2%)
52	RV	0.17	0/790	0.70	0/1057
52	YV	0.19	0/790	0.68	0/1057
53	RW	0.14	0/911	0.59	0/1220
53	YW	0.17	0/911	0.65	0/1220
54	RX	0.27	0/739	0.67	1/993 (0.1%)
54	YX	0.16	0/739	0.64	0/993
55	RY	0.19	0/798	0.74	0/1064
55	YY	0.19	0/798	0.78	0/1064
56	RZ	0.15	0/1493	0.65	1/2026 (0.0%)
56	YZ	0.18	0/1493	0.75	1/2026 (0.0%)
All	All	0.30	59/323346 (0.0%)	0.51	170/483882 (0.0%)

The worst 5 of 59 bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	YF	199	TRP	CD2-CE3	54.49	2.27	1.40
40	YF	199	TRP	CE2-CZ2	39.35	2.22	1.39
40	RF	199	TRP	NE1-CE2	33.31	1.74	1.37
44	YN	42	TRP	CG-CD2	33.21	2.03	1.43
44	YN	42	TRP	CD2-CE3	-26.63	0.97	1.40

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	XH	138	TRP	CB-CG-CD2	16.90	150.46	126.80
8	XH	138	TRP	CG-CD2-CE3	-16.80	117.10	133.90
44	YN	42	TRP	CE2-CD2-CE3	16.13	134.93	118.80
16	XP	40	ASP	CA-C-N	15.96	135.67	119.56
16	XP	40	ASP	C-N-CA	15.96	135.67	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	520	0
1	XA	32249	0	16278	485	0
2	QB	1924	0	1975	34	0
2	XB	1924	0	1975	57	0
3	QC	1605	0	1668	44	0
3	XC	1605	0	1668	38	0
4	QD	1674	0	1716	35	0
4	XD	1674	0	1718	38	0
5	QE	1155	0	1213	24	0
5	XE	1155	0	1213	17	0
6	QF	843	0	857	7	0
6	XF	843	0	857	25	0
7	QG	1257	0	1296	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	32	0
8	QH	1116	0	1177	35	0
8	XH	1116	0	1177	30	0
9	QI	1010	0	1037	30	0
9	XI	1010	0	1037	30	0
10	QJ	801	0	849	24	0
10	XJ	801	0	849	34	0
11	QK	885	0	904	38	0
11	XK	885	0	904	38	0
12	QL	975	0	1062	21	0
12	XL	975	0	1062	23	0
13	QM	964	0	1034	27	0
13	XM	964	0	1034	25	0
14	QN	492	0	532	23	0
14	XN	492	0	529	20	0
15	QO	734	0	771	14	0
15	XO	734	0	771	11	0
16	QP	705	0	725	17	0
16	XP	705	0	725	26	0
17	QQ	834	0	904	10	0
17	XQ	834	0	904	19	0
18	QR	574	0	644	12	0
18	XR	574	0	644	12	0
19	QS	674	0	699	32	0
19	XS	674	0	699	27	0
20	QT	763	0	861	16	0
20	XT	763	0	861	23	0
21	QU	217	0	234	10	0
21	XU	217	0	234	5	0
22	QV	1640	0	837	9	0
22	XV	1640	0	837	9	0
23	QW	1627	0	823	20	0
23	XW	1627	0	823	39	0
24	QX	416	0	208	4	0
24	XX	394	0	197	9	0
25	QY	1603	0	811	24	0
25	XY	1603	0	811	24	0
26	R0	648	0	672	10	0
26	Y0	648	0	672	19	0
27	R1	763	0	848	17	0
27	Y1	763	0	848	19	0
28	R2	581	0	629	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Y2	581	0	629	8	0
29	R3	469	0	518	11	0
29	Y3	469	0	518	11	0
30	R4	581	0	577	24	0
30	Y4	581	0	577	19	0
31	R5	459	0	480	22	0
31	Y5	459	0	480	8	0
32	R6	424	0	450	20	0
32	Y6	424	0	450	17	0
33	R7	430	0	480	11	0
33	Y7	430	0	480	21	0
34	R8	517	0	582	36	0
34	Y8	517	0	582	28	0
35	R9	307	0	338	7	0
35	Y9	307	0	338	7	0
36	RA	62071	0	31289	871	0
36	YA	62091	0	31301	801	0
37	RB	2573	0	1306	33	0
37	YB	2573	0	1306	22	0
38	RD	2115	0	2195	71	0
38	YD	2145	0	2234	36	0
39	RE	1568	0	1633	56	0
39	YE	1568	0	1634	56	0
40	RF	1585	0	1632	45	0
40	YF	1585	0	1632	46	0
41	RG	1474	0	1535	36	0
41	YG	1474	0	1535	34	0
42	RH	1307	0	1382	30	0
42	YH	1307	0	1381	47	0
43	RI	1136	0	1223	18	0
43	YI	1136	0	1223	31	0
44	RN	1104	0	1180	27	0
44	YN	1104	0	1180	31	0
45	RO	933	0	996	26	0
45	YO	933	0	996	23	0
46	RP	1145	0	1227	53	0
46	YP	1145	0	1227	56	0
47	RQ	1122	0	1179	48	0
47	YQ	1122	0	1179	42	0
48	RR	968	0	1033	19	0
48	YR	968	0	1033	24	0
49	RS	882	0	943	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	YS	882	0	943	22	0
50	RT	1141	0	1202	34	0
50	YT	1141	0	1202	35	0
51	RU	964	0	1022	26	0
51	YU	964	0	1022	33	0
52	RV	779	0	852	19	0
52	YV	779	0	852	22	0
53	RW	900	0	964	19	0
53	YW	900	0	964	21	0
54	RX	725	0	778	11	0
54	YX	725	0	778	10	0
55	RY	785	0	878	29	0
55	YY	785	0	878	33	0
56	RZ	1461	0	1493	44	0
56	YZ	1461	0	1493	45	0
57	QA	124	0	0	0	0
57	QD	1	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QK	2	0	0	0	0
57	QL	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	6	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R1	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	R9	1	0	0	0	0
57	RA	378	0	0	0	0
57	RB	4	0	0	0	0
57	RD	2	0	0	0	0
57	RE	8	0	0	0	0
57	RF	2	0	0	0	0
57	RG	1	0	0	0	0
57	RI	1	0	0	0	0
57	RP	3	0	0	0	0
57	RR	2	0	0	0	0
57	RT	2	0	0	0	0
57	XA	123	0	0	0	0
57	XB	2	0	0	0	0
57	XD	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XF	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XK	1	0	0	0	0
57	XL	2	0	0	0	0
57	XM	1	0	0	0	0
57	XV	7	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	3	0	0	0	0
57	Y2	3	0	0	0	0
57	Y3	1	0	0	0	0
57	Y4	2	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	Y8	3	0	0	0	0
57	YA	457	0	0	0	0
57	YB	8	0	0	0	0
57	YD	4	0	0	0	0
57	YE	6	0	0	0	0
57	YF	5	0	0	0	0
57	YG	2	0	0	0	0
57	YH	5	0	0	0	0
57	YI	1	0	0	0	0
57	YN	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	7	0	0	0	0
57	YQ	4	0	0	0	0
57	YR	2	0	0	0	0
57	YT	2	0	0	0	0
57	YU	1	0	0	0	0
57	YV	1	0	0	0	0
57	YW	1	0	0	0	0
57	YX	2	0	0	0	0
57	YY	5	0	0	0	0
58	QA	42	0	45	1	0
58	XA	42	0	45	2	0
59	QD	8	0	0	0	0
59	XD	8	0	0	0	0
60	QN	1	0	0	0	0
60	XN	1	0	0	0	0
61	QY	22	0	12	1	0
62	QA	1	0	0	0	0
62	QX	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	298675	0	201403	4712	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4712 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)
40:YF:199:TRP:CH2	40:YF:199:TRP:CZ3	1.78	1.69
8:XH:138:TRP:CE3	8:XH:138:TRP:CZ3	1.75	1.64
40:YF:199:TRP:CG	40:YF:199:TRP:CD1	1.86	1.62
44:YN:42:TRP:CE2	44:YN:42:TRP:CZ2	1.86	1.62
40:YF:199:TRP:CE2	40:YF:199:TRP:CD2	1.85	1.61

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	212 (90%)	21 (9%)	2 (1%)	14	47
2	XB	235/256 (92%)	208 (88%)	27 (12%)	0	100	100
3	QC	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
3	XC	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	QD	206/209 (99%)	203 (98%)	3 (2%)	0	100	100
4	XD	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
5	QE	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
5	XE	149/162 (92%)	143 (96%)	6 (4%)	0	100	100
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	XF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
8	QH	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
8	XH	136/138 (99%)	127 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	16	50
9	XI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
10	QJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
10	XJ	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
11	QK	117/129 (91%)	104 (89%)	13 (11%)	0	100	100
11	XK	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
12	QL	123/131 (94%)	110 (89%)	13 (11%)	0	100	100
12	XL	123/131 (94%)	114 (93%)	9 (7%)	0	100	100
13	QM	119/126 (94%)	98 (82%)	21 (18%)	0	100	100
13	XM	119/126 (94%)	98 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	35
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	35
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	QP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
17	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	82/93 (88%)	73 (89%)	7 (8%)	2 (2%)	4	28
19	XS	82/93 (88%)	72 (88%)	10 (12%)	0	100	100
20	QT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
20	XT	97/106 (92%)	87 (90%)	10 (10%)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	R0	80/85 (94%)	74 (92%)	6 (8%)	0	100	100
26	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
27	R1	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	11	43
27	Y1	95/98 (97%)	85 (90%)	9 (10%)	1 (1%)	11	43
28	R2	67/72 (93%)	64 (96%)	3 (4%)	0	100	100
28	Y2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	8	37
29	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	Y3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
30	R4	69/71 (97%)	41 (59%)	25 (36%)	3 (4%)	2	16
30	Y4	69/71 (97%)	45 (65%)	21 (30%)	3 (4%)	2	16
31	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
31	Y5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
32	R6	47/54 (87%)	30 (64%)	17 (36%)	0	100	100
32	Y6	47/54 (87%)	35 (74%)	12 (26%)	0	100	100
33	R7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
33	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
34	R8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	7	36
34	Y8	62/65 (95%)	49 (79%)	13 (21%)	0	100	100
35	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
35	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
38	RD	270/276 (98%)	245 (91%)	24 (9%)	1 (0%)	30	62
38	YD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
39	RE	203/206 (98%)	170 (84%)	28 (14%)	5 (2%)	4	27
39	YE	203/206 (98%)	166 (82%)	35 (17%)	2 (1%)	12	45
40	RF	200/210 (95%)	185 (92%)	12 (6%)	3 (2%)	8	37
40	YF	200/210 (95%)	187 (94%)	13 (6%)	0	100	100
41	RG	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	21	56
41	YG	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	21	56
42	RH	168/180 (93%)	157 (94%)	11 (6%)	0	100	100
42	YH	168/180 (93%)	143 (85%)	22 (13%)	3 (2%)	6	34
43	RI	144/148 (97%)	132 (92%)	12 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YI	144/148 (97%)	121 (84%)	23 (16%)	0	100	100
44	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	52
44	YN	136/140 (97%)	125 (92%)	11 (8%)	0	100	100
45	RO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	50
45	YO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
46	RP	148/150 (99%)	131 (88%)	16 (11%)	1 (1%)	18	52
46	YP	148/150 (99%)	117 (79%)	30 (20%)	1 (1%)	18	52
47	RQ	139/141 (99%)	113 (81%)	26 (19%)	0	100	100
47	YQ	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	5	29
48	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
48	YR	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
49	RS	109/112 (97%)	96 (88%)	13 (12%)	0	100	100
49	YS	109/112 (97%)	92 (84%)	17 (16%)	0	100	100
50	RT	135/146 (92%)	119 (88%)	16 (12%)	0	100	100
50	YT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
51	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	47
