



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2024 – 04:51 AM EST

PDB ID : 5VPP
Title : The 70S P-site tRNA SufA6 complex
Authors : Hong, S.; Sunita, S.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2017-05-05
Resolution : 3.90 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

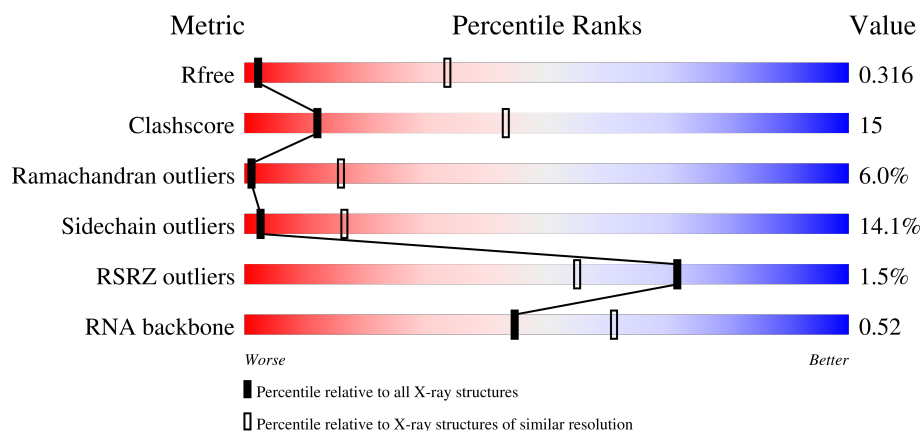
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.






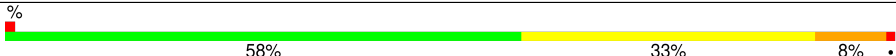
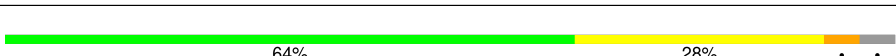
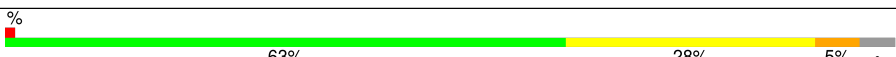
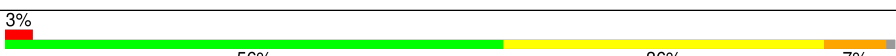
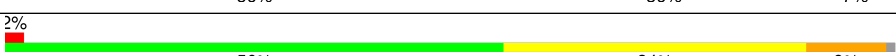
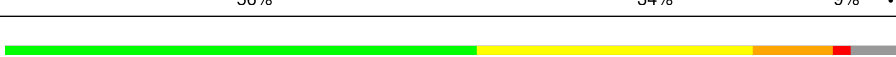


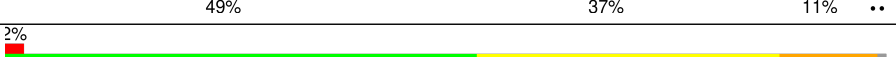

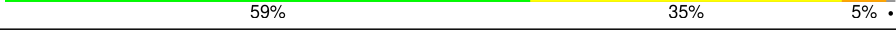
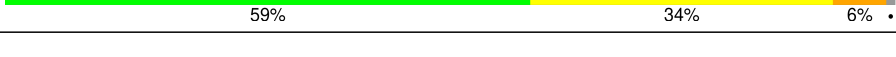




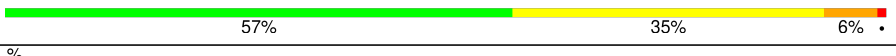

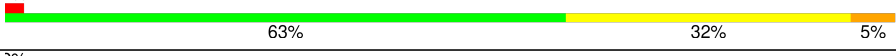



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1157 (4.10-3.70)
Clashscore	180529	1219 (4.10-3.70)
Ramachandran outliers	177936	1177 (4.10-3.70)
Sidechain outliers	177891	1169 (4.10-3.70)
RSRZ outliers	164620	1157 (4.10-3.70)
RNA backbone	3690	1135 (4.76-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	RA	2915	
1	YA	2915	
2	RB	122	
2	YB	122	






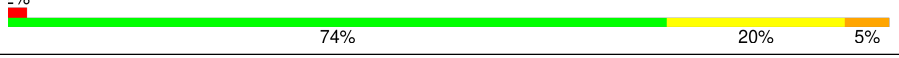

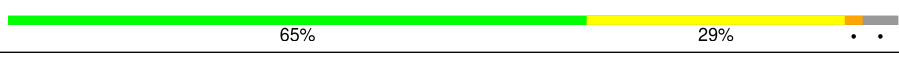
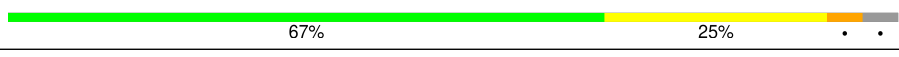
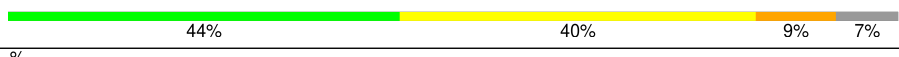
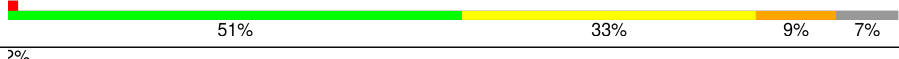
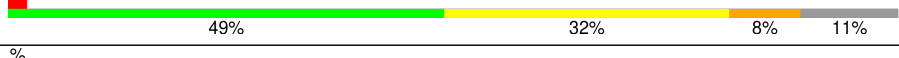







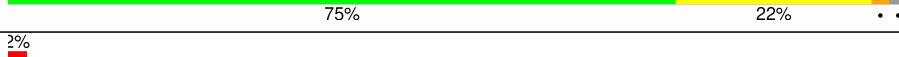
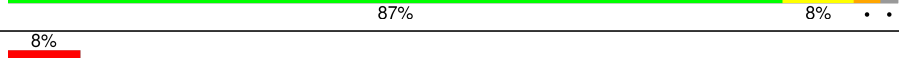


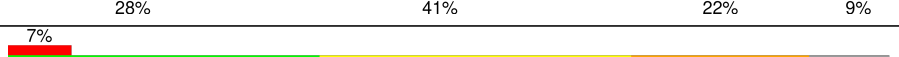
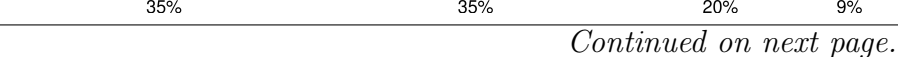
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Mol	Chain	Length	Quality of chain
3	RD	276	
3	YD	276	
4	RE	206	
4	YE	206	
5	RF	210	
5	YF	210	
6	RG	182	
6	YG	182	
7	RH	180	
7	YH	180	
8	RI	148	
8	YI	148	
9	RN	140	
9	YN	140	
10	RO	122	
10	YO	122	
11	RP	150	
11	YP	150	
12	RQ	141	
12	YQ	141	
13	RR	118	
13	YR	118	
14	RS	112	
14	YS	112	
15	RT	146	







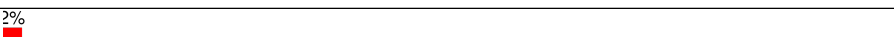
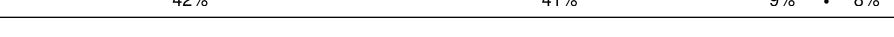
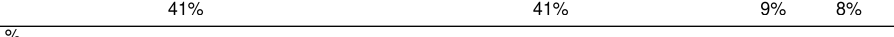
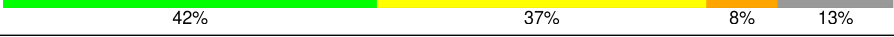
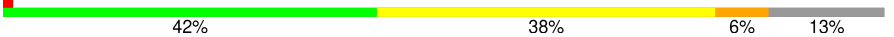
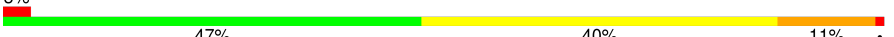









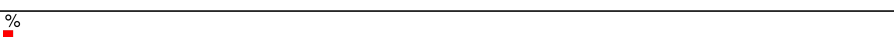

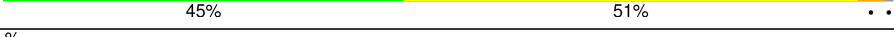

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Mol	Chain	Length	Quality of chain
15	YT	146	
16	RU	118	
16	YU	118	
17	RV	101	
17	YV	101	
18	RW	113	
18	YW	113	
19	RX	96	
19	YX	96	
20	RY	110	
20	YY	110	
21	RZ	206	
21	YZ	206	
22	R0	85	
22	Y0	85	
23	R1	98	
23	Y1	98	
24	R2	72	
24	Y2	72	
25	R3	60	
25	Y3	60	
26	R5	60	
26	Y5	60	
27	R6	54	
27	Y6	54	

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Mol	Chain	Length	Quality of chain
28	R7	49	
28	Y7	49	
29	R8	65	
29	Y8	65	
30	R9	37	
30	Y9	37	
31	QB	256	
31	XB	256	
32	QC	239	
32	XC	239	
33	QD	209	
33	XD	209	
34	QE	162	
34	XE	162	
35	QF	101	
35	XF	101	
36	QG	156	
36	XG	156	
37	QH	138	
37	XH	138	
38	QI	128	
38	XI	128	
39	QJ	105	
39	XJ	105	
40	QK	129	

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Mol	Chain	Length	Quality of chain
40	XK	129	
41	QL	132	
41	XL	132	
42	QM	126	
42	XM	126	
43	QN	61	
43	XN	61	
44	QO	89	
44	XO	89	
45	QP	88	
45	XP	88	
46	QQ	105	
46	XQ	105	
47	QR	88	
47	XR	88	
48	QT	106	
48	XT	106	
49	QA	1521	
49	XA	1521	
50	QS	93	
50	XS	93	
51	R4	71	
51	Y4	71	
52	QX	19	
52	XX	19	

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Mol	Chain	Length	Quality of chain
53	QV	78	<div><div>%</div><div><div></div><div>49%</div><div>32%</div><div>13%</div><div>6%</div></div></div>
53	XV	78	<div><div>3%</div><div><div></div><div>47%</div><div>37%</div><div>13%</div><div></div></div><div></div></div>

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 291660 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 23S rRNA.

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

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
22	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L33.

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

- Molecule 28 is a protein called 50S ribosomal protein L34.

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

- Molecule 29 is a protein called 50S ribosomal protein L35.

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

- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	QB	235	Total	C	N	O	S	0	0	0
			1909	1218	342	344	5			
31	XB	235	Total	C	N	O	S	0	0	0
			1909	1218	342	344	5			

- Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QC	207	Total	C	N	O	S	0	0	0
			1620	1022	315	282	1			
32	XC	207	Total	C	N	O	S	0	0	0
			1620	1022	315	282	1			

- Molecule 33 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
33	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 34 is a protein called 30S ribosomal protein S5.

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

- Molecule 35 is a protein called 30S ribosomal protein S6.

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

- Molecule 36 is a protein called 30S ribosomal protein S7.

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

- Molecule 37 is a protein called 30S ribosomal protein S8.

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

- Molecule 38 is a protein called 30S ribosomal protein S9.

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

- Molecule 39 is a protein called 30S ribosomal protein S10.

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

- Molecule 40 is a protein called 30S ribosomal protein S11.

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

- Molecule 41 is a protein called 30S ribosomal protein S12.

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

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

- Molecule 43 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 44 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
44	XO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 45 is a protein called 30S ribosomal protein S16.

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

- Molecule 46 is a protein called 30S ribosomal protein S17.

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

- Molecule 47 is a protein called 30S ribosomal protein S18.

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

- Molecule 48 is a protein called 30S ribosomal protein S20.

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

- Molecule 49 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	QA	1511	Total	C	N	O	P	0	0	0
			32472	14454	6013	10495	1510			
49	XA	1515	Total	C	N	O	P	0	0	0
			32554	14491	6024	10525	1514			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	458C	G	C	conflict	GB 55771382
XA	458C	G	C	conflict	GB 55771382

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	XS	79	Total	C	N	O	S	0	0	0
			633	405	115	111	2			
50	QS	79	Total	C	N	O	S	0	0	0
			633	405	115	111	2			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R4	34	Total	C	N	O	S	0	0	0
			262	169	43	48	2			
51	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 52 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	XX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	QX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

- Molecule 53 is a RNA chain called P-site tRNA SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	XV	78	Total	C	N	O	P	0	0	0
			1670	744	300	548	78			
53	QV	78	Total	C	N	O	P	0	0	0
			1670	744	300	548	78			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XV	38	1MG	-	insertion	GB 1151176235
QV	38	1MG	-	insertion	GB 1151176235

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	RA	562	Total	Mg	0	0
			562	562		
54	RB	15	Total	Mg	0	0
			15	15		
54	RD	10	Total	Mg	0	0
			10	10		
54	RE	7	Total	Mg	0	0
			7	7		
54	RF	4	Total	Mg	0	0
			4	4		
54	RI	1	Total	Mg	0	0
			1	1		
54	RO	2	Total	Mg	0	0
			2	2		
54	RQ	2	Total	Mg	0	0
			2	2		
54	RR	3	Total	Mg	0	0
			3	3		
54	RT	3	Total	Mg	0	0
			3	3		
54	RU	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	RX	2	Total 2	Mg 2	0	0
54	RY	1	Total 1	Mg 1	0	0
54	R0	2	Total 2	Mg 2	0	0
54	R1	3	Total 3	Mg 3	0	0
54	R3	1	Total 1	Mg 1	0	0
54	R6	1	Total 1	Mg 1	0	0
54	R8	3	Total 3	Mg 3	0	0
54	YA	379	Total 379	Mg 379	0	0
54	YB	10	Total 10	Mg 10	0	0
54	YD	4	Total 4	Mg 4	0	0
54	YE	5	Total 5	Mg 5	0	0
54	YI	1	Total 1	Mg 1	0	0
54	YP	1	Total 1	Mg 1	0	0
54	YQ	1	Total 1	Mg 1	0	0
54	YR	1	Total 1	Mg 1	0	0
54	YT	2	Total 2	Mg 2	0	0
54	YU	1	Total 1	Mg 1	0	0
54	YX	1	Total 1	Mg 1	0	0
54	YY	1	Total 1	Mg 1	0	0
54	Y0	1	Total 1	Mg 1	0	0
54	Y1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	Y8	1	Total 1	Mg 1	0	0
54	QC	1	Total 1	Mg 1	0	0
54	QD	3	Total 3	Mg 3	0	0
54	QE	1	Total 1	Mg 1	0	0
54	QL	3	Total 3	Mg 3	0	0
54	QP	2	Total 2	Mg 2	0	0
54	QQ	2	Total 2	Mg 2	0	0
54	QT	2	Total 2	Mg 2	0	0
54	QA	131	Total 131	Mg 131	0	0
54	XC	1	Total 1	Mg 1	0	0
54	XD	1	Total 1	Mg 1	0	0
54	XE	1	Total 1	Mg 1	0	0
54	XK	1	Total 1	Mg 1	0	0
54	XL	2	Total 2	Mg 2	0	0
54	XM	1	Total 1	Mg 1	0	0
54	XO	1	Total 1	Mg 1	0	0
54	XP	1	Total 1	Mg 1	0	0
54	XA	128	Total 128	Mg 128	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

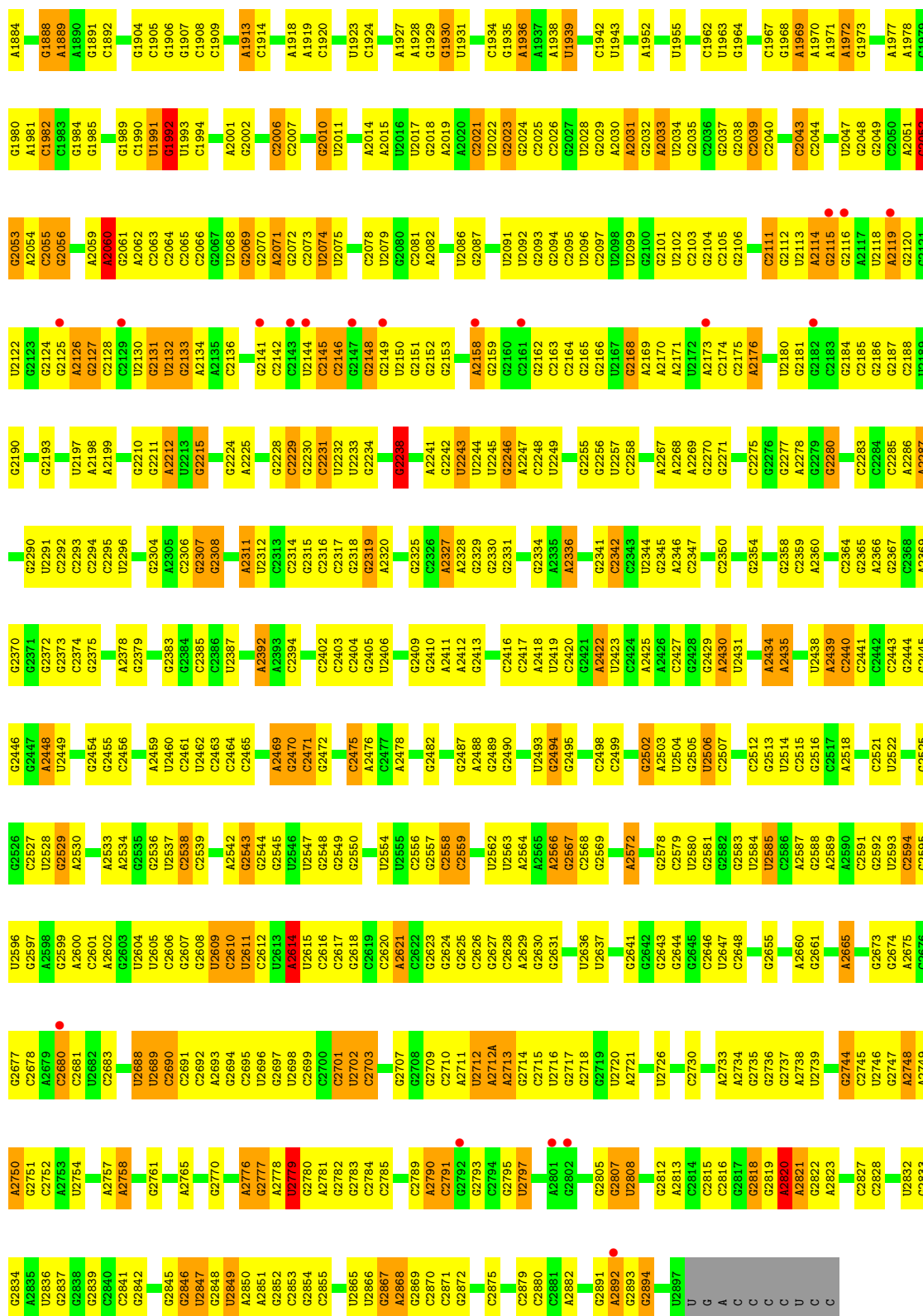
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	Y9	1	Total 1	Zn 1	0	0

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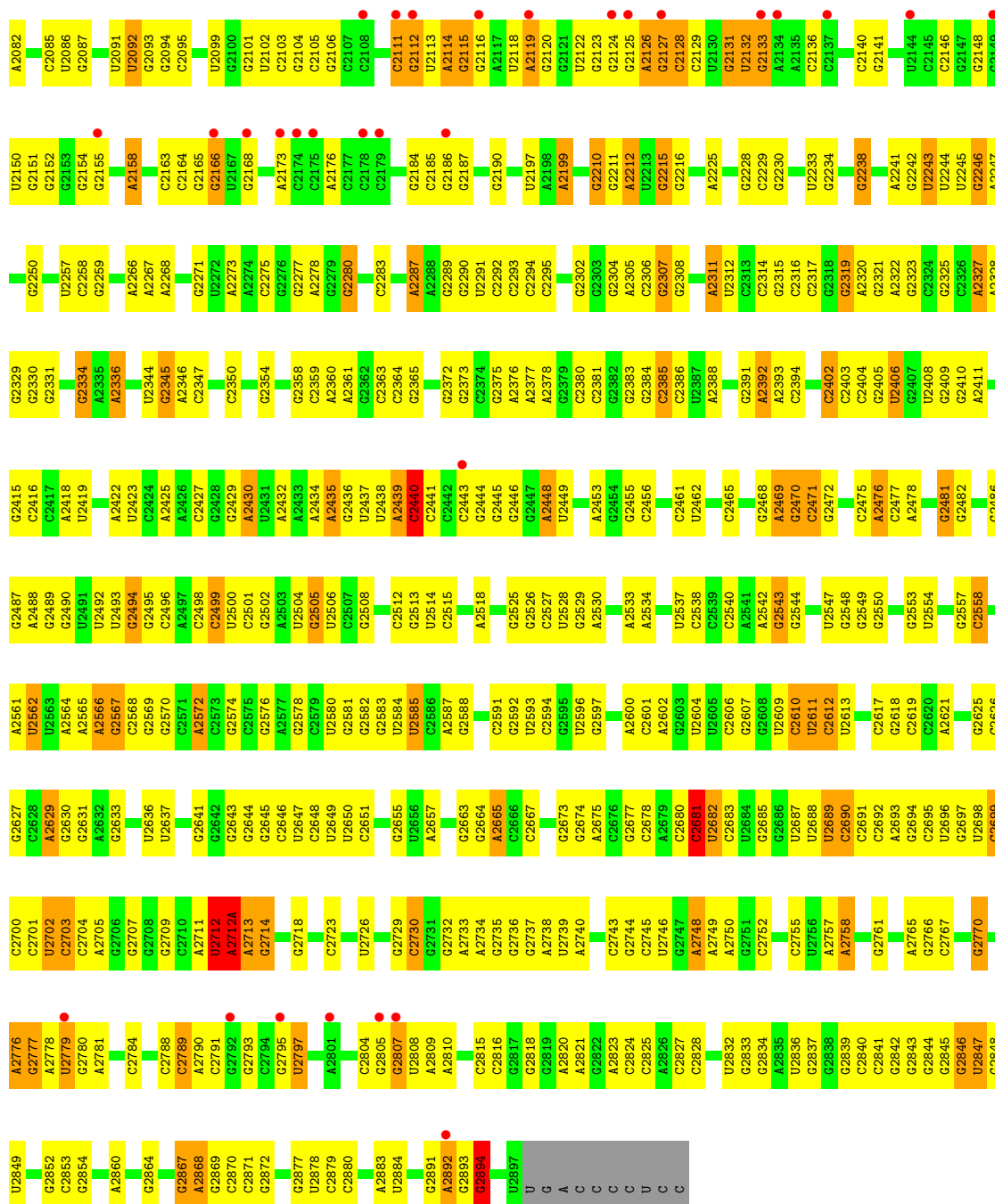
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QD	2	Total 2	Zn 2	0	0
55	XD	1	Total 1	Zn 1	0	0

A1803	C1804	U1805	C1806	G1807	C1808	G1809	C1810	G1811	C1812	U1813	C1814	G1815	C1816	G1817	C1818	A1819	C1820	G1821	C1822	U1823	C1824	G1825	U1826	C1827	G1828	C1829	G1830	C1831	G1832	U1833	C1834	G1835	C1836	U1837	C1838	G1839	C1840	U1841	C1842	G1843	C1844	G1845	C1846	U1847	C1848	G1849	U1850	C1851	G1852	C1853	G1854	C1855	C1856	U1857	C1858	G1859	U1860	C1861	G1862	C1863	G1864	C1865	C1866	U1867	C1868	G1869	C1870	U1871	C1872	G1873	C1874	U1875	C1876	G1877	C1878	U1879	C1880	C1881	G1882	C1883	U1884	C1885	G1886	C1887	U1888	C1889	G1890	C1891	U1892	C1893	G1894	C1895	U1896	C1897	G1898	C1899	U1900	C1901	G1902	C1903	U1904	C1905	G1906	C1907	U1908	C1909	G1910	C1911	U1912	C1913	G1914	C1915	U1916	C1917	G1918	C1919	U1920	C1921	G1922	C1923	U1924	C1925	G1926	C1927	U1928	C1929	G1930	C1931	U1932	C1933	G1934	C1935	U1936	C1937	G1938	C1939	U1940	C1941	G1942	C1943	U1944	C1945	G1946	C1947	U1948	C1949	G1950	C1951	U1952	C1953	G1954	C1955	U1956	C1957	G1958	C1959	U1960	C1961	G1962	C1963	U1964	C1965	G1966	C1967	U1968	C1969	G1970	C1971	U1972	C1973	G1974	C1975	U1976	C1977	G1978	C1979	U1980	C1981	G1982	C1983	U1984	C1985	G1986	C1987	U1988	C1989	G1990	C1991	U1992	C1993	G1994	C1995	U1996	C1997	G1998	C1999	U2000	C2001	G2002	C2003	U2004	C2005	G2006	C2007	U2008	C2009	G2010	C2011	U2012	C2013	G2014	C2015	U2016	C2017	G2018	C2019	U2020	C2021	G2022	C2023	U2024	C2025	G2026	C2027	U2028	C2029	G2030	C2031	U2032	C2033	G2034	C2035	U2036	C2037	G2038	C2039	U2040	C2041	G2042	C2043	U2044	C2045	G2046	C2047	U2048	C2049	G2050	C2051	U2052	C2053	G2054	C2055	U2056	C2057	G2058	C2059	U2060	C2061	G2062	C2063	U2064	C2065	G2066	C2067	U2068	C2069	G2070	C2071	U2072	C2073	G2074	C2075	U2076	C2077	G2078	C2079	U2080	C2081	G2082	C2083	U2084	C2085	G2086	C2087	U2088	C2089	G2090	C2091	U2092	C2093	G2094	C2095	U2096	C2097	G2098	C2099	U2100	C2101	G2102	C2103	U2104	C2105	G2106	C2107	U2108	C2109	G2110	C2111	U2112	C2113	G2114	C2115	U2116	C2117	G2118	C2119	U2120	C2121	G2122	C2123	U2124	C2125	G2126	C2127	U2128	C2129	G2130	C2131	U2132	C2133	G2134	C2135	U2136	C2137	G2138	C2139	U2140	C2141	G2142	C2143	U2144	C2145	G2146	C2147	U2148	C2149	G2150	C2151	U2152	C2153	G2154	C2155	U2156	C2157	G2158	C2159	U2160	C2161	G2162	C2163	U2164	C2165	G2166	C2167	U2168	C2169	G2170	C2171	U2172	C2173	G2174	C2175	U2176	C2177	G2178	C2179	U2180	C2181	G2182	C2183	U2184	C2185	G2186	C2187	U2188	C2189	G2190	C2191	U2192	C2193	G2194	C2195	U2196	C2197	G2198	C2199	U2200	C2201	G2202	C2203	U2204	C2205	G2206	C2207	U2208	C2209	G2210	C2211	U2212	C2213	G2214	C2215	U2216	C2217	G2218	C2219	U2220	C2221	G2222	C2223	U2224	C2225	G2226	C2227	U2228	C2229	G2230	C2231	U2232	C2233	G2234	C2235	U2236	C2237	G2238	C2239	U2240	C2241	G2242	C2243	U2244	C2245	G2246	C2247	U2248	C2249	G2250	C2251	U2252	C2253	G2254	C2255	U2256	C2257	G2258	C2259	U2260	C2261	G2262	C2263	U2264	C2265	G2266	C2267	U2268	C2269	G2270	C2271	U2272	C2273	G2274	C2275	U2276	C2277	G2278	C2279	U2280	C2281	G2282	C2283	U2284	C2285	G2286	C2287	U2288	C2289	G2290	C2291	U2292	C2293	G2294	C2295	U2296	C2297	G2298	C2299	U2300	C2301	G2302	C2303	U2304	C2305	G2306	C2307	U2308	C2309	G2310	C2311	U2312	C2313	G2314	C2315	U2316	C2317	G2318	C2319	U2320	C2321	G2322	C2323	U2324	C2325	G2326	C2327	U2328	C2329	G2330	C2331	U2332	C2333	G2334	C2335	U2336	C2337	G2338	C2339	U2340	C2341	G2342	C2343	U2344	C2345	G2346	C2347	U2348	C2349	G2350	C2351	U2352	C2353	G2354	C2355	U2356	C2357	G2358	C2359	U2360	C2361	G2362	C2363	U2364	C2365	G2366	C2367	U2368	C2369	G2370	C2371	U2372	C2373	G2374	C2375	U2376	C2377	G2378	C2379	U2380	C2381	G2382	C2383	U2384	C2385	G2386	C2387	U2388	C2389	G2390	C2391	U2392	C2393	G2394	C2395	U2396	C2397	G2398	C2399	U2400	C2401	G2402	C2403	U2404	C2405	G2406	C2407	U2408	C2409	G2410	C2411	U2412	C2413	G2414	C2415	U2416	C2417	G2418	C2419	U2420	C2421	G2422	C2423	U2424	C2425	G2426	C2427	U2428	C2429	G2430	C2431	U2432	C2433	U2434	C2435	U2436	C2437	U2438	C2439	U2440	C2441	U2442	C2443	U2444	C2445	U2446	C2447	U2448	C2449	U2450	C2451	U2452	C2453	U2454	C2455	U2456	C2457	U2458	C2459	U2460	C2461	U2462	C2463	U2464	C2465	U2466	C2467	U2468	C2469	U2470	C2471	U2472	C2473	U2474	C2475	U2476	C2477	U2478	C2479	U2480	C2481	U2482	C2483	U2484	C2485	U2486	C2487	U2488	C2489	U2490	C2491	U2492	C2493	U2494	C2495	U2496	C2497	U2498	C2499	U2500	C2501	U2502	C2503	U2504	C2505	U2506	C2507	U2508	C2509	U2510	C2511	U2512	C2513	U2514	C2515	U2516	C2517	U2518	C2519	U2520	C2521	U2522	C2523	U2524	C2525	U2526	C2527	U2528	C2529	U2530	C2531	U2532	C2533	U2534	C2535	U2536	C2537	U2538	C2539	U2540	C2541	U2542	C2543	U2544	C2545	U2546	C2547	U2548	C2549	U2550	C2551	U2552	C2553	U2554	C2555	U2556	C2557	U2558	C2559	U2560	C2561	U2562	C2563	U2564	C2565	U2566	C2567	U2568	C2569	U2570	C2571	U2572	C2573	U2574	C2575	U2576	C2577	U2578	C2579	U2580	C2581	U2582	C2583	U2584	C2585	U2586	C2587	U2588	C2589	U2590	C2591	U2592	C2593	U2594	C2595	U2596	C2597	U2598	C2599	U2600	C2601	U2602	C2603	U2604	C2605	U2606	C2607	U2608	C2609	U2610	C2611	U2612	C2613	U2614	C2615	U2616	C2617	U2618	C2619	U2620	C2621	U2622	C2623	U2624	C2625	U2626	C2627	U2628	C2629	U2630	C2631	U2632	C2633	U2634	C2635	U2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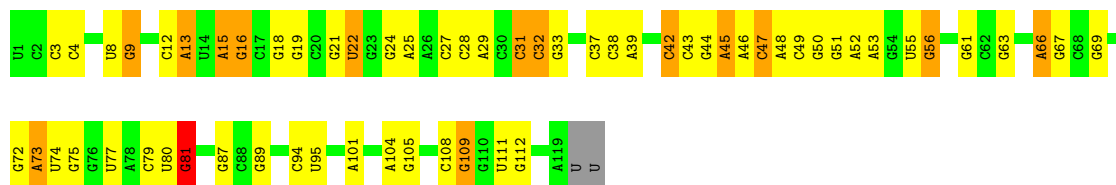
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U943	G855	G786	G713	C	A590	C516	G441	G363B	C250	C250	G178	A84	A6
G944	C857	A788	U714	C	C591	C517	A443	C287	A251	A251	G181	G89	U9
A945	G858	G789	U715	A	U594	G520	A445	C364	G252	G252	A181	G92	G15
G946	G859	C790	A716	C	A596	G521	G446	A371	A256	A256	G184	G93	G16
G947	U860	A793	G717	C	G596	G521	A447	G372	C297	C297	C184	G94	G17
G948	A861	A793	A718	C	U597	G521	A448	U373	A298	A298	U185	G94	C18
C949	G862	C797	C719	C	G598	G521	U448	A374	A299	A299	G186	G95	C19
G950	A863	C797	C720	G	G598	G521	U448	A374	A300	A300	G187	G96	C20
G951	G864	G798	G721	C	A603	A526	A454	C375	G301	A262	G188	G99	A21
G952	C865	G799	A722	C	G604	A527	C455	C376	C302	A262	A192	U99	G24
A953	A866	G801	G723	C	C905	A528	A457	C377	U303	C264	G101	G102	U25
G954	G867	A802	U724	C	U606	G530	G458	G378	G304	G194	G103	G26	G26
G955	U877	G805	G725	G	U607	G531	U459	G379	U305	G195	A103	G27	G27
G956	A878	C806	G726	C	A608	C532	A460	U380	U306	A196	U108	A28	A28
G957	G879	U807	A727	C	A609	G533	G463	G381	G307	A197	U109	U29	U29
U958	G880	G808	G728	C	G609A	U534	U464	U383	G308	C198	G110	G30	G30
A959	G881	C809	G729	C	C910	C535	G465	U384	G309	C199	A111	C31	C31
G960	G882	U810	C730	C	U614	A536	A466	C385	A310	A270B	U112	C32	C32
C961	C884	U811	C731	C	G615	A537	G467	G386	A311	C270C	G113	U33	U33
C964	C888	C812	G732	C	A616	C537	G468	U387	G317	U270F	U114	C34	C34
C965	U888	U813	G733	C	G617	G539	G469	A390	C318	C270G	G117	G35	G35
G966	G889	C814	A734	C	G618	G540	A470	G391	C319	C270H	A118	G36	G36
G967	A890	G815	C735	C	G618	C541	A471	C392	A320	G270I	A119	C37	C37
U968	G892	C816	U740	C	G620	C542	A472	C393	A321	C210	U120	A38	A38
U969	C893	C817	G741	C	A621	C546	U475	C394	A322	G212	G125	C46	C46
C970	G894	U819	G742	C	G626	A547	G476	U395	A323	G215	A126	C47	C47
C971	U895	A820	G743	C	U626	A548	G476	G396	A324	G216	A127	G48	G48
A973	A896	A821	A746	C	A627	G552	A479	G397	A325	G217	C128	A49	A49
G974	C897	U822	U747	C	G628	U553	A480	G398	G326	G219	G131	U50	U50
C974A	A899	C823	G748	C	G629	U554	G481	G399	U328	A218	G137A	G55	G55
G975	A900	A824	G748	C	G630	U557	A482	G400	G329	G219	G138	U59	U59
C976	A901	A824	A752	C	A631	G558	A483	A401	A330	G220	A141	G60	G60
G977	C902	U827	C753	C	C634	G563	C487	U403	A331	A221	G142	G61	G61
G978	C903	U828	C754	C	G635	C564	C488	U404	A332	A222	G143	G62	G62
C904	U905	G831	C755	C	G636	C565	C489	U405	A333	A223	C144	U63	U63
G980	G906	G832	C756	C	A637	U566	G491	C409	C334	G224	C144	G66	G66
C982	U907	U833	G760	C	G638	C566	G494	G410	C335	A225	U147	U67	U67
A983	A910	A835	A761	C	U639	G570	G495	G411	C336	G226	C148	G68	G68
G987	C915	G836	U762	C	C641	A571	C496	G412	A340	A228	A149	G69	G69
A988	G916	U839	A764	C	G642	A572	C497	C413	G342	U230	C151	G70	G70
G989	A917	C840	G765	C	C645	G573	G498	C414	A345	C231	U161	A73	A73
A918	U918	A841	G771	C	G646	C574	U499	A415	A346	G232	U162	A74	A74
C994	U922	G843	G774	C	G647	U576	G500	C416	A347	A233	U	G75	G75
C995	G943	C844	A775	C	G647	U577	G501	C417	A347	C234	C151	U72	U72
A996	G944	G845	G776	C	G651	A578	U504	U427	G348	U235	C236	A75	A75
G997	C923	C846	G777	C	C852	G579	A505	A428	G352	C274	C237	A76	A76
A1000	A925	C847	A777	C	A653	C580	G506	A430	G353	G275	A241	G76	G76
A1001	A926	C848	G778	C	A654	C581	A507	G430	G354	C277	G242	U	U



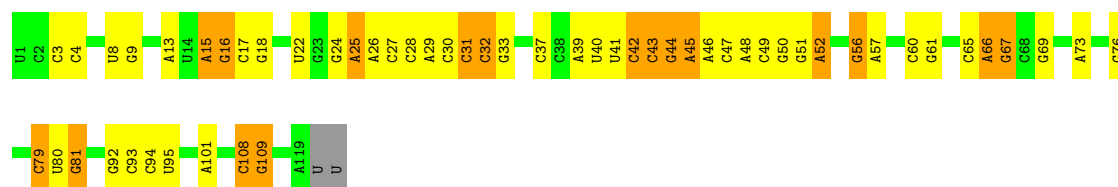


• Molecule 2: 5S rRNA

Chain RB: 48% 38% 11% ..

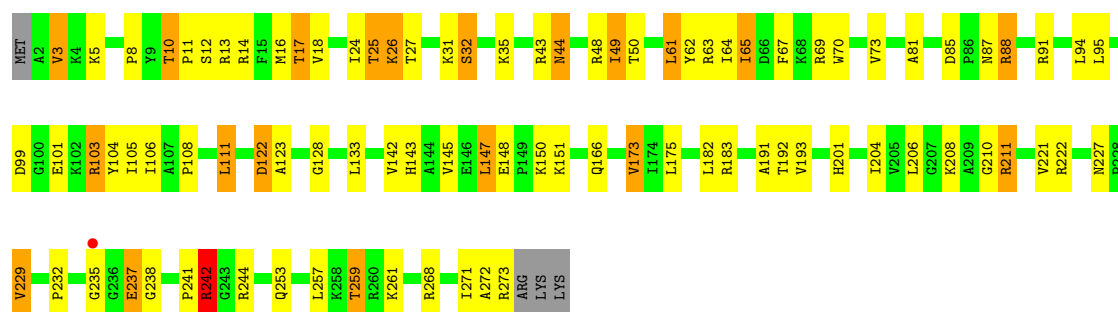


Chain YB: 

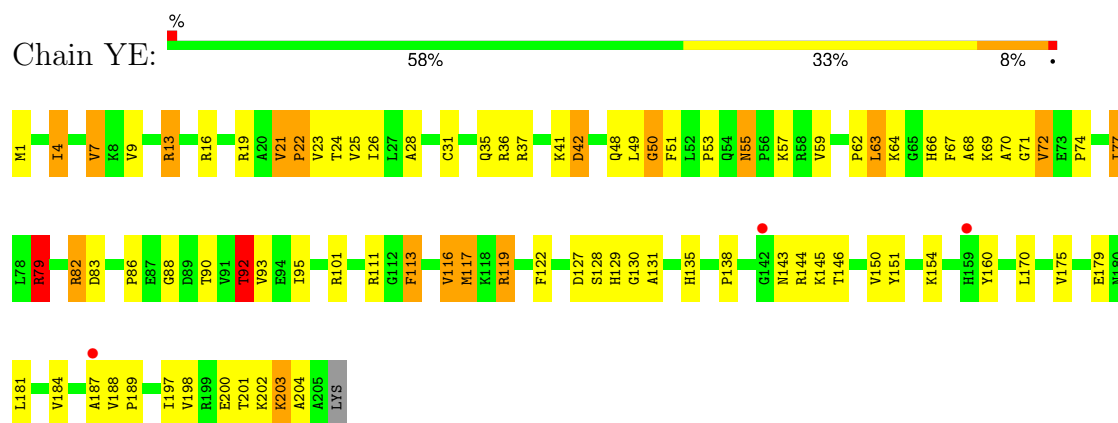


• Molecule 3: 50S ribosomal protein L2

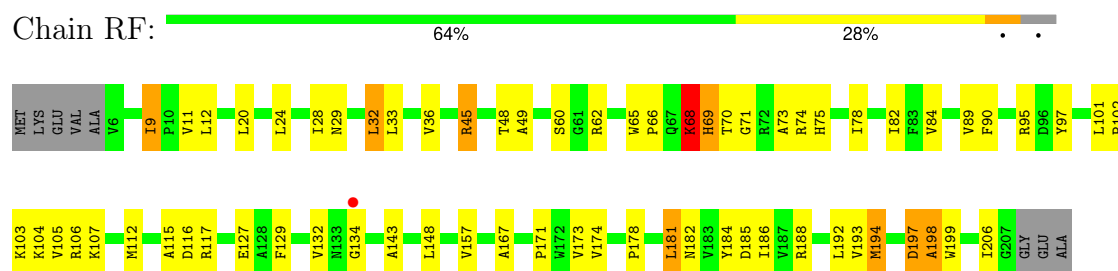
Chain RD: 



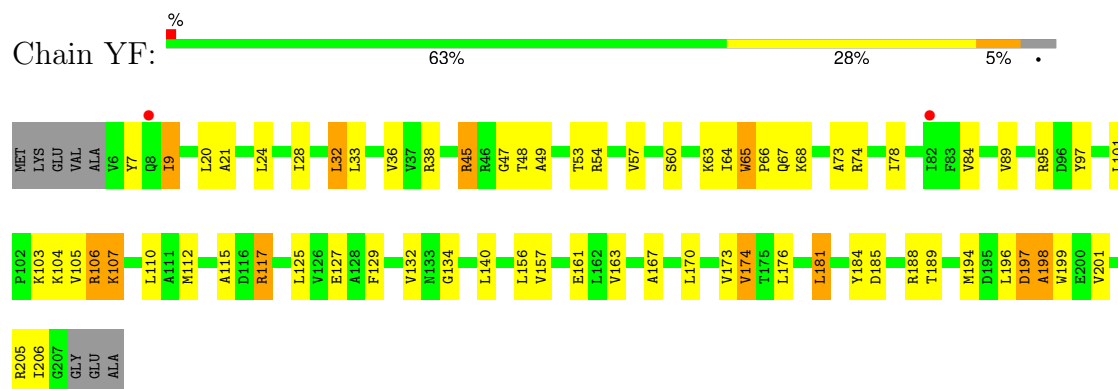
- Molecule 4: 50S ribosomal protein L3



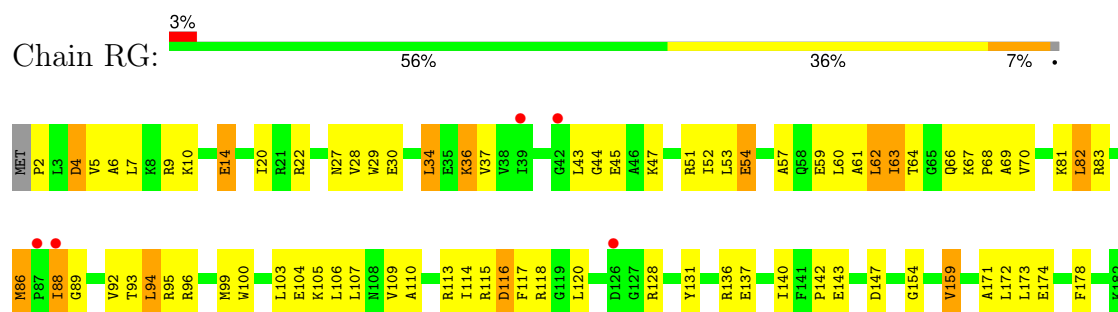
- Molecule 5: 50S ribosomal protein L4



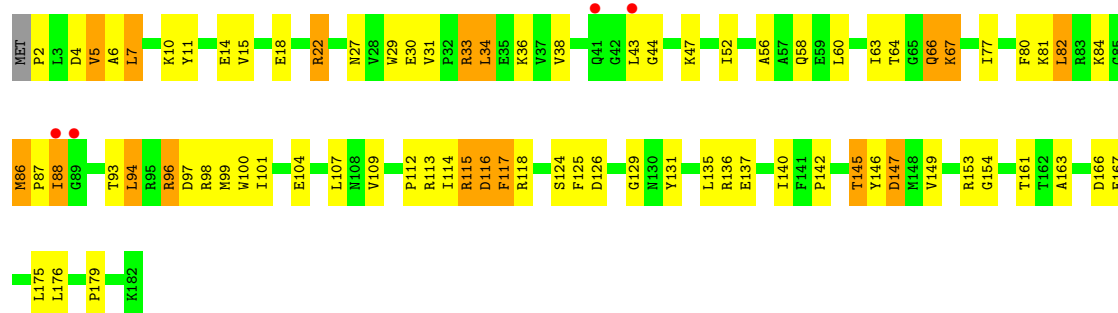
- Molecule 5: 50S ribosomal protein L4



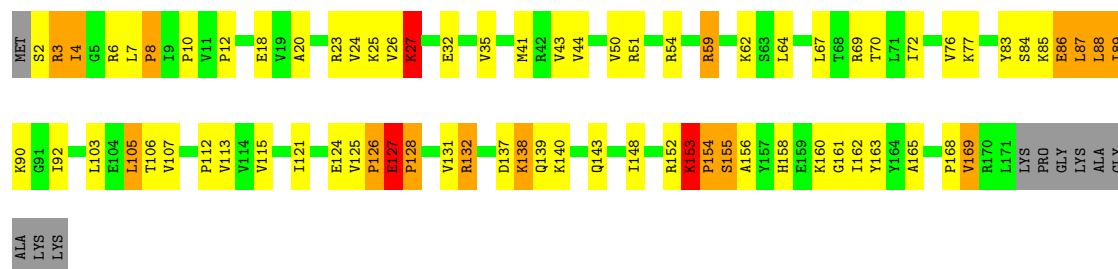
- Molecule 6: 50S ribosomal protein L5



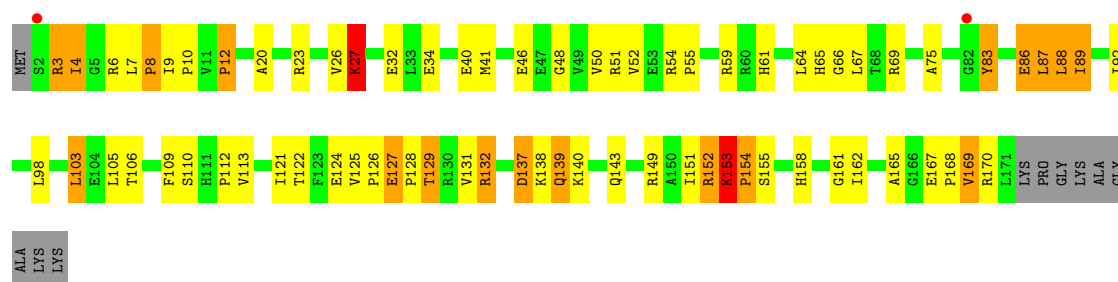
- Molecule 6: 50S ribosomal protein L5



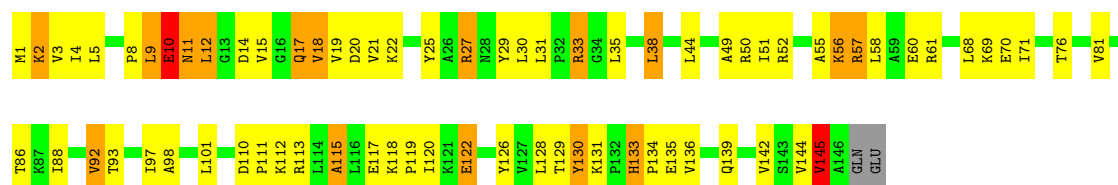
• Molecule 7: 50S ribosomal protein L6



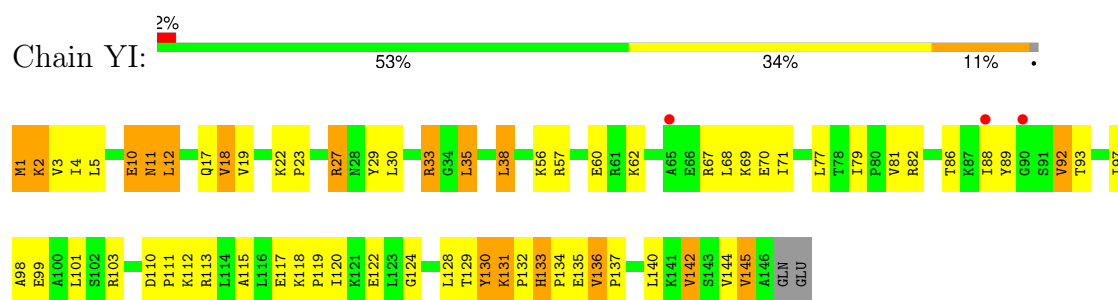
• Molecule 7: 50S ribosomal protein L6



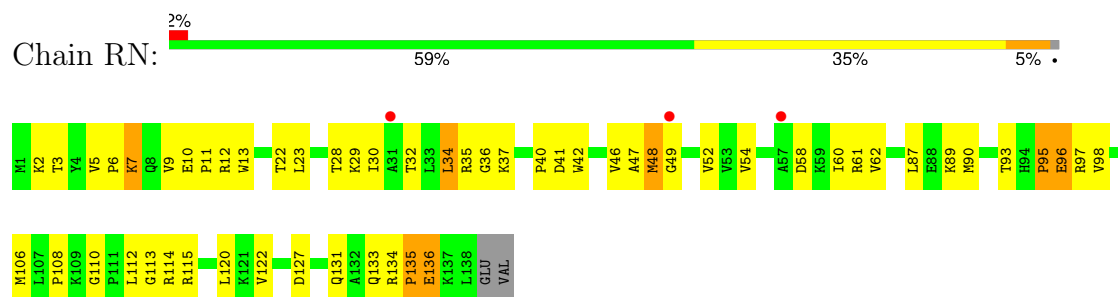
• Molecule 8: 50S ribosomal protein L9



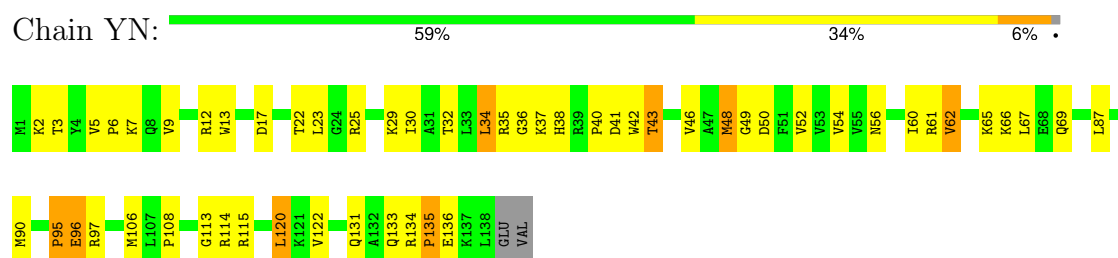
• Molecule 8: 50S ribosomal protein L9



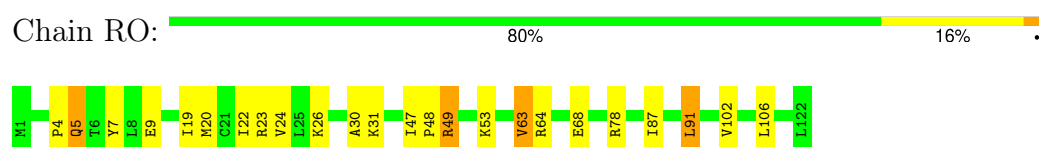
- Molecule 9: 50S ribosomal protein L13



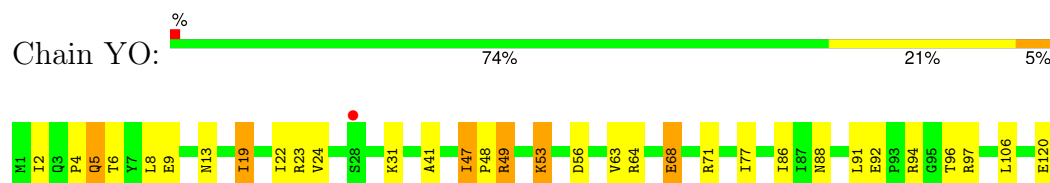
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