51	YU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	47
52	RV	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
52	YV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
53	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
53	YW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
54	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
54	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
55	RY	100/110 (91%)	75 (75%)	24 (24%)	1 (1%)	12	45
55	YY	100/110 (91%)	76 (76%)	22 (22%)	2 (2%)	6	31
56	RZ	181/206 (88%)	155 (86%)	24 (13%)	2 (1%)	11	43
56	YZ	181/206 (88%)	147 (81%)	29 (16%)	5 (3%)	4	25
All	All	11473/12126 (95%)	10363 (90%)	1058 (9%)	52 (0%)	24	59

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	RN	22	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	RU	92	ARG
30	Y4	24	THR
42	YH	128	PRO
47	YQ	105	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	205 (100%)	0	100	100
2	XB	205/220 (93%)	205 (100%)	0	100	100
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	173 (100%)	0	100	100
4	XD	173/181 (96%)	173 (100%)	0	100	100
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	98/99 (99%)	98 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	89 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	90/99 (91%)	90 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	QL	104/108 (96%)	104 (100%)	0	100	100
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	97 (100%)	0	100	100
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	73 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	R0	65/67 (97%)	65 (100%)	0	100	100
26	Y0	65/67 (97%)	65 (100%)	0	100	100
27	R1	82/83 (99%)	82 (100%)	0	100	100
27	Y1	82/83 (99%)	82 (100%)	0	100	100
28	R2	64/67 (96%)	64 (100%)	0	100	100
28	Y2	64/67 (96%)	64 (100%)	0	100	100
29	R3	51/52 (98%)	51 (100%)	0	100	100
29	Y3	51/52 (98%)	51 (100%)	0	100	100
30	R4	63/63 (100%)	63 (100%)	0	100	100
30	Y4	63/63 (100%)	63 (100%)	0	100	100
31	R5	51/52 (98%)	51 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Y5	51/52 (98%)	51 (100%)	0	100	100
32	R6	48/52 (92%)	48 (100%)	0	100	100
32	Y6	48/52 (92%)	48 (100%)	0	100	100
33	R7	42/42 (100%)	42 (100%)	0	100	100
33	Y7	42/42 (100%)	42 (100%)	0	100	100
34	R8	54/55 (98%)	54 (100%)	0	100	100
34	Y8	54/55 (98%)	54 (100%)	0	100	100
35	R9	34/34 (100%)	34 (100%)	0	100	100
35	Y9	34/34 (100%)	34 (100%)	0	100	100
38	RD	214/218 (98%)	214 (100%)	0	100	100
38	YD	217/218 (100%)	217 (100%)	0	100	100
39	RE	165/166 (99%)	165 (100%)	0	100	100
39	YE	165/166 (99%)	165 (100%)	0	100	100
40	RF	161/166 (97%)	161 (100%)	0	100	100
40	YF	161/166 (97%)	161 (100%)	0	100	100
41	RG	155/156 (99%)	155 (100%)	0	100	100
41	YG	155/156 (99%)	155 (100%)	0	100	100
42	RH	142/148 (96%)	142 (100%)	0	100	100
42	YH	142/148 (96%)	142 (100%)	0	100	100
43	RI	122/124 (98%)	122 (100%)	0	100	100
43	YI	122/124 (98%)	122 (100%)	0	100	100
44	RN	117/119 (98%)	117 (100%)	0	100	100
44	YN	117/119 (98%)	117 (100%)	0	100	100
45	RO	100/100 (100%)	100 (100%)	0	100	100
45	YO	100/100 (100%)	100 (100%)	0	100	100
46	RP	116/116 (100%)	116 (100%)	0	100	100
46	YP	116/116 (100%)	116 (100%)	0	100	100
47	RQ	111/111 (100%)	111 (100%)	0	100	100
47	YQ	111/111 (100%)	111 (100%)	0	100	100
48	RR	101/101 (100%)	101 (100%)	0	100	100
48	YR	101/101 (100%)	101 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	RS	87/88 (99%)	87 (100%)	0	100	100
49	YS	87/88 (99%)	87 (100%)	0	100	100
50	RT	120/127 (94%)	120 (100%)	0	100	100
50	YT	120/127 (94%)	120 (100%)	0	100	100
51	RU	93/94 (99%)	93 (100%)	0	100	100
51	YU	93/94 (99%)	93 (100%)	0	100	100
52	RV	82/82 (100%)	82 (100%)	0	100	100
52	YV	82/82 (100%)	82 (100%)	0	100	100
53	RW	92/92 (100%)	92 (100%)	0	100	100
53	YW	92/92 (100%)	92 (100%)	0	100	100
54	RX	74/78 (95%)	74 (100%)	0	100	100
54	YX	74/78 (95%)	74 (100%)	0	100	100
55	RY	85/91 (93%)	85 (100%)	0	100	100
55	YY	85/91 (93%)	85 (100%)	0	100	100
56	RZ	162/179 (90%)	162 (100%)	0	100	100
56	YZ	162/179 (90%)	162 (100%)	0	100	100
All	All	9691/10064 (96%)	9691 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
48	YR	11	ASN
48	YR	50	HIS
56	YZ	32	HIS
41	RG	79	ASN
41	RG	58	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	262 (17%)	31 (2%)
1	XA	1498/1522 (98%)	258 (17%)	30 (2%)
22	QV	76/77 (98%)	11 (14%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XV	76/77 (98%)	11 (14%)	0
23	QW	75/76 (98%)	25 (33%)	2 (2%)
23	XW	75/76 (98%)	33 (44%)	7 (9%)
24	QX	18/19 (94%)	9 (50%)	1 (5%)
24	XX	17/19 (89%)	7 (41%)	1 (5%)
25	QY	74/76 (97%)	22 (29%)	0
25	XY	74/76 (97%)	31 (41%)	1 (1%)
36	RA	2879/2915 (98%)	543 (18%)	44 (1%)
36	YA	2880/2915 (98%)	541 (18%)	45 (1%)
37	RB	119/122 (97%)	18 (15%)	2 (1%)
37	YB	119/122 (97%)	20 (16%)	1 (0%)
All	All	9478/9614 (98%)	1791 (18%)	165 (1%)

5 of 1791 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	22	G
1	QA	32	A

5 of 165 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	XW	59	U
36	YA	1427	A
36	YA	99	U
36	YA	637	A
36	YA	1930	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1222 ligands modelled in this entry, 1217 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	QA	1711	-	44,45,45	0.53	0	63,67,67	0.90	1 (1%)
59	SF4	QD	501	4	0,12,12	-	-	-		
61	AMP	QY	101	-	21,24,25	0.28	0	30,35,38	0.47	0
58	PAR	XA	1717	-	44,45,45	0.53	0	63,67,67	0.86	1 (1%)
59	SF4	XD	501	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
58	PAR	QA	1711	-	-	3/18/94/94	0/4/4/4
59	SF4	QD	501	4	-	-	0/6/5/5
61	AMP	QY	101	-	-	0/7/25/26	0/3/3/3
58	PAR	XA	1717	-	-	2/18/94/94	0/4/4/4
59	SF4	XD	501	4	-	-	0/6/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1711	PAR	C13-O52-C52	-2.95	110.99	117.98
58	XA	1717	PAR	C13-O52-C52	-2.83	111.26	117.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

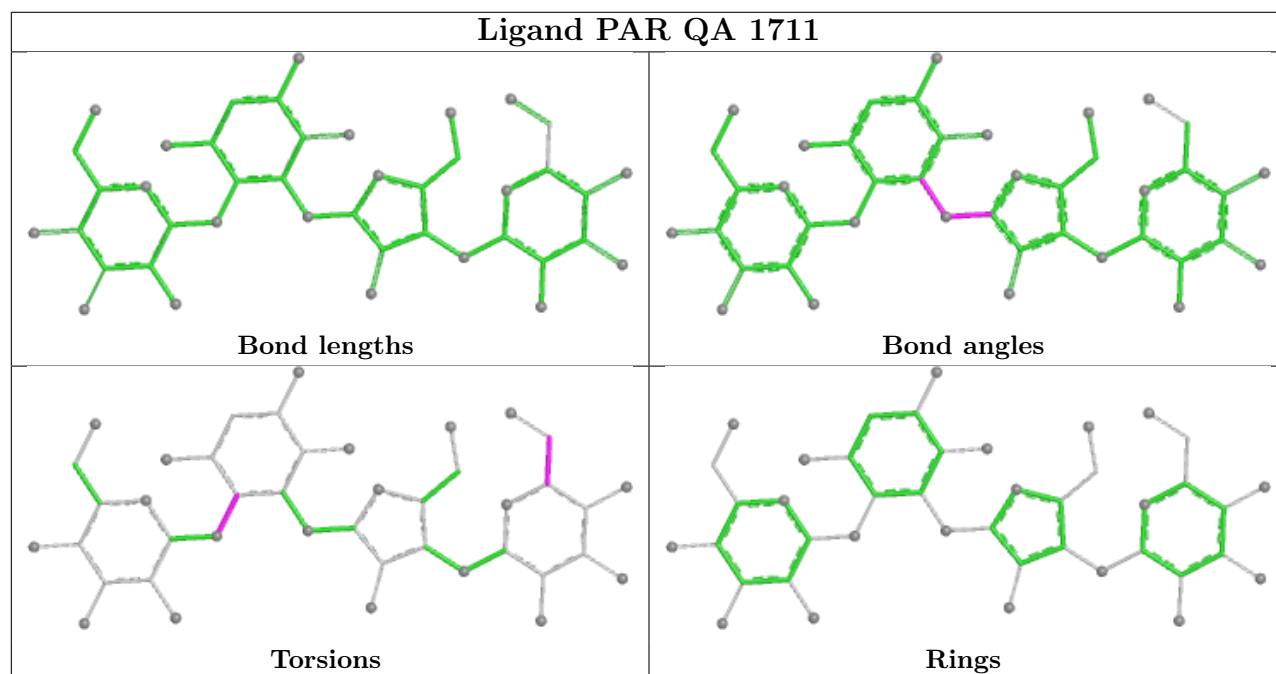
Mol	Chain	Res	Type	Atoms
58	QA	1711	PAR	O54-C54-C64-N64
58	XA	1717	PAR	C23-C33-O33-C14
58	QA	1711	PAR	C52-C42-O11-C11
58	XA	1717	PAR	C52-C42-O11-C11
58	QA	1711	PAR	C44-C54-C64-N64

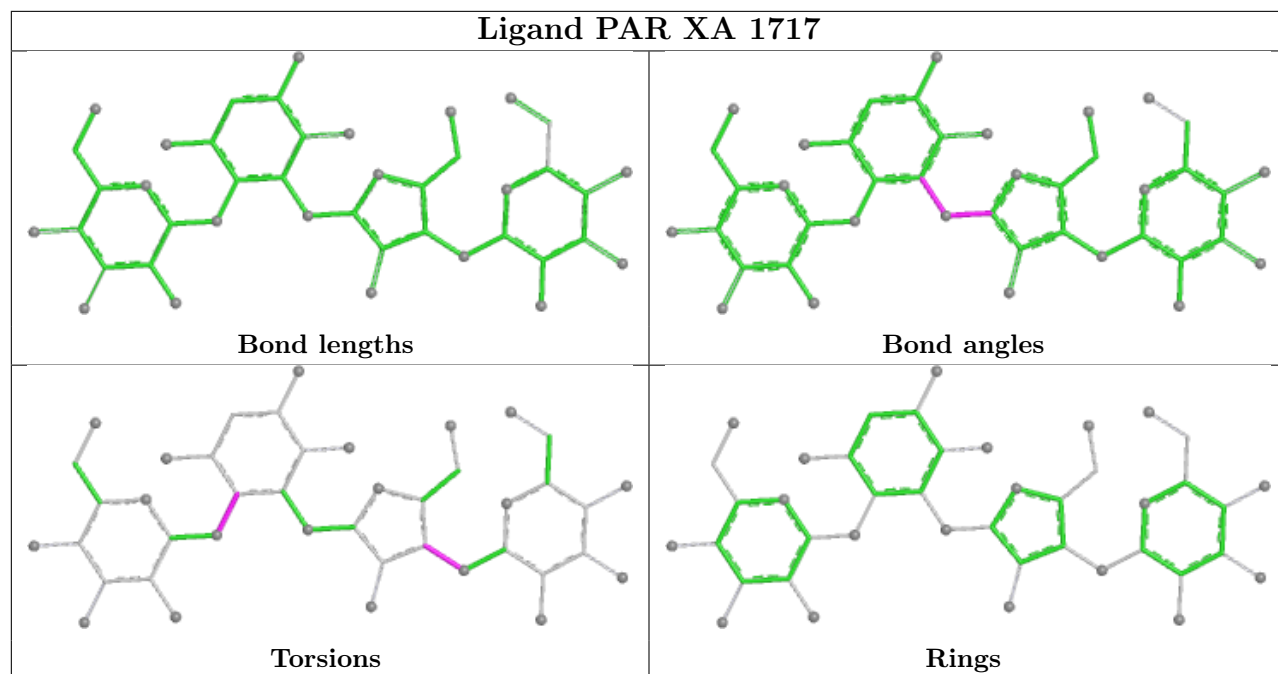
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1711	PAR	1	0
61	QY	101	AMP	1	0
58	XA	1717	PAR	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	-0.00	32 (2%) 63 43	50, 86, 165, 319	0
1	XA	1500/1522 (98%)	0.01	25 (1%) 69 49	44, 83, 171, 304	0
2	QB	237/256 (92%)	0.69	25 (10%) 11 8	81, 123, 178, 221	0
2	XB	237/256 (92%)	0.64	20 (8%) 17 11	83, 116, 166, 197	0
3	QC	205/239 (85%)	0.72	22 (10%) 11 7	93, 122, 161, 210	0
3	XC	205/239 (85%)	0.41	11 (5%) 31 20	69, 101, 144, 222	0
4	QD	208/209 (99%)	0.18	8 (3%) 44 27	57, 74, 105, 133	0
4	XD	208/209 (99%)	0.25	7 (3%) 48 30	64, 81, 117, 193	0
5	QE	151/162 (93%)	0.23	7 (4%) 37 23	65, 94, 132, 164	0
5	XE	151/162 (93%)	0.32	6 (3%) 42 26	56, 84, 127, 206	0
6	QF	101/101 (100%)	-0.04	0 100 100	68, 82, 110, 150	0
6	XF	101/101 (100%)	-0.04	0 100 100	59, 79, 106, 162	0
7	QG	155/156 (99%)	0.37	7 (4%) 38 24	80, 99, 135, 209	0
7	XG	155/156 (99%)	0.52	15 (9%) 13 9	78, 100, 143, 177	0
8	QH	138/138 (100%)	0.43	7 (5%) 33 21	68, 93, 129, 145	0
8	XH	138/138 (100%)	0.32	8 (5%) 29 18	62, 86, 114, 130	0
9	QI	127/128 (99%)	0.81	13 (10%) 12 8	77, 120, 157, 184	0
9	XI	127/128 (99%)	0.70	11 (8%) 16 11	72, 119, 161, 179	0
10	QJ	99/105 (94%)	1.05	18 (18%) 3 3	100, 135, 178, 190	0
10	XJ	99/105 (94%)	0.97	16 (16%) 4 3	85, 128, 170, 183	0
11	QK	119/129 (92%)	0.60	13 (10%) 10 7	61, 84, 131, 191	0
11	XK	119/129 (92%)	0.39	7 (5%) 28 18	59, 82, 126, 175	0
12	QL	125/131 (95%)	0.77	11 (8%) 15 10	61, 85, 133, 201	0
12	XL	125/131 (95%)	0.40	9 (7%) 21 14	49, 67, 121, 168	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.76	14 (11%) 9 7	78, 113, 154, 201	0
13	XM	121/126 (96%)	0.82	15 (12%) 8 6	80, 106, 154, 223	0
14	QN	60/61 (98%)	1.32	13 (21%) 2 2	104, 120, 160, 181	0
14	XN	60/61 (98%)	0.77	7 (11%) 9 6	75, 97, 139, 194	0
15	QO	88/89 (98%)	0.22	2 (2%) 61 41	58, 79, 111, 122	0
15	XO	88/89 (98%)	0.18	0 100 100	54, 77, 112, 132	0
16	QP	84/88 (95%)	0.48	6 (7%) 22 14	58, 77, 115, 157	0
16	XP	84/88 (95%)	0.55	7 (8%) 17 11	69, 92, 135, 169	0
17	QQ	100/105 (95%)	0.46	5 (5%) 34 22	64, 86, 125, 145	0
17	XQ	100/105 (95%)	0.54	7 (7%) 22 14	57, 84, 112, 129	0
18	QR	70/88 (79%)	0.12	1 (1%) 73 54	62, 82, 125, 145	0
18	XR	70/88 (79%)	0.05	1 (1%) 73 54	57, 83, 124, 148	0
19	QS	84/93 (90%)	1.26	16 (19%) 3 2	97, 135, 177, 242	0
19	XS	84/93 (90%)	1.15	19 (22%) 2 2	93, 119, 158, 206	0
20	QT	99/106 (93%)	0.84	12 (12%) 8 6	65, 97, 155, 183	0
20	XT	99/106 (93%)	0.90	15 (15%) 5 4	81, 106, 157, 185	0
21	QU	25/27 (92%)	1.08	3 (12%) 9 6	82, 105, 139, 150	0
21	XU	25/27 (92%)	0.96	4 (16%) 5 3	82, 97, 121, 135	0
22	QV	77/77 (100%)	0.13	4 (5%) 33 21	68, 107, 144, 184	0
22	XV	77/77 (100%)	-0.09	2 (2%) 57 37	61, 91, 133, 174	0
23	QW	76/76 (100%)	1.27	19 (25%) 2 2	87, 201, 260, 298	0
23	XW	76/76 (100%)	1.46	24 (31%) 1 1	72, 216, 282, 293	0
24	QX	19/19 (100%)	1.00	3 (15%) 5 4	73, 137, 257, 258	0
24	XX	18/19 (94%)	1.16	4 (22%) 2 2	59, 141, 233, 233	0
25	QY	75/76 (98%)	1.61	28 (37%) 1 1	92, 218, 273, 304	0
25	XY	75/76 (98%)	1.29	20 (26%) 1 1	80, 196, 262, 284	0
26	R0	82/85 (96%)	0.83	10 (12%) 8 6	59, 77, 116, 189	0
26	Y0	82/85 (96%)	0.44	6 (7%) 21 13	44, 62, 89, 130	0
27	R1	97/98 (98%)	0.49	8 (8%) 17 11	43, 63, 127, 177	0
27	Y1	97/98 (98%)	0.43	6 (6%) 26 17	39, 59, 129, 160	0
28	R2	69/72 (95%)	0.55	5 (7%) 21 14	61, 79, 141, 197	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y2	69/72 (95%)	0.39	5 (7%) 21 14	54, 67, 126, 180	0
29	R3	59/60 (98%)	0.38	2 (3%) 48 30	67, 87, 125, 143	0
29	Y3	59/60 (98%)	0.08	1 (1%) 69 49	47, 62, 110, 135	0
30	R4	71/71 (100%)	1.30	16 (22%) 2 2	95, 143, 218, 262	0
30	Y4	71/71 (100%)	1.19	12 (16%) 4 3	98, 146, 221, 235	0
31	R5	59/60 (98%)	0.70	11 (18%) 3 3	51, 73, 187, 215	0
31	Y5	59/60 (98%)	0.62	7 (11%) 9 6	37, 65, 183, 200	0
32	R6	49/54 (90%)	3.40	34 (69%) 0 0	121, 168, 217, 225	0
32	Y6	49/54 (90%)	2.80	24 (48%) 0 1	129, 162, 210, 239	0
33	R7	49/49 (100%)	0.16	3 (6%) 27 17	37, 51, 125, 177	0
33	Y7	49/49 (100%)	0.78	10 (20%) 3 2	31, 45, 140, 169	0
34	R8	64/65 (98%)	1.11	14 (21%) 2 2	50, 69, 126, 175	0
34	Y8	64/65 (98%)	1.05	15 (23%) 2 2	44, 62, 113, 195	0
35	R9	37/37 (100%)	2.40	20 (54%) 0 0	151, 187, 223, 236	0
35	Y9	37/37 (100%)	4.39	31 (83%) 0 0	130, 195, 223, 237	0
36	RA	2882/2915 (98%)	-0.08	71 (2%) 58 39	41, 70, 193, 312	0
36	YA	2883/2915 (98%)	-0.22	56 (1%) 66 46	30, 57, 185, 306	0
37	RB	120/122 (98%)	0.10	0 100 100	85, 104, 132, 152	0
37	YB	120/122 (98%)	0.06	4 (3%) 49 30	64, 86, 111, 140	0
38	RD	272/276 (98%)	0.37	27 (9%) 13 8	39, 56, 87, 225	0
38	YD	275/276 (99%)	-0.06	0 100 100	33, 48, 73, 160	0
39	RE	205/206 (99%)	0.57	15 (7%) 21 13	46, 82, 142, 230	0
39	YE	205/206 (99%)	0.49	17 (8%) 17 11	38, 70, 144, 192	0
40	RF	202/210 (96%)	0.47	13 (6%) 25 16	41, 77, 136, 181	0
40	YF	202/210 (96%)	0.20	5 (2%) 58 39	36, 61, 111, 174	0
41	RG	181/182 (99%)	0.49	9 (4%) 34 22	77, 99, 138, 181	0
41	YG	181/182 (99%)	0.58	15 (8%) 17 11	71, 91, 136, 171	0
42	RH	170/180 (94%)	1.28	34 (20%) 3 2	115, 164, 200, 231	0
42	YH	170/180 (94%)	0.65	18 (10%) 11 8	65, 88, 142, 214	0
43	RI	146/148 (98%)	0.51	8 (5%) 30 19	66, 99, 138, 221	0
43	YI	146/148 (98%)	0.51	6 (4%) 41 25	61, 103, 136, 185	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	RN	138/140 (98%)	0.42	4 (2%)	53	35	60, 91, 130, 160	0
44	YN	138/140 (98%)	0.34	5 (3%)	46	28	42, 69, 115, 163	0
45	RO	122/122 (100%)	0.10	1 (0%)	82	67	55, 72, 97, 130	0
45	YO	122/122 (100%)	-0.24	0	100	100	40, 60, 81, 93	0
46	RP	150/150 (100%)	0.99	25 (16%)	4	3	46, 85, 136, 194	0
46	YP	150/150 (100%)	0.83	19 (12%)	8	6	36, 75, 123, 207	0
47	RQ	141/141 (100%)	1.11	21 (14%)	5	4	69, 94, 156, 223	0
47	YQ	141/141 (100%)	0.56	14 (9%)	13	8	49, 69, 133, 188	0
48	RR	118/118 (100%)	0.35	6 (5%)	33	21	53, 65, 96, 143	0
48	YR	118/118 (100%)	0.31	3 (2%)	58	39	43, 66, 92, 148	0
49	RS	111/112 (99%)	0.84	9 (8%)	18	11	66, 95, 141, 211	0
49	YS	111/112 (99%)	0.62	7 (6%)	26	17	68, 87, 122, 225	0
50	RT	137/146 (93%)	0.38	7 (5%)	33	21	61, 83, 161, 224	0
50	YT	137/146 (93%)	0.48	8 (5%)	29	18	55, 72, 139, 176	0
51	RU	117/118 (99%)	0.77	13 (11%)	10	7	44, 86, 141, 229	0
51	YU	117/118 (99%)	0.24	6 (5%)	33	21	39, 63, 107, 191	0
52	RV	101/101 (100%)	0.59	6 (5%)	28	18	52, 102, 139, 241	0
52	YV	101/101 (100%)	0.36	5 (4%)	34	22	39, 77, 124, 209	0
53	RW	113/113 (100%)	0.16	7 (6%)	26	17	49, 64, 105, 187	0
53	YW	113/113 (100%)	0.14	2 (1%)	67	48	42, 54, 94, 176	0
54	RX	92/96 (95%)	0.40	3 (3%)	49	30	50, 66, 92, 125	0
54	YX	92/96 (95%)	0.26	1 (1%)	78	61	46, 56, 84, 128	0
55	RY	102/110 (92%)	1.28	26 (25%)	1	2	67, 95, 162, 213	0
55	YY	102/110 (92%)	1.03	15 (14%)	6	4	48, 81, 172, 197	0
56	RZ	183/206 (88%)	1.27	36 (19%)	3	2	97, 144, 217, 255	0
56	YZ	183/206 (88%)	1.24	40 (21%)	2	2	69, 115, 199, 232	0
All	All	21167/21740 (97%)	0.31	1376 (6%)	25	16	30, 82, 180, 319	0

The worst 5 of 1376 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	Y6	40	CYS	12.8
35	Y9	23	VAL	10.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	Y9	7	VAL	10.3
46	RP	13	ASN	10.0
32	R6	42	TRP	9.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	XM	201	1/1	-0.07	0.42	139,139,139,139	0
57	MG	XA	1710	1/1	-0.01	0.60	139,139,139,139	0
57	MG	XA	1689	1/1	0.24	0.47	124,124,124,124	0
57	MG	RA	3195	1/1	0.28	0.28	91,91,91,91	0
57	MG	YA	3399	1/1	0.30	0.17	85,85,85,85	0
57	MG	YA	3166	1/1	0.37	0.46	134,134,134,134	0
57	MG	YA	3379	1/1	0.39	0.25	115,115,115,115	0
57	MG	YA	3281	1/1	0.39	0.54	86,86,86,86	0
57	MG	RA	3366	1/1	0.41	0.51	85,85,85,85	0
57	MG	RA	3125	1/1	0.42	0.52	98,98,98,98	0
57	MG	QA	1659	1/1	0.44	0.37	134,134,134,134	0
57	MG	YA	3350	1/1	0.44	0.43	90,90,90,90	0
57	MG	YA	3105	1/1	0.45	0.98	126,126,126,126	0
57	MG	XA	1668	1/1	0.45	0.25	142,142,142,142	0
57	MG	RA	3225	1/1	0.46	0.77	107,107,107,107	0
57	MG	RA	3361	1/1	0.47	0.95	179,179,179,179	0
57	MG	XA	1608	1/1	0.47	0.20	136,136,136,136	0
57	MG	RA	3269	1/1	0.49	0.45	106,106,106,106	0
57	MG	QA	1681	1/1	0.49	0.24	149,149,149,149	0
57	MG	YA	3437	1/1	0.49	0.91	116,116,116,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3170	1/1	0.51	0.39	104,104,104,104	0
57	MG	QA	1644	1/1	0.51	0.48	122,122,122,122	0
57	MG	YY	205	1/1	0.51	0.30	167,167,167,167	0
57	MG	QA	1710	1/1	0.52	0.38	112,112,112,112	0
57	MG	RA	3258	1/1	0.54	0.35	116,116,116,116	0
57	MG	QA	1610	1/1	0.54	0.83	129,129,129,129	0
57	MG	XA	1694	1/1	0.55	0.54	136,136,136,136	0
57	MG	RA	3157	1/1	0.56	0.30	65,65,65,65	0
57	MG	YA	3342	1/1	0.57	0.48	135,135,135,135	0
57	MG	XA	1711	1/1	0.57	0.55	118,118,118,118	0
57	MG	XA	1703	1/1	0.58	0.32	124,124,124,124	0
57	MG	QA	1612	1/1	0.59	0.59	98,98,98,98	0
57	MG	RA	3323	1/1	0.59	0.51	95,95,95,95	0
57	MG	YH	205	1/1	0.60	0.14	105,105,105,105	0
57	MG	YA	3332	1/1	0.60	0.41	126,126,126,126	0
57	MG	YA	3413	1/1	0.61	0.72	162,162,162,162	0
57	MG	YA	3382	1/1	0.62	0.46	108,108,108,108	0
57	MG	RA	3277	1/1	0.62	0.56	90,90,90,90	0
57	MG	RA	3187	1/1	0.62	0.34	165,165,165,165	0
57	MG	YA	3231	1/1	0.63	0.55	89,89,89,89	0
57	MG	QA	1615	1/1	0.63	0.26	111,111,111,111	0
57	MG	YA	3356	1/1	0.64	0.50	93,93,93,93	0
57	MG	YA	3191	1/1	0.64	0.59	125,125,125,125	0
57	MG	RA	3307	1/1	0.64	0.49	110,110,110,110	0
57	MG	XA	1691	1/1	0.64	0.34	88,88,88,88	0
57	MG	RA	3294	1/1	0.65	0.22	107,107,107,107	0
57	MG	QA	1619	1/1	0.65	0.72	74,74,74,74	0
57	MG	RA	3196	1/1	0.65	0.43	88,88,88,88	0
57	MG	RA	3344	1/1	0.65	0.34	106,106,106,106	0
57	MG	QA	1662	1/1	0.66	0.64	100,100,100,100	0
57	MG	YA	3172	1/1	0.66	0.48	51,51,51,51	0
57	MG	RA	3205	1/1	0.66	0.55	100,100,100,100	0
57	MG	XA	1674	1/1	0.66	0.35	91,91,91,91	0
57	MG	XA	1610	1/1	0.67	0.30	67,67,67,67	0
57	MG	RA	3166	1/1	0.67	0.25	81,81,81,81	0
57	MG	QA	1706	1/1	0.67	0.62	89,89,89,89	0
57	MG	RA	3143	1/1	0.67	0.15	73,73,73,73	0
57	MG	QA	1627	1/1	0.67	0.20	101,101,101,101	0
57	MG	XV	103	1/1	0.67	0.62	146,146,146,146	0
57	MG	XA	1712	1/1	0.68	0.31	80,80,80,80	0
57	MG	YA	3203	1/1	0.68	0.67	117,117,117,117	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3302	1/1	0.68	0.49	94,94,94,94	0
57	MG	QA	1623	1/1	0.68	0.31	89,89,89,89	0
57	MG	YA	3013	1/1	0.68	0.50	54,54,54,54	0
57	MG	YA	3324	1/1	0.69	0.38	101,101,101,101	0
57	MG	XA	1720	1/1	0.69	0.29	89,89,89,89	0
57	MG	XA	1665	1/1	0.69	0.27	55,55,55,55	0
57	MG	YA	3168	1/1	0.69	0.19	74,74,74,74	0
57	MG	QA	1647	1/1	0.70	0.46	100,100,100,100	0
57	MG	QA	1618	1/1	0.70	0.71	66,66,66,66	0
57	MG	YA	3348	1/1	0.70	0.21	84,84,84,84	0
57	MG	RA	3206	1/1	0.70	0.34	74,74,74,74	0
57	MG	YA	3305	1/1	0.70	1.01	104,104,104,104	0
57	MG	RA	3115	1/1	0.70	0.47	71,71,71,71	0
57	MG	YA	3201	1/1	0.71	0.34	68,68,68,68	0
57	MG	QA	1654	1/1	0.71	0.45	106,106,106,106	0
57	MG	YA	3368	1/1	0.71	0.43	87,87,87,87	0
57	MG	QA	1649	1/1	0.71	0.43	80,80,80,80	0
57	MG	YA	3109	1/1	0.71	0.29	78,78,78,78	0
57	MG	RA	3185	1/1	0.71	0.33	92,92,92,92	0
57	MG	QA	1713	1/1	0.71	0.26	95,95,95,95	0
57	MG	XV	101	1/1	0.71	0.32	142,142,142,142	0
57	MG	XA	1682	1/1	0.71	0.53	101,101,101,101	0
57	MG	YA	3003	1/1	0.71	0.17	71,71,71,71	0
57	MG	XA	1692	1/1	0.72	0.42	122,122,122,122	0
57	MG	RA	3319	1/1	0.72	0.84	111,111,111,111	0
57	MG	XA	1614	1/1	0.72	0.50	94,94,94,94	0
57	MG	YA	3301	1/1	0.72	0.34	80,80,80,80	0
57	MG	QA	1617	1/1	0.72	0.70	117,117,117,117	0
57	MG	YB	201	1/1	0.72	0.41	98,98,98,98	0
57	MG	YA	3362	1/1	0.72	0.82	100,100,100,100	0
57	MG	YO	201	1/1	0.72	0.25	62,62,62,62	0
57	MG	RA	3249	1/1	0.72	0.30	67,67,67,67	0
57	MG	YA	3426	1/1	0.73	0.29	104,104,104,104	0
57	MG	YA	3228	1/1	0.73	0.30	81,81,81,81	0
57	MG	QA	1704	1/1	0.73	0.23	90,90,90,90	0
57	MG	YG	202	1/1	0.73	0.26	79,79,79,79	0
57	MG	YA	3352	1/1	0.73	0.27	100,100,100,100	0
57	MG	RA	3112	1/1	0.73	0.27	120,120,120,120	0
57	MG	RA	3370	1/1	0.73	0.35	74,74,74,74	0
57	MG	YA	3244	1/1	0.74	0.19	79,79,79,79	0
57	MG	YA	3439	1/1	0.74	0.21	120,120,120,120	0
57	MG	YA	3444	1/1	0.74	0.52	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3250	1/1	0.74	0.78	86,86,86,86	0
57	MG	QA	1712	1/1	0.74	0.22	67,67,67,67	0
57	MG	RA	3184	1/1	0.74	0.32	70,70,70,70	0
57	MG	YA	3414	1/1	0.74	0.39	89,89,89,89	0
57	MG	YA	3349	1/1	0.74	0.23	103,103,103,103	0
57	MG	QA	1688	1/1	0.75	0.44	106,106,106,106	0
57	MG	QA	1638	1/1	0.75	0.43	83,83,83,83	0
57	MG	YA	3346	1/1	0.75	0.69	90,90,90,90	0
57	MG	YA	3274	1/1	0.75	0.26	81,81,81,81	0
57	MG	XA	1702	1/1	0.75	0.29	86,86,86,86	0
57	MG	YA	3162	1/1	0.75	0.54	75,75,75,75	0
57	MG	Y0	101	1/1	0.75	0.30	99,99,99,99	0
57	MG	YQ	202	1/1	0.75	0.48	100,100,100,100	0
57	MG	YX	101	1/1	0.75	0.55	149,149,149,149	0
57	MG	RI	201	1/1	0.75	0.19	129,129,129,129	0
57	MG	YA	3180	1/1	0.76	0.28	103,103,103,103	0
57	MG	YA	3312	1/1	0.76	0.60	100,100,100,100	0
57	MG	RA	3264	1/1	0.76	0.22	71,71,71,71	0
57	MG	QV	103	1/1	0.76	0.47	118,118,118,118	0
57	MG	RA	3272	1/1	0.76	0.36	115,115,115,115	0
57	MG	YA	3289	1/1	0.76	0.49	79,79,79,79	0
57	MG	QA	1723	1/1	0.76	0.30	123,123,123,123	0
57	MG	YA	3440	1/1	0.76	0.25	82,82,82,82	0
57	MG	QA	1667	1/1	0.77	0.39	71,71,71,71	0
57	MG	RA	3042	1/1	0.77	0.33	75,75,75,75	0
57	MG	RA	3079	1/1	0.77	0.28	89,89,89,89	0
57	MG	YE	304	1/1	0.77	0.20	112,112,112,112	0
57	MG	QA	1696	1/1	0.77	0.38	91,91,91,91	0
57	MG	YH	202	1/1	0.77	0.24	96,96,96,96	0
57	MG	YA	3236	1/1	0.77	0.21	86,86,86,86	0
57	MG	RA	3280	1/1	0.77	0.16	53,53,53,53	0
57	MG	RA	3290	1/1	0.77	0.36	89,89,89,89	0