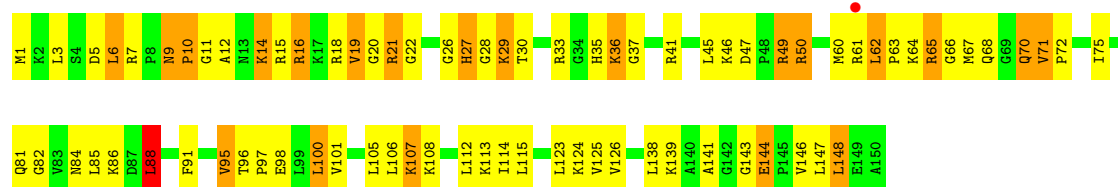


- Molecule 10: 50S ribosomal protein L14

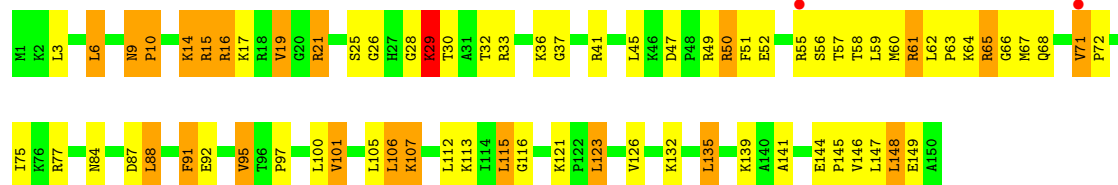


- Molecule 11: 50S ribosomal protein L15

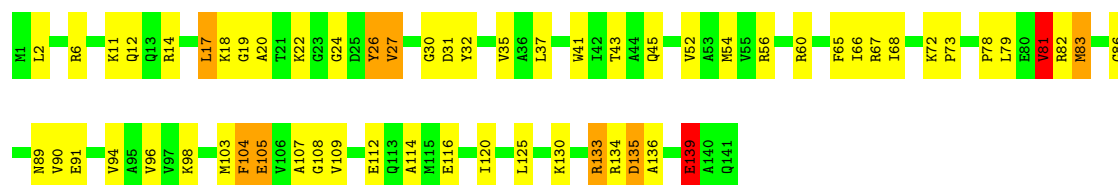




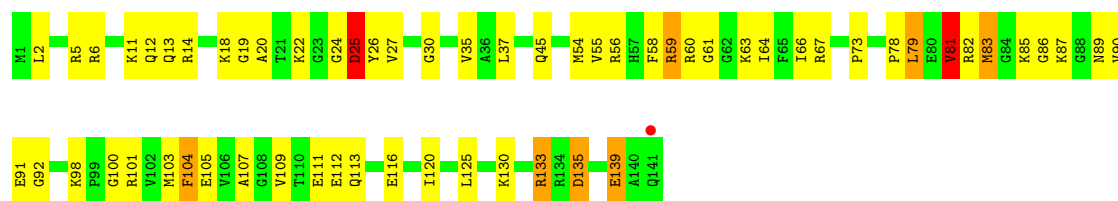
• Molecule 11: 50S ribosomal protein L15



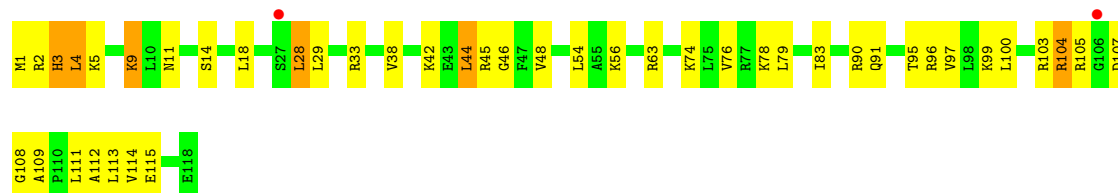
• Molecule 12: 50S ribosomal protein L16



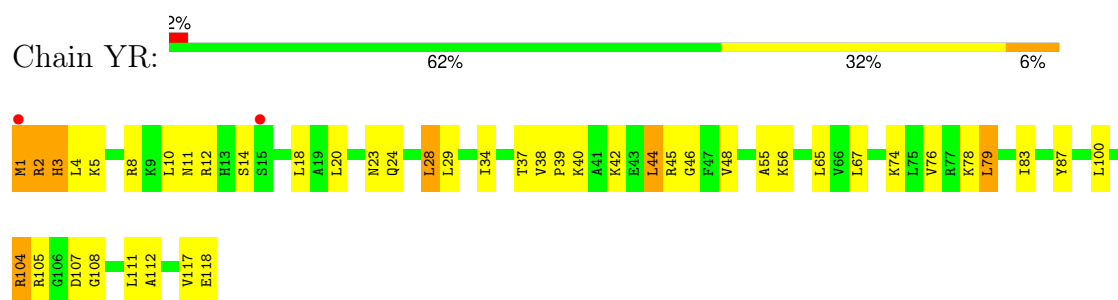
• Molecule 12: 50S ribosomal protein L16



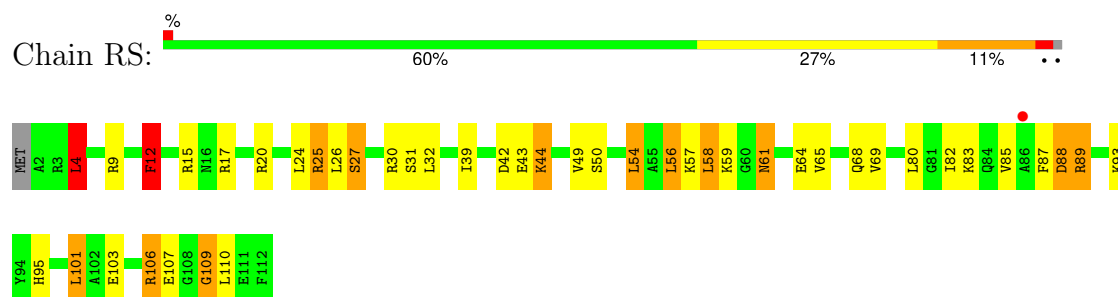
• Molecule 13: 50S ribosomal protein L17



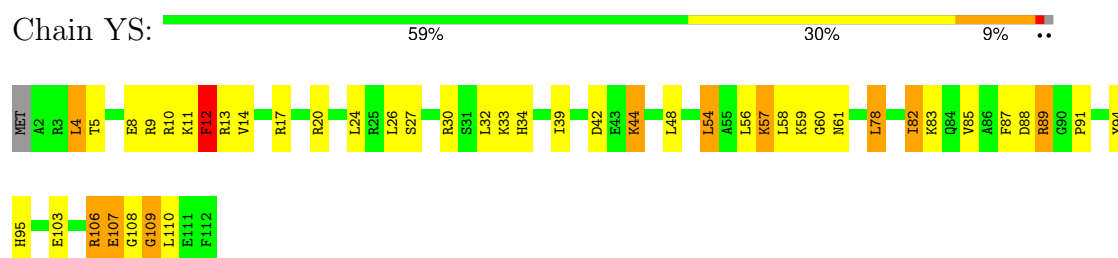
• Molecule 13: 50S ribosomal protein L17



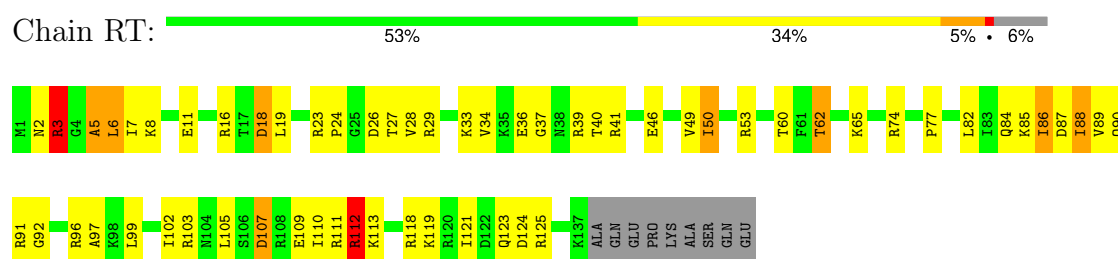
• Molecule 14: 50S ribosomal protein L18



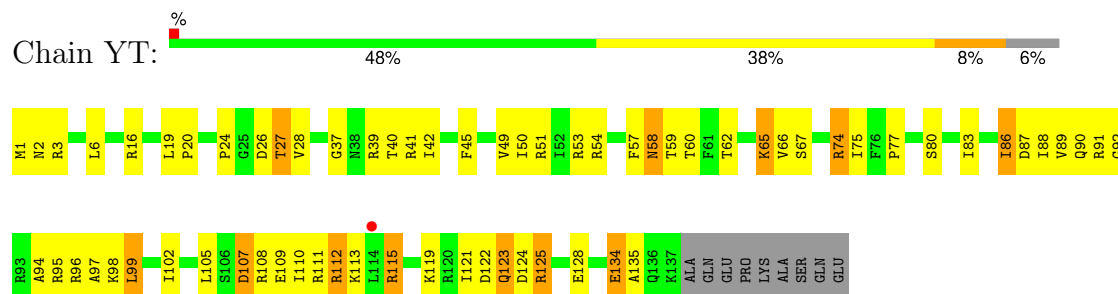
• Molecule 14: 50S ribosomal protein L18



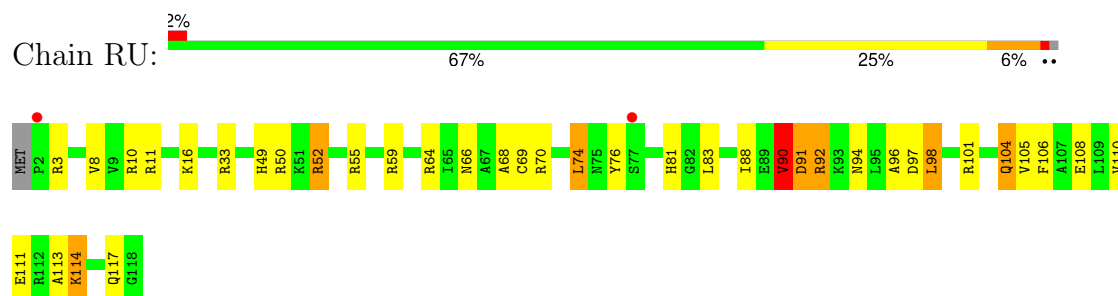
• Molecule 15: 50S ribosomal protein L19



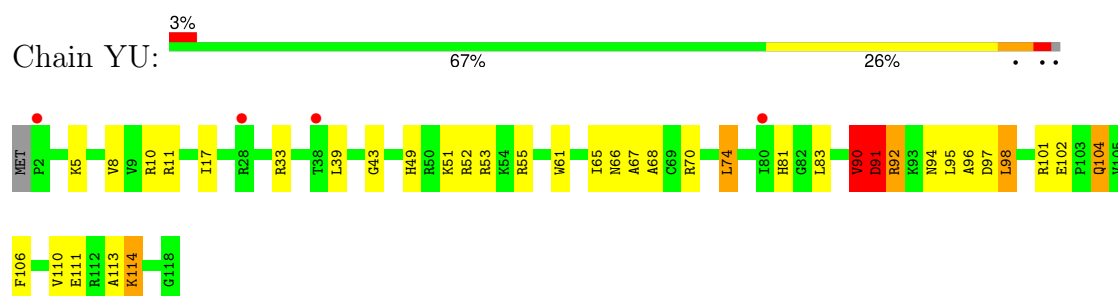
• Molecule 15: 50S ribosomal protein L19



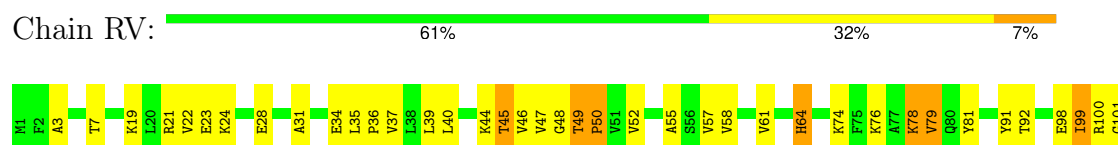
- Molecule 16: 50S ribosomal protein L20



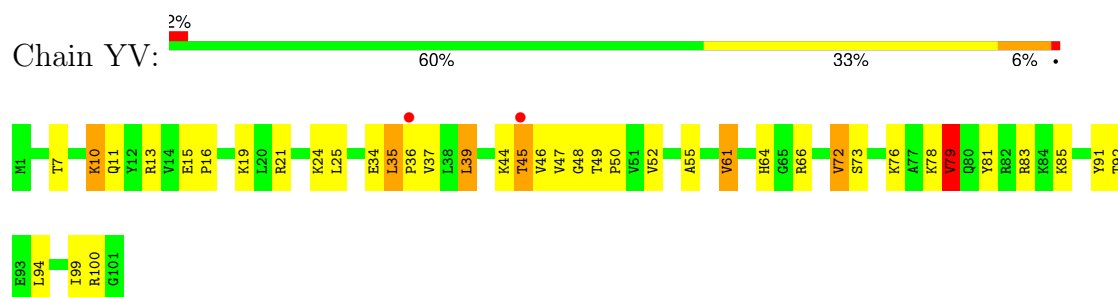
- Molecule 16: 50S ribosomal protein L20



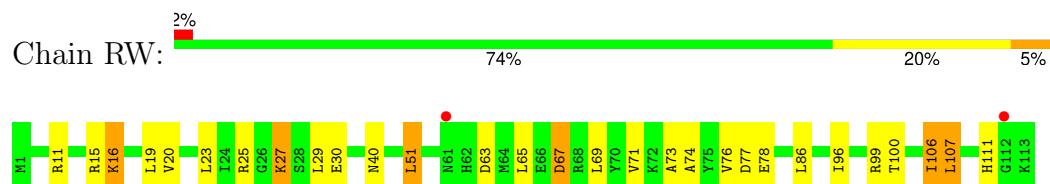
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



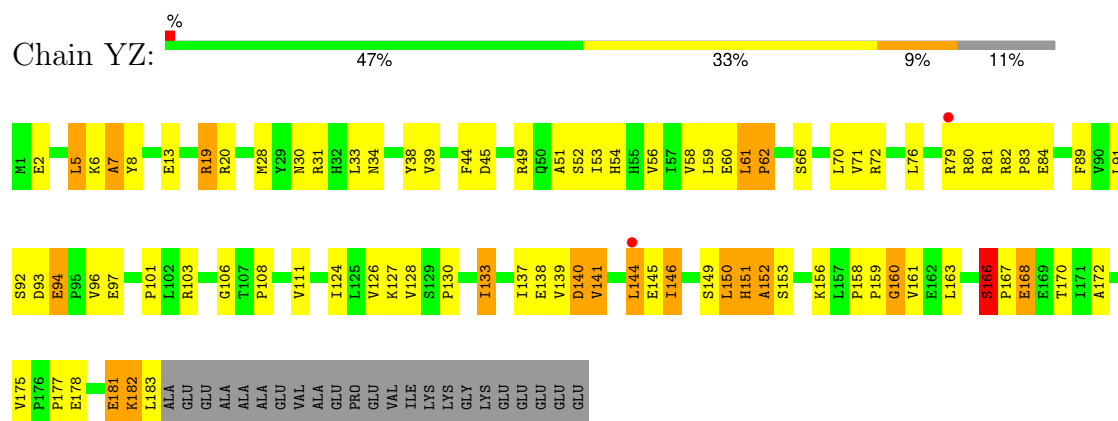
- Molecule 18: 50S ribosomal protein L22



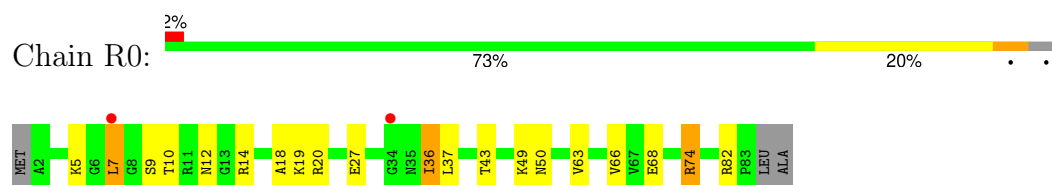
- Molecule 18: 50S ribosomal protein L22



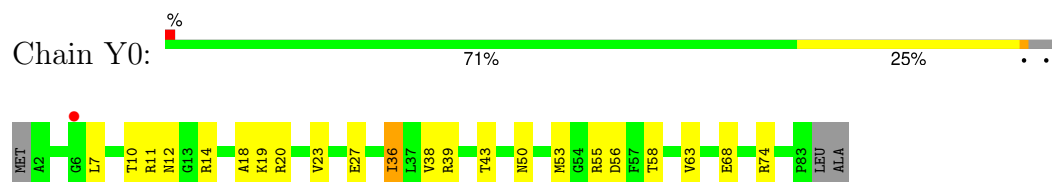
- Molecule 21: 50S ribosomal protein L25



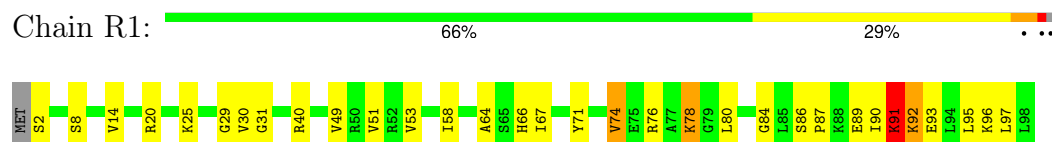
- Molecule 22: 50S ribosomal protein L27



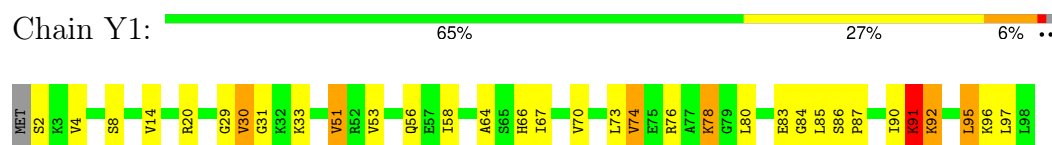
- Molecule 22: 50S ribosomal protein L27



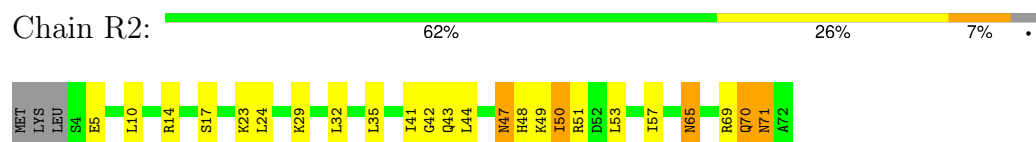
- Molecule 23: 50S ribosomal protein L28



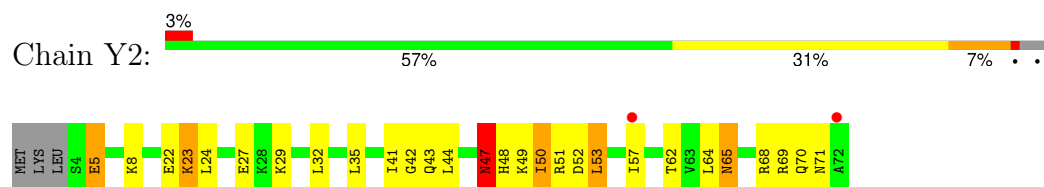
- Molecule 23: 50S ribosomal protein L28



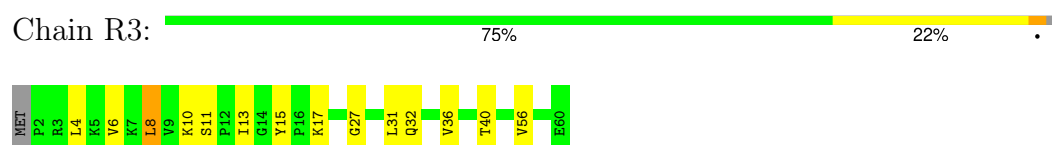
- Molecule 24: 50S ribosomal protein L29



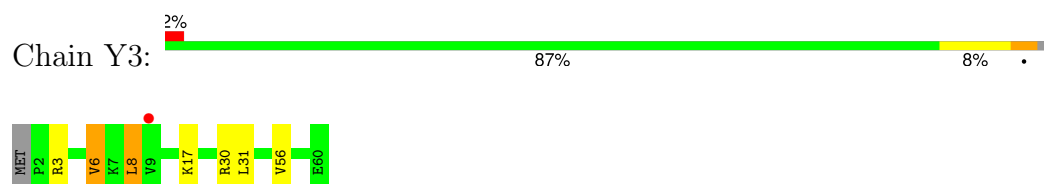
- Molecule 24: 50S ribosomal protein L29



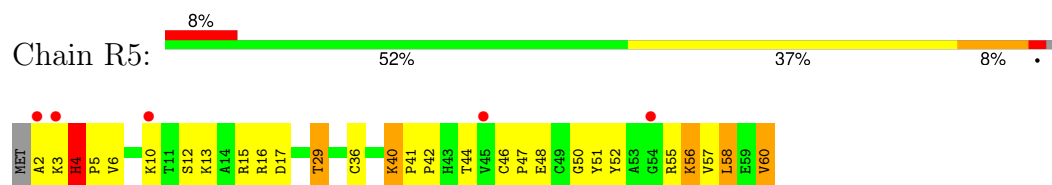
- Molecule 25: 50S ribosomal protein L30



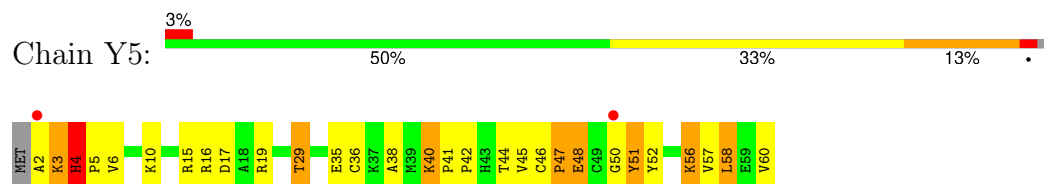
- Molecule 25: 50S ribosomal protein L30



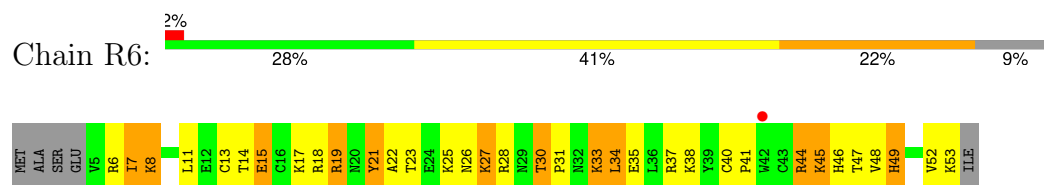
- Molecule 26: 50S ribosomal protein L32



- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33

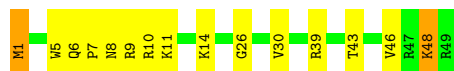


- Molecule 27: 50S ribosomal protein L33

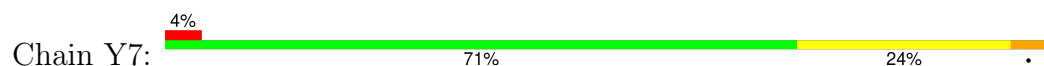




- Molecule 28: 50S ribosomal protein L34



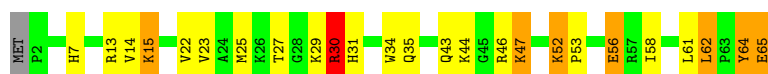
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



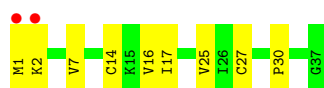
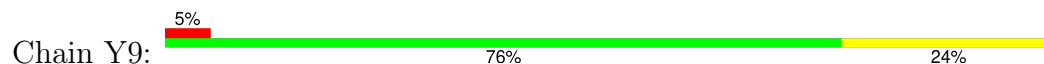
- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36

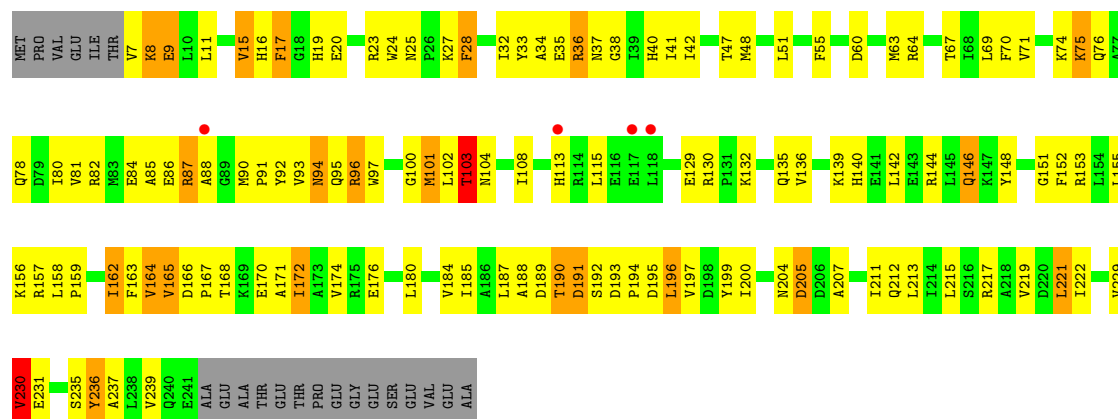


- Molecule 30: 50S ribosomal protein L36



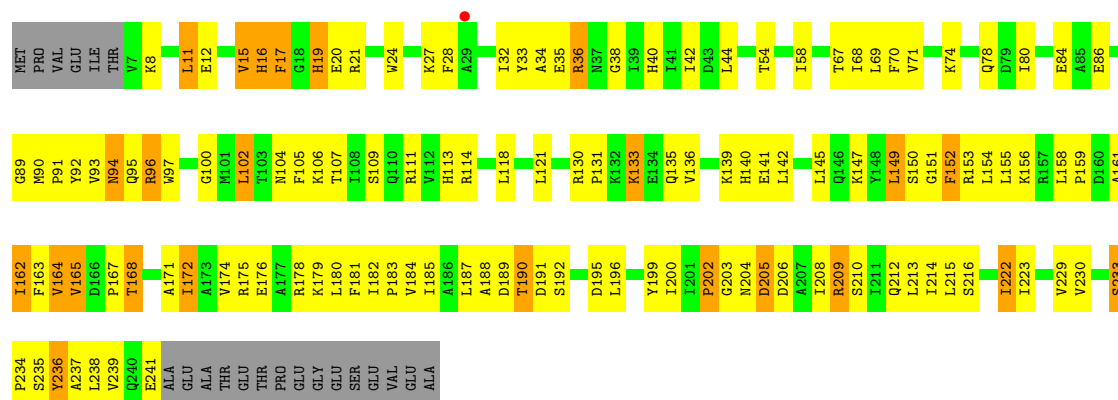
- Molecule 31: 30S ribosomal protein S2





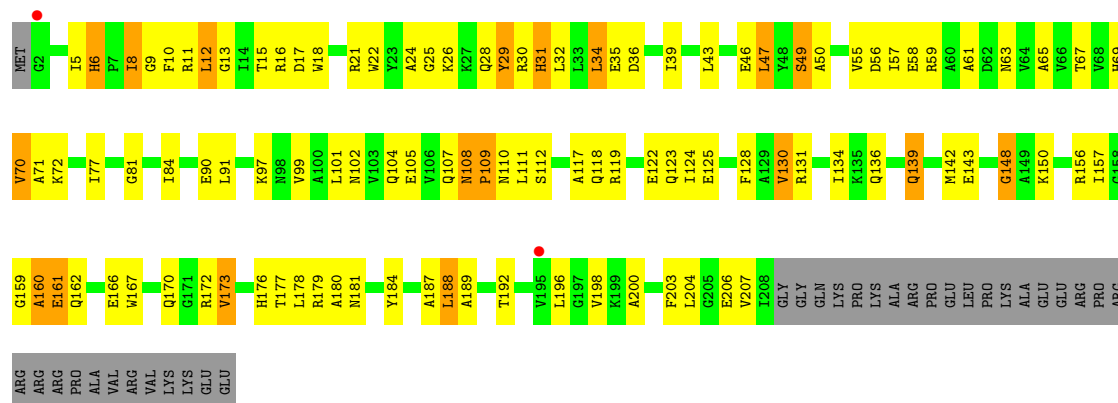
• Molecule 31: 30S ribosomal protein S2

Chain XB: 41% 41% 9% 8%



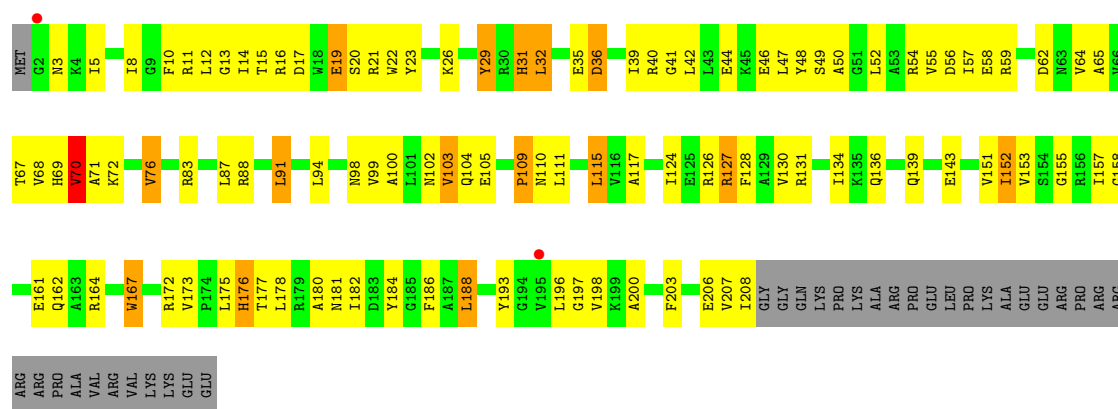
• Molecule 32: 30S ribosomal protein S3

Chain QC: 42% 37% 8% 13%

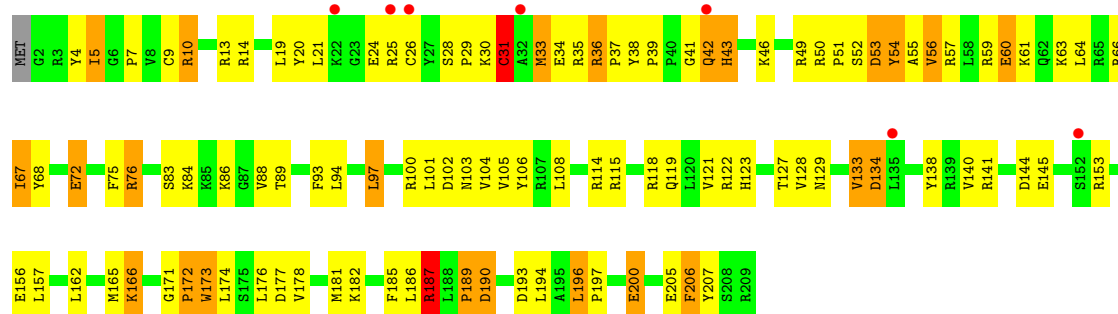


• Molecule 32: 30S ribosomal protein S3

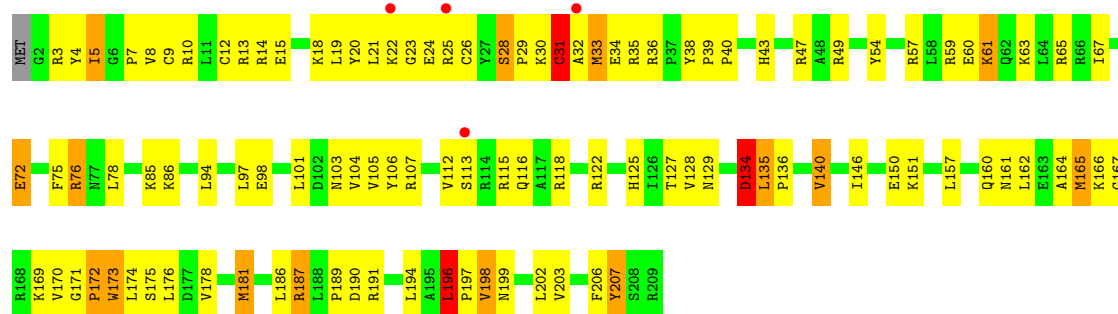
Chain XC: 42% 38% 6% 13%



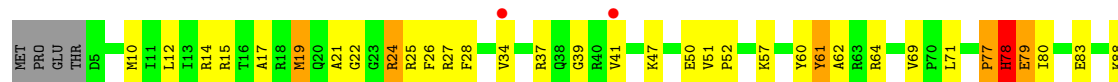
• Molecule 33: 30S ribosomal protein S4



• Molecule 33: 30S ribosomal protein S4



• Molecule 34: 30S ribosomal protein S5

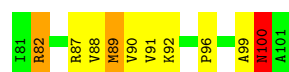
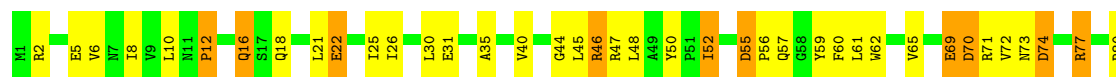




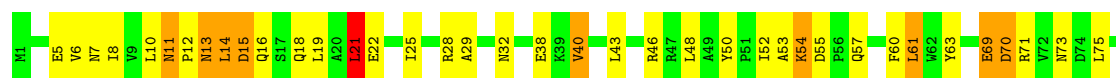
- Molecule 34: 30S ribosomal protein S5



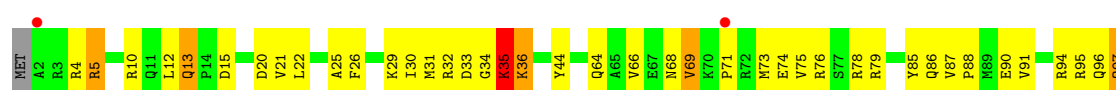
- Molecule 35: 30S ribosomal protein S6



- Molecule 35: 30S ribosomal protein S6

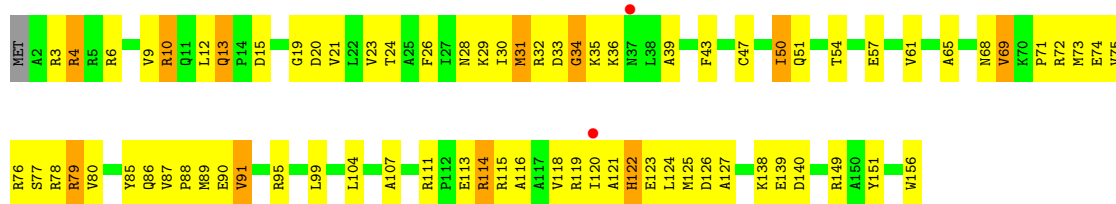


- Molecule 36: 30S ribosomal protein S7

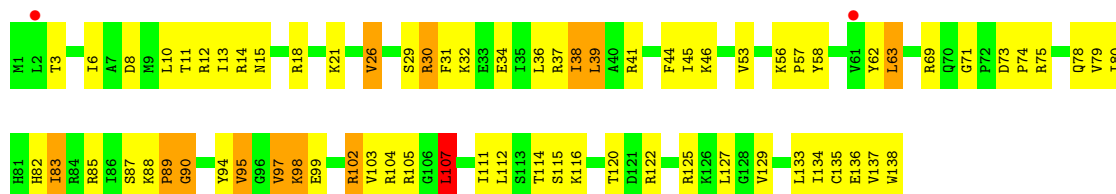


- Molecule 36: 30S ribosomal protein S7

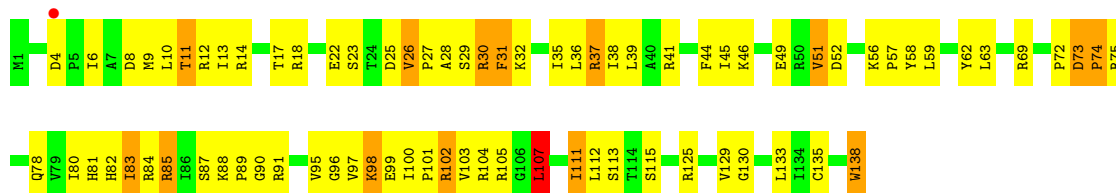
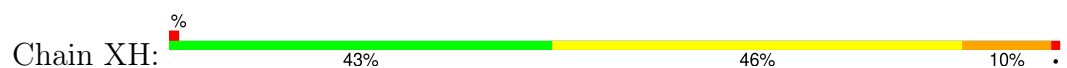




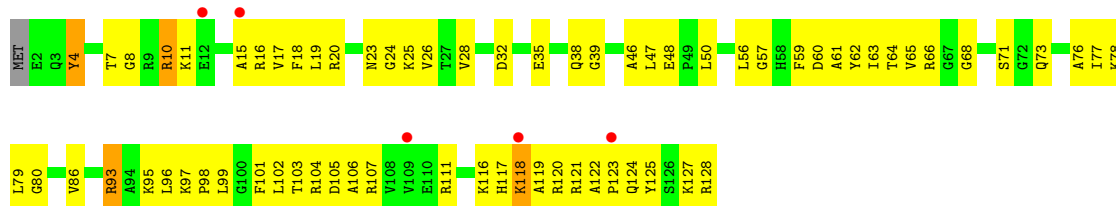
• Molecule 37: 30S ribosomal protein S8



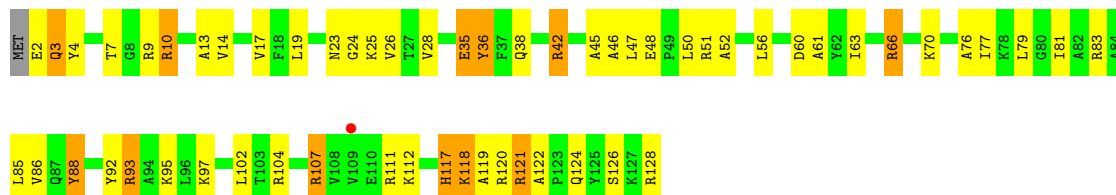
• Molecule 37: 30S ribosomal protein S8



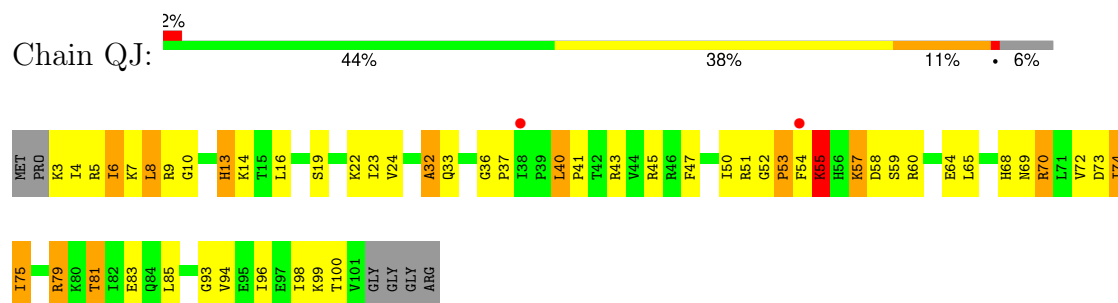
• Molecule 38: 30S ribosomal protein S9



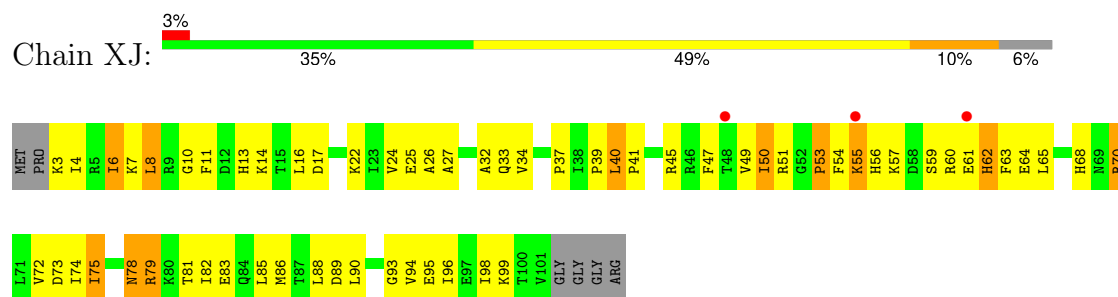
• Molecule 38: 30S ribosomal protein S9



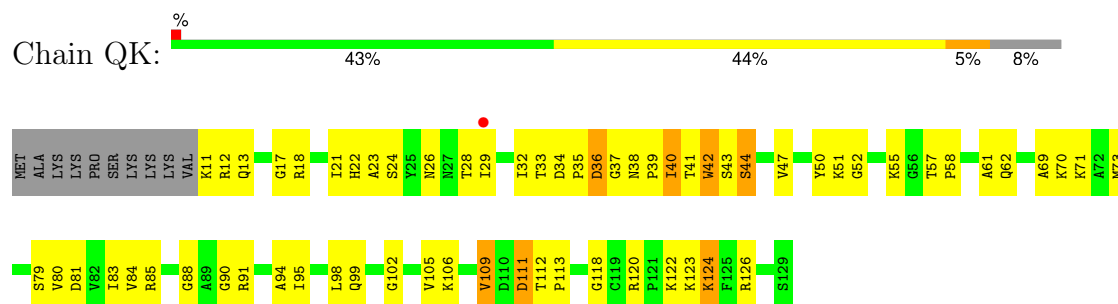
• Molecule 39: 30S ribosomal protein S10



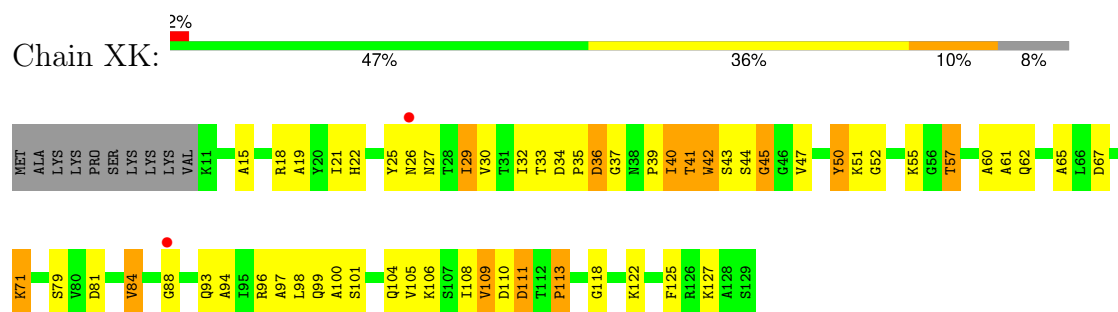
• Molecule 39: 30S ribosomal protein S10



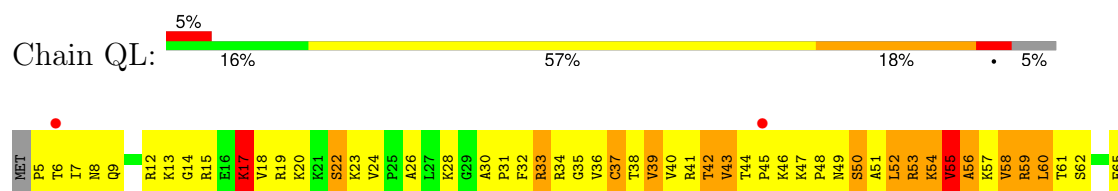
• Molecule 40: 30S ribosomal protein S11



• Molecule 40: 30S ribosomal protein S11

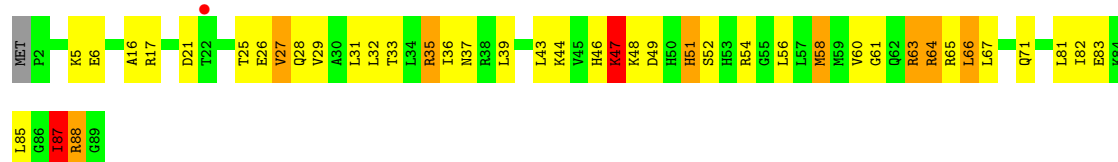


• Molecule 41: 30S ribosomal protein S12





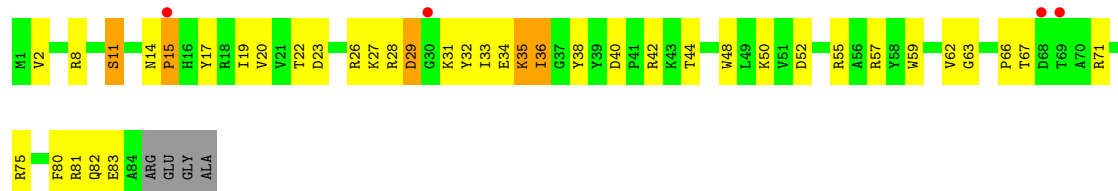
- Molecule 44: 30S ribosomal protein S15



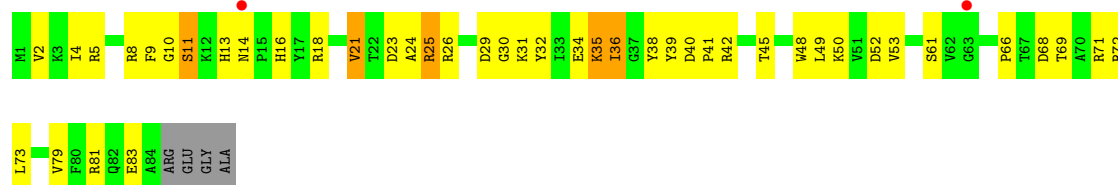
- Molecule 44: 30S ribosomal protein S15



- Molecule 45: 30S ribosomal protein S16

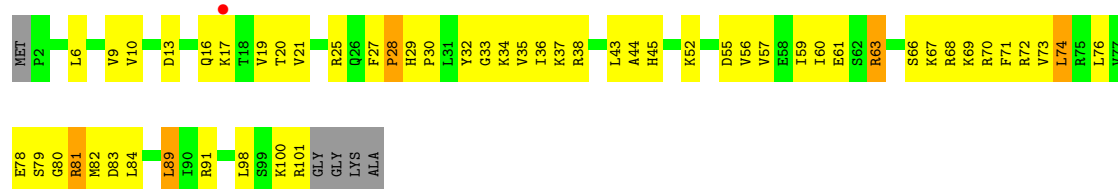


- Molecule 45: 30S ribosomal protein S16

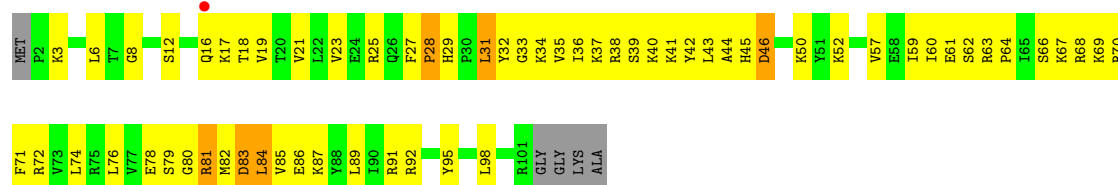
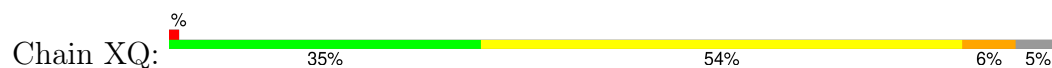


- Molecule 46: 30S ribosomal protein S17





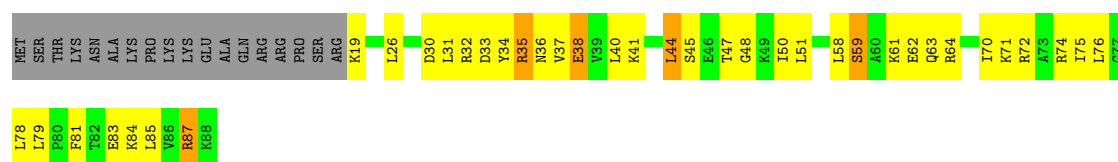
- Molecule 46: 30S ribosomal protein S17



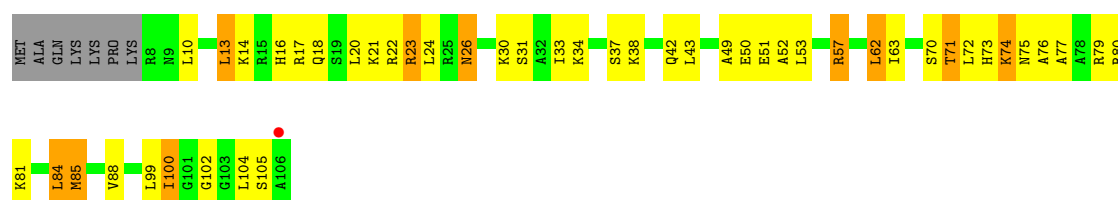
- Molecule 47: 30S ribosomal protein S18



- Molecule 47: 30S ribosomal protein S18



- Molecule 48: 30S ribosomal protein S20

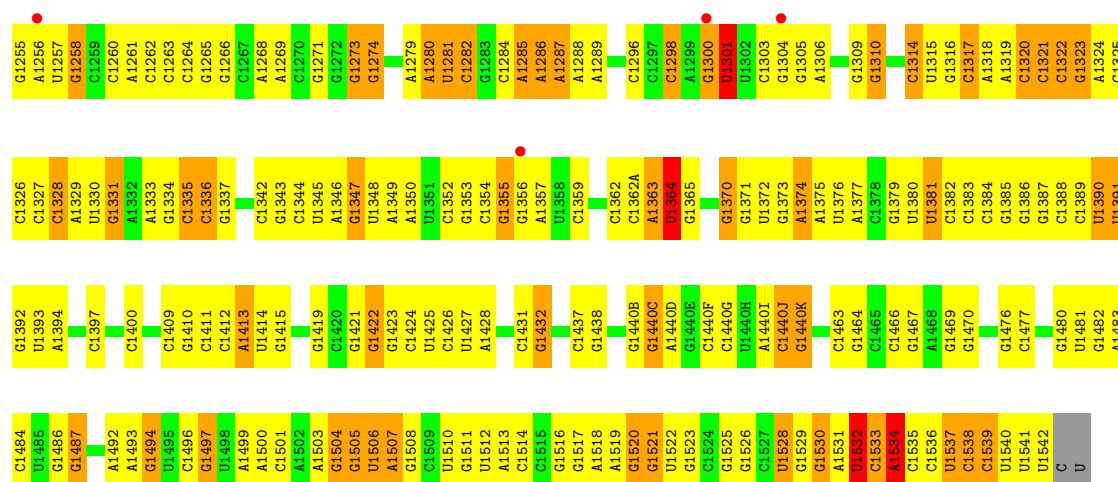


- Molecule 48: 30S ribosomal protein S20

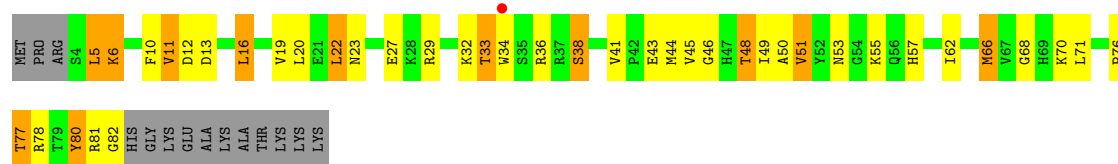
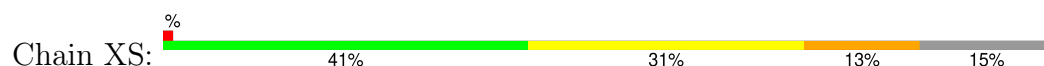