57	MG	YA	3339	1/1	0.77	0.57	147,147,147,147	0
57	MG	YA	3363	1/1	0.77	0.23	97,97,97,97	0
57	MG	RA	3182	1/1	0.78	0.40	84,84,84,84	0
57	MG	RA	3010	1/1	0.78	0.51	103,103,103,103	0
57	MG	YA	3286	1/1	0.78	0.35	116,116,116,116	0
57	MG	QA	1725	1/1	0.78	0.96	107,107,107,107	0
57	MG	QA	1655	1/1	0.78	0.34	162,162,162,162	0
57	MG	RA	3191	1/1	0.78	0.27	68,68,68,68	0
57	MG	RA	3167	1/1	0.78	0.19	89,89,89,89	0
57	MG	YA	3320	1/1	0.78	0.39	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3241	1/1	0.78	0.42	93,93,93,93	0
57	MG	RA	3286	1/1	0.78	0.22	103,103,103,103	0
57	MG	QA	1676	1/1	0.79	0.36	75,75,75,75	0
57	MG	XA	1618	1/1	0.79	0.56	68,68,68,68	0
57	MG	XA	1706	1/1	0.79	0.19	133,133,133,133	0
57	MG	QA	1636	1/1	0.79	0.44	87,87,87,87	0
57	MG	YA	3141	1/1	0.79	0.43	129,129,129,129	0
57	MG	YA	3142	1/1	0.79	0.21	50,50,50,50	0
57	MG	YA	3248	1/1	0.79	0.57	107,107,107,107	0
57	MG	QA	1621	1/1	0.79	0.19	84,84,84,84	0
57	MG	RA	3291	1/1	0.79	0.35	80,80,80,80	0
57	MG	QA	1692	1/1	0.79	0.40	94,94,94,94	0
57	MG	RF	302	1/1	0.79	0.33	79,79,79,79	0
57	MG	RA	3152	1/1	0.79	0.39	64,64,64,64	0
57	MG	RA	3212	1/1	0.79	0.17	85,85,85,85	0
57	MG	XV	105	1/1	0.79	0.35	133,133,133,133	0
57	MG	RA	3098	1/1	0.79	0.54	96,96,96,96	0
57	MG	YA	3323	1/1	0.79	0.57	88,88,88,88	0
57	MG	RA	3063	1/1	0.80	0.38	55,55,55,55	0
57	MG	QA	1680	1/1	0.80	0.21	97,97,97,97	0
57	MG	XA	1644	1/1	0.80	0.29	73,73,73,73	0
57	MG	YA	3442	1/1	0.80	0.58	99,99,99,99	0
57	MG	XA	1645	1/1	0.80	0.25	79,79,79,79	0
57	MG	RA	3299	1/1	0.80	0.38	82,82,82,82	0
57	MG	QA	1607	1/1	0.80	0.15	28,28,28,28	0
57	MG	RB	203	1/1	0.80	0.25	69,69,69,69	0
57	MG	YA	3327	1/1	0.80	0.36	76,76,76,76	0
57	MG	RE	301	1/1	0.80	0.44	126,126,126,126	0
57	MG	RA	3305	1/1	0.80	0.32	80,80,80,80	0
57	MG	RA	3198	1/1	0.80	0.38	89,89,89,89	0
57	MG	QA	1656	1/1	0.80	0.46	103,103,103,103	0
57	MG	QA	1689	1/1	0.80	0.32	73,73,73,73	0
57	MG	RA	3068	1/1	0.81	0.39	90,90,90,90	0
57	MG	RA	3210	1/1	0.81	0.30	80,80,80,80	0
57	MG	XA	1693	1/1	0.81	0.55	87,87,87,87	0
57	MG	RA	3332	1/1	0.81	0.35	83,83,83,83	0
57	MG	RE	307	1/1	0.81	0.20	68,68,68,68	0
57	MG	YF	302	1/1	0.81	0.55	108,108,108,108	0
57	MG	RA	3340	1/1	0.81	0.36	78,78,78,78	0
57	MG	QA	1626	1/1	0.81	0.20	78,78,78,78	0
57	MG	YA	3008	1/1	0.81	0.29	80,80,80,80	0
57	MG	RR	201	1/1	0.81	0.21	121,121,121,121	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3050	1/1	0.81	0.45	76,76,76,76	0
57	MG	RA	3174	1/1	0.81	0.22	101,101,101,101	0
57	MG	QA	1673	1/1	0.81	0.23	96,96,96,96	0
57	MG	YA	3223	1/1	0.82	0.33	62,62,62,62	0
57	MG	RA	3188	1/1	0.82	0.15	111,111,111,111	0
57	MG	YA	3419	1/1	0.82	0.34	100,100,100,100	0
57	MG	QA	1613	1/1	0.82	0.36	71,71,71,71	0
57	MG	QA	1620	1/1	0.82	0.25	78,78,78,78	0
57	MG	YA	3240	1/1	0.82	0.24	104,104,104,104	0
57	MG	QA	1693	1/1	0.82	0.35	101,101,101,101	0
57	MG	XA	1671	1/1	0.82	0.20	48,48,48,48	0
57	MG	YA	3161	1/1	0.82	0.37	109,109,109,109	0
57	MG	QA	1632	1/1	0.82	0.24	105,105,105,105	0
57	MG	YB	204	1/1	0.82	0.08	28,28,28,28	0
57	MG	QA	1625	1/1	0.82	0.28	58,58,58,58	0
57	MG	RA	3176	1/1	0.82	0.54	76,76,76,76	0
57	MG	QK	201	1/1	0.82	0.32	138,138,138,138	0
57	MG	QA	1705	1/1	0.82	0.28	68,68,68,68	0
57	MG	YA	3365	1/1	0.82	0.33	78,78,78,78	0
57	MG	RA	3008	1/1	0.82	0.44	96,96,96,96	0
57	MG	YP	207	1/1	0.82	0.18	71,71,71,71	0
57	MG	QA	1637	1/1	0.82	0.24	64,64,64,64	0
57	MG	XA	1697	1/1	0.82	0.30	97,97,97,97	0
57	MG	XA	1643	1/1	0.82	0.28	100,100,100,100	0
57	MG	RA	3336	1/1	0.83	0.69	82,82,82,82	0
57	MG	YA	3188	1/1	0.83	0.28	86,86,86,86	0
57	MG	YA	3043	1/1	0.83	0.48	101,101,101,101	0
57	MG	YA	3048	1/1	0.83	0.14	17,17,17,17	0
57	MG	RG	201	1/1	0.83	0.27	81,81,81,81	0
57	MG	RA	3251	1/1	0.83	0.22	71,71,71,71	0
57	MG	YA	3293	1/1	0.83	0.26	48,48,48,48	0
57	MG	YA	3298	1/1	0.83	0.32	61,61,61,61	0
57	MG	QH	201	1/1	0.83	0.22	69,69,69,69	0
57	MG	YA	3115	1/1	0.83	0.35	74,74,74,74	0
57	MG	YA	3129	1/1	0.83	0.22	69,69,69,69	0
57	MG	YA	3175	1/1	0.83	0.30	101,101,101,101	0
57	MG	YA	3179	1/1	0.83	0.58	79,79,79,79	0
57	MG	RA	3077	1/1	0.84	0.46	60,60,60,60	0
57	MG	R8	101	1/1	0.84	0.17	39,39,39,39	0
57	MG	Y5	101	1/1	0.84	0.24	60,60,60,60	0
57	MG	YA	3428	1/1	0.84	0.52	72,72,72,72	0
57	MG	YA	3243	1/1	0.84	0.10	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
57	MG	RA	3204	1/1	0.84	0.25	72,72,72,72	0
57	MG	RA	3365	1/1	0.84	0.34	72,72,72,72	0
57	MG	YA	3266	1/1	0.84	0.49	83,83,83,83	0
57	MG	YA	3443	1/1	0.84	0.39	106,106,106,106	0
57	MG	QA	1677	1/1	0.84	0.23	66,66,66,66	0
57	MG	RA	3149	1/1	0.84	0.49	83,83,83,83	0
57	MG	RA	3377	1/1	0.84	0.54	73,73,73,73	0
57	MG	YB	206	1/1	0.84	0.30	91,91,91,91	0
57	MG	YB	208	1/1	0.84	0.46	114,114,114,114	0
57	MG	YA	3287	1/1	0.84	0.25	54,54,54,54	0
57	MG	RA	3209	1/1	0.84	0.26	44,44,44,44	0
57	MG	RA	3308	1/1	0.84	0.43	67,67,67,67	0
57	MG	QA	1678	1/1	0.84	0.35	55,55,55,55	0
57	MG	YH	204	1/1	0.84	0.12	103,103,103,103	0
57	MG	RA	3177	1/1	0.84	0.14	55,55,55,55	0
57	MG	RA	3330	1/1	0.84	0.37	64,64,64,64	0
57	MG	YA	3380	1/1	0.84	0.53	69,69,69,69	0
57	MG	RA	3193	1/1	0.84	0.09	63,63,63,63	0
57	MG	RA	3179	1/1	0.84	0.16	99,99,99,99	0
57	MG	YA	3155	1/1	0.84	0.26	49,49,49,49	0
57	MG	RA	3172	1/1	0.85	0.26	59,59,59,59	0
57	MG	QA	1630	1/1	0.85	0.21	61,61,61,61	0
57	MG	YA	3216	1/1	0.85	0.11	66,66,66,66	0
57	MG	XA	1624	1/1	0.85	0.25	45,45,45,45	0
57	MG	YA	3114	1/1	0.85	0.19	23,23,23,23	0
57	MG	XA	1635	1/1	0.85	0.37	73,73,73,73	0
57	MG	QA	1721	1/1	0.85	0.22	52,52,52,52	0
57	MG	QA	1601	1/1	0.85	0.53	107,107,107,107	0
57	MG	RA	3312	1/1	0.85	0.36	68,68,68,68	0
57	MG	YA	3149	1/1	0.85	0.15	30,30,30,30	0
57	MG	YB	203	1/1	0.85	0.17	62,62,62,62	0
57	MG	XA	1651	1/1	0.85	0.14	141,141,141,141	0
57	MG	XA	1663	1/1	0.85	0.28	75,75,75,75	0
57	MG	RA	3316	1/1	0.85	0.46	78,78,78,78	0
57	MG	QA	1650	1/1	0.85	0.15	50,50,50,50	0
57	MG	RE	306	1/1	0.85	0.22	40,40,40,40	0
57	MG	QA	1646	1/1	0.85	0.42	69,69,69,69	0
57	MG	QA	1697	1/1	0.85	0.25	79,79,79,79	0
57	MG	RA	3120	1/1	0.85	0.34	70,70,70,70	0
57	MG	RA	3295	1/1	0.85	0.35	88,88,88,88	0
57	MG	YA	3295	1/1	0.85	0.39	71,71,71,71	0
57	MG	YA	3297	1/1	0.85	0.23	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3171	1/1	0.85	0.56	81,81,81,81	0
57	MG	RA	3300	1/1	0.85	0.23	67,67,67,67	0
57	MG	RA	3356	1/1	0.85	0.32	101,101,101,101	0
57	MG	YA	3445	1/1	0.86	0.45	68,68,68,68	0
57	MG	YA	3452	1/1	0.86	0.29	100,100,100,100	0
57	MG	XF	301	1/1	0.86	0.25	64,64,64,64	0
57	MG	RA	3238	1/1	0.86	0.29	117,117,117,117	0
57	MG	YA	3336	1/1	0.86	0.13	42,42,42,42	0
57	MG	XA	1612	1/1	0.86	0.23	53,53,53,53	0
57	MG	RA	3298	1/1	0.86	0.15	36,36,36,36	0
57	MG	YD	302	1/1	0.86	0.39	97,97,97,97	0
57	MG	QA	1701	1/1	0.86	0.17	75,75,75,75	0
57	MG	QA	1639	1/1	0.86	0.46	73,73,73,73	0
57	MG	YA	3127	1/1	0.86	0.36	51,51,51,51	0
57	MG	XA	1629	1/1	0.86	0.16	73,73,73,73	0
57	MG	YA	3131	1/1	0.86	0.25	60,60,60,60	0
57	MG	YA	3355	1/1	0.86	0.49	95,95,95,95	0
57	MG	RA	3181	1/1	0.86	0.31	88,88,88,88	0
57	MG	YA	3357	1/1	0.86	0.21	73,73,73,73	0
57	MG	RA	3213	1/1	0.86	0.23	86,86,86,86	0
57	MG	YQ	203	1/1	0.86	0.45	102,102,102,102	0
57	MG	RA	3219	1/1	0.86	0.52	159,159,159,159	0
57	MG	QA	1648	1/1	0.86	0.18	69,69,69,69	0
61	AMP	QY	101	22/23	0.86	0.18	121,122,134,149	0
57	MG	RA	3375	1/1	0.87	0.30	83,83,83,83	0
57	MG	YA	3232	1/1	0.87	0.20	83,83,83,83	0
57	MG	QA	1708	1/1	0.87	0.38	79,79,79,79	0
57	MG	QA	1643	1/1	0.87	0.15	63,63,63,63	0
57	MG	RA	3072	1/1	0.87	0.13	36,36,36,36	0
57	MG	YA	3375	1/1	0.87	0.51	75,75,75,75	0
57	MG	YA	3376	1/1	0.87	0.21	57,57,57,57	0
57	MG	RE	305	1/1	0.87	0.21	54,54,54,54	0
57	MG	XA	1683	1/1	0.87	0.24	72,72,72,72	0
57	MG	RA	3310	1/1	0.87	0.19	74,74,74,74	0
57	MG	YA	3388	1/1	0.87	0.31	75,75,75,75	0
57	MG	YA	3262	1/1	0.87	0.31	37,37,37,37	0
57	MG	QA	1669	1/1	0.87	0.19	48,48,48,48	0
57	MG	YA	3118	1/1	0.87	0.34	86,86,86,86	0
57	MG	RA	3313	1/1	0.87	0.23	70,70,70,70	0
57	MG	YA	3420	1/1	0.87	0.24	48,48,48,48	0
57	MG	YA	3282	1/1	0.87	0.24	57,57,57,57	0
57	MG	QA	1682	1/1	0.87	0.53	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3429	1/1	0.87	0.16	48,48,48,48	0
57	MG	YA	3431	1/1	0.87	0.29	79,79,79,79	0
57	MG	RA	3202	1/1	0.87	0.33	86,86,86,86	0
57	MG	RA	3087	1/1	0.87	0.09	35,35,35,35	0
57	MG	RA	3328	1/1	0.87	0.19	63,63,63,63	0
57	MG	QA	1717	1/1	0.87	0.23	69,69,69,69	0
57	MG	QA	1695	1/1	0.87	0.38	89,89,89,89	0
57	MG	RA	3114	1/1	0.87	0.21	62,62,62,62	0
57	MG	RA	3009	1/1	0.87	0.10	43,43,43,43	0
57	MG	YA	3446	1/1	0.87	0.33	75,75,75,75	0
57	MG	QA	1722	1/1	0.87	0.09	122,122,122,122	0
57	MG	RA	3351	1/1	0.87	0.15	58,58,58,58	0
57	MG	YB	202	1/1	0.87	0.44	57,57,57,57	0
57	MG	YA	3315	1/1	0.87	0.66	100,100,100,100	0
57	MG	QA	1608	1/1	0.87	0.18	63,63,63,63	0
57	MG	XA	1637	1/1	0.87	0.08	43,43,43,43	0
57	MG	XA	1638	1/1	0.87	0.08	55,55,55,55	0
57	MG	RA	3358	1/1	0.87	0.13	91,91,91,91	0
57	MG	YA	3328	1/1	0.87	0.32	46,46,46,46	0
57	MG	RA	3130	1/1	0.87	0.26	53,53,53,53	0
57	MG	YA	3182	1/1	0.87	0.10	14,14,14,14	0
57	MG	XV	106	1/1	0.87	0.35	90,90,90,90	0
57	MG	YA	3189	1/1	0.87	0.31	71,71,71,71	0
57	MG	YA	3344	1/1	0.87	0.28	72,72,72,72	0
57	MG	XX	101	1/1	0.87	0.28	65,65,65,65	0
57	MG	RA	3051	1/1	0.87	0.17	12,12,12,12	0
57	MG	Y4	101	1/1	0.87	0.16	103,103,103,103	0
57	MG	YA	3204	1/1	0.87	0.32	75,75,75,75	0
57	MG	RA	3147	1/1	0.87	0.36	58,58,58,58	0
57	MG	YY	202	1/1	0.87	0.28	147,147,147,147	0
57	MG	XA	1656	1/1	0.87	0.38	59,59,59,59	0
57	MG	RA	3060	1/1	0.87	0.21	80,80,80,80	0
57	MG	YA	3009	1/1	0.88	0.26	39,39,39,39	0
57	MG	YA	3195	1/1	0.88	0.40	54,54,54,54	0
57	MG	RA	3190	1/1	0.88	0.19	121,121,121,121	0
57	MG	XA	1620	1/1	0.88	0.23	79,79,79,79	0
57	MG	RA	3150	1/1	0.88	0.32	92,92,92,92	0
57	MG	XA	1695	1/1	0.88	0.26	75,75,75,75	0
57	MG	YA	3072	1/1	0.88	0.32	90,90,90,90	0
57	MG	RA	3192	1/1	0.88	0.67	88,88,88,88	0
57	MG	XA	1630	1/1	0.88	0.14	37,37,37,37	0
57	MG	RA	3007	1/1	0.88	0.06	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3218	1/1	0.88	0.15	69,69,69,69	0
57	MG	YA	3117	1/1	0.88	0.54	80,80,80,80	0
57	MG	XA	1708	1/1	0.88	0.24	69,69,69,69	0
57	MG	RA	3284	1/1	0.88	0.46	86,86,86,86	0
57	MG	RB	204	1/1	0.88	0.23	54,54,54,54	0
57	MG	RA	3062	1/1	0.88	0.54	86,86,86,86	0
57	MG	RA	3287	1/1	0.88	0.24	83,83,83,83	0
57	MG	XA	1721	1/1	0.88	0.29	58,58,58,58	0
57	MG	RA	3164	1/1	0.88	0.11	35,35,35,35	0
57	MG	RA	3227	1/1	0.88	0.56	80,80,80,80	0
57	MG	RA	3135	1/1	0.88	0.11	79,79,79,79	0
57	MG	YF	301	1/1	0.88	0.15	49,49,49,49	0
57	MG	XV	102	1/1	0.88	0.37	83,83,83,83	0
57	MG	YG	201	1/1	0.88	0.23	60,60,60,60	0
57	MG	RA	3240	1/1	0.88	0.28	59,59,59,59	0
57	MG	QA	1635	1/1	0.88	0.42	62,62,62,62	0
57	MG	YA	3292	1/1	0.88	0.24	55,55,55,55	0
57	MG	XA	1669	1/1	0.88	0.37	64,64,64,64	0
57	MG	RA	3146	1/1	0.88	0.14	62,62,62,62	0
57	MG	XA	1606	1/1	0.88	0.29	37,37,37,37	0
57	MG	YA	3396	1/1	0.88	0.29	108,108,108,108	0
57	MG	Y2	101	1/1	0.88	0.11	50,50,50,50	0
57	MG	RA	3083	1/1	0.88	0.14	46,46,46,46	0
57	MG	RA	3253	1/1	0.88	0.37	80,80,80,80	0
57	MG	RA	3303	1/1	0.88	0.51	104,104,104,104	0
57	MG	QA	1687	1/1	0.88	0.17	75,75,75,75	0
57	MG	RA	3082	1/1	0.89	0.29	41,41,41,41	0
57	MG	XA	1713	1/1	0.89	0.23	67,67,67,67	0
57	MG	YA	3314	1/1	0.89	0.35	83,83,83,83	0
57	MG	RA	3180	1/1	0.89	0.29	51,51,51,51	0
57	MG	RA	3232	1/1	0.89	0.23	68,68,68,68	0
57	MG	YA	3322	1/1	0.89	0.08	74,74,74,74	0
57	MG	YA	3205	1/1	0.89	0.17	66,66,66,66	0
57	MG	YA	3116	1/1	0.89	0.18	44,44,44,44	0
57	MG	YA	3220	1/1	0.89	0.11	41,41,41,41	0
57	MG	QA	1684	1/1	0.89	0.18	59,59,59,59	0
57	MG	XA	1623	1/1	0.89	0.15	51,51,51,51	0
57	MG	YA	3334	1/1	0.89	0.42	85,85,85,85	0
57	MG	YA	3229	1/1	0.89	0.20	28,28,28,28	0
57	MG	YA	3122	1/1	0.89	0.44	74,74,74,74	0
57	MG	YA	3341	1/1	0.89	0.35	100,100,100,100	0
57	MG	XA	1675	1/1	0.89	0.21	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1602	1/1	0.89	0.53	86,86,86,86	0
57	MG	YA	3237	1/1	0.89	0.31	92,92,92,92	0
57	MG	YA	3239	1/1	0.89	0.11	48,48,48,48	0
57	MG	RA	3281	1/1	0.89	0.22	36,36,36,36	0
57	MG	QA	1628	1/1	0.89	0.41	71,71,71,71	0
57	MG	XA	1690	1/1	0.89	0.29	60,60,60,60	0
57	MG	XA	1631	1/1	0.89	0.26	57,57,57,57	0
57	MG	XA	1634	1/1	0.89	0.12	79,79,79,79	0
57	MG	QA	1683	1/1	0.89	0.08	31,31,31,31	0
57	MG	Y2	102	1/1	0.89	0.34	53,53,53,53	0
57	MG	RA	3309	1/1	0.89	0.34	53,53,53,53	0
57	MG	QL	201	1/1	0.89	0.08	24,24,24,24	0
57	MG	XA	1639	1/1	0.89	0.23	68,68,68,68	0
57	MG	RA	3252	1/1	0.89	0.27	73,73,73,73	0
57	MG	RA	3364	1/1	0.89	0.40	62,62,62,62	0
57	MG	XA	1704	1/1	0.89	0.22	56,56,56,56	0
57	MG	YP	201	1/1	0.89	0.22	35,35,35,35	0
57	MG	YA	3020	1/1	0.89	0.33	72,72,72,72	0
57	MG	RR	202	1/1	0.89	0.17	38,38,38,38	0
57	MG	YA	3183	1/1	0.89	0.15	60,60,60,60	0
57	MG	YU	201	1/1	0.89	0.17	59,59,59,59	0
57	MG	YA	3395	1/1	0.89	0.17	54,54,54,54	0
57	MG	RA	3199	1/1	0.89	0.12	43,43,43,43	0
57	MG	RA	3144	1/1	0.89	0.17	35,35,35,35	0
57	MG	RA	3262	1/1	0.89	0.06	49,49,49,49	0
57	MG	QA	1675	1/1	0.90	0.46	97,97,97,97	0
57	MG	RA	3334	1/1	0.90	0.31	68,68,68,68	0
57	MG	YA	3387	1/1	0.90	0.09	22,22,22,22	0
57	MG	XA	1684	1/1	0.90	0.23	41,41,41,41	0
57	MG	RA	3335	1/1	0.90	0.44	68,68,68,68	0
57	MG	RA	3054	1/1	0.90	0.34	79,79,79,79	0
57	MG	QA	1634	1/1	0.90	0.14	92,92,92,92	0
57	MG	YA	3404	1/1	0.90	0.34	67,67,67,67	0
57	MG	RA	3341	1/1	0.90	0.42	104,104,104,104	0
57	MG	RA	3104	1/1	0.90	0.07	58,58,58,58	0
57	MG	RA	3111	1/1	0.90	0.31	81,81,81,81	0
57	MG	YA	3309	1/1	0.90	0.17	47,47,47,47	0
57	MG	YA	3421	1/1	0.90	0.33	82,82,82,82	0
57	MG	RA	3352	1/1	0.90	0.25	90,90,90,90	0
57	MG	R9	101	1/1	0.90	0.29	98,98,98,98	0
57	MG	XA	1700	1/1	0.90	0.21	68,68,68,68	0
57	MG	YA	3070	1/1	0.90	0.02	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3434	1/1	0.90	0.39	66,66,66,66	0
57	MG	RA	3301	1/1	0.90	0.29	50,50,50,50	0
57	MG	YA	3215	1/1	0.90	0.21	96,96,96,96	0
57	MG	YA	3077	1/1	0.90	0.13	12,12,12,12	0
57	MG	YA	3218	1/1	0.90	0.12	63,63,63,63	0
57	MG	QA	1691	1/1	0.90	0.15	89,89,89,89	0
57	MG	QA	1660	1/1	0.90	0.12	119,119,119,119	0
57	MG	RA	3211	1/1	0.90	0.20	72,72,72,72	0
57	MG	RA	3162	1/1	0.90	0.27	95,95,95,95	0
57	MG	YA	3451	1/1	0.90	0.34	55,55,55,55	0
57	MG	RA	3116	1/1	0.90	0.18	43,43,43,43	0
57	MG	RA	3273	1/1	0.90	0.10	44,44,44,44	0
57	MG	RA	3275	1/1	0.90	0.40	74,74,74,74	0
57	MG	YA	3343	1/1	0.90	0.22	77,77,77,77	0
57	MG	RA	3311	1/1	0.90	0.14	50,50,50,50	0
57	MG	YA	3238	1/1	0.90	0.17	66,66,66,66	0
57	MG	RA	3117	1/1	0.90	0.46	63,63,63,63	0
57	MG	QA	1624	1/1	0.90	0.27	82,82,82,82	0
57	MG	YE	301	1/1	0.90	0.11	21,21,21,21	0
57	MG	RA	3314	1/1	0.90	0.20	59,59,59,59	0
57	MG	XA	1662	1/1	0.90	0.21	88,88,88,88	0
57	MG	YA	3354	1/1	0.90	0.14	60,60,60,60	0
57	MG	RA	3169	1/1	0.90	0.13	69,69,69,69	0
57	MG	RA	3317	1/1	0.90	0.23	46,46,46,46	0
57	MG	YH	201	1/1	0.90	0.13	29,29,29,29	0
57	MG	YA	3259	1/1	0.90	0.42	66,66,66,66	0
57	MG	YA	3358	1/1	0.90	0.16	64,64,64,64	0
57	MG	QA	1674	1/1	0.90	0.46	85,85,85,85	0
57	MG	YA	3263	1/1	0.90	0.27	48,48,48,48	0
57	MG	RA	3019	1/1	0.90	0.17	30,30,30,30	0
57	MG	YA	3366	1/1	0.90	0.19	63,63,63,63	0
57	MG	YA	3367	1/1	0.90	0.42	96,96,96,96	0
57	MG	RA	3326	1/1	0.90	0.07	32,32,32,32	0
57	MG	YA	3370	1/1	0.90	0.19	70,70,70,70	0
57	MG	YA	3374	1/1	0.90	0.51	84,84,84,84	0
57	MG	YY	201	1/1	0.90	0.19	54,54,54,54	0
57	MG	RA	3236	1/1	0.90	0.09	40,40,40,40	0
57	MG	QV	102	1/1	0.90	0.28	78,78,78,78	0
57	MG	Y0	103	1/1	0.90	0.23	118,118,118,118	0
57	MG	YA	3302	1/1	0.91	0.29	60,60,60,60	0
57	MG	RA	3134	1/1	0.91	0.15	32,32,32,32	0
57	MG	RA	3254	1/1	0.91	0.23	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3010	1/1	0.91	0.10	20,20,20,20	0
57	MG	RB	202	1/1	0.91	0.15	55,55,55,55	0
57	MG	RA	3327	1/1	0.91	0.27	12,12,12,12	0
57	MG	YA	3318	1/1	0.91	0.17	30,30,30,30	0
57	MG	YA	3424	1/1	0.91	0.28	110,110,110,110	0
57	MG	YA	3319	1/1	0.91	0.35	57,57,57,57	0
57	MG	QA	1699	1/1	0.91	0.56	91,91,91,91	0
57	MG	QA	1690	1/1	0.91	0.23	51,51,51,51	0
57	MG	YA	3430	1/1	0.91	0.31	149,149,149,149	0
57	MG	RA	3106	1/1	0.91	0.09	33,33,33,33	0
57	MG	RA	3333	1/1	0.91	0.26	63,63,63,63	0
57	MG	RA	3145	1/1	0.91	0.23	66,66,66,66	0
57	MG	YA	3075	1/1	0.91	0.51	70,70,70,70	0
57	MG	RA	3173	1/1	0.91	0.30	81,81,81,81	0
57	MG	YA	3096	1/1	0.91	0.29	35,35,35,35	0
57	MG	XA	1646	1/1	0.91	0.21	68,68,68,68	0
57	MG	YA	3338	1/1	0.91	0.17	54,54,54,54	0
57	MG	QA	1719	1/1	0.91	0.30	51,51,51,51	0
57	MG	RA	3337	1/1	0.91	0.09	34,34,34,34	0
57	MG	YA	3450	1/1	0.91	0.20	43,43,43,43	0
57	MG	XA	1659	1/1	0.91	0.07	40,40,40,40	0
57	MG	RP	202	1/1	0.91	0.16	96,96,96,96	0
57	MG	RA	3121	1/1	0.91	0.13	25,25,25,25	0
57	MG	XB	301	1/1	0.91	0.22	96,96,96,96	0
57	MG	RA	3122	1/1	0.91	0.19	51,51,51,51	0
57	MG	YA	3124	1/1	0.91	0.25	25,25,25,25	0
57	MG	YA	3125	1/1	0.91	0.15	32,32,32,32	0
57	MG	XK	201	1/1	0.91	0.09	35,35,35,35	0
57	MG	RA	3124	1/1	0.91	0.15	47,47,47,47	0
57	MG	XA	1607	1/1	0.91	0.15	59,59,59,59	0
57	MG	RA	3200	1/1	0.91	0.23	55,55,55,55	0
57	MG	YE	305	1/1	0.91	0.13	89,89,89,89	0
57	MG	YA	3249	1/1	0.91	0.24	33,33,33,33	0
57	MG	XA	1673	1/1	0.91	0.64	60,60,60,60	0
57	MG	QA	1702	1/1	0.91	0.10	50,50,50,50	0
57	MG	RA	3285	1/1	0.91	0.19	56,56,56,56	0
57	MG	YA	3160	1/1	0.91	0.19	34,34,34,34	0
57	MG	RA	3247	1/1	0.91	0.24	44,44,44,44	0
57	MG	YA	3280	1/1	0.91	0.44	50,50,50,50	0
57	MG	RA	3153	1/1	0.91	0.39	52,52,52,52	0
57	MG	RA	3127	1/1	0.91	0.27	95,95,95,95	0
57	MG	XA	1685	1/1	0.91	0.23	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1622	1/1	0.91	0.16	49,49,49,49	0
57	MG	RA	3096	1/1	0.91	0.08	25,25,25,25	0
57	MG	YA	3174	1/1	0.91	0.15	38,38,38,38	0
57	MG	RA	3132	1/1	0.91	0.36	79,79,79,79	0
57	MG	YA	3294	1/1	0.91	0.61	64,64,64,64	0
57	MG	Y8	102	1/1	0.91	0.21	106,106,106,106	0
57	MG	YA	3001	1/1	0.91	0.28	119,119,119,119	0
57	MG	YA	3181	1/1	0.91	0.20	54,54,54,54	0
57	MG	RA	3320	1/1	0.91	0.54	111,111,111,111	0
57	MG	RA	3186	1/1	0.92	0.07	28,28,28,28	0
57	MG	XA	1718	1/1	0.92	0.27	53,53,53,53	0
57	MG	QA	1651	1/1	0.92	0.18	64,64,64,64	0
57	MG	YA	3340	1/1	0.92	0.17	74,74,74,74	0
57	MG	RA	3207	1/1	0.92	0.19	61,61,61,61	0
57	MG	YA	3055	1/1	0.92	0.44	94,94,94,94	0
57	MG	YA	3059	1/1	0.92	0.22	41,41,41,41	0
57	MG	QA	1622	1/1	0.92	0.15	62,62,62,62	0
57	MG	XA	1676	1/1	0.92	0.45	60,60,60,60	0
57	MG	RA	3085	1/1	0.92	0.25	62,62,62,62	0
57	MG	XA	1633	1/1	0.92	0.15	39,39,39,39	0
57	MG	RA	3086	1/1	0.92	0.07	23,23,23,23	0
57	MG	RA	3342	1/1	0.92	0.16	33,33,33,33	0
57	MG	YA	3285	1/1	0.92	0.24	37,37,37,37	0
57	MG	QA	1604	1/1	0.92	0.13	16,16,16,16	0
57	MG	RA	3043	1/1	0.92	0.10	20,20,20,20	0
57	MG	YA	3288	1/1	0.92	0.28	57,57,57,57	0
57	MG	YA	3194	1/1	0.92	0.26	101,101,101,101	0
57	MG	RA	3318	1/1	0.92	0.15	77,77,77,77	0
57	MG	YA	3196	1/1	0.92	0.18	34,34,34,34	0
57	MG	RA	3217	1/1	0.92	0.13	43,43,43,43	0
57	MG	RA	3119	1/1	0.92	0.14	54,54,54,54	0
57	MG	YA	3296	1/1	0.92	0.36	78,78,78,78	0
57	MG	RA	3359	1/1	0.92	0.15	41,41,41,41	0
57	MG	YA	3120	1/1	0.92	0.08	27,27,27,27	0
57	MG	YE	303	1/1	0.92	0.06	38,38,38,38	0
57	MG	YA	3208	1/1	0.92	0.24	113,113,113,113	0
57	MG	YA	3210	1/1	0.92	0.10	50,50,50,50	0
57	MG	RA	3160	1/1	0.92	0.27	61,61,61,61	0
57	MG	XA	1650	1/1	0.92	0.17	65,65,65,65	0
57	MG	RA	3142	1/1	0.92	0.30	65,65,65,65	0
57	MG	YA	3126	1/1	0.92	0.32	56,56,56,56	0
57	MG	XA	1655	1/1	0.92	0.22	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3048	1/1	0.92	0.28	53,53,53,53	0
57	MG	YA	3389	1/1	0.92	0.21	16,16,16,16	0
57	MG	QA	1716	1/1	0.92	0.09	40,40,40,40	0
57	MG	YA	3133	1/1	0.92	0.09	29,29,29,29	0
57	MG	RA	3368	1/1	0.92	0.07	30,30,30,30	0
57	MG	YA	3402	1/1	0.92	0.13	49,49,49,49	0
57	MG	QA	1670	1/1	0.92	0.14	44,44,44,44	0