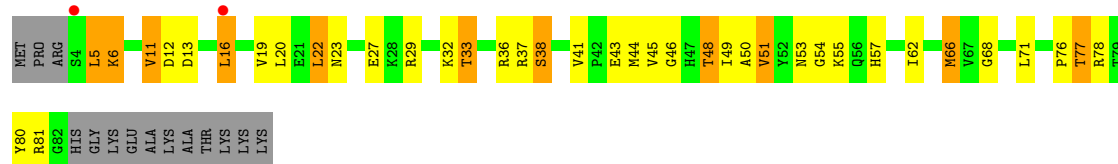
G1181	G1106	G1028H	G971	G902	U820	C744	G673	G604	U534	C436	C366	G299	G226
G1182	C1107	G1033	G972	G903	G821	C745	G674	U605	A535	U437	U367	A300	G227
A1183	G1108	G1034	G973	G906	G824	C748	A675	G606	C536	G438	C370	G306	A228
	C1109	A1035	A974	A975	G825	C749	A676	A607	G537	A440	G371	C307	U229
	G1112	G1036	G975	A908	C826	G750	U677	A609	G538	C443	C372	G308	G230
		G1037	G976	A909	U827	G751	C680	G610	A539	C444	A373	C309	G231
	C1115	C1038	A977	C910	A828	G752	C681	A611	G540	C445	A374	C310	G232
	C1116	C1039	A978	U911	G829	G753	G682	C612	G541	C446	U375	G311	C233
	G1117	U1040	G979			A754	G683	C613	G542		G376	C312	C237
	C1118	A1041	G980	A914		G755	G684	A614	C545	A452	G377	A313	G238
	C1119	G1042	U981			G756	G685	G615	G546	A453	G378	C314	U239
	G1120	G1043	U982	A918		G757	G686	G616	A547		C379	A315	C240
	U1121	A1044	A983	A919	U835	G758	A687	G617		G458A	G380	A316	C241
		G1045	C984	U920			C688	G618	U551	A458B	C381	G316	U244
	G1124	A1046	C985	U921	U838A	A759	C689	U619	U552	A458C	A382	G317	
	U1125	G1047	A986	U922	C838B	G760	C690	C620	A553	G458D	A383	G318	C245
	U1126	U1048	G987	G922	U838C	G761	C691	A621	C554	A458E	A384	G319	A246
	A1201	U1049	G988	A923	C848	G762	U692	A622	C555	G474	C385	C320	G247
	U1127	G1050		C924	C849	G763	G693	G623	C556			A321	
	C1128	U1051	U992	G925	C850	G764	A693	C624	C557	U480	G388	A322	A250
	G1129	G1052	A993	G926	U850	G765	A694	C625	G557	A481	A389	U323	G251
	A1130	U1053	A994	G927	G851	A766	A695	G626	G558	A482		G324	U252
	G1131	C1054	C995	G928	G852	A767		U626	A559	G483		A325	
		A1055	A996	G929	G853	G768	C701	G627	U560	G484	G392		U253
	U1135	U1056		C930	G854	G769	A702		U561	G485	A393		G254
	U1136	G1057	C988A	C931	G855	C770	G703	G633	C562		G394	C326	G255
	C1137	U1058	U999	G932	C856	C771	A704	C634	A563		C395	A329	U256
	G1138	C1059	A1000	G933	C857		U705	G635	C564	G491	G396	C330	G257
	U1139	G1060	G1001	C934	G858	A777	A706		U565	A498	A397	G331	U258
	C1140	G1061	G1002	A935	A859	G778	C707	G638	G566	G493	G398	G332	G259
		U1062	G1003			G779	C708	G639	G567	U494	G399	G333	
	G1145	U1063	A1004	G939	A864	A780		G640	G568	A495	C400	G334	U261
	A1146	G1064		C940	A865	A781	G711	A642	C401	A497	C401	C335	A262
	C1147	U1065	C1007	G941	C866		A712	C643	G570	U498	G402	C336	G263
	U1148	G1066	C1008		G867	C784	G713	G644	U571	G500	G403	C337	U264
	G1149	A1067	G1009	A946	C868		G714	C645	A572	C501	U405	A338	G265
	U1150	G1070	G1010	G947	G869	A787	A715	U646	A573		U406	C339	G266
	A1151	U1073	G1011	C948	U870	U788	A716	C647	A574	G505	G406	U340	C267
	A1152	G1074	U1012	A949	A872	U789	C717	A648	G575	G508	G407	C341	C268
		U1075	U950	C948		A790	G718	G649	G576	A509	A408	C342	C269
	G1157	G1076	G951	U950		G791	C719	G650	G577	C508	G409	U343	A270
	U1159	U1077	A1015	U952	C875	A792	C720	C651	U580	A510		A344	C271
	G1160	U1078	A1016	G953	G876	U793	G721	A652	G581	C511	A412	C345	C272
	C1161	G1079	G1017	G954	C877	A794	A722	A653	U582	U512	G413	G346	G273
		A1080	U955	U955	G878		U723	G654	A583	C513	A414	G347	
	G1166	G1081	C1018	U956	C879	G799		G658	G584	C514		G348	G278
	U1235	U1082	C1019	U957	C880	G800	G727	U659	G585	G515	C422	A349	A279
	A1167	U1083	G1021	U958	G881		A728	G660	G586	G518	G423	G350	C280
	C1237	G1084	U1022	A959	G888	C806	A729	G661	C590	C519	G425	C351	G281
	A1238		G1023	U960	A889	A807	G730	G662		A520	G426	A353	G289
	G1171	U1094	U1024	U961	G890	C811	G731	A663	G595	G521	U427	G354	C290
	U1240	U1095	G1025	C962	G890	C812	G732	A664	C596	C522	G428		G291
	G1172	C1096	G1026	G963	C933	U813	A733	A665	G597	U429	U429	G352	G292
	C1242	C1097	C1027	A964	C933	A814	G734	G666	G599	A523	A430	A360	G293
	G1173	G1098	C1028	A965	C936	A815	C735	G667	C600	G524	A431	G361	U294
	A1175	G1099	C1028A	G966	C936	A816	C736	G667	C601	C525	A432	G362	C295
	C1244	G1100	C1028B	C967	C939	A817	A737	G668	A602	A532	C433	A363	U296
	A1245	A1101	G1028C	A968	A900	C817	C738				U434		G297
				A969	A901	A819	U743			A533	C435		A298
	G1179	A1105	G1028G	C970									



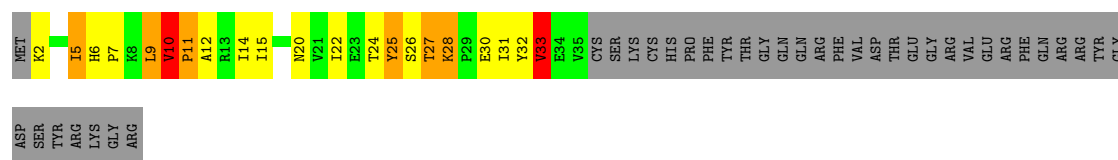
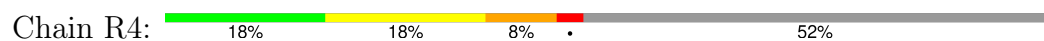
• Molecule 50: 30S ribosomal protein S19



• Molecule 50: 30S ribosomal protein S19

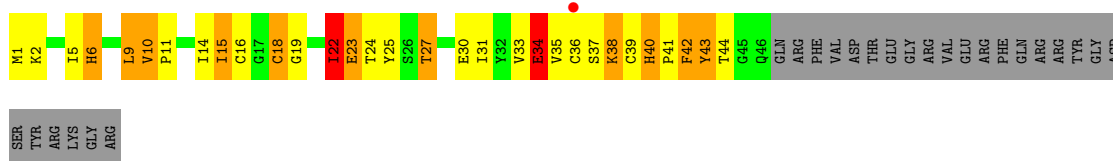


• Molecule 51: 50S ribosomal protein L31



• Molecule 51: 50S ribosomal protein L31





- Molecule 52: messenger RNA

Chain XX: 68% 26% 5%



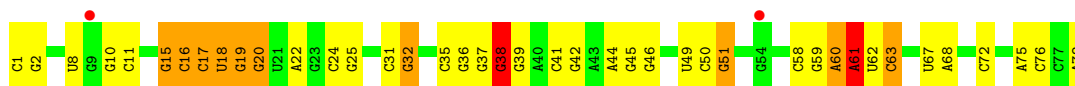
- Molecule 52: messenger RNA

Chain QX: 63% 32% 5%



- Molecule 53: P-site tRNA SufA6

Chain XV: 3% 47% 37% 13%



- Molecule 53: P-site tRNA SufA6

Chain QV: 49% 32% 13% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.75Å 450.05Å 626.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.60 – 3.90 16.60 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (16.60-3.90) 96.8 (16.60-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.272 , 0.316	Depositor DCC
R_{free} test set	22947 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	291660	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	RA	0.31	11/69520 (0.0%)	0.97	171/108525 (0.2%)
1	YA	0.29	1/69543 (0.0%)	0.96	137/108563 (0.1%)
2	RB	0.29	0/2878	0.99	11/4490 (0.2%)
2	YB	0.29	0/2878	0.99	9/4490 (0.2%)
3	RD	0.28	0/2165	0.54	0/2919
3	YD	0.27	0/2165	0.53	0/2919
4	RE	0.29	0/1601	0.60	2/2160 (0.1%)
4	YE	0.32	1/1601 (0.1%)	0.59	1/2160 (0.0%)
5	RF	0.28	0/1620	0.55	1/2194 (0.0%)
5	YF	0.27	0/1620	0.51	0/2194
6	RG	0.28	0/1499	0.55	0/2016
6	YG	0.26	0/1499	0.51	0/2016
7	RH	0.28	0/1332	0.56	0/1802
7	YH	0.30	0/1332	0.61	1/1802 (0.1%)
8	RI	0.26	0/1151	0.61	0/1558
8	YI	0.27	0/1151	0.60	0/1558
9	RN	0.26	0/1131	0.51	0/1525
9	YN	0.26	0/1131	0.50	0/1525
10	RO	0.26	0/943	0.51	0/1269
10	YO	0.26	0/943	0.51	0/1269
11	RP	0.28	0/1162	0.65	1/1544 (0.1%)
11	YP	0.28	0/1162	0.63	0/1544
12	RQ	0.31	0/1143	0.58	0/1527
12	YQ	0.28	0/1143	0.55	0/1527
13	RR	0.26	0/982	0.55	0/1312
13	YR	0.29	0/982	0.57	0/1312
14	RS	0.27	0/892	0.58	0/1187
14	YS	0.27	0/892	0.60	0/1187
15	RT	0.35	0/1155	0.65	2/1542 (0.1%)
15	YT	0.32	0/1155	0.59	0/1542
16	RU	0.28	0/982	0.54	0/1306
16	YU	0.25	0/982	0.47	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	RV	0.26	0/790	0.55	0/1057
17	YV	0.27	0/790	0.58	1/1057 (0.1%)
18	RW	0.26	0/911	0.48	0/1220
18	YW	0.26	0/911	0.51	0/1220
19	RX	0.28	0/739	0.49	0/993
19	YX	0.30	0/739	0.51	0/993
20	RY	0.31	0/798	0.61	0/1064
20	YY	0.30	0/798	0.60	0/1064
21	RZ	0.28	0/1493	0.57	0/2026
21	YZ	0.27	0/1493	0.58	1/2026 (0.0%)
22	R0	0.26	0/657	0.53	0/874
22	Y0	0.33	0/657	0.56	0/874
23	R1	0.31	0/770	0.58	0/1022
23	Y1	0.29	0/770	0.55	0/1022
24	R2	0.25	0/583	0.53	0/771
24	Y2	0.23	0/583	0.49	0/771
25	R3	0.27	0/474	0.51	0/635
25	Y3	0.22	0/474	0.44	0/635
26	R5	0.26	0/473	0.57	0/639
26	Y5	0.27	0/473	0.55	0/639
27	R6	0.27	0/431	0.63	0/575
27	Y6	0.25	0/431	0.61	0/575
28	R7	0.24	0/438	0.48	0/575
28	Y7	0.23	0/438	0.45	0/575
29	R8	0.27	0/525	0.58	0/691
29	Y8	0.33	0/525	0.60	0/691
30	R9	0.24	0/310	0.51	0/407
30	Y9	0.23	0/310	0.48	0/407
31	QB	0.28	0/1944	0.58	0/2621
31	XB	0.27	0/1944	0.59	0/2621
32	QC	0.26	0/1644	0.57	0/2216
32	XC	0.27	0/1644	0.60	0/2216
33	QD	0.45	2/1733 (0.1%)	0.70	4/2318 (0.2%)
33	XD	0.30	0/1733	0.62	0/2318
34	QE	0.28	0/1171	0.58	0/1576
34	XE	0.26	0/1171	0.58	1/1576 (0.1%)
35	QF	0.25	0/856	0.59	0/1154
35	XF	0.27	0/856	0.60	1/1154 (0.1%)
36	QG	0.25	0/1276	0.51	0/1709
36	XG	0.26	0/1276	0.51	0/1709
37	QH	0.26	0/1136	0.58	0/1527
37	XH	0.27	0/1136	0.58	0/1527
38	QI	0.29	0/1029	0.55	0/1379

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	XI	0.26	0/1029	0.55	0/1379
39	QJ	0.26	0/814	0.53	0/1095
39	XJ	0.26	0/814	0.57	0/1095
40	QK	0.28	0/900	0.54	0/1213
40	XK	0.27	0/900	0.54	0/1213
41	QL	0.28	0/991	0.68	0/1327
41	XL	0.30	0/991	0.74	1/1327 (0.1%)
42	QM	0.25	0/924	0.57	0/1238
42	XM	0.29	0/924	0.64	0/1238
43	QN	0.28	0/501	0.56	0/664
43	XN	0.30	0/501	0.59	0/664
44	QO	0.24	0/745	0.55	0/992
44	XO	0.34	1/745 (0.1%)	0.55	0/992
45	QP	0.26	0/721	0.62	0/970
45	XP	0.26	0/721	0.60	0/970
46	QQ	0.28	0/847	0.61	0/1131
46	XQ	0.27	0/847	0.59	0/1131
47	QR	0.28	0/579	0.62	0/768
47	XR	0.28	0/579	0.65	0/768
48	QT	0.23	0/765	0.53	0/1007
48	XT	0.24	0/765	0.50	0/1007
49	QA	0.25	0/36347	0.90	37/56727 (0.1%)
49	XA	0.31	6/36439 (0.0%)	0.96	86/56872 (0.2%)
50	QS	0.23	0/646	0.49	0/870
50	XS	0.24	0/646	0.49	0/870
51	R4	0.34	0/267	0.63	0/362
51	Y4	0.27	0/366	0.57	0/495
52	QX	0.22	0/459	0.89	2/715 (0.3%)
52	XX	0.21	0/459	0.89	2/715 (0.3%)
53	QV	0.22	0/1839	0.87	9/2866 (0.3%)
53	XV	0.17	0/1839	0.78	2/2866 (0.1%)
All	All	0.29	22/315578 (0.0%)	0.87	483/472056 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	RA	0	2
3	RD	0	1
7	RH	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	YH	0	2
11	RP	0	1
15	RT	0	1
21	YZ	0	1
23	R1	0	1
29	R8	0	1
33	QD	0	1
33	XD	0	1
49	XA	0	2
53	QV	0	1
All	All	0	17

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	XA	771	G	C1'-N9	18.11	1.75	1.48
1	RA	1558	A	C1'-N9	17.07	1.74	1.48
1	RA	1913	A	C5'-C4'	16.54	1.71	1.51
49	XA	771	G	C4'-O4'	14.31	1.64	1.45
1	RA	1463	C	C5'-C4'	12.46	1.66	1.51

The worst 5 of 483 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	XA	771	G	O4'-C1'-N9	26.71	129.57	108.20
1	RA	1558	A	C8-N9-C1'	-26.16	80.62	127.70
1	RA	1558	A	O4'-C1'-N9	-24.62	88.50	108.20
1	RA	1463	C	C2-N1-C1'	24.24	145.47	118.80
1	RA	1762	A	N1-C6-N6	-24.02	104.19	118.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	RA	1558	A	Sidechain
1	RA	1765	C	Sidechain
3	RD	235	GLY	Mainchain
7	RH	127	GLU	Peptide
7	RH	153	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	62071	0	31249	1298	0
1	YA	62091	0	31283	1245	0
2	RB	2573	0	1299	53	0
2	YB	2573	0	1304	49	0
3	RD	2115	0	2191	68	0
3	YD	2115	0	2194	63	0
4	RE	1568	0	1632	58	0
4	YE	1568	0	1633	51	0
5	RF	1585	0	1630	48	0
5	YF	1585	0	1632	53	0
6	RG	1474	0	1535	68	0
6	YG	1474	0	1535	56	0
7	RH	1307	0	1382	54	0
7	YH	1307	0	1382	54	0
8	RI	1136	0	1223	44	0
8	YI	1136	0	1223	42	0
9	RN	1104	0	1180	33	0
9	YN	1104	0	1180	35	0
10	RO	933	0	995	13	0
10	YO	933	0	996	22	0
11	RP	1145	0	1228	54	0
11	YP	1145	0	1228	69	0
12	RQ	1122	0	1179	39	0
12	YQ	1122	0	1179	35	0
13	RR	968	0	1032	34	0
13	YR	968	0	1031	28	0
14	RS	882	0	943	33	0
14	YS	882	0	943	36	0
15	RT	1141	0	1200	39	0
15	YT	1141	0	1201	45	0
16	RU	964	0	1022	30	0
16	YU	964	0	1022	32	0
17	RV	779	0	852	22	0
17	YV	779	0	852	22	0
18	RW	900	0	964	13	0
18	YW	900	0	964	21	0
19	RX	725	0	778	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	YX	725	0	778	21	0
20	RY	785	0	877	30	0
20	YY	785	0	877	30	0
21	RZ	1461	0	1493	46	0
21	YZ	1461	0	1493	51	0
22	R0	648	0	671	18	0
22	Y0	648	0	672	18	0
23	R1	763	0	846	21	0
23	Y1	763	0	847	26	0
24	R2	581	0	629	15	0
24	Y2	581	0	629	14	0
25	R3	469	0	518	10	0
25	Y3	469	0	518	3	0
26	R5	459	0	480	25	0
26	Y5	459	0	479	25	0
27	R6	424	0	450	26	0
27	Y6	424	0	450	23	0
28	R7	430	0	480	11	0
28	Y7	430	0	480	12	0
29	R8	517	0	582	23	0
29	Y8	517	0	582	24	0
30	R9	307	0	338	7	0
30	Y9	307	0	335	5	0
31	QB	1909	0	1957	99	0
31	XB	1909	0	1957	100	0
32	QC	1620	0	1688	63	0
32	XC	1620	0	1687	74	0
33	QD	1703	0	1762	97	0
33	XD	1703	0	1765	83	0
34	QE	1155	0	1213	52	0
34	XE	1155	0	1213	47	0
35	QF	843	0	857	32	0
35	XF	843	0	857	42	0
36	QG	1257	0	1296	34	0
36	XG	1257	0	1296	56	0
37	QH	1116	0	1177	52	0
37	XH	1116	0	1177	73	0
38	QI	1010	0	1035	58	0
38	XI	1010	0	1037	55	0
39	QJ	801	0	849	51	0
39	XJ	801	0	849	46	0
40	QK	885	0	904	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	XK	885	0	904	47	0
41	QL	975	0	1062	109	0
41	XL	975	0	1061	88	0
42	QM	914	0	971	33	0
42	XM	914	0	971	54	0
43	QN	492	0	533	26	0
43	XN	492	0	533	34	0
44	QO	734	0	771	39	0
44	XO	734	0	768	27	0
45	QP	705	0	724	38	0
45	XP	705	0	725	39	0
46	QQ	834	0	903	48	0
46	XQ	834	0	904	59	0
47	QR	574	0	644	35	0
47	XR	574	0	644	40	0
48	QT	763	0	861	33	0
48	XT	763	0	861	44	0
49	QA	32472	0	16387	843	0
49	XA	32554	0	16414	909	0
50	QS	633	0	655	28	0
50	XS	633	0	655	28	0
51	R4	262	0	272	25	0
51	Y4	357	0	362	29	0
52	QX	409	0	209	49	0
52	XX	409	0	209	53	0
53	QV	1670	0	845	49	0
53	XV	1670	0	845	30	0
54	QA	131	0	0	0	0
54	QC	1	0	0	0	0
54	QD	3	0	0	0	0
54	QE	1	0	0	0	0
54	QL	3	0	0	0	0
54	QP	2	0	0	0	0
54	QQ	2	0	0	0	0
54	QT	2	0	0	0	0
54	R0	2	0	0	0	0
54	R1	3	0	0	0	0
54	R3	1	0	0	0	0
54	R6	1	0	0	0	0
54	R8	3	0	0	0	0
54	RA	562	0	0	0	0
54	RB	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	RD	10	0	0	0	0
54	RE	7	0	0	0	0
54	RF	4	0	0	0	0
54	RI	1	0	0	0	0
54	RO	2	0	0	0	0
54	RQ	2	0	0	0	0
54	RR	3	0	0	0	0
54	RT	3	0	0	0	0
54	RU	1	0	0	0	0
54	RX	2	0	0	0	0
54	RY	1	0	0	0	0
54	XA	128	0	0	0	0
54	XC	1	0	0	0	0
54	XD	1	0	0	0	0
54	XE	1	0	0	0	0
54	XK	1	0	0	0	0
54	XL	2	0	0	0	0
54	XM	1	0	0	0	0
54	XO	1	0	0	0	0
54	XP	1	0	0	0	0
54	Y0	1	0	0	0	0
54	Y1	1	0	0	0	0
54	Y8	1	0	0	0	0
54	YA	379	0	0	0	0
54	YB	10	0	0	0	0
54	YD	4	0	0	0	0
54	YE	5	0	0	0	0
54	YI	1	0	0	0	0
54	YP	1	0	0	0	0
54	YQ	1	0	0	0	0
54	YR	1	0	0	0	0
54	YT	2	0	0	0	0
54	YU	1	0	0	0	0
54	YX	1	0	0	0	0
54	YY	1	0	0	0	0
55	QD	2	0	0	0	0
55	XD	1	0	0	0	0
55	Y9	1	0	0	0	0
All	All	291660	0	197069	7411	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 15.