57	MG	YA	3408	1/1	0.92	0.16	67,67,67,67	0
57	MG	YT	201	1/1	0.92	0.16	79,79,79,79	0
57	MG	RA	3203	1/1	0.92	0.06	37,37,37,37	0
57	MG	YV	301	1/1	0.92	0.10	59,59,59,59	0
57	MG	YW	201	1/1	0.92	0.17	61,61,61,61	0
57	MG	RA	3168	1/1	0.92	0.12	36,36,36,36	0
57	MG	RA	3378	1/1	0.92	0.36	81,81,81,81	0
57	MG	YA	3017	1/1	0.92	0.21	12,12,12,12	0
57	MG	YA	3019	1/1	0.92	0.12	28,28,28,28	0
57	MG	YA	3335	1/1	0.92	0.08	18,18,18,18	0
57	MG	RE	308	1/1	0.93	0.07	69,69,69,69	0
57	MG	YA	3173	1/1	0.93	0.07	60,60,60,60	0
57	MG	YA	3291	1/1	0.93	0.08	28,28,28,28	0
57	MG	YA	3394	1/1	0.93	0.07	42,42,42,42	0
57	MG	RA	3141	1/1	0.93	0.14	33,33,33,33	0
57	MG	XA	1699	1/1	0.93	0.25	51,51,51,51	0
57	MG	YA	3176	1/1	0.93	0.39	76,76,76,76	0
57	MG	YA	3178	1/1	0.93	0.44	83,83,83,83	0
57	MG	RA	3109	1/1	0.93	0.13	12,12,12,12	0
57	MG	QA	1698	1/1	0.93	0.19	53,53,53,53	0
57	MG	XA	1648	1/1	0.93	0.14	53,53,53,53	0
57	MG	YA	3031	1/1	0.93	0.12	44,44,44,44	0
57	MG	XA	1649	1/1	0.93	0.40	68,68,68,68	0
57	MG	YA	3304	1/1	0.93	0.06	24,24,24,24	0
57	MG	RA	3214	1/1	0.93	0.10	55,55,55,55	0
57	MG	RA	3289	1/1	0.93	0.38	85,85,85,85	0
57	MG	YA	3425	1/1	0.93	0.23	121,121,121,121	0
57	MG	YA	3190	1/1	0.93	0.15	41,41,41,41	0
57	MG	YA	3313	1/1	0.93	0.28	51,51,51,51	0
57	MG	XA	1709	1/1	0.93	0.35	77,77,77,77	0
57	MG	XA	1654	1/1	0.93	0.15	50,50,50,50	0
57	MG	YA	3067	1/1	0.93	0.13	34,34,34,34	0
57	MG	QA	1715	1/1	0.93	0.19	63,63,63,63	0
57	MG	YA	3436	1/1	0.93	0.20	54,54,54,54	0
57	MG	RA	3001	1/1	0.93	0.11	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3073	1/1	0.93	0.21	18,18,18,18	0
57	MG	RA	3293	1/1	0.93	0.25	71,71,71,71	0
57	MG	RA	3052	1/1	0.93	0.23	50,50,50,50	0
57	MG	YA	3325	1/1	0.93	0.35	66,66,66,66	0
57	MG	YA	3093	1/1	0.93	0.15	12,12,12,12	0
57	MG	XA	1609	1/1	0.93	0.21	42,42,42,42	0
57	MG	YA	3097	1/1	0.93	0.05	12,12,12,12	0
57	MG	RA	3321	1/1	0.93	0.14	85,85,85,85	0
57	MG	XA	1667	1/1	0.93	0.16	51,51,51,51	0
57	MG	XB	302	1/1	0.93	0.09	80,80,80,80	0
57	MG	YA	3455	1/1	0.93	0.24	52,52,52,52	0
57	MG	RA	3224	1/1	0.93	0.24	48,48,48,48	0
57	MG	XJ	301	1/1	0.93	0.13	55,55,55,55	0
57	MG	RA	3012	1/1	0.93	0.11	33,33,33,33	0
57	MG	YA	3230	1/1	0.93	0.10	31,31,31,31	0
57	MG	XL	202	1/1	0.93	0.16	27,27,27,27	0
57	MG	RA	3268	1/1	0.93	0.21	49,49,49,49	0
57	MG	RA	3369	1/1	0.93	0.14	33,33,33,33	0
57	MG	RA	3002	1/1	0.93	0.21	56,56,56,56	0
57	MG	RA	3371	1/1	0.93	0.32	84,84,84,84	0
57	MG	RA	3133	1/1	0.93	0.27	44,44,44,44	0
57	MG	RA	3331	1/1	0.93	0.07	56,56,56,56	0
57	MG	YA	3351	1/1	0.93	0.26	68,68,68,68	0
57	MG	QV	104	1/1	0.93	0.14	54,54,54,54	0
57	MG	RA	3108	1/1	0.93	0.17	74,74,74,74	0
57	MG	YA	3132	1/1	0.93	0.18	51,51,51,51	0
57	MG	RA	3276	1/1	0.93	0.27	58,58,58,58	0
57	MG	XA	1687	1/1	0.93	0.17	42,42,42,42	0
57	MG	XA	1688	1/1	0.93	0.15	38,38,38,38	0
57	MG	YA	3147	1/1	0.93	0.10	34,34,34,34	0
57	MG	Y3	101	1/1	0.93	0.20	119,119,119,119	0
57	MG	YA	3265	1/1	0.93	0.10	31,31,31,31	0
57	MG	YA	3151	1/1	0.93	0.19	62,62,62,62	0
57	MG	YA	3269	1/1	0.93	0.07	27,27,27,27	0
57	MG	RA	3140	1/1	0.93	0.10	25,25,25,25	0
57	MG	RA	3279	1/1	0.93	0.15	64,64,64,64	0
57	MG	RA	3243	1/1	0.93	0.28	60,60,60,60	0
57	MG	RA	3339	1/1	0.93	0.08	22,22,22,22	0
57	MG	YA	3284	1/1	0.93	0.30	52,52,52,52	0
57	MG	RA	3158	1/1	0.93	0.25	57,57,57,57	0
57	MG	YX	102	1/1	0.93	0.11	55,55,55,55	0
57	MG	YA	3005	1/1	0.93	0.18	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1641	1/1	0.93	0.18	40,40,40,40	0
57	MG	YA	3385	1/1	0.93	0.07	19,19,19,19	0
57	MG	YA	3386	1/1	0.93	0.16	41,41,41,41	0
57	MG	YA	3390	1/1	0.94	0.20	65,65,65,65	0
57	MG	XA	1657	1/1	0.94	0.21	44,44,44,44	0
57	MG	RA	3229	1/1	0.94	0.24	62,62,62,62	0
57	MG	XA	1661	1/1	0.94	0.13	57,57,57,57	0
57	MG	YA	3398	1/1	0.94	0.15	36,36,36,36	0
57	MG	XA	1714	1/1	0.94	0.27	61,61,61,61	0
57	MG	YA	3068	1/1	0.94	0.17	25,25,25,25	0
57	MG	YA	3184	1/1	0.94	0.20	82,82,82,82	0
57	MG	XA	1715	1/1	0.94	0.20	62,62,62,62	0
57	MG	YA	3410	1/1	0.94	0.24	73,73,73,73	0
57	MG	YA	3412	1/1	0.94	0.14	80,80,80,80	0
57	MG	RA	3231	1/1	0.94	0.06	13,13,13,13	0
57	MG	YA	3303	1/1	0.94	0.34	52,52,52,52	0
57	MG	YA	3415	1/1	0.94	0.17	53,53,53,53	0
57	MG	XA	1719	1/1	0.94	0.24	48,48,48,48	0
57	MG	RA	3353	1/1	0.94	0.22	159,159,159,159	0
57	MG	YA	3076	1/1	0.94	0.18	12,12,12,12	0
57	MG	YA	3422	1/1	0.94	0.13	62,62,62,62	0
57	MG	XA	1664	1/1	0.94	0.14	75,75,75,75	0
57	MG	QA	1640	1/1	0.94	0.16	47,47,47,47	0
57	MG	RA	3278	1/1	0.94	0.15	59,59,59,59	0
57	MG	RA	3011	1/1	0.94	0.36	57,57,57,57	0
57	MG	YA	3101	1/1	0.94	0.18	32,32,32,32	0
57	MG	YA	3102	1/1	0.94	0.08	36,36,36,36	0
57	MG	RA	3360	1/1	0.94	0.17	59,59,59,59	0
57	MG	YA	3433	1/1	0.94	0.52	80,80,80,80	0
57	MG	YA	3106	1/1	0.94	0.11	12,12,12,12	0
57	MG	RA	3237	1/1	0.94	0.06	18,18,18,18	0
57	MG	QA	1652	1/1	0.94	0.18	62,62,62,62	0
57	MG	YA	3438	1/1	0.94	0.08	18,18,18,18	0
57	MG	QA	1679	1/1	0.94	0.34	70,70,70,70	0
57	MG	RA	3241	1/1	0.94	0.20	33,33,33,33	0
57	MG	YA	3221	1/1	0.94	0.12	15,15,15,15	0
57	MG	YA	3329	1/1	0.94	0.14	44,44,44,44	0
57	MG	YA	3330	1/1	0.94	0.16	56,56,56,56	0
57	MG	RA	3242	1/1	0.94	0.19	35,35,35,35	0
57	MG	RA	3093	1/1	0.94	0.23	40,40,40,40	0
57	MG	YA	3447	1/1	0.94	0.27	37,37,37,37	0
57	MG	RA	3288	1/1	0.94	0.07	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
57	MG	YA	3121	1/1	0.94	0.07	29,29,29,29	0
57	MG	RA	3024	1/1	0.94	0.12	20,20,20,20	0
57	MG	YA	3123	1/1	0.94	0.26	44,44,44,44	0
57	MG	RA	3097	1/1	0.94	0.09	27,27,27,27	0
57	MG	RA	3041	1/1	0.94	0.21	33,33,33,33	0
57	MG	RA	3170	1/1	0.94	0.18	71,71,71,71	0
57	MG	RA	3099	1/1	0.94	0.11	27,27,27,27	0
57	MG	QA	1614	1/1	0.94	0.18	37,37,37,37	0
57	MG	RA	3297	1/1	0.94	0.05	41,41,41,41	0
57	MG	RA	3105	1/1	0.94	0.17	30,30,30,30	0
57	MG	RA	3194	1/1	0.94	0.23	62,62,62,62	0
57	MG	Y7	101	1/1	0.94	0.09	51,51,51,51	0
57	MG	QA	1700	1/1	0.94	0.31	50,50,50,50	0
57	MG	YA	3252	1/1	0.94	0.21	64,64,64,64	0
57	MG	YA	3254	1/1	0.94	0.30	55,55,55,55	0
57	MG	YA	3257	1/1	0.94	0.16	27,27,27,27	0
57	MG	YF	304	1/1	0.94	0.29	85,85,85,85	0
57	MG	RA	3175	1/1	0.94	0.15	51,51,51,51	0
57	MG	YA	3148	1/1	0.94	0.11	65,65,65,65	0
57	MG	XA	1696	1/1	0.94	0.13	70,70,70,70	0
57	MG	RA	3267	1/1	0.94	0.18	54,54,54,54	0
57	MG	YH	203	1/1	0.94	0.14	89,89,89,89	0
57	MG	XA	1698	1/1	0.94	0.15	43,43,43,43	0
57	MG	RF	301	1/1	0.94	0.05	21,21,21,21	0
57	MG	YI	201	1/1	0.94	0.08	69,69,69,69	0
57	MG	YA	3273	1/1	0.94	0.30	53,53,53,53	0
57	MG	RA	3220	1/1	0.94	0.19	44,44,44,44	0
57	MG	YA	3277	1/1	0.94	0.22	58,58,58,58	0
57	MG	YA	3279	1/1	0.94	0.16	48,48,48,48	0
57	MG	RA	3078	1/1	0.94	0.13	19,19,19,19	0
57	MG	YA	3163	1/1	0.94	0.12	35,35,35,35	0
57	MG	RA	3306	1/1	0.94	0.26	53,53,53,53	0
57	MG	YA	3018	1/1	0.94	0.18	36,36,36,36	0
57	MG	XA	1652	1/1	0.94	0.24	55,55,55,55	0
57	MG	XA	1653	1/1	0.94	0.08	36,36,36,36	0
57	MG	YA	3027	1/1	0.94	0.22	42,42,42,42	0
57	MG	QA	1707	1/1	0.94	0.28	54,54,54,54	0
57	MG	YA	3032	1/1	0.94	0.05	14,14,14,14	0
57	MG	YY	204	1/1	0.94	0.05	48,48,48,48	0
57	MG	QV	105	1/1	0.94	0.09	32,32,32,32	0
58	PAR	QA	1711	42/42	0.94	0.10	62,62,86,94	0
57	MG	RA	3347	1/1	0.94	0.19	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3256	1/1	0.95	0.14	59,59,59,59	0
57	MG	RA	3315	1/1	0.95	0.14	19,19,19,19	0
57	MG	YA	3258	1/1	0.95	0.08	40,40,40,40	0
57	MG	RA	3131	1/1	0.95	0.21	58,58,58,58	0
57	MG	YA	3130	1/1	0.95	0.12	41,41,41,41	0
57	MG	RA	3094	1/1	0.95	0.15	12,12,12,12	0
57	MG	RA	3270	1/1	0.95	0.05	49,49,49,49	0
57	MG	RE	302	1/1	0.95	0.08	15,15,15,15	0
57	MG	YA	3134	1/1	0.95	0.09	15,15,15,15	0
57	MG	YA	3270	1/1	0.95	0.14	19,19,19,19	0
57	MG	RA	3271	1/1	0.95	0.09	29,29,29,29	0
57	MG	QA	1665	1/1	0.95	0.14	35,35,35,35	0
57	MG	YA	3275	1/1	0.95	0.20	33,33,33,33	0
57	MG	YA	3391	1/1	0.95	0.25	58,58,58,58	0
57	MG	YA	3393	1/1	0.95	0.08	31,31,31,31	0
57	MG	YA	3145	1/1	0.95	0.15	12,12,12,12	0
57	MG	YA	3278	1/1	0.95	0.28	49,49,49,49	0
57	MG	YA	3146	1/1	0.95	0.12	27,27,27,27	0
57	MG	QA	1657	1/1	0.95	0.06	18,18,18,18	0
57	MG	RA	3274	1/1	0.95	0.07	21,21,21,21	0
57	MG	YA	3401	1/1	0.95	0.21	12,12,12,12	0
57	MG	RA	3324	1/1	0.95	0.17	42,42,42,42	0
57	MG	YA	3403	1/1	0.95	0.24	65,65,65,65	0
57	MG	YA	3150	1/1	0.95	0.10	50,50,50,50	0
57	MG	YA	3406	1/1	0.95	0.20	68,68,68,68	0
57	MG	QA	1668	1/1	0.95	0.21	62,62,62,62	0
57	MG	RA	3137	1/1	0.95	0.09	16,16,16,16	0
57	MG	YA	3158	1/1	0.95	0.06	21,21,21,21	0
57	MG	Y8	101	1/1	0.95	0.09	70,70,70,70	0
57	MG	RA	3139	1/1	0.95	0.10	20,20,20,20	0
57	MG	YA	3290	1/1	0.95	0.21	39,39,39,39	0
57	MG	YA	3417	1/1	0.95	0.10	26,26,26,26	0
57	MG	YA	3418	1/1	0.95	0.15	82,82,82,82	0
57	MG	RP	201	1/1	0.95	0.47	63,63,63,63	0
57	MG	XA	1680	1/1	0.95	0.15	48,48,48,48	0
57	MG	QA	1709	1/1	0.95	0.18	40,40,40,40	0
57	MG	RA	3103	1/1	0.95	0.14	43,43,43,43	0
57	MG	YA	3423	1/1	0.95	0.30	49,49,49,49	0
57	MG	RA	3222	1/1	0.95	0.14	67,67,67,67	0
57	MG	RT	201	1/1	0.95	0.06	52,52,52,52	0
57	MG	XA	1686	1/1	0.95	0.06	22,22,22,22	0
57	MG	XA	1605	1/1	0.95	0.30	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3299	1/1	0.95	0.17	61,61,61,61	0
57	MG	YA	3300	1/1	0.95	0.10	13,13,13,13	0
57	MG	QV	106	1/1	0.95	0.09	28,28,28,28	0
57	MG	RA	3018	1/1	0.95	0.08	14,14,14,14	0
57	MG	RA	3066	1/1	0.95	0.12	18,18,18,18	0
57	MG	YA	3025	1/1	0.95	0.17	12,12,12,12	0
57	MG	RA	3228	1/1	0.95	0.03	15,15,15,15	0
57	MG	YA	3308	1/1	0.95	0.11	41,41,41,41	0
57	MG	QX	101	1/1	0.95	0.14	33,33,33,33	0
57	MG	YA	3311	1/1	0.95	0.17	44,44,44,44	0
57	MG	YA	3441	1/1	0.95	0.18	54,54,54,54	0
57	MG	XA	1611	1/1	0.95	0.10	27,27,27,27	0
57	MG	YA	3042	1/1	0.95	0.21	12,12,12,12	0
57	MG	RA	3338	1/1	0.95	0.25	69,69,69,69	0
57	MG	RA	3071	1/1	0.95	0.10	21,21,21,21	0
57	MG	YA	3316	1/1	0.95	0.08	46,46,46,46	0
57	MG	RA	3021	1/1	0.95	0.12	17,17,17,17	0
57	MG	XA	1619	1/1	0.95	0.13	37,37,37,37	0
57	MG	RA	3073	1/1	0.95	0.19	68,68,68,68	0
57	MG	YA	3066	1/1	0.95	0.11	31,31,31,31	0
57	MG	RA	3074	1/1	0.95	0.15	20,20,20,20	0
57	MG	QA	1631	1/1	0.95	0.04	31,31,31,31	0
57	MG	YA	3197	1/1	0.95	0.23	48,48,48,48	0
57	MG	YA	3069	1/1	0.95	0.11	21,21,21,21	0
57	MG	RA	3029	1/1	0.95	0.13	25,25,25,25	0
57	MG	RA	3349	1/1	0.95	0.11	30,30,30,30	0
57	MG	RA	3350	1/1	0.95	0.07	51,51,51,51	0
57	MG	YA	3331	1/1	0.95	0.08	56,56,56,56	0
57	MG	RA	3033	1/1	0.95	0.12	18,18,18,18	0
57	MG	RA	3036	1/1	0.95	0.09	20,20,20,20	0
57	MG	YA	3211	1/1	0.95	0.14	37,37,37,37	0
57	MG	RA	3159	1/1	0.95	0.17	48,48,48,48	0
57	MG	YE	306	1/1	0.95	0.15	55,55,55,55	0
57	MG	YA	3087	1/1	0.95	0.09	21,21,21,21	0
57	MG	YA	3217	1/1	0.95	0.06	19,19,19,19	0
57	MG	RA	3354	1/1	0.95	0.21	133,133,133,133	0
57	MG	YA	3219	1/1	0.95	0.12	47,47,47,47	0
57	MG	QA	1616	1/1	0.95	0.18	34,34,34,34	0
57	MG	RA	3248	1/1	0.95	0.12	40,40,40,40	0
57	MG	YA	3100	1/1	0.95	0.16	12,12,12,12	0
57	MG	RA	3161	1/1	0.95	0.09	36,36,36,36	0
57	MG	YA	3347	1/1	0.95	0.20	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1703	1/1	0.95	0.15	83,83,83,83	0
57	MG	QA	1672	1/1	0.95	0.22	69,69,69,69	0
57	MG	YN	201	1/1	0.95	0.09	31,31,31,31	0
57	MG	RA	3362	1/1	0.95	0.42	32,32,32,32	0
57	MG	RA	3363	1/1	0.95	0.15	35,35,35,35	0
57	MG	YP	202	1/1	0.95	0.06	38,38,38,38	0
57	MG	YP	204	1/1	0.95	0.11	44,44,44,44	0
57	MG	RA	3045	1/1	0.95	0.26	35,35,35,35	0
57	MG	YQ	201	1/1	0.95	0.15	61,61,61,61	0
57	MG	RA	3088	1/1	0.95	0.15	17,17,17,17	0
57	MG	XA	1722	1/1	0.95	0.13	58,58,58,58	0
57	MG	RA	3126	1/1	0.95	0.15	42,42,42,42	0
57	MG	RA	3255	1/1	0.95	0.42	52,52,52,52	0
57	MG	RA	3090	1/1	0.95	0.09	15,15,15,15	0
57	MG	YA	3360	1/1	0.95	0.26	55,55,55,55	0
57	MG	YA	3361	1/1	0.95	0.43	80,80,80,80	0
57	MG	RA	3261	1/1	0.95	0.25	53,53,53,53	0
57	MG	RA	3128	1/1	0.95	0.05	18,18,18,18	0
57	MG	RA	3208	1/1	0.95	0.07	48,48,48,48	0
57	MG	RA	3376	1/1	0.95	0.14	23,23,23,23	0
57	MG	RA	3266	1/1	0.95	0.13	52,52,52,52	0
57	MG	QA	1603	1/1	0.95	0.34	55,55,55,55	0
58	PAR	XA	1717	42/42	0.95	0.15	62,62,79,86	0
57	MG	YA	3369	1/1	0.95	0.17	51,51,51,51	0
57	MG	YA	3022	1/1	0.96	0.14	12,12,12,12	0
57	MG	YA	3024	1/1	0.96	0.13	13,13,13,13	0
57	MG	YA	3276	1/1	0.96	0.24	43,43,43,43	0
57	MG	YA	3153	1/1	0.96	0.07	35,35,35,35	0
57	MG	YA	3154	1/1	0.96	0.06	27,27,27,27	0
57	MG	RA	3178	1/1	0.96	0.14	29,29,29,29	0
57	MG	YA	3156	1/1	0.96	0.07	17,17,17,17	0
57	MG	YA	3157	1/1	0.96	0.09	12,12,12,12	0
57	MG	XA	1707	1/1	0.96	0.35	92,92,92,92	0
57	MG	QD	502	1/1	0.96	0.05	54,54,54,54	0
57	MG	YA	3400	1/1	0.96	0.23	40,40,40,40	0
57	MG	RA	3355	1/1	0.96	0.12	32,32,32,32	0
57	MG	YA	3037	1/1	0.96	0.13	12,12,12,12	0
57	MG	RA	3151	1/1	0.96	0.29	52,52,52,52	0
57	MG	YA	3165	1/1	0.96	0.17	41,41,41,41	0
57	MG	RT	202	1/1	0.96	0.05	54,54,54,54	0
57	MG	YA	3407	1/1	0.96	0.07	26,26,26,26	0
57	MG	YA	3046	1/1	0.96	0.12	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3047	1/1	0.96	0.08	19,19,19,19	0
57	MG	XA	1658	1/1	0.96	0.20	53,53,53,53	0
57	MG	XA	1601	1/1	0.96	0.10	15,15,15,15	0
57	MG	XA	1660	1/1	0.96	0.10	52,52,52,52	0
57	MG	QA	1671	1/1	0.96	0.15	36,36,36,36	0
57	MG	YA	3416	1/1	0.96	0.10	35,35,35,35	0
57	MG	YA	3062	1/1	0.96	0.16	32,32,32,32	0
57	MG	YA	3065	1/1	0.96	0.05	12,12,12,12	0
57	MG	RA	3034	1/1	0.96	0.10	29,29,29,29	0
57	MG	QA	1642	1/1	0.96	0.11	39,39,39,39	0
57	MG	RA	3129	1/1	0.96	0.04	21,21,21,21	0
57	MG	RA	3215	1/1	0.96	0.22	55,55,55,55	0
57	MG	RA	3039	1/1	0.96	0.12	14,14,14,14	0
57	MG	XA	1724	1/1	0.96	0.17	31,31,31,31	0
57	MG	YA	3185	1/1	0.96	0.04	39,39,39,39	0
57	MG	YA	3187	1/1	0.96	0.12	42,42,42,42	0
57	MG	RA	3256	1/1	0.96	0.15	45,45,45,45	0
57	MG	RA	3292	1/1	0.96	0.10	61,61,61,61	0
57	MG	YA	3310	1/1	0.96	0.32	69,69,69,69	0
57	MG	XD	502	1/1	0.96	0.12	74,74,74,74	0
57	MG	XA	1613	1/1	0.96	0.05	12,12,12,12	0
57	MG	YA	3083	1/1	0.96	0.06	16,16,16,16	0
57	MG	YA	3084	1/1	0.96	0.09	12,12,12,12	0
57	MG	XA	1672	1/1	0.96	0.11	21,21,21,21	0
57	MG	YA	3091	1/1	0.96	0.09	47,47,47,47	0
57	MG	YA	3199	1/1	0.96	0.06	53,53,53,53	0
57	MG	YA	3092	1/1	0.96	0.14	25,25,25,25	0
57	MG	QK	202	1/1	0.96	0.06	43,43,43,43	0
57	MG	RA	3367	1/1	0.96	0.24	68,68,68,68	0
57	MG	QA	1685	1/1	0.96	0.16	37,37,37,37	0
57	MG	YA	3207	1/1	0.96	0.04	42,42,42,42	0
57	MG	RA	3107	1/1	0.96	0.07	26,26,26,26	0
57	MG	YA	3209	1/1	0.96	0.07	28,28,28,28	0
57	MG	XA	1677	1/1	0.96	0.21	49,49,49,49	0
57	MG	YA	3449	1/1	0.96	0.04	30,30,30,30	0
57	MG	XA	1678	1/1	0.96	0.19	34,34,34,34	0
57	MG	YA	3212	1/1	0.96	0.06	32,32,32,32	0
57	MG	YA	3213	1/1	0.96	0.04	22,22,22,22	0
57	MG	YA	3453	1/1	0.96	0.15	17,17,17,17	0
57	MG	YA	3454	1/1	0.96	0.26	80,80,80,80	0
57	MG	YA	3214	1/1	0.96	0.04	25,25,25,25	0
57	MG	YA	3456	1/1	0.96	0.20	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3457	1/1	0.96	0.11	28,28,28,28	0
57	MG	RA	3296	1/1	0.96	0.06	33,33,33,33	0
57	MG	XA	1681	1/1	0.96	0.05	27,27,27,27	0
57	MG	RA	3263	1/1	0.96	0.85	76,76,76,76	0
57	MG	YA	3337	1/1	0.96	0.09	21,21,21,21	0
57	MG	YA	3113	1/1	0.96	0.15	17,17,17,17	0
57	MG	YB	207	1/1	0.96	0.11	30,30,30,30	0
57	MG	RA	3373	1/1	0.96	0.06	34,34,34,34	0
57	MG	YD	301	1/1	0.96	0.15	58,58,58,58	0
57	MG	XA	1625	1/1	0.96	0.12	60,60,60,60	0
57	MG	RA	3163	1/1	0.96	0.27	69,69,69,69	0
57	MG	YA	3222	1/1	0.96	0.10	12,12,12,12	0
57	MG	QV	101	1/1	0.96	0.07	23,23,23,23	0
57	MG	Y2	103	1/1	0.96	0.07	19,19,19,19	0
57	MG	RA	3165	1/1	0.96	0.04	34,34,34,34	0
57	MG	QA	1633	1/1	0.96	0.25	50,50,50,50	0
57	MG	Y4	102	1/1	0.96	0.11	29,29,29,29	0
57	MG	RB	201	1/1	0.96	0.08	52,52,52,52	0
57	MG	QA	1720	1/1	0.96	0.05	41,41,41,41	0
57	MG	RA	3049	1/1	0.96	0.07	21,21,21,21	0
57	MG	RA	3304	1/1	0.96	0.07	43,43,43,43	0
57	MG	YA	3353	1/1	0.96	0.12	115,115,115,115	0
57	MG	QA	1661	1/1	0.96	0.06	69,69,69,69	0
57	MG	YA	3002	1/1	0.96	0.24	66,66,66,66	0
57	MG	QA	1658	1/1	0.96	0.07	40,40,40,40	0
57	MG	RA	3053	1/1	0.96	0.02	12,12,12,12	0
57	MG	YA	3006	1/1	0.96	0.16	12,12,12,12	0
57	MG	YA	3359	1/1	0.96	0.09	46,46,46,46	0
57	MG	YA	3246	1/1	0.96	0.33	64,64,64,64	0
57	MG	QA	1664	1/1	0.96	0.15	50,50,50,50	0
57	MG	RA	3346	1/1	0.96	0.33	67,67,67,67	0
57	MG	YA	3135	1/1	0.96	0.05	25,25,25,25	0
57	MG	YA	3136	1/1	0.96	0.61	75,75,75,75	0
57	MG	YA	3255	1/1	0.96	0.17	12,12,12,12	0
57	MG	YA	3137	1/1	0.96	0.16	56,56,56,56	0
57	MG	YQ	204	1/1	0.96	0.13	18,18,18,18	0
57	MG	YA	3138	1/1	0.96	0.05	25,25,25,25	0
57	MG	YA	3139	1/1	0.96	0.06	34,34,34,34	0
57	MG	RA	3089	1/1	0.96	0.10	29,29,29,29	0
57	MG	YA	3261	1/1	0.96	0.15	18,18,18,18	0
57	MG	YA	3011	1/1	0.96	0.16	12,12,12,12	0
57	MG	YA	3143	1/1	0.96	0.05	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
57	MG	YA	3377	1/1	0.96	0.12	27,27,27,27	0
57	MG	YA	3264	1/1	0.96	0.23	47,47,47,47	0
57	MG	YY	203	1/1	0.96	0.05	62,62,62,62	0
57	MG	RA	3348	1/1	0.96	0.12	25,25,25,25	0
57	MG	RA	3056	1/1	0.96	0.14	53,53,53,53	0
57	MG	RA	3020	1/1	0.96	0.11	12,12,12,12	0
57	MG	QA	1724	1/1	0.96	0.08	25,25,25,25	0
57	MG	QA	1714	1/1	0.96	0.13	47,47,47,47	0
57	MG	YA	3167	1/1	0.97	0.05	33,33,33,33	0
57	MG	RA	3091	1/1	0.97	0.12	14,14,14,14	0
57	MG	YA	3392	1/1	0.97	0.10	42,42,42,42	0
57	MG	YA	3169	1/1	0.97	0.04	26,26,26,26	0
57	MG	RA	3092	1/1	0.97	0.07	19,19,19,19	0
57	MG	RA	3057	1/1	0.97	0.11	28,28,28,28	0
57	MG	QA	1666	1/1	0.97	0.17	48,48,48,48	0
57	MG	YA	3397	1/1	0.97	0.12	12,12,12,12	0
57	MG	YA	3283	1/1	0.97	0.29	48,48,48,48	0
57	MG	RA	3095	1/1	0.97	0.12	12,12,12,12	0
57	MG	RA	3013	1/1	0.97	0.11	12,12,12,12	0
57	MG	RA	3037	1/1	0.97	0.19	18,18,18,18	0
57	MG	YA	3177	1/1	0.97	0.13	20,20,20,20	0
57	MG	RA	3038	1/1	0.97	0.14	12,12,12,12	0
57	MG	YA	3082	1/1	0.97	0.05	14,14,14,14	0
57	MG	RA	3015	1/1	0.97	0.13	14,14,14,14	0
57	MG	RA	3100	1/1	0.97	0.04	12,12,12,12	0
57	MG	YA	3085	1/1	0.97	0.09	12,12,12,12	0
57	MG	YA	3409	1/1	0.97	0.09	36,36,36,36	0
57	MG	YA	3086	1/1	0.97	0.08	14,14,14,14	0
57	MG	YA	3411	1/1	0.97	0.07	50,50,50,50	0
57	MG	RA	3322	1/1	0.97	0.09	22,22,22,22	0
57	MG	YA	3090	1/1	0.97	0.20	45,45,45,45	0
57	MG	YA	3186	1/1	0.97	0.04	28,28,28,28	0
57	MG	RA	3282	1/1	0.97	0.15	45,45,45,45	0
57	MG	RA	3283	1/1	0.97	0.16	59,59,59,59	0
57	MG	RA	3069	1/1	0.97	0.11	26,26,26,26	0
57	MG	YA	3095	1/1	0.97	0.10	15,15,15,15	0
57	MG	XA	1626	1/1	0.97	0.07	24,24,24,24	0
57	MG	YA	3193	1/1	0.97	0.09	39,39,39,39	0
57	MG	XA	1628	1/1	0.97	0.08	25,25,25,25	0
57	MG	YA	3099	1/1	0.97	0.12	26,26,26,26	0
57	MG	RA	3372	1/1	0.97	0.13	12,12,12,12	0
57	MG	YA	3306	1/1	0.97	0.03	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
57	MG	RA	3040	1/1	0.97	0.12	17,17,17,17	0
57	MG	YA	3198	1/1	0.97	0.03	55,55,55,55	0
57	MG	RA	3374	1/1	0.97	0.12	34,34,34,34	0
57	MG	YA	3103	1/1	0.97	0.12	12,12,12,12	0
57	MG	YA	3202	1/1	0.97	0.07	23,23,23,23	0
57	MG	RA	3244	1/1	0.97	0.05	35,35,35,35	0
57	MG	YA	3432	1/1	0.97	0.09	50,50,50,50	0
57	MG	RA	3245	1/1	0.97	0.18	30,30,30,30	0
57	MG	YA	3107	1/1	0.97	0.11	12,12,12,12	0
57	MG	YA	3108	1/1	0.97	0.22	21,21,21,21	0
57	MG	RA	3016	1/1	0.97	0.05	16,16,16,16	0
57	MG	QA	1653	1/1	0.97	0.04	41,41,41,41	0
57	MG	QA	1606	1/1	0.97	0.05	19,19,19,19	0
57	MG	YA	3321	1/1	0.97	0.25	55,55,55,55	0
57	MG	QA	1645	1/1	0.97	0.12	53,53,53,53	0
57	MG	RA	3046	1/1	0.97	0.11	12,12,12,12	0
57	MG	XA	1642	1/1	0.97	0.13	26,26,26,26	0
57	MG	RA	3047	1/1	0.97	0.18	15,15,15,15	0
57	MG	YA	3326	1/1	0.97	0.22	48,48,48,48	0
57	MG	RD	302	1/1	0.97	0.16	45,45,45,45	0
57	MG	RA	3080	1/1	0.97	0.06	12,12,12,12	0
57	MG	RA	3081	1/1	0.97	0.15	19,19,19,19	0
57	MG	XA	1647	1/1	0.97	0.20	58,58,58,58	0
57	MG	YA	3016	1/1	0.97	0.18	12,12,12,12	0
57	MG	QA	1605	1/1	0.97	0.20	22,22,22,22	0
57	MG	XA	1705	1/1	0.97	0.13	51,51,51,51	0
57	MG	RA	3148	1/1	0.97	0.08	16,16,16,16	0
57	MG	YA	3128	1/1	0.97	0.09	22,22,22,22	0