The worst 5 of 7411 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)
49:QA:1339:A:C2	53:QV:32:G:H1'	1.41	1.52
1:RA:1558:A:N9	1:RA:1558:A:C1'	1.74	1.48
49:XA:771:G:N9	49:XA:771:G:C1'	1.75	1.46
49:XA:1531:A:C5	49:XA:1532:U:O4	1.70	1.42
49:XA:771:G:C4'	49:XA:771:G:O4'	1.64	1.41

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	
3	RD	270/276 (98%)	235 (87%)	28 (10%)	7 (3%)	4	29
3	YD	270/276 (98%)	234 (87%)	30 (11%)	6 (2%)	5	32
4	RE	203/206 (98%)	158 (78%)	29 (14%)	16 (8%)	1	12
4	YE	203/206 (98%)	154 (76%)	33 (16%)	16 (8%)	1	12
5	RF	200/210 (95%)	173 (86%)	21 (10%)	6 (3%)	3	27
5	YF	200/210 (95%)	177 (88%)	18 (9%)	5 (2%)	4	30
6	RG	179/182 (98%)	149 (83%)	20 (11%)	10 (6%)	1	17
6	YG	179/182 (98%)	151 (84%)	18 (10%)	10 (6%)	1	17
7	RH	168/180 (93%)	129 (77%)	22 (13%)	17 (10%)	0	8
7	YH	168/180 (93%)	126 (75%)	25 (15%)	17 (10%)	0	8
8	RI	144/148 (97%)	109 (76%)	25 (17%)	10 (7%)	1	14
8	YI	144/148 (97%)	108 (75%)	28 (19%)	8 (6%)	1	17
9	RN	136/140 (97%)	113 (83%)	15 (11%)	8 (6%)	1	16
9	YN	136/140 (97%)	114 (84%)	13 (10%)	9 (7%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	RO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	51
10	YO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	51
11	RP	148/150 (99%)	105 (71%)	32 (22%)	11 (7%)	1	13
11	YP	148/150 (99%)	106 (72%)	32 (22%)	10 (7%)	1	14
12	RQ	139/141 (99%)	104 (75%)	21 (15%)	14 (10%)	0	8
12	YQ	139/141 (99%)	105 (76%)	17 (12%)	17 (12%)	0	5
13	RR	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	7	36
13	YR	116/118 (98%)	104 (90%)	9 (8%)	3 (3%)	4	29
14	RS	109/112 (97%)	81 (74%)	19 (17%)	9 (8%)	0	11
14	YS	109/112 (97%)	83 (76%)	17 (16%)	9 (8%)	0	11
15	RT	135/146 (92%)	109 (81%)	19 (14%)	7 (5%)	1	18
15	YT	135/146 (92%)	110 (82%)	19 (14%)	6 (4%)	2	21
16	RU	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	7	36
16	YU	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	7	36
17	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	16
17	YV	99/101 (98%)	84 (85%)	9 (9%)	6 (6%)	1	16
18	RW	111/113 (98%)	105 (95%)	4 (4%)	2 (2%)	7	35
18	YW	111/113 (98%)	105 (95%)	4 (4%)	2 (2%)	7	35
19	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
19	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
20	RY	100/110 (91%)	73 (73%)	16 (16%)	11 (11%)	0	6
20	YY	100/110 (91%)	73 (73%)	17 (17%)	10 (10%)	0	8
21	RZ	181/206 (88%)	133 (74%)	29 (16%)	19 (10%)	0	7
21	YZ	181/206 (88%)	139 (77%)	26 (14%)	16 (9%)	0	10
22	R0	80/85 (94%)	74 (92%)	6 (8%)	0	100	100
22	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
23	R1	95/98 (97%)	75 (79%)	15 (16%)	5 (5%)	1	18
23	Y1	95/98 (97%)	75 (79%)	15 (16%)	5 (5%)	1	18
24	R2	67/72 (93%)	58 (87%)	4 (6%)	5 (8%)	1	13
24	Y2	67/72 (93%)	58 (87%)	4 (6%)	5 (8%)	1	13
25	R3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	7	35
26	R5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	7	35
26	Y5	57/60 (95%)	48 (84%)	7 (12%)	2 (4%)	3	24
27	R6	47/54 (87%)	21 (45%)	18 (38%)	8 (17%)	0	2
27	Y6	47/54 (87%)	24 (51%)	17 (36%)	6 (13%)	0	4
28	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	33
28	Y7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	33
29	R8	62/65 (95%)	53 (86%)	5 (8%)	4 (6%)	1	15
29	Y8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2	19
30	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
30	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
31	QB	233/256 (91%)	181 (78%)	38 (16%)	14 (6%)	1	16
31	XB	233/256 (91%)	190 (82%)	31 (13%)	12 (5%)	1	18
32	QC	205/239 (86%)	152 (74%)	33 (16%)	20 (10%)	0	8
32	XC	205/239 (86%)	157 (77%)	34 (17%)	14 (7%)	1	14
33	QD	206/209 (99%)	153 (74%)	40 (19%)	13 (6%)	1	16
33	XD	206/209 (99%)	149 (72%)	41 (20%)	16 (8%)	1	12
34	QE	149/162 (92%)	128 (86%)	17 (11%)	4 (3%)	4	29
34	XE	149/162 (92%)	123 (83%)	18 (12%)	8 (5%)	1	18
35	QF	99/101 (98%)	80 (81%)	15 (15%)	4 (4%)	2	22
35	XF	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	1	18
36	QG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	4	29
36	XG	153/156 (98%)	127 (83%)	18 (12%)	8 (5%)	1	18
37	QH	136/138 (99%)	105 (77%)	25 (18%)	6 (4%)	2	21
37	XH	136/138 (99%)	106 (78%)	24 (18%)	6 (4%)	2	21
38	QI	125/128 (98%)	106 (85%)	16 (13%)	3 (2%)	5	30
38	XI	125/128 (98%)	102 (82%)	19 (15%)	4 (3%)	3	26
39	QJ	97/105 (92%)	77 (79%)	15 (16%)	5 (5%)	1	18
39	XJ	97/105 (92%)	77 (79%)	16 (16%)	4 (4%)	2	22
40	QK	117/129 (91%)	86 (74%)	22 (19%)	9 (8%)	1	12
40	XK	117/129 (91%)	84 (72%)	23 (20%)	10 (8%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	QL	123/132 (93%)	44 (36%)	47 (38%)	32 (26%)	0	1
41	XL	123/132 (93%)	47 (38%)	44 (36%)	32 (26%)	0	1
42	QM	112/126 (89%)	95 (85%)	11 (10%)	6 (5%)	1	18
42	XM	112/126 (89%)	96 (86%)	10 (9%)	6 (5%)	1	18
43	QN	58/61 (95%)	44 (76%)	11 (19%)	3 (5%)	1	18
43	XN	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	7
44	QO	86/89 (97%)	74 (86%)	9 (10%)	3 (4%)	3	24
44	XO	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	11	43
45	QP	82/88 (93%)	62 (76%)	13 (16%)	7 (8%)	0	10
45	XP	82/88 (93%)	62 (76%)	14 (17%)	6 (7%)	1	13
46	QQ	98/105 (93%)	80 (82%)	17 (17%)	1 (1%)	13	46
46	XQ	98/105 (93%)	82 (84%)	13 (13%)	3 (3%)	3	26
47	QR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	13
47	XR	68/88 (77%)	54 (79%)	11 (16%)	3 (4%)	2	21
48	QT	97/106 (92%)	81 (84%)	13 (13%)	3 (3%)	3	26
48	XT	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	5	33
50	QS	77/93 (83%)	43 (56%)	25 (32%)	9 (12%)	0	5
50	XS	77/93 (83%)	43 (56%)	25 (32%)	9 (12%)	0	5
51	R4	32/71 (45%)	16 (50%)	13 (41%)	3 (9%)	0	9
51	Y4	44/71 (62%)	22 (50%)	11 (25%)	11 (25%)	0	1
All	All	11338/12074 (94%)	9058 (80%)	1601 (14%)	679 (6%)	1	16

5 of 679 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	RD	26	LYS
3	RD	122	ASP
3	RD	242	ARG
4	RE	22	PRO
4	RE	53	PRO

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	
3	RD	214/218 (98%)	184 (86%)	30 (14%)	3	17
3	YD	214/218 (98%)	187 (87%)	27 (13%)	3	18
4	RE	165/166 (99%)	137 (83%)	28 (17%)	1	11
4	YE	165/166 (99%)	142 (86%)	23 (14%)	3	17
5	RF	161/166 (97%)	147 (91%)	14 (9%)	8	30
5	YF	161/166 (97%)	145 (90%)	16 (10%)	6	24
6	RG	155/156 (99%)	141 (91%)	14 (9%)	8	28
6	YG	155/156 (99%)	135 (87%)	20 (13%)	3	18
7	RH	142/148 (96%)	126 (89%)	16 (11%)	4	21
7	YH	142/148 (96%)	123 (87%)	19 (13%)	3	17
8	RI	122/124 (98%)	99 (81%)	23 (19%)	1	8
8	YI	122/124 (98%)	102 (84%)	20 (16%)	2	12
9	RN	117/119 (98%)	102 (87%)	15 (13%)	3	18
9	YN	117/119 (98%)	103 (88%)	14 (12%)	4	19
10	RO	100/100 (100%)	92 (92%)	8 (8%)	10	33
10	YO	100/100 (100%)	91 (91%)	9 (9%)	8	28
11	RP	116/116 (100%)	88 (76%)	28 (24%)	0	4
11	YP	116/116 (100%)	92 (79%)	24 (21%)	1	5
12	RQ	111/111 (100%)	97 (87%)	14 (13%)	3	18
12	YQ	111/111 (100%)	98 (88%)	13 (12%)	4	20
13	RR	101/101 (100%)	89 (88%)	12 (12%)	4	20
13	YR	101/101 (100%)	90 (89%)	11 (11%)	5	22
14	RS	87/88 (99%)	72 (83%)	15 (17%)	1	11
14	YS	87/88 (99%)	75 (86%)	12 (14%)	3	17
15	RT	120/127 (94%)	107 (89%)	13 (11%)	5	22
15	YT	120/127 (94%)	102 (85%)	18 (15%)	2	14
16	RU	93/94 (99%)	82 (88%)	11 (12%)	4	20
16	YU	93/94 (99%)	84 (90%)	9 (10%)	6	25
17	RV	82/82 (100%)	70 (85%)	12 (15%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	YV	82/82 (100%)	69 (84%)	13 (16%)	2	13
18	RW	92/92 (100%)	78 (85%)	14 (15%)	2	14
18	YW	92/92 (100%)	79 (86%)	13 (14%)	3	16
19	RX	74/78 (95%)	64 (86%)	10 (14%)	3	17
19	YX	74/78 (95%)	63 (85%)	11 (15%)	2	14
20	RY	85/91 (93%)	66 (78%)	19 (22%)	1	5
20	YY	85/91 (93%)	70 (82%)	15 (18%)	1	10
21	RZ	162/179 (90%)	140 (86%)	22 (14%)	3	17
21	YZ	162/179 (90%)	139 (86%)	23 (14%)	2	16
22	R0	65/67 (97%)	60 (92%)	5 (8%)	10	34
22	Y0	65/67 (97%)	63 (97%)	2 (3%)	35	56
23	R1	82/83 (99%)	77 (94%)	5 (6%)	15	41
23	Y1	82/83 (99%)	75 (92%)	7 (8%)	8	31
24	R2	64/67 (96%)	58 (91%)	6 (9%)	7	26
24	Y2	64/67 (96%)	52 (81%)	12 (19%)	1	8
25	R3	51/52 (98%)	46 (90%)	5 (10%)	6	24
25	Y3	51/52 (98%)	48 (94%)	3 (6%)	16	41
26	R5	51/52 (98%)	40 (78%)	11 (22%)	1	5
26	Y5	51/52 (98%)	39 (76%)	12 (24%)	0	4
27	R6	48/52 (92%)	38 (79%)	10 (21%)	1	5
27	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	5
28	R7	42/42 (100%)	38 (90%)	4 (10%)	7	25
28	Y7	42/42 (100%)	38 (90%)	4 (10%)	7	25
29	R8	54/55 (98%)	45 (83%)	9 (17%)	2	12
29	Y8	54/55 (98%)	42 (78%)	12 (22%)	1	5
30	R9	34/34 (100%)	32 (94%)	2 (6%)	16	41
30	Y9	34/34 (100%)	32 (94%)	2 (6%)	16	41
31	QB	203/220 (92%)	170 (84%)	33 (16%)	2	12
31	XB	203/220 (92%)	169 (83%)	34 (17%)	2	12
32	QC	161/188 (86%)	141 (88%)	20 (12%)	4	18
32	XC	161/188 (86%)	136 (84%)	25 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	QD	180/181 (99%)	154 (86%)	26 (14%)	2	16
33	XD	180/181 (99%)	155 (86%)	25 (14%)	3	17
34	QE	116/123 (94%)	100 (86%)	16 (14%)	3	17
34	XE	116/123 (94%)	98 (84%)	18 (16%)	2	13
35	QF	90/90 (100%)	73 (81%)	17 (19%)	1	8
35	XF	90/90 (100%)	75 (83%)	15 (17%)	2	12
36	QG	126/127 (99%)	111 (88%)	15 (12%)	4	20
36	XG	126/127 (99%)	115 (91%)	11 (9%)	8	30
37	QH	119/119 (100%)	101 (85%)	18 (15%)	2	14
37	XH	119/119 (100%)	102 (86%)	17 (14%)	2	16
38	QI	98/99 (99%)	89 (91%)	9 (9%)	7	27
38	XI	98/99 (99%)	83 (85%)	15 (15%)	2	13
39	QJ	89/92 (97%)	74 (83%)	15 (17%)	1	11
39	XJ	89/92 (97%)	72 (81%)	17 (19%)	1	7
40	QK	90/99 (91%)	83 (92%)	7 (8%)	10	33
40	XK	90/99 (91%)	80 (89%)	10 (11%)	5	21
41	QL	104/109 (95%)	83 (80%)	21 (20%)	1	6
41	XL	104/109 (95%)	85 (82%)	19 (18%)	1	9
42	QM	92/101 (91%)	80 (87%)	12 (13%)	3	18
42	XM	92/101 (91%)	75 (82%)	17 (18%)	1	8
43	QN	49/50 (98%)	42 (86%)	7 (14%)	2	16
43	XN	49/50 (98%)	36 (74%)	13 (26%)	0	3
44	QO	79/80 (99%)	60 (76%)	19 (24%)	0	4
44	XO	79/80 (99%)	71 (90%)	8 (10%)	6	24
45	QP	72/74 (97%)	71 (99%)	1 (1%)	62	75
45	XP	72/74 (97%)	65 (90%)	7 (10%)	6	25
46	QQ	95/97 (98%)	86 (90%)	9 (10%)	7	25
46	XQ	95/97 (98%)	84 (88%)	11 (12%)	4	20
47	QR	61/77 (79%)	49 (80%)	12 (20%)	1	7
47	XR	61/77 (79%)	55 (90%)	6 (10%)	6	24
48	QT	76/82 (93%)	63 (83%)	13 (17%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	XT	76/82 (93%)	60 (79%)	16 (21%)	1	5
50	QS	69/80 (86%)	55 (80%)	14 (20%)	1	6
50	XS	69/80 (86%)	55 (80%)	14 (20%)	1	6
51	R4	30/63 (48%)	20 (67%)	10 (33%)	0	1
51	Y4	41/63 (65%)	32 (78%)	9 (22%)	1	5
All	All	9589/10022 (96%)	8239 (86%)	1350 (14%)	3	16

5 of 1350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	QL	18	VAL
36	XG	149	ARG
42	QM	56	LEU
41	QL	17	LYS
31	XB	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
32	XC	104	GLN
46	XQ	16	GLN
42	XM	92	HIS
15	YT	58	ASN
31	XB	212	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2878/2915 (98%)	573 (19%)	52 (1%)
1	YA	2880/2915 (98%)	590 (20%)	55 (1%)
2	RB	119/122 (97%)	19 (15%)	2 (1%)
2	YB	119/122 (97%)	20 (16%)	2 (1%)
49	QA	1509/1521 (99%)	296 (19%)	15 (0%)
49	XA	1514/1521 (99%)	288 (19%)	19 (1%)
52	QX	18/19 (94%)	7 (38%)	1 (5%)
52	XX	18/19 (94%)	7 (38%)	1 (5%)
53	QV	77/78 (98%)	27 (35%)	4 (5%)
53	XV	77/78 (98%)	26 (33%)	5 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9209/9310 (98%)	1853 (20%)	156 (1%)

5 of 1853 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	9	U
1	RA	15	G
1	RA	28	A
1	RA	34	C
1	RA	35	G

5 of 156 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	QA	748	C
49	XA	1504	G
49	QA	1300	G
49	XA	748	C
53	XV	75	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	1MG	XV	38	53	19,26,27	0.83	1 (5%)	18,39,42	1.29	2 (11%)
53	1MG	QV	38	53	19,26,27	0.82	1 (5%)	18,39,42	1.27	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	1MG	XV	38	53	-	3/3/25/26	0/3/3/3
53	1MG	QV	38	53	-	3/3/25/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	XV	38	1MG	C2-N1	2.26	1.41	1.37
53	QV	38	1MG	C2-N1	2.20	1.41	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	XV	38	1MG	C8-N7-C5	2.82	107.35	102.55
53	XV	38	1MG	C5-C6-N1	2.82	118.03	113.96
53	QV	38	1MG	C5-C6-N1	2.81	118.02	113.96
53	QV	38	1MG	C8-N7-C5	2.79	107.30	102.55

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	XV	38	1MG	C4'-C5'-O5'-P
53	QV	38	1MG	C4'-C5'-O5'-P
53	XV	38	1MG	O4'-C4'-C5'-O5'
53	QV	38	1MG	O4'-C4'-C5'-O5'
53	XV	38	1MG	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	XV	38	1MG	2	0
53	QV	38	1MG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1319 ligands modelled in this entry, 1319 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	RA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	RA	1052:C	O3'	1053:C	P	3.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.2724, which does not match the depositor's R factor of 0.0. Please interpret the results in this section carefully.

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	RA	2882/2915 (98%)	-0.00	41 (1%) 73 57	94, 115, 163, 199	0
1	YA	2883/2915 (98%)	0.20	64 (2%) 62 46	91, 101, 157, 189	0
2	RB	120/122 (98%)	0.11	0 100 100	111, 133, 146, 156	0
2	YB	120/122 (98%)	-0.09	0 100 100	92, 110, 128, 155	0
3	RD	272/276 (98%)	-0.10	1 (0%) 89 78	92, 110, 128, 149	0
3	YD	272/276 (98%)	0.19	8 (2%) 54 40	91, 103, 121, 147	0
4	RE	205/206 (99%)	-0.05	4 (1%) 64 49	93, 122, 141, 157	0
4	YE	205/206 (99%)	0.06	3 (1%) 71 55	91, 103, 128, 170	0
5	RF	202/210 (96%)	-0.27	1 (0%) 87 75	96, 119, 138, 160	0
5	YF	202/210 (96%)	-0.00	2 (0%) 79 64	90, 101, 130, 153	0
6	RG	181/182 (99%)	0.20	5 (2%) 55 41	114, 142, 165, 174	0
6	YG	181/182 (99%)	0.05	4 (2%) 62 46	99, 129, 155, 168	0
7	RH	170/180 (94%)	-0.13	0 100 100	99, 141, 162, 191	0
7	YH	170/180 (94%)	0.02	2 (1%) 76 60	94, 108, 134, 148	0
8	RI	146/148 (98%)	-0.21	0 100 100	113, 132, 147, 158	0
8	YI	146/148 (98%)	0.07	3 (2%) 63 48	98, 130, 155, 167	0
9	RN	138/140 (98%)	-0.24	3 (2%) 62 46	97, 122, 141, 156	0
9	YN	138/140 (98%)	0.03	0 100 100	91, 101, 125, 158	0
10	RO	122/122 (100%)	-0.22	0 100 100	94, 116, 137, 144	0
10	YO	122/122 (100%)	-0.14	1 (0%) 82 69	92, 102, 120, 138	0
11	RP	150/150 (100%)	-0.21	1 (0%) 84 71	96, 122, 144, 169	0
11	YP	150/150 (100%)	0.07	2 (1%) 74 58	92, 105, 134, 168	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	RQ	141/141 (100%)	-0.16	0 100 100	98, 124, 144, 157	0
12	YQ	141/141 (100%)	-0.11	1 (0%) 84 71	91, 106, 132, 154	0
13	RR	118/118 (100%)	-0.14	2 (1%) 69 52	93, 109, 129, 148	0
13	YR	118/118 (100%)	0.18	2 (1%) 69 52	92, 103, 120, 129	0
14	RS	111/112 (99%)	-0.09	1 (0%) 81 66	108, 130, 150, 161	0
14	YS	111/112 (99%)	-0.26	0 100 100	93, 107, 133, 158	0
15	RT	137/146 (93%)	-0.29	0 100 100	101, 123, 146, 172	0
15	YT	137/146 (93%)	-0.14	1 (0%) 84 71	96, 109, 139, 158	0
16	RU	117/118 (99%)	-0.12	2 (1%) 69 52	94, 116, 143, 151	0
16	YU	117/118 (99%)	0.33	4 (3%) 48 37	91, 99, 116, 164	0
17	RV	101/101 (100%)	-0.34	0 100 100	96, 125, 146, 160	0
17	YV	101/101 (100%)	-0.04	2 (1%) 64 49	91, 101, 124, 162	0
18	RW	113/113 (100%)	-0.11	2 (1%) 67 50	92, 105, 126, 155	0
18	YW	113/113 (100%)	-0.00	0 100 100	90, 97, 115, 147	0
19	RX	92/96 (95%)	-0.23	0 100 100	93, 108, 130, 140	0
19	YX	92/96 (95%)	0.05	0 100 100	91, 98, 116, 130	0
20	RY	102/110 (92%)	0.00	0 100 100	98, 124, 148, 166	0
20	YY	102/110 (92%)	0.07	1 (0%) 79 64	92, 109, 132, 146	0
21	RZ	183/206 (88%)	0.17	5 (2%) 56 42	107, 139, 160, 168	0
21	YZ	183/206 (88%)	-0.09	2 (1%) 77 62	94, 112, 147, 167	0
22	R0	82/85 (96%)	-0.08	2 (2%) 59 45	95, 120, 158, 175	0
22	Y0	82/85 (96%)	0.07	1 (1%) 76 60	92, 103, 140, 172	0
23	R1	97/98 (98%)	-0.18	0 100 100	98, 116, 139, 165	0
23	Y1	97/98 (98%)	0.08	0 100 100	92, 105, 133, 149	0
24	R2	69/72 (95%)	-0.27	0 100 100	96, 117, 135, 164	0
24	Y2	69/72 (95%)	0.21	2 (2%) 54 40	92, 107, 130, 138	0
25	R3	59/60 (98%)	-0.22	0 100 100	105, 124, 145, 158	0
25	Y3	59/60 (98%)	-0.09	1 (1%) 69 52	91, 102, 122, 129	0
26	R5	59/60 (98%)	0.29	5 (8%) 18 18	93, 113, 147, 160	0
26	Y5	59/60 (98%)	0.62	2 (3%) 48 37	91, 104, 152, 161	0
27	R6	49/54 (90%)	0.30	1 (2%) 64 49	100, 128, 156, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	Y6	49/54 (90%)	0.48	4 (8%) 19 18	95, 116, 146, 154	0
28	R7	49/49 (100%)	0.05	0 100 100	91, 106, 125, 157	0
28	Y7	49/49 (100%)	0.30	2 (4%) 42 34	91, 96, 117, 147	0
29	R8	64/65 (98%)	-0.20	0 100 100	100, 117, 133, 140	0
29	Y8	64/65 (98%)	0.10	0 100 100	93, 103, 123, 139	0
30	R9	37/37 (100%)	0.29	1 (2%) 56 42	111, 125, 144, 167	0
30	Y9	37/37 (100%)	0.28	2 (5%) 32 27	91, 104, 129, 129	0
31	QB	235/256 (91%)	0.12	4 (1%) 69 52	112, 142, 167, 180	0
31	XB	235/256 (91%)	-0.02	1 (0%) 89 78	105, 139, 163, 179	0
32	QC	207/239 (86%)	0.06	2 (0%) 79 64	115, 147, 163, 187	0
32	XC	207/239 (86%)	0.03	2 (0%) 79 64	112, 143, 164, 185	0
33	QD	208/209 (99%)	0.21	7 (3%) 48 37	109, 138, 161, 176	0
33	XD	208/209 (99%)	0.15	4 (1%) 66 49	107, 138, 158, 170	0
34	QE	151/162 (93%)	0.18	3 (1%) 64 49	112, 141, 163, 173	0
34	XE	151/162 (93%)	0.00	2 (1%) 74 58	98, 128, 152, 160	0
35	QF	101/101 (100%)	-0.03	0 100 100	109, 139, 163, 170	0
35	XF	101/101 (100%)	-0.03	0 100 100	102, 131, 154, 165	0
36	QG	155/156 (99%)	0.20	2 (1%) 74 58	123, 148, 171, 188	0
36	XG	155/156 (99%)	0.15	2 (1%) 74 58	120, 149, 166, 170	0
37	QH	138/138 (100%)	0.02	2 (1%) 73 57	103, 136, 159, 171	0
37	XH	138/138 (100%)	-0.01	1 (0%) 84 71	108, 133, 154, 175	0
38	QI	127/128 (99%)	0.41	5 (3%) 44 35	128, 150, 167, 175	0
38	XI	127/128 (99%)	0.22	1 (0%) 82 69	112, 146, 167, 173	0
39	QJ	99/105 (94%)	0.40	2 (2%) 64 49	129, 152, 167, 175	0
39	XJ	99/105 (94%)	0.38	3 (3%) 52 40	111, 152, 167, 175	0
40	QK	119/129 (92%)	0.20	1 (0%) 82 69	105, 140, 158, 176	0
40	XK	119/129 (92%)	0.17	2 (1%) 69 52	98, 133, 156, 185	0
41	QL	125/132 (94%)	0.44	7 (5%) 31 27	106, 141, 162, 181	0
41	XL	125/132 (94%)	0.37	6 (4%) 36 30	100, 133, 156, 166	0
42	QM	114/126 (90%)	0.31	4 (3%) 47 37	115, 152, 177, 189	0
42	XM	114/126 (90%)	0.19	2 (1%) 67 50	112, 150, 169, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	QN	60/61 (98%)	0.49	1 (1%) 69 52	133, 149, 169, 174	0
43	XN	60/61 (98%)	0.31	2 (3%) 49 38	117, 150, 164, 171	0
44	QO	88/89 (98%)	-0.15	1 (1%) 77 62	96, 129, 150, 157	0
44	XO	88/89 (98%)	0.05	0 100 100	104, 127, 150, 160	0
45	QP	84/88 (95%)	0.27	4 (4%) 36 30	103, 138, 166, 173	0
45	XP	84/88 (95%)	0.28	2 (2%) 59 45	104, 136, 156, 164	0
46	QQ	100/105 (95%)	0.02	1 (1%) 79 64	108, 132, 153, 161	0
46	XQ	100/105 (95%)	0.04	1 (1%) 79 64	105, 129, 151, 161	0
47	QR	70/88 (79%)	-0.15	1 (1%) 73 57	113, 132, 151, 158	0
47	XR	70/88 (79%)	-0.07	0 100 100	101, 130, 151, 167	0
48	QT	99/106 (93%)	-0.04	1 (1%) 79 64	107, 131, 155, 163	0
48	XT	99/106 (93%)	-0.08	1 (1%) 79 64	102, 129, 154, 168	0
49	QA	1511/1521 (99%)	0.20	20 (1%) 74 58	102, 135, 167, 186	0
49	XA	1515/1521 (99%)	0.12	21 (1%) 73 57	96, 130, 164, 192	0
50	QS	79/93 (84%)	0.47	2 (2%) 58 44	133, 155, 173, 185	0
50	XS	79/93 (84%)	0.26	1 (1%) 74 58	121, 152, 169, 174	0
51	R4	34/71 (47%)	0.15	0 100 100	113, 153, 169, 176	0
51	Y4	46/71 (64%)	0.11	1 (2%) 62 46	110, 145, 171, 184	0
52	QX	19/19 (100%)	0.64	0 100 100	135, 162, 170, 174	0
52	XX	19/19 (100%)	0.28	0 100 100	135, 156, 175, 178	0
53	QV	77/78 (98%)	0.65	1 (1%) 74 58	121, 158, 174, 187	0
53	XV	77/78 (98%)	0.43	2 (2%) 57 43	97, 153, 174, 194	0
All	All	20753/21384 (97%)	0.08	321 (1%) 71 55	90, 122, 161, 199	0