57	MG	YA	3224	1/1	0.97	0.05	19,19,19,19	0
57	MG	YA	3227	1/1	0.97	0.05	29,29,29,29	0
57	MG	RA	3257	1/1	0.97	0.08	19,19,19,19	0
57	MG	RA	3022	1/1	0.97	0.19	23,23,23,23	0
57	MG	RA	3259	1/1	0.97	0.16	164,164,164,164	0
57	MG	RA	3345	1/1	0.97	0.07	26,26,26,26	0
57	MG	YA	3026	1/1	0.97	0.06	17,17,17,17	0
57	MG	YA	3233	1/1	0.97	0.16	37,37,37,37	0
57	MG	YA	3345	1/1	0.97	0.10	35,35,35,35	0
57	MG	YA	3235	1/1	0.97	0.13	108,108,108,108	0
57	MG	RA	3216	1/1	0.97	0.06	45,45,45,45	0
57	MG	YD	303	1/1	0.97	0.06	12,12,12,12	0
57	MG	YD	304	1/1	0.97	0.06	16,16,16,16	0
57	MG	YA	3028	1/1	0.97	0.22	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3030	1/1	0.97	0.08	12,12,12,12	0
57	MG	RA	3050	1/1	0.97	0.12	19,19,19,19	0
57	MG	QM	201	1/1	0.97	0.05	53,53,53,53	0
57	MG	RA	3027	1/1	0.97	0.04	19,19,19,19	0
57	MG	YA	3242	1/1	0.97	0.43	80,80,80,80	0
57	MG	YA	3038	1/1	0.97	0.11	12,12,12,12	0
57	MG	YA	3039	1/1	0.97	0.16	12,12,12,12	0
57	MG	YF	305	1/1	0.97	0.08	31,31,31,31	0
57	MG	RP	203	1/1	0.97	0.12	12,12,12,12	0
57	MG	YA	3247	1/1	0.97	0.17	12,12,12,12	0
57	MG	XA	1716	1/1	0.97	0.18	43,43,43,43	0
57	MG	YA	3044	1/1	0.97	0.15	18,18,18,18	0
57	MG	YA	3045	1/1	0.97	0.07	12,12,12,12	0
57	MG	RA	3265	1/1	0.97	0.07	30,30,30,30	0
57	MG	RA	3028	1/1	0.97	0.05	12,12,12,12	0
57	MG	RA	3155	1/1	0.97	0.07	18,18,18,18	0
57	MG	YA	3364	1/1	0.97	0.10	14,14,14,14	0
57	MG	YA	3049	1/1	0.97	0.14	12,12,12,12	0
57	MG	YA	3152	1/1	0.97	0.07	17,17,17,17	0
57	MG	RA	3223	1/1	0.97	0.18	35,35,35,35	0
57	MG	YA	3260	1/1	0.97	0.10	28,28,28,28	0
57	MG	YP	206	1/1	0.97	0.07	21,21,21,21	0
57	MG	YA	3051	1/1	0.97	0.10	12,12,12,12	0
57	MG	YA	3054	1/1	0.97	0.16	28,28,28,28	0
57	MG	YA	3371	1/1	0.97	0.34	68,68,68,68	0
57	MG	YA	3373	1/1	0.97	0.11	12,12,12,12	0
57	MG	R0	101	1/1	0.97	0.06	34,34,34,34	0
57	MG	YR	202	1/1	0.97	0.07	18,18,18,18	0
57	MG	YA	3056	1/1	0.97	0.15	12,12,12,12	0
57	MG	XA	1603	1/1	0.97	0.10	12,12,12,12	0
57	MG	YA	3159	1/1	0.97	0.11	36,36,36,36	0
57	MG	YA	3378	1/1	0.97	0.31	52,52,52,52	0
57	MG	YA	3268	1/1	0.97	0.15	18,18,18,18	0
57	MG	YA	3061	1/1	0.97	0.12	12,12,12,12	0
57	MG	YA	3381	1/1	0.97	0.22	59,59,59,59	0
57	MG	QA	1686	1/1	0.97	0.05	36,36,36,36	0
57	MG	YA	3383	1/1	0.97	0.20	59,59,59,59	0
57	MG	YA	3272	1/1	0.97	0.16	71,71,71,71	0
57	MG	YA	3064	1/1	0.97	0.04	30,30,30,30	0
57	MG	XA	1666	1/1	0.97	0.23	42,42,42,42	0
57	MG	RA	3226	1/1	0.97	0.08	16,16,16,16	0
57	MG	RA	3357	1/1	0.97	0.14	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1616	1/1	0.98	0.12	13,13,13,13	0
57	MG	XL	201	1/1	0.98	0.04	21,21,21,21	0
57	MG	YA	3052	1/1	0.98	0.15	14,14,14,14	0
57	MG	YA	3144	1/1	0.98	0.17	32,32,32,32	0
57	MG	YA	3053	1/1	0.98	0.11	12,12,12,12	0
57	MG	XA	1617	1/1	0.98	0.05	12,12,12,12	0
57	MG	YA	3234	1/1	0.98	0.06	28,28,28,28	0
57	MG	RA	3061	1/1	0.98	0.23	12,12,12,12	0
57	MG	QA	1694	1/1	0.98	0.08	53,53,53,53	0
57	MG	YA	3058	1/1	0.98	0.12	12,12,12,12	0
57	MG	RA	3003	1/1	0.98	0.04	24,24,24,24	0
57	MG	RA	3064	1/1	0.98	0.07	24,24,24,24	0
57	MG	YA	3427	1/1	0.98	0.08	37,37,37,37	0
57	MG	RA	3329	1/1	0.98	0.05	23,23,23,23	0
57	MG	RA	3006	1/1	0.98	0.17	15,15,15,15	0
57	MG	XV	107	1/1	0.98	0.09	52,52,52,52	0
57	MG	RA	3201	1/1	0.98	0.06	30,30,30,30	0
57	MG	RA	3067	1/1	0.98	0.31	52,52,52,52	0
57	MG	YA	3245	1/1	0.98	0.05	34,34,34,34	0
57	MG	Y0	102	1/1	0.98	0.04	20,20,20,20	0
57	MG	YA	3435	1/1	0.98	0.11	30,30,30,30	0
57	MG	XA	1627	1/1	0.98	0.04	20,20,20,20	0
57	MG	QA	1611	1/1	0.98	0.12	27,27,27,27	0
57	MG	QA	1609	1/1	0.98	0.06	24,24,24,24	0
57	MG	YA	3250	1/1	0.98	0.12	13,13,13,13	0
57	MG	YA	3251	1/1	0.98	0.08	12,12,12,12	0
57	MG	RA	3070	1/1	0.98	0.03	19,19,19,19	0
57	MG	YA	3253	1/1	0.98	0.13	12,12,12,12	0
57	MG	YA	3074	1/1	0.98	0.04	21,21,21,21	0
57	MG	RA	3044	1/1	0.98	0.04	14,14,14,14	0
57	MG	XA	1632	1/1	0.98	0.07	14,14,14,14	0
57	MG	QA	1641	1/1	0.98	0.04	29,29,29,29	0
57	MG	RA	3101	1/1	0.98	0.10	13,13,13,13	0
57	MG	RD	301	1/1	0.98	0.12	14,14,14,14	0
57	MG	XA	1636	1/1	0.98	0.10	18,18,18,18	0
57	MG	RA	3136	1/1	0.98	0.14	39,39,39,39	0
57	MG	Y8	103	1/1	0.98	0.12	27,27,27,27	0
57	MG	RA	3102	1/1	0.98	0.11	18,18,18,18	0
57	MG	YA	3088	1/1	0.98	0.10	13,13,13,13	0
57	MG	YA	3089	1/1	0.98	0.10	12,12,12,12	0
57	MG	RA	3138	1/1	0.98	0.06	18,18,18,18	0
57	MG	YA	3267	1/1	0.98	0.06	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1640	1/1	0.98	0.05	19,19,19,19	0
57	MG	YA	3004	1/1	0.98	0.09	24,24,24,24	0
57	MG	RE	303	1/1	0.98	0.09	27,27,27,27	0
57	MG	YA	3094	1/1	0.98	0.09	18,18,18,18	0
57	MG	YB	205	1/1	0.98	0.18	39,39,39,39	0
57	MG	RA	3025	1/1	0.98	0.06	26,26,26,26	0
57	MG	RA	3343	1/1	0.98	0.10	88,88,88,88	0
57	MG	RA	3026	1/1	0.98	0.09	12,12,12,12	0
57	MG	XA	1701	1/1	0.98	0.06	27,27,27,27	0
57	MG	RA	3075	1/1	0.98	0.08	18,18,18,18	0
57	MG	RA	3076	1/1	0.98	0.05	35,35,35,35	0
57	MG	YA	3015	1/1	0.98	0.11	14,14,14,14	0
57	MG	YA	3372	1/1	0.98	0.29	24,24,24,24	0
57	MG	YE	302	1/1	0.98	0.10	29,29,29,29	0
57	MG	RA	3260	1/1	0.98	0.09	18,18,18,18	0
57	MG	QA	1629	1/1	0.98	0.07	30,30,30,30	0
57	MG	R1	101	1/1	0.98	0.11	40,40,40,40	0
57	MG	R5	101	1/1	0.98	0.08	19,19,19,19	0
57	MG	YA	3192	1/1	0.98	0.11	28,28,28,28	0
57	MG	RA	3031	1/1	0.98	0.16	34,34,34,34	0
57	MG	YA	3021	1/1	0.98	0.05	15,15,15,15	0
57	MG	YA	3112	1/1	0.98	0.12	29,29,29,29	0
57	MG	RA	3032	1/1	0.98	0.06	12,12,12,12	0
57	MG	YA	3023	1/1	0.98	0.10	12,12,12,12	0
57	MG	RA	3221	1/1	0.98	0.16	16,16,16,16	0
57	MG	YA	3384	1/1	0.98	0.12	55,55,55,55	0
57	MG	RA	3183	1/1	0.98	0.05	22,22,22,22	0
57	MG	RA	3113	1/1	0.98	0.03	45,45,45,45	0
57	MG	QA	1718	1/1	0.98	0.15	72,72,72,72	0
57	MG	YA	3119	1/1	0.98	0.08	27,27,27,27	0
57	MG	RA	3014	1/1	0.98	0.18	12,12,12,12	0
57	MG	XA	1602	1/1	0.98	0.07	29,29,29,29	0
57	MG	YA	3206	1/1	0.98	0.08	26,26,26,26	0
57	MG	RA	3084	1/1	0.98	0.15	21,21,21,21	0
57	MG	YP	203	1/1	0.98	0.16	50,50,50,50	0
57	MG	XA	1604	1/1	0.98	0.27	44,44,44,44	0
57	MG	YP	205	1/1	0.98	0.04	45,45,45,45	0
57	MG	YA	3034	1/1	0.98	0.11	12,12,12,12	0
57	MG	YA	3035	1/1	0.98	0.09	23,23,23,23	0
57	MG	YA	3036	1/1	0.98	0.10	13,13,13,13	0
57	MG	QA	1663	1/1	0.98	0.08	18,18,18,18	0
57	MG	RA	3189	1/1	0.98	0.04	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
57	MG	QF	301	1/1	0.98	0.03	43,43,43,43	0
57	MG	YA	3040	1/1	0.98	0.10	12,12,12,12	0
57	MG	YA	3307	1/1	0.98	0.04	22,22,22,22	0
57	MG	YT	202	1/1	0.98	0.03	38,38,38,38	0
57	MG	YA	3041	1/1	0.98	0.04	12,12,12,12	0
57	MG	RA	3230	1/1	0.98	0.10	20,20,20,20	0
57	MG	XA	1723	1/1	0.98	0.15	38,38,38,38	0
57	MG	YA	3405	1/1	0.98	0.07	22,22,22,22	0
57	MG	RA	3058	1/1	0.98	0.08	12,12,12,12	0
57	MG	RA	3156	1/1	0.98	0.05	17,17,17,17	0
57	MG	RA	3233	1/1	0.98	0.12	27,27,27,27	0
57	MG	RA	3234	1/1	0.98	0.05	12,12,12,12	0
57	MG	RA	3059	1/1	0.98	0.08	13,13,13,13	0
57	MG	RA	3017	1/1	0.98	0.04	21,21,21,21	0
57	MG	YA	3317	1/1	0.98	0.04	36,36,36,36	0
57	MG	YA	3226	1/1	0.98	0.06	38,38,38,38	0
59	SF4	QD	501	8/8	0.98	0.05	62,62,74,92	0
60	ZN	QN	101	1/1	0.98	0.05	79,79,79,79	0
57	MG	YA	3140	1/1	0.98	0.05	20,20,20,20	0
57	MG	YA	3012	1/1	0.99	0.06	12,12,12,12	0
57	MG	YA	3104	1/1	0.99	0.07	12,12,12,12	0
57	MG	XA	1679	1/1	0.99	0.20	42,42,42,42	0
57	MG	YF	303	1/1	0.99	0.09	23,23,23,23	0
57	MG	YA	3014	1/1	0.99	0.03	12,12,12,12	0
57	MG	YA	3071	1/1	0.99	0.04	12,12,12,12	0
57	MG	XA	1621	1/1	0.99	0.06	17,17,17,17	0
57	MG	YA	3225	1/1	0.99	0.04	34,34,34,34	0
57	MG	RA	3123	1/1	0.99	0.07	32,32,32,32	0
57	MG	YA	3110	1/1	0.99	0.04	31,31,31,31	0
57	MG	YA	3111	1/1	0.99	0.03	19,19,19,19	0
57	MG	RA	3325	1/1	0.99	0.05	28,28,28,28	0
57	MG	YA	3271	1/1	0.99	0.08	14,14,14,14	0
57	MG	RA	3235	1/1	0.99	0.03	22,22,22,22	0
57	MG	RA	3154	1/1	0.99	0.04	39,39,39,39	0
57	MG	RA	3004	1/1	0.99	0.03	16,16,16,16	0
57	MG	YA	3078	1/1	0.99	0.06	14,14,14,14	0
57	MG	YA	3079	1/1	0.99	0.04	12,12,12,12	0
57	MG	YA	3448	1/1	0.99	0.10	12,12,12,12	0
57	MG	YA	3081	1/1	0.99	0.10	12,12,12,12	0
57	MG	RA	3065	1/1	0.99	0.07	24,24,24,24	0
57	MG	RA	3239	1/1	0.99	0.30	26,26,26,26	0
57	MG	RA	3023	1/1	0.99	0.04	17,17,17,17	0

Continued on next page...

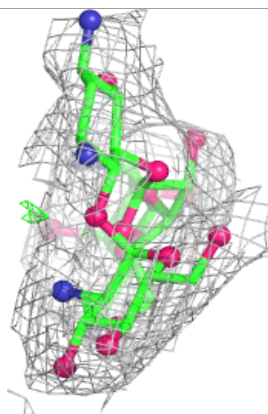
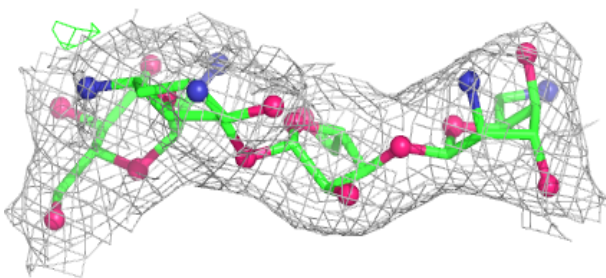
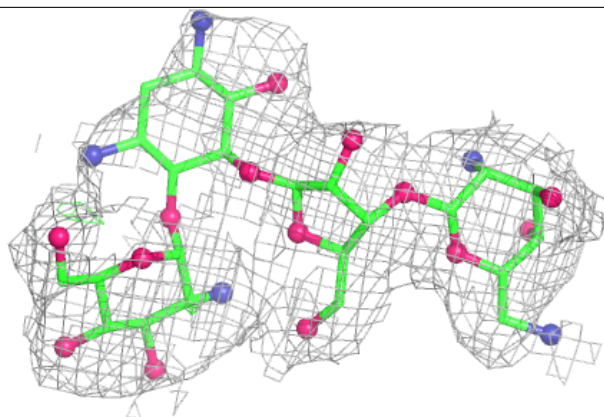
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3030	1/1	0.99	0.09	18,18,18,18	0
57	MG	RA	3118	1/1	0.99	0.04	24,24,24,24	0
57	MG	YA	3200	1/1	0.99	0.04	16,16,16,16	0
57	MG	XA	1670	1/1	0.99	0.08	31,31,31,31	0
57	MG	YR	201	1/1	0.99	0.05	25,25,25,25	0
57	MG	RA	3110	1/1	0.99	0.10	16,16,16,16	0
57	MG	RA	3055	1/1	0.99	0.06	12,12,12,12	0
57	MG	YA	3164	1/1	0.99	0.04	13,13,13,13	0
57	MG	YA	3029	1/1	0.99	0.04	20,20,20,20	0
57	MG	YA	3057	1/1	0.99	0.05	15,15,15,15	0
57	MG	XV	104	1/1	0.99	0.09	54,54,54,54	0
57	MG	YA	3333	1/1	0.99	0.03	26,26,26,26	0
57	MG	XA	1615	1/1	0.99	0.07	12,12,12,12	0
57	MG	YA	3060	1/1	0.99	0.06	14,14,14,14	0
57	MG	RA	3035	1/1	0.99	0.05	15,15,15,15	0
57	MG	YA	3171	1/1	0.99	0.18	38,38,38,38	0
57	MG	YA	3007	1/1	0.99	0.09	12,12,12,12	0
57	MG	YA	3063	1/1	0.99	0.04	12,12,12,12	0
57	MG	YA	3098	1/1	0.99	0.12	16,16,16,16	0
57	MG	RA	3246	1/1	0.99	0.04	22,22,22,22	0
57	MG	RA	3005	1/1	0.99	0.11	16,16,16,16	0
59	SF4	XD	501	8/8	0.99	0.05	62,62,66,70	0
57	MG	RA	3197	1/1	0.99	0.04	19,19,19,19	0
57	MG	RE	304	1/1	0.99	0.04	19,19,19,19	0
57	MG	YA	3080	1/1	1.00	0.17	12,12,12,12	0
60	ZN	XN	101	1/1	1.00	0.02	76,76,76,76	0
57	MG	YA	3033	1/1	1.00	0.09	15,15,15,15	0

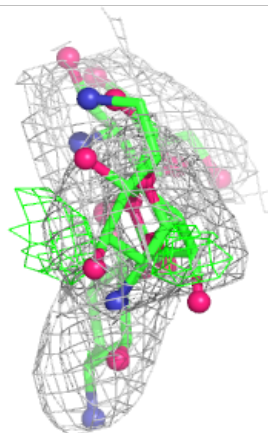
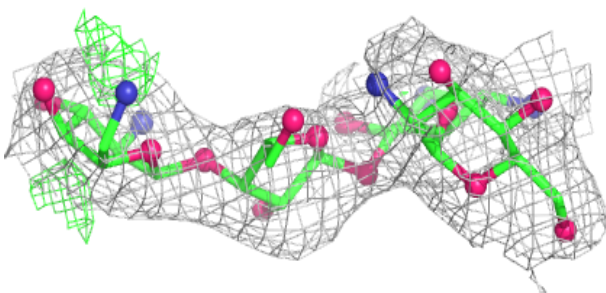
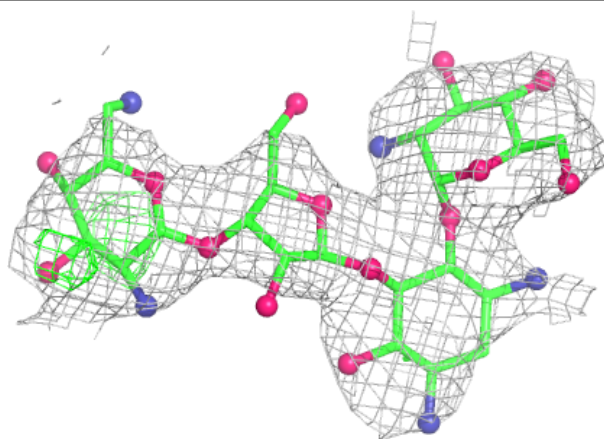
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR QA 1711:

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

**Electron density around PAR XA 1717:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.