The worst 5 of 321 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Y5	2	ALA	10.5
33	QD	25	ARG	7.8
6	YG	43	LEU	6.3
7	YH	2	SER	6.1
30	Y9	1	MET	5.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
53	1MG	QV	38	24/25	0.58	0.11	139,172,202,204	0
53	1MG	XV	38	24/25	0.61	0.11	108,152,169,192	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
54	MG	QA	1724	1/1	-0.43	0.19	160,160,160,160	0
54	MG	XA	1677	1/1	-0.21	0.64	99,99,99,99	0
54	MG	XA	1714	1/1	-0.20	0.18	90,90,90,90	0
54	MG	XA	1674	1/1	-0.11	0.15	90,90,90,90	0
54	MG	XA	1709	1/1	-0.10	0.22	94,94,94,94	0
54	MG	QA	1663	1/1	-0.09	0.27	95,95,95,95	0
54	MG	YA	3876	1/1	-0.09	0.15	138,138,138,138	0
54	MG	QA	1657	1/1	-0.08	0.21	90,90,90,90	0
54	MG	RT	201	1/1	-0.07	0.22	144,144,144,144	0
54	MG	RA	3100	1/1	-0.07	0.40	90,90,90,90	0
54	MG	RA	3427	1/1	-0.07	0.16	176,176,176,176	0
54	MG	RA	3298	1/1	-0.05	0.27	106,106,106,106	0
54	MG	QA	1677	1/1	-0.04	0.23	90,90,90,90	0
54	MG	RA	3347	1/1	-0.04	0.28	94,94,94,94	0
54	MG	RA	3380	1/1	0.02	0.11	148,148,148,148	0
54	MG	QA	1709	1/1	0.03	0.24	97,97,97,97	0
54	MG	YA	3737	1/1	0.03	0.59	90,90,90,90	0
54	MG	QA	1693	1/1	0.03	0.15	123,123,123,123	0
54	MG	RA	3535	1/1	0.04	0.11	92,92,92,92	0
54	MG	XA	1711	1/1	0.06	0.18	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	QA	1616	1/1	0.06	0.25	156,156,156,156	0
54	MG	RA	3466	1/1	0.07	0.22	128,128,128,128	0
54	MG	RA	3129	1/1	0.08	0.31	96,96,96,96	0
54	MG	R3	101	1/1	0.08	0.24	170,170,170,170	0
54	MG	RA	3135	1/1	0.08	0.22	90,90,90,90	0
54	MG	RA	3546	1/1	0.08	0.19	106,106,106,106	0
54	MG	QA	1721	1/1	0.09	0.13	128,128,128,128	0
54	MG	YA	3836	1/1	0.10	0.33	90,90,90,90	0
54	MG	YA	3766	1/1	0.10	0.26	90,90,90,90	0
54	MG	QA	1727	1/1	0.10	0.12	182,182,182,182	0
54	MG	QA	1715	1/1	0.10	0.27	95,95,95,95	0
54	MG	YA	3942	1/1	0.11	0.35	90,90,90,90	0
54	MG	YA	3709	1/1	0.11	0.36	90,90,90,90	0
54	MG	XA	1611	1/1	0.11	0.43	110,110,110,110	0
54	MG	YA	3832	1/1	0.11	0.58	96,96,96,96	0
54	MG	RI	201	1/1	0.12	0.27	161,161,161,161	0
54	MG	RA	3043	1/1	0.12	0.41	90,90,90,90	0
54	MG	YA	3704	1/1	0.13	0.28	91,91,91,91	0
54	MG	RA	3039	1/1	0.13	0.24	96,96,96,96	0
54	MG	YA	3648	1/1	0.13	0.21	151,151,151,151	0
54	MG	QE	201	1/1	0.14	0.10	166,166,166,166	0
54	MG	RA	3361	1/1	0.15	0.16	136,136,136,136	0
54	MG	QA	1668	1/1	0.15	0.42	90,90,90,90	0
54	MG	QL	201	1/1	0.15	0.11	188,188,188,188	0
54	MG	QA	1725	1/1	0.16	0.17	106,106,106,106	0
54	MG	RA	3166	1/1	0.16	0.31	90,90,90,90	0
54	MG	YA	3874	1/1	0.17	0.40	90,90,90,90	0
54	MG	Y0	101	1/1	0.17	0.28	96,96,96,96	0
54	MG	XA	1623	1/1	0.17	0.14	125,125,125,125	0
54	MG	RA	3437	1/1	0.17	0.93	134,134,134,134	0
54	MG	QA	1611	1/1	0.18	0.42	114,114,114,114	0
54	MG	YA	3974	1/1	0.18	0.15	94,94,94,94	0
54	MG	QA	1645	1/1	0.19	0.23	92,92,92,92	0
54	MG	XA	1624	1/1	0.20	0.14	141,141,141,141	0
54	MG	XA	1669	1/1	0.21	0.27	118,118,118,118	0
54	MG	RA	3113	1/1	0.21	0.22	97,97,97,97	0
54	MG	YA	3604	1/1	0.22	0.25	131,131,131,131	0
54	MG	RA	3553	1/1	0.22	0.19	90,90,90,90	0
54	MG	RA	3025	1/1	0.22	0.37	90,90,90,90	0
54	MG	YA	3814	1/1	0.22	0.22	92,92,92,92	0
54	MG	QC	301	1/1	0.23	0.15	154,154,154,154	0
54	MG	YA	3783	1/1	0.23	0.21	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	YA	3943	1/1	0.23	0.12	133,133,133,133	0
54	MG	RA	3413	1/1	0.23	0.21	136,136,136,136	0
54	MG	YA	3679	1/1	0.23	0.24	90,90,90,90	0
54	MG	XA	1668	1/1	0.23	0.32	172,172,172,172	0
54	MG	YI	201	1/1	0.24	0.20	104,104,104,104	0
54	MG	XA	1629	1/1	0.25	0.23	164,164,164,164	0
54	MG	RA	3561	1/1	0.26	0.40	92,92,92,92	0
54	MG	RA	3247	1/1	0.27	0.14	99,99,99,99	0
54	MG	YA	3891	1/1	0.28	0.51	90,90,90,90	0
54	MG	QA	1669	1/1	0.28	0.18	97,97,97,97	0
54	MG	RA	3066	1/1	0.28	0.26	100,100,100,100	0
54	MG	YA	3776	1/1	0.29	0.53	90,90,90,90	0
54	MG	RA	3185	1/1	0.29	0.21	129,129,129,129	0
54	MG	QA	1690	1/1	0.29	0.28	103,103,103,103	0
54	MG	RA	3525	1/1	0.30	0.14	100,100,100,100	0
54	MG	YA	3724	1/1	0.30	0.17	97,97,97,97	0
54	MG	YA	3653	1/1	0.30	0.28	106,106,106,106	0
54	MG	YA	3670	1/1	0.30	0.23	110,110,110,110	0
54	MG	RA	3171	1/1	0.30	0.24	92,92,92,92	0
54	MG	XA	1703	1/1	0.30	0.16	91,91,91,91	0
54	MG	YA	3698	1/1	0.30	0.45	91,91,91,91	0
54	MG	RA	3279	1/1	0.30	0.17	148,148,148,148	0
54	MG	YA	3828	1/1	0.30	0.26	90,90,90,90	0
54	MG	RA	3286	1/1	0.31	0.19	90,90,90,90	0
54	MG	RA	3312	1/1	0.31	0.34	113,113,113,113	0
54	MG	R1	102	1/1	0.31	0.15	149,149,149,149	0
54	MG	RA	3384	1/1	0.32	0.24	97,97,97,97	0
54	MG	RA	3246	1/1	0.32	0.31	90,90,90,90	0
54	MG	YA	3755	1/1	0.33	0.26	90,90,90,90	0
54	MG	RA	3180	1/1	0.33	0.29	90,90,90,90	0
54	MG	YA	3774	1/1	0.33	0.27	90,90,90,90	0
54	MG	RA	3449	1/1	0.33	0.39	90,90,90,90	0
54	MG	YA	3613	1/1	0.34	0.24	90,90,90,90	0
54	MG	YA	3953	1/1	0.34	0.23	125,125,125,125	0
54	MG	QA	1706	1/1	0.34	0.08	94,94,94,94	0
54	MG	RA	3418	1/1	0.35	0.20	134,134,134,134	0
54	MG	RE	306	1/1	0.35	0.15	90,90,90,90	0
54	MG	RA	3545	1/1	0.35	0.21	93,93,93,93	0
54	MG	XA	1700	1/1	0.35	0.11	91,91,91,91	0
54	MG	RA	3087	1/1	0.35	0.16	174,174,174,174	0
54	MG	R0	102	1/1	0.35	0.18	103,103,103,103	0
54	MG	RA	3301	1/1	0.35	0.47	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	YA	3671	1/1	0.35	0.40	90,90,90,90	0
54	MG	XA	1723	1/1	0.35	0.22	96,96,96,96	0
54	MG	QA	1700	1/1	0.36	0.39	90,90,90,90	0
54	MG	QA	1628	1/1	0.37	0.16	92,92,92,92	0
54	MG	QA	1640	1/1	0.37	0.19	97,97,97,97	0
54	MG	RA	3159	1/1	0.37	0.23	98,98,98,98	0
54	MG	QP	101	1/1	0.37	0.41	120,120,120,120	0
54	MG	YA	3731	1/1	0.38	0.59	90,90,90,90	0
54	MG	YA	3625	1/1	0.38	0.61	125,125,125,125	0
54	MG	YA	3769	1/1	0.39	0.36	90,90,90,90	0
54	MG	QA	1618	1/1	0.39	0.09	96,96,96,96	0
54	MG	QA	1664	1/1	0.39	0.11	114,114,114,114	0
54	MG	YA	3794	1/1	0.39	0.47	168,168,168,168	0
54	MG	RA	3299	1/1	0.39	0.18	90,90,90,90	0
54	MG	RA	3539	1/1	0.39	0.24	90,90,90,90	0
54	MG	YA	3879	1/1	0.40	0.16	153,153,153,153	0
54	MG	YA	3615	1/1	0.40	0.34	90,90,90,90	0
54	MG	XA	1652	1/1	0.41	0.18	121,121,121,121	0
54	MG	RA	3452	1/1	0.41	0.28	110,110,110,110	0
54	MG	RA	3248	1/1	0.41	0.20	90,90,90,90	0
54	MG	RA	3005	1/1	0.41	0.19	95,95,95,95	0
54	MG	XA	1676	1/1	0.41	0.34	90,90,90,90	0
54	MG	RA	3032	1/1	0.41	0.14	94,94,94,94	0
54	MG	XA	1688	1/1	0.41	0.17	92,92,92,92	0
54	MG	YA	3967	1/1	0.41	0.24	135,135,135,135	0
54	MG	YA	3854	1/1	0.41	0.65	90,90,90,90	0
54	MG	RA	3125	1/1	0.41	0.32	90,90,90,90	0
54	MG	QA	1638	1/1	0.41	0.40	90,90,90,90	0
54	MG	YA	3787	1/1	0.41	0.28	90,90,90,90	0
54	MG	YA	3703	1/1	0.41	0.34	90,90,90,90	0
54	MG	RA	3451	1/1	0.42	0.39	90,90,90,90	0
54	MG	XA	1627	1/1	0.42	0.13	94,94,94,94	0
54	MG	RA	3370	1/1	0.42	0.23	127,127,127,127	0
54	MG	QA	1655	1/1	0.42	0.12	102,102,102,102	0
54	MG	RA	3329	1/1	0.42	0.22	91,91,91,91	0
54	MG	YA	3760	1/1	0.42	0.44	90,90,90,90	0
54	MG	RA	3223	1/1	0.42	0.18	106,106,106,106	0
54	MG	RA	3162	1/1	0.42	0.70	90,90,90,90	0
54	MG	YA	3747	1/1	0.43	0.26	90,90,90,90	0
54	MG	RA	3558	1/1	0.43	0.38	90,90,90,90	0
54	MG	RA	3297	1/1	0.43	0.18	136,136,136,136	0
54	MG	YA	3643	1/1	0.43	0.34	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3036	1/1	0.44	0.15	144,144,144,144	0
54	MG	RA	3253	1/1	0.44	0.31	90,90,90,90	0
54	MG	YA	3935	1/1	0.44	0.19	90,90,90,90	0
54	MG	YA	3846	1/1	0.44	0.15	94,94,94,94	0
54	MG	RA	3428	1/1	0.44	0.37	102,102,102,102	0
54	MG	RA	3415	1/1	0.44	0.24	100,100,100,100	0
54	MG	RB	212	1/1	0.44	0.25	99,99,99,99	0
54	MG	QA	1652	1/1	0.45	0.25	91,91,91,91	0
54	MG	RA	3228	1/1	0.45	0.10	145,145,145,145	0
54	MG	QA	1625	1/1	0.45	0.35	98,98,98,98	0
54	MG	RB	205	1/1	0.45	0.17	179,179,179,179	0
54	MG	QA	1631	1/1	0.45	0.18	95,95,95,95	0
54	MG	QA	1666	1/1	0.45	0.17	91,91,91,91	0
54	MG	RA	3270	1/1	0.45	0.36	90,90,90,90	0
54	MG	XA	1653	1/1	0.45	0.16	91,91,91,91	0
54	MG	YA	3685	1/1	0.45	0.31	90,90,90,90	0
54	MG	YA	3619	1/1	0.45	0.17	146,146,146,146	0
54	MG	YA	3707	1/1	0.46	0.22	94,94,94,94	0
54	MG	XA	1638	1/1	0.46	0.20	91,91,91,91	0
54	MG	RA	3337	1/1	0.46	0.75	90,90,90,90	0
54	MG	YA	3612	1/1	0.46	0.31	90,90,90,90	0
54	MG	YE	304	1/1	0.46	0.21	118,118,118,118	0
54	MG	YA	3765	1/1	0.46	0.37	90,90,90,90	0
54	MG	RA	3335	1/1	0.46	0.51	121,121,121,121	0
54	MG	RA	3350	1/1	0.46	0.13	90,90,90,90	0
54	MG	YA	3905	1/1	0.47	0.20	90,90,90,90	0
54	MG	YA	3921	1/1	0.47	0.45	90,90,90,90	0
54	MG	RA	3196	1/1	0.47	0.17	107,107,107,107	0
54	MG	RA	3386	1/1	0.47	0.13	100,100,100,100	0
54	MG	RA	3323	1/1	0.47	0.58	90,90,90,90	0
54	MG	RA	3339	1/1	0.47	0.21	130,130,130,130	0
54	MG	RA	3059	1/1	0.47	0.20	97,97,97,97	0
54	MG	YA	3644	1/1	0.48	0.35	173,173,173,173	0
54	MG	YA	3687	1/1	0.48	0.41	90,90,90,90	0
54	MG	RA	3400	1/1	0.48	0.37	93,93,93,93	0
54	MG	RA	3346	1/1	0.48	0.55	96,96,96,96	0
54	MG	QA	1681	1/1	0.48	0.13	97,97,97,97	0
54	MG	QA	1680	1/1	0.49	0.14	151,151,151,151	0
54	MG	RA	3447	1/1	0.49	0.31	100,100,100,100	0
54	MG	RA	3481	1/1	0.49	0.20	90,90,90,90	0
54	MG	YA	3919	1/1	0.49	0.18	90,90,90,90	0
54	MG	RE	303	1/1	0.49	0.14	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	QA	1705	1/1	0.49	0.21	90,90,90,90	0
54	MG	RA	3215	1/1	0.49	0.46	90,90,90,90	0
54	MG	RA	3392	1/1	0.49	0.21	108,108,108,108	0
54	MG	RA	3376	1/1	0.49	0.37	93,93,93,93	0
54	MG	YA	3692	1/1	0.49	0.29	94,94,94,94	0
54	MG	YA	3958	1/1	0.49	0.27	90,90,90,90	0
54	MG	RA	3041	1/1	0.50	0.24	181,181,181,181	0
54	MG	RD	303	1/1	0.50	0.38	90,90,90,90	0
54	MG	YD	302	1/1	0.50	0.42	90,90,90,90	0
54	MG	YA	3817	1/1	0.50	0.14	90,90,90,90	0
54	MG	QA	1603	1/1	0.50	0.19	98,98,98,98	0
54	MG	YA	3700	1/1	0.50	0.25	90,90,90,90	0
54	MG	RB	206	1/1	0.50	0.77	178,178,178,178	0
54	MG	RA	3441	1/1	0.51	0.13	90,90,90,90	0
54	MG	XA	1699	1/1	0.51	0.43	90,90,90,90	0
54	MG	QA	1708	1/1	0.51	0.20	95,95,95,95	0
54	MG	RA	3192	1/1	0.51	0.18	92,92,92,92	0
54	MG	QA	1620	1/1	0.51	0.22	96,96,96,96	0
54	MG	YA	3835	1/1	0.51	0.22	90,90,90,90	0
54	MG	RA	3249	1/1	0.51	0.12	140,140,140,140	0
54	MG	RA	3230	1/1	0.51	0.45	91,91,91,91	0
54	MG	YA	3923	1/1	0.52	0.27	94,94,94,94	0
54	MG	RA	3331	1/1	0.52	0.17	110,110,110,110	0
54	MG	RA	3503	1/1	0.52	0.36	94,94,94,94	0
54	MG	RA	3201	1/1	0.52	0.58	90,90,90,90	0
54	MG	RA	3111	1/1	0.52	0.11	90,90,90,90	0
54	MG	QA	1696	1/1	0.52	0.21	129,129,129,129	0
54	MG	XA	1689	1/1	0.52	0.21	182,182,182,182	0
54	MG	QA	1609	1/1	0.53	0.22	90,90,90,90	0
54	MG	RA	3306	1/1	0.53	0.29	92,92,92,92	0
54	MG	YA	3899	1/1	0.53	0.32	90,90,90,90	0
54	MG	YA	3851	1/1	0.53	0.32	90,90,90,90	0
54	MG	QA	1660	1/1	0.53	0.35	96,96,96,96	0
54	MG	YA	3933	1/1	0.53	0.07	107,107,107,107	0
54	MG	YA	3637	1/1	0.54	0.39	98,98,98,98	0
54	MG	YA	3902	1/1	0.54	0.20	93,93,93,93	0
54	MG	RA	3470	1/1	0.54	0.17	124,124,124,124	0
54	MG	YA	3693	1/1	0.54	0.17	94,94,94,94	0
54	MG	YA	3761	1/1	0.54	1.04	90,90,90,90	0
54	MG	RA	3303	1/1	0.54	0.16	145,145,145,145	0
54	MG	Y1	101	1/1	0.54	0.14	96,96,96,96	0
54	MG	YB	204	1/1	0.55	0.13	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3362	1/1	0.55	0.20	120,120,120,120	0
54	MG	RA	3148	1/1	0.55	0.35	90,90,90,90	0
54	MG	QA	1612	1/1	0.55	0.13	90,90,90,90	0
54	MG	RA	3155	1/1	0.55	0.17	90,90,90,90	0
54	MG	XA	1719	1/1	0.55	0.14	114,114,114,114	0
54	MG	YA	3978	1/1	0.55	0.21	90,90,90,90	0
54	MG	YA	3778	1/1	0.56	0.17	191,191,191,191	0
54	MG	XA	1631	1/1	0.56	0.09	91,91,91,91	0
54	MG	RA	3011	1/1	0.56	0.30	96,96,96,96	0
54	MG	YA	3750	1/1	0.56	0.31	90,90,90,90	0
54	MG	RA	3294	1/1	0.56	0.21	120,120,120,120	0
54	MG	RA	3262	1/1	0.56	0.38	99,99,99,99	0
54	MG	YA	3924	1/1	0.56	0.30	90,90,90,90	0
54	MG	YA	3969	1/1	0.56	0.12	94,94,94,94	0
54	MG	RA	3283	1/1	0.56	0.36	91,91,91,91	0
54	MG	QD	303	1/1	0.56	0.15	128,128,128,128	0
54	MG	RD	307	1/1	0.57	0.10	93,93,93,93	0
54	MG	XA	1690	1/1	0.57	0.21	125,125,125,125	0
54	MG	YA	3779	1/1	0.57	0.17	90,90,90,90	0
54	MG	RA	3550	1/1	0.57	0.21	94,94,94,94	0
54	MG	RA	3319	1/1	0.57	0.22	90,90,90,90	0
54	MG	QA	1648	1/1	0.57	0.59	127,127,127,127	0
54	MG	RA	3214	1/1	0.57	0.22	90,90,90,90	0
54	MG	YE	303	1/1	0.57	0.14	98,98,98,98	0
54	MG	YA	3880	1/1	0.57	0.19	95,95,95,95	0
54	MG	RA	3238	1/1	0.57	0.13	113,113,113,113	0
54	MG	YA	3686	1/1	0.58	0.54	90,90,90,90	0
54	MG	RA	3510	1/1	0.58	0.23	125,125,125,125	0
54	MG	R0	101	1/1	0.58	0.43	92,92,92,92	0
54	MG	YA	3909	1/1	0.58	0.18	90,90,90,90	0
54	MG	YA	3944	1/1	0.58	0.17	101,101,101,101	0
54	MG	RA	3518	1/1	0.58	0.21	109,109,109,109	0
54	MG	QA	1606	1/1	0.58	0.15	94,94,94,94	0
54	MG	RA	3381	1/1	0.58	0.25	95,95,95,95	0
54	MG	RA	3526	1/1	0.58	0.21	100,100,100,100	0
54	MG	YA	3897	1/1	0.58	0.23	90,90,90,90	0
54	MG	YA	3710	1/1	0.59	0.27	158,158,158,158	0
54	MG	RA	3366	1/1	0.59	0.13	99,99,99,99	0
54	MG	QA	1622	1/1	0.59	0.23	114,114,114,114	0
54	MG	RA	3123	1/1	0.59	0.17	94,94,94,94	0
54	MG	YA	3654	1/1	0.59	0.29	90,90,90,90	0
54	MG	YA	3666	1/1	0.59	0.25	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	QA	1635	1/1	0.59	0.29	102,102,102,102	0
54	MG	RA	3394	1/1	0.59	0.19	100,100,100,100	0
54	MG	RA	3509	1/1	0.59	0.28	132,132,132,132	0
54	MG	YA	3603	1/1	0.59	0.16	98,98,98,98	0
54	MG	YA	3793	1/1	0.59	0.14	98,98,98,98	0
54	MG	RO	201	1/1	0.59	0.15	103,103,103,103	0
54	MG	YA	3809	1/1	0.59	0.57	90,90,90,90	0
54	MG	RA	3288	1/1	0.59	0.27	90,90,90,90	0
54	MG	YA	3885	1/1	0.59	0.23	93,93,93,93	0
54	MG	XA	1664	1/1	0.59	0.16	90,90,90,90	0
54	MG	XA	1610	1/1	0.60	0.07	90,90,90,90	0
54	MG	XA	1697	1/1	0.60	0.28	95,95,95,95	0
54	MG	YA	3617	1/1	0.60	0.45	90,90,90,90	0
54	MG	YA	3744	1/1	0.60	0.26	90,90,90,90	0
54	MG	YA	3929	1/1	0.60	0.13	94,94,94,94	0
54	MG	YB	208	1/1	0.60	0.36	90,90,90,90	0
54	MG	RA	3131	1/1	0.60	0.19	97,97,97,97	0
54	MG	RA	3229	1/1	0.60	0.09	144,144,144,144	0
54	MG	QA	1704	1/1	0.60	0.15	98,98,98,98	0
54	MG	YA	3901	1/1	0.60	0.46	94,94,94,94	0
54	MG	RA	3430	1/1	0.61	0.19	90,90,90,90	0
54	MG	RA	3048	1/1	0.61	0.25	90,90,90,90	0
54	MG	YA	3723	1/1	0.61	0.29	90,90,90,90	0
54	MG	QA	1614	1/1	0.61	0.23	95,95,95,95	0
54	MG	RA	3173	1/1	0.61	0.24	90,90,90,90	0
54	MG	RA	3468	1/1	0.61	0.27	121,121,121,121	0
54	MG	YA	3881	1/1	0.61	0.34	90,90,90,90	0
54	MG	QA	1719	1/1	0.61	0.17	92,92,92,92	0
54	MG	RA	3356	1/1	0.61	0.22	109,109,109,109	0
54	MG	XA	1706	1/1	0.61	0.29	112,112,112,112	0
54	MG	RA	3336	1/1	0.61	0.22	90,90,90,90	0
54	MG	YA	3665	1/1	0.61	0.38	90,90,90,90	0
54	MG	QA	1661	1/1	0.61	0.10	106,106,106,106	0
54	MG	XE	201	1/1	0.61	0.18	95,95,95,95	0
54	MG	XO	101	1/1	0.61	0.13	147,147,147,147	0
54	MG	QD	302	1/1	0.62	0.08	96,96,96,96	0
54	MG	RA	3357	1/1	0.62	0.46	171,171,171,171	0
54	MG	YA	3734	1/1	0.62	0.30	93,93,93,93	0
54	MG	RA	3393	1/1	0.62	0.07	91,91,91,91	0
54	MG	XA	1636	1/1	0.62	0.09	103,103,103,103	0
54	MG	RA	3074	1/1	0.62	0.24	90,90,90,90	0
54	MG	YA	3690	1/1	0.62	0.12	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	YA	3945	1/1	0.62	0.11	90,90,90,90	0
54	MG	RA	3397	1/1	0.62	0.20	94,94,94,94	0
54	MG	RA	3031	1/1	0.63	0.11	122,122,122,122	0
54	MG	RA	3071	1/1	0.63	0.47	90,90,90,90	0
54	MG	YA	3884	1/1	0.63	0.18	90,90,90,90	0
54	MG	RA	3363	1/1	0.63	0.10	90,90,90,90	0
54	MG	RA	3385	1/1	0.63	0.19	170,170,170,170	0
54	MG	RA	3107	1/1	0.63	0.27	116,116,116,116	0
54	MG	RA	3450	1/1	0.63	0.24	90,90,90,90	0
54	MG	RA	3515	1/1	0.63	0.24	90,90,90,90	0
54	MG	YA	3850	1/1	0.63	0.23	90,90,90,90	0
54	MG	RA	3390	1/1	0.63	0.34	152,152,152,152	0
54	MG	QA	1665	1/1	0.63	0.12	96,96,96,96	0
54	MG	YA	3754	1/1	0.63	0.23	93,93,93,93	0
54	MG	RA	3014	1/1	0.63	0.23	90,90,90,90	0
54	MG	RA	3342	1/1	0.63	0.16	90,90,90,90	0
54	MG	QL	202	1/1	0.63	0.17	113,113,113,113	0
54	MG	RB	207	1/1	0.63	0.68	262,262,262,262	0
54	MG	YA	3741	1/1	0.64	0.72	90,90,90,90	0
54	MG	YA	3875	1/1	0.64	0.26	90,90,90,90	0
54	MG	XA	1620	1/1	0.64	0.36	90,90,90,90	0
54	MG	YE	301	1/1	0.64	0.26	90,90,90,90	0
54	MG	RA	3130	1/1	0.64	0.98	90,90,90,90	0
54	MG	QA	1604	1/1	0.64	0.27	158,158,158,158	0
54	MG	RA	3015	1/1	0.64	0.17	93,93,93,93	0
54	MG	RA	3396	1/1	0.64	0.23	113,113,113,113	0
54	MG	RA	3500	1/1	0.64	0.18	94,94,94,94	0
54	MG	QA	1678	1/1	0.64	0.09	91,91,91,91	0
54	MG	RA	3026	1/1	0.64	0.58	94,94,94,94	0
54	MG	RA	3259	1/1	0.64	0.43	90,90,90,90	0
54	MG	RA	3434	1/1	0.64	0.07	92,92,92,92	0
54	MG	RA	3020	1/1	0.64	0.16	119,119,119,119	0
54	MG	RA	3516	1/1	0.64	0.33	90,90,90,90	0
54	MG	XA	1670	1/1	0.64	0.17	91,91,91,91	0
54	MG	YA	3912	1/1	0.65	0.14	123,123,123,123	0
54	MG	YA	3658	1/1	0.65	0.42	90,90,90,90	0
54	MG	YA	3714	1/1	0.65	0.36	90,90,90,90	0
54	MG	QA	1694	1/1	0.65	0.12	129,129,129,129	0
54	MG	RA	3022	1/1	0.65	0.28	90,90,90,90	0
54	MG	XA	1613	1/1	0.65	0.39	90,90,90,90	0
54	MG	YA	3838	1/1	0.65	0.14	158,158,158,158	0
54	MG	QA	1621	1/1	0.65	0.45	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	RA	3504	1/1	0.65	0.26	256,256,256,256	0
54	MG	YA	3640	1/1	0.65	0.48	90,90,90,90	0
54	MG	RA	3431	1/1	0.65	0.14	137,137,137,137	0
54	MG	RA	3555	1/1	0.65	0.30	90,90,90,90	0
54	MG	QA	1711	1/1	0.65	0.36	92,92,92,92	0
54	MG	QA	1632	1/1	0.65	0.14	133,133,133,133	0
54	MG	YA	3865	1/1	0.65	0.37	152,152,152,152	0
54	MG	RA	3314	1/1	0.65	0.14	187,187,187,187	0
54	MG	RA	3315	1/1	0.65	0.12	113,113,113,113	0
54	MG	RA	3126	1/1	0.65	0.55	121,121,121,121	0
54	MG	YA	3861	1/1	0.66	0.32	107,107,107,107	0
54	MG	RA	3033	1/1	0.66	0.65	90,90,90,90	0
54	MG	RA	3517	1/1	0.66	0.26	120,120,120,120	0
54	MG	YA	3962	1/1	0.66	0.25	100,100,100,100	0
54	MG	QA	1633	1/1	0.66	0.16	90,90,90,90	0
54	MG	YA	3763	1/1	0.66	0.22	91,91,91,91	0
54	MG	RA	3002	1/1	0.66	0.11	133,133,133,133	0
54	MG	XA	1687	1/1	0.66	0.09	91,91,91,91	0
54	MG	RA	3044	1/1	0.66	0.28	140,140,140,140	0
54	MG	YA	3922	1/1	0.66	0.40	90,90,90,90	0
54	MG	RA	3045	1/1	0.66	0.25	111,111,111,111	0
54	MG	RA	3467	1/1	0.66	0.22	90,90,90,90	0
54	MG	YA	3927	1/1	0.66	0.26	90,90,90,90	0
54	MG	YA	3743	1/1	0.66	0.40	90,90,90,90	0
54	MG	XA	1628	1/1	0.66	0.23	114,114,114,114	0
54	MG	YA	3932	1/1	0.66	0.18	90,90,90,90	0
54	MG	YA	3610	1/1	0.66	0.44	90,90,90,90	0
54	MG	RB	202	1/1	0.66	0.26	99,99,99,99	0
54	MG	RA	3233	1/1	0.66	0.42	90,90,90,90	0
54	MG	YA	3711	1/1	0.66	0.20	90,90,90,90	0
54	MG	RA	3023	1/1	0.66	0.23	100,100,100,100	0
54	MG	QQ	202	1/1	0.67	0.24	167,167,167,167	0
54	MG	YR	201	1/1	0.67	0.15	112,112,112,112	0
54	MG	RA	3146	1/1	0.67	0.16	130,130,130,130	0
54	MG	YA	3845	1/1	0.67	0.36	90,90,90,90	0
54	MG	YA	3738	1/1	0.67	0.12	102,102,102,102	0
54	MG	RA	3037	1/1	0.67	0.36	124,124,124,124	0
54	MG	R1	103	1/1	0.67	0.11	113,113,113,113	0
54	MG	RA	3332	1/1	0.67	0.14	104,104,104,104	0
54	MG	XA	1625	1/1	0.67	0.18	174,174,174,174	0
54	MG	XA	1626	1/1	0.67	0.35	90,90,90,90	0
54	MG	YA	3941	1/1	0.67	0.14	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3145	1/1	0.67	0.29	90,90,90,90	0
54	MG	YA	3972	1/1	0.67	0.20	126,126,126,126	0
54	MG	RA	3158	1/1	0.68	0.35	118,118,118,118	0
54	MG	RA	3038	1/1	0.68	0.13	171,171,171,171	0
54	MG	YA	3784	1/1	0.68	0.19	121,121,121,121	0
54	MG	RF	301	1/1	0.68	0.17	115,115,115,115	0
54	MG	YA	3758	1/1	0.68	0.22	90,90,90,90	0
54	MG	RA	3389	1/1	0.68	0.14	109,109,109,109	0
54	MG	RA	3426	1/1	0.68	0.17	90,90,90,90	0
54	MG	YA	3638	1/1	0.68	0.32	90,90,90,90	0
54	MG	RA	3086	1/1	0.68	0.12	131,131,131,131	0
54	MG	YA	3739	1/1	0.68	0.18	95,95,95,95	0
54	MG	QA	1646	1/1	0.68	0.15	107,107,107,107	0
54	MG	YA	3611	1/1	0.68	0.33	90,90,90,90	0
54	MG	RA	3195	1/1	0.68	0.26	94,94,94,94	0
54	MG	YA	3646	1/1	0.68	0.75	90,90,90,90	0
54	MG	RA	3429	1/1	0.68	0.25	183,183,183,183	0
54	MG	QA	1698	1/1	0.68	0.38	90,90,90,90	0
54	MG	YA	3842	1/1	0.68	0.18	95,95,95,95	0
54	MG	RA	3120	1/1	0.69	0.35	96,96,96,96	0
54	MG	YA	3917	1/1	0.69	0.60	90,90,90,90	0
54	MG	RA	3419	1/1	0.69	0.17	142,142,142,142	0
54	MG	QA	1686	1/1	0.69	0.19	93,93,93,93	0
54	MG	RB	204	1/1	0.69	0.55	158,158,158,158	0
54	MG	YA	3668	1/1	0.69	0.47	90,90,90,90	0
54	MG	RA	3305	1/1	0.69	0.54	93,93,93,93	0
54	MG	RA	3269	1/1	0.69	0.22	117,117,117,117	0
54	MG	XA	1651	1/1	0.69	0.17	99,99,99,99	0
54	MG	YA	3672	1/1	0.69	0.12	100,100,100,100	0
54	MG	RA	3076	1/1	0.69	0.27	92,92,92,92	0
54	MG	RA	3222	1/1	0.69	0.49	134,134,134,134	0
54	MG	RD	301	1/1	0.69	0.20	124,124,124,124	0
54	MG	RA	3096	1/1	0.69	0.15	98,98,98,98	0
54	MG	QA	1673	1/1	0.69	0.66	90,90,90,90	0
54	MG	RA	3210	1/1	0.69	0.18	123,123,123,123	0
54	MG	QA	1674	1/1	0.70	0.15	90,90,90,90	0
54	MG	QA	1676	1/1	0.70	0.39	90,90,90,90	0
54	MG	YA	3914	1/1	0.70	0.26	90,90,90,90	0
54	MG	XA	1684	1/1	0.70	0.77	90,90,90,90	0
54	MG	RA	3405	1/1	0.70	0.17	90,90,90,90	0
54	MG	RA	3522	1/1	0.70	0.16	145,145,145,145	0
54	MG	RA	3213	1/1	0.70	0.17	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	QL	203	1/1	0.70	0.13	126,126,126,126	0
54	MG	RA	3160	1/1	0.70	0.59	90,90,90,90	0
54	MG	XA	1698	1/1	0.70	0.29	90,90,90,90	0
54	MG	RA	3264	1/1	0.70	0.29	90,90,90,90	0
54	MG	YA	3867	1/1	0.70	0.37	90,90,90,90	0
54	MG	RA	3121	1/1	0.70	0.23	90,90,90,90	0
54	MG	YA	3966	1/1	0.70	0.20	90,90,90,90	0
54	MG	XA	1660	1/1	0.70	0.19	90,90,90,90	0
54	MG	RA	3295	1/1	0.70	0.45	108,108,108,108	0
54	MG	RA	3056	1/1	0.70	0.30	116,116,116,116	0
54	MG	YA	3607	1/1	0.70	0.29	90,90,90,90	0
54	MG	RA	3138	1/1	0.70	0.35	90,90,90,90	0
54	MG	YA	3918	1/1	0.71	0.24	90,90,90,90	0
54	MG	RA	3021	1/1	0.71	0.21	112,112,112,112	0
54	MG	QA	1723	1/1	0.71	0.12	149,149,149,149	0
54	MG	YA	3759	1/1	0.71	0.51	90,90,90,90	0
54	MG	RA	3052	1/1	0.71	0.20	98,98,98,98	0
54	MG	YA	3790	1/1	0.71	0.21	90,90,90,90	0
54	MG	QA	1679	1/1	0.71	0.09	108,108,108,108	0
54	MG	YA	3886	1/1	0.71	0.21	162,162,162,162	0
54	MG	YA	3888	1/1	0.71	0.41	90,90,90,90	0
54	MG	YA	3614	1/1	0.71	0.56	90,90,90,90	0
54	MG	QA	1688	1/1	0.71	0.09	173,173,173,173	0
54	MG	RA	3338	1/1	0.71	0.10	129,129,129,129	0
54	MG	YB	205	1/1	0.71	0.49	97,97,97,97	0
54	MG	YB	207	1/1	0.71	0.19	109,109,109,109	0
54	MG	RA	3199	1/1	0.71	0.26	148,148,148,148	0
54	MG	YA	3813	1/1	0.71	0.39	111,111,111,111	0
54	MG	RA	3265	1/1	0.71	0.30	90,90,90,90	0
54	MG	YA	3655	1/1	0.71	0.39	90,90,90,90	0
54	MG	RA	3250	1/1	0.71	0.10	121,121,121,121	0
54	MG	RA	3035	1/1	0.71	0.16	94,94,94,94	0
54	MG	RA	3273	1/1	0.71	0.20	90,90,90,90	0
54	MG	YA	3947	1/1	0.71	0.43	90,90,90,90	0
54	MG	XA	1644	1/1	0.71	0.40	91,91,91,91	0
54	MG	RA	3313	1/1	0.71	0.11	90,90,90,90	0
54	MG	YA	3956	1/1	0.71	0.45	93,93,93,93	0
54	MG	YB	201	1/1	0.72	0.19	90,90,90,90	0
54	MG	RA	3486	1/1	0.72	0.21	90,90,90,90	0
54	MG	QQ	201	1/1	0.72	0.08	106,106,106,106	0
54	MG	YA	3632	1/1	0.72	0.20	91,91,91,91	0
54	MG	QT	201	1/1	0.72	0.34	205,205,205,205	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3549	1/1	0.72	0.17	121,121,121,121	0
54	MG	YA	3868	1/1	0.72	0.41	154,154,154,154	0
54	MG	RA	3257	1/1	0.72	0.14	102,102,102,102	0
54	MG	YA	3910	1/1	0.72	0.25	91,91,91,91	0
54	MG	QA	1656	1/1	0.72	0.21	90,90,90,90	0
54	MG	RA	3457	1/1	0.72	0.27	90,90,90,90	0
54	MG	RA	3206	1/1	0.72	0.40	134,134,134,134	0
54	MG	XA	1691	1/1	0.72	0.09	121,121,121,121	0
54	MG	RA	3351	1/1	0.72	0.13	90,90,90,90	0
54	MG	RA	3334	1/1	0.72	0.14	95,95,95,95	0
54	MG	YA	3682	1/1	0.72	0.22	90,90,90,90	0
54	MG	RD	308	1/1	0.72	0.12	94,94,94,94	0
54	MG	YA	3652	1/1	0.72	0.34	90,90,90,90	0
54	MG	RA	3200	1/1	0.72	0.30	90,90,90,90	0
54	MG	YA	3618	1/1	0.72	0.41	90,90,90,90	0
54	MG	RA	3193	1/1	0.72	0.11	91,91,91,91	0
54	MG	QA	1630	1/1	0.72	0.32	120,120,120,120	0
54	MG	YA	3895	1/1	0.72	0.35	90,90,90,90	0
54	MG	YA	3796	1/1	0.72	0.90	90,90,90,90	0
54	MG	YA	3649	1/1	0.73	0.31	90,90,90,90	0
54	MG	RA	3465	1/1	0.73	0.31	90,90,90,90	0
54	MG	RA	3085	1/1	0.73	0.10	126,126,126,126	0
54	MG	RA	3411	1/1	0.73	0.14	90,90,90,90	0
54	MG	RA	3091	1/1	0.73	0.19	99,99,99,99	0
54	MG	YA	3725	1/1	0.73	0.35	92,92,92,92	0
54	MG	YA	3636	1/1	0.73	0.56	113,113,113,113	0
54	MG	XA	1696	1/1	0.73	0.10	101,101,101,101	0
54	MG	RA	3271	1/1	0.73	0.17	98,98,98,98	0
54	MG	QP	102	1/1	0.73	0.88	145,145,145,145	0
54	MG	RA	3479	1/1	0.73	0.52	154,154,154,154	0
54	MG	RA	3292	1/1	0.73	0.18	96,96,96,96	0
54	MG	QA	1697	1/1	0.73	0.37	116,116,116,116	0
54	MG	RB	214	1/1	0.73	0.27	106,106,106,106	0
54	MG	RA	3485	1/1	0.73	0.50	90,90,90,90	0
54	MG	XA	1710	1/1	0.73	0.21	129,129,129,129	0
54	MG	YA	3896	1/1	0.73	0.14	93,93,93,93	0
54	MG	RA	3004	1/1	0.73	0.38	109,109,109,109	0
54	MG	YA	3898	1/1	0.73	0.28	145,145,145,145	0
54	MG	RA	3268	1/1	0.73	0.41	90,90,90,90	0
54	MG	RA	3444	1/1	0.74	0.25	119,119,119,119	0
54	MG	QA	1714	1/1	0.74	0.25	174,174,174,174	0
54	MG	YA	3862	1/1	0.74	0.30	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3316	1/1	0.74	0.12	92,92,92,92	0
54	MG	RA	3412	1/1	0.74	0.37	90,90,90,90	0
54	MG	RA	3399	1/1	0.74	0.14	158,158,158,158	0
54	MG	YA	3916	1/1	0.74	0.31	91,91,91,91	0
54	MG	YA	3869	1/1	0.74	0.74	90,90,90,90	0
54	MG	QA	1726	1/1	0.74	0.28	195,195,195,195	0
54	MG	XA	1640	1/1	0.74	0.05	126,126,126,126	0
54	MG	YA	3827	1/1	0.74	0.16	91,91,91,91	0
54	MG	QA	1730	1/1	0.74	0.12	112,112,112,112	0
54	MG	YA	3847	1/1	0.74	0.26	90,90,90,90	0
54	MG	XL	201	1/1	0.74	0.11	99,99,99,99	0
54	MG	YA	3848	1/1	0.74	0.45	90,90,90,90	0
54	MG	RA	3047	1/1	0.74	0.12	93,93,93,93	0
54	MG	RA	3341	1/1	0.74	0.08	92,92,92,92	0
54	MG	YA	3954	1/1	0.74	0.17	134,134,134,134	0
54	MG	XA	1712	1/1	0.74	0.06	96,96,96,96	0
54	MG	RA	3471	1/1	0.74	0.16	90,90,90,90	0
54	MG	YA	3925	1/1	0.74	0.38	90,90,90,90	0
54	MG	XA	1675	1/1	0.74	0.26	93,93,93,93	0
54	MG	RR	202	1/1	0.75	0.11	108,108,108,108	0
54	MG	RA	3260	1/1	0.75	0.45	90,90,90,90	0
54	MG	RA	3009	1/1	0.75	0.17	91,91,91,91	0
54	MG	RA	3274	1/1	0.75	0.14	90,90,90,90	0
54	MG	R1	101	1/1	0.75	0.08	154,154,154,154	0
54	MG	YA	3745	1/1	0.75	0.25	90,90,90,90	0
54	MG	RA	3168	1/1	0.75	0.34	90,90,90,90	0
54	MG	YA	3806	1/1	0.75	0.47	90,90,90,90	0
54	MG	RA	3219	1/1	0.75	0.33	112,112,112,112	0
54	MG	QA	1682	1/1	0.75	0.14	90,90,90,90	0
54	MG	QA	1636	1/1	0.75	0.14	138,138,138,138	0
54	MG	QA	1687	1/1	0.75	0.40	90,90,90,90	0
54	MG	YA	3706	1/1	0.75	0.17	118,118,118,118	0
54	MG	RA	3489	1/1	0.75	0.22	92,92,92,92	0
54	MG	YA	3635	1/1	0.75	0.21	152,152,152,152	0
54	MG	R6	101	1/1	0.75	0.29	159,159,159,159	0
54	MG	RA	3266	1/1	0.75	0.31	90,90,90,90	0
54	MG	RE	305	1/1	0.75	0.28	91,91,91,91	0
54	MG	QA	1653	1/1	0.75	0.14	95,95,95,95	0
54	MG	YA	3678	1/1	0.75	0.18	94,94,94,94	0
54	MG	XA	1701	1/1	0.75	0.09	120,120,120,120	0
54	MG	RA	3207	1/1	0.75	0.23	90,90,90,90	0
54	MG	YA	3608	1/1	0.75	0.21	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3055	1/1	0.75	0.25	136,136,136,136	0
54	MG	YA	3931	1/1	0.75	0.17	122,122,122,122	0
54	MG	YA	3843	1/1	0.75	0.29	174,174,174,174	0
54	MG	YA	3732	1/1	0.75	0.26	221,221,221,221	0
54	MG	RA	3293	1/1	0.75	0.10	118,118,118,118	0
54	MG	YA	3736	1/1	0.75	0.28	90,90,90,90	0
54	MG	RA	3080	1/1	0.75	0.18	100,100,100,100	0
54	MG	RA	3277	1/1	0.76	0.13	92,92,92,92	0
54	MG	RA	3501	1/1	0.76	0.37	90,90,90,90	0
54	MG	QA	1695	1/1	0.76	0.56	131,131,131,131	0
54	MG	RA	3245	1/1	0.76	0.25	92,92,92,92	0
54	MG	RA	3019	1/1	0.76	0.41	132,132,132,132	0
54	MG	YA	3650	1/1	0.76	0.74	155,155,155,155	0
54	MG	RA	3175	1/1	0.76	0.15	97,97,97,97	0
54	MG	RA	3554	1/1	0.76	0.11	103,103,103,103	0
54	MG	RA	3069	1/1	0.76	0.05	90,90,90,90	0
54	MG	QA	1629	1/1	0.76	0.10	105,105,105,105	0
54	MG	RA	3512	1/1	0.76	0.17	105,105,105,105	0
54	MG	RA	3513	1/1	0.76	0.18	137,137,137,137	0
54	MG	RA	3562	1/1	0.76	0.20	90,90,90,90	0
54	MG	RA	3101	1/1	0.76	0.14	123,123,123,123	0
54	MG	QA	1634	1/1	0.76	0.59	99,99,99,99	0
54	MG	RA	3164	1/1	0.76	0.18	90,90,90,90	0
54	MG	RA	3358	1/1	0.76	0.10	155,155,155,155	0
54	MG	RA	3414	1/1	0.76	0.08	112,112,112,112	0
54	MG	QA	1639	1/1	0.76	0.15	91,91,91,91	0
54	MG	RA	3209	1/1	0.76	0.32	106,106,106,106	0
54	MG	RA	3151	1/1	0.76	0.41	90,90,90,90	0
54	MG	RA	3114	1/1	0.76	0.27	90,90,90,90	0
54	MG	YA	3871	1/1	0.76	0.28	90,90,90,90	0
54	MG	XA	1715	1/1	0.76	0.19	144,144,144,144	0
54	MG	RA	3116	1/1	0.76	0.13	90,90,90,90	0
54	MG	RA	3499	1/1	0.76	0.10	92,92,92,92	0
54	MG	YA	3767	1/1	0.77	0.44	90,90,90,90	0
54	MG	RA	3492	1/1	0.77	0.23	92,92,92,92	0
54	MG	YA	3772	1/1	0.77	0.66	90,90,90,90	0
54	MG	RA	3498	1/1	0.77	0.24	90,90,90,90	0
54	MG	YA	3860	1/1	0.77	0.21	90,90,90,90	0
54	MG	RA	3383	1/1	0.77	0.10	133,133,133,133	0
54	MG	YA	3889	1/1	0.77	0.22	90,90,90,90	0
54	MG	XA	1648	1/1	0.77	0.14	95,95,95,95	0
54	MG	RA	3042	1/1	0.77	0.33	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3254	1/1	0.77	0.22	149,149,149,149	0
54	MG	RA	3472	1/1	0.77	0.21	90,90,90,90	0
54	MG	QA	1670	1/1	0.77	0.14	94,94,94,94	0
54	MG	RA	3178	1/1	0.77	0.19	94,94,94,94	0
54	MG	RA	3340	1/1	0.77	0.14	97,97,97,97	0
54	MG	QA	1675	1/1	0.77	0.13	125,125,125,125	0
54	MG	RA	3202	1/1	0.77	0.22	90,90,90,90	0
54	MG	RA	3541	1/1	0.77	0.19	90,90,90,90	0
54	MG	RA	3040	1/1	0.77	0.23	91,91,91,91	0
54	MG	RF	304	1/1	0.77	0.13	91,91,91,91	0
54	MG	YA	3878	1/1	0.77	0.26	90,90,90,90	0
54	MG	RA	3289	1/1	0.77	0.26	94,94,94,94	0
54	MG	RA	3211	1/1	0.78	0.27	92,92,92,92	0
54	MG	RE	307	1/1	0.78	0.23	90,90,90,90	0
54	MG	YB	206	1/1	0.78	0.45	90,90,90,90	0
54	MG	RA	3520	1/1	0.78	0.18	156,156,156,156	0
54	MG	YA	3623	1/1	0.78	0.12	113,113,113,113	0
54	MG	RA	3105	1/1	0.78	0.19	92,92,92,92	0
54	MG	RA	3343	1/1	0.78	0.16	151,151,151,151	0
54	MG	RA	3425	1/1	0.78	0.06	133,133,133,133	0
54	MG	XD	302	1/1	0.78	0.11	142,142,142,142	0
54	MG	YA	3959	1/1	0.78	0.53	111,111,111,111	0
54	MG	RO	202	1/1	0.78	0.09	108,108,108,108	0
54	MG	YA	3858	1/1	0.78	0.78	90,90,90,90	0
54	MG	RA	3497	1/1	0.78	0.25	90,90,90,90	0
54	MG	XA	1707	1/1	0.78	0.15	134,134,134,134	0
54	MG	RA	3560	1/1	0.78	0.24	90,90,90,90	0
54	MG	RA	3310	1/1	0.78	0.11	92,92,92,92	0
54	MG	QA	1615	1/1	0.78	0.09	142,142,142,142	0
54	MG	RA	3143	1/1	0.78	0.15	90,90,90,90	0
54	MG	QA	1617	1/1	0.78	0.26	92,92,92,92	0
54	MG	YA	3976	1/1	0.78	0.24	92,92,92,92	0
54	MG	RA	3464	1/1	0.78	0.12	105,105,105,105	0
54	MG	RA	3240	1/1	0.78	0.11	91,91,91,91	0
54	MG	YA	3977	1/1	0.79	0.19	90,90,90,90	0
54	MG	YA	3781	1/1	0.79	0.16	90,90,90,90	0
54	MG	YA	3742	1/1	0.79	0.31	90,90,90,90	0
54	MG	YB	202	1/1	0.79	0.11	106,106,106,106	0
54	MG	YA	3948	1/1	0.79	0.50	90,90,90,90	0
54	MG	YA	3949	1/1	0.79	0.08	90,90,90,90	0
54	MG	RA	3079	1/1	0.79	0.17	93,93,93,93	0
54	MG	XA	1645	1/1	0.79	0.10	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3244	1/1	0.79	0.19	90,90,90,90	0
54	MG	RA	3227	1/1	0.79	0.19	148,148,148,148	0
54	MG	RA	3176	1/1	0.79	0.60	90,90,90,90	0
54	MG	RA	3017	1/1	0.79	0.27	91,91,91,91	0
54	MG	YA	3841	1/1	0.79	0.36	90,90,90,90	0
54	MG	QA	1605	1/1	0.79	0.19	90,90,90,90	0
54	MG	RA	3290	1/1	0.79	0.09	153,153,153,153	0
54	MG	RA	3058	1/1	0.79	0.14	122,122,122,122	0
54	MG	YQ	201	1/1	0.79	0.15	90,90,90,90	0
54	MG	RA	3078	1/1	0.79	0.29	96,96,96,96	0
54	MG	YA	3721	1/1	0.79	0.35	90,90,90,90	0
54	MG	RA	3191	1/1	0.79	0.18	90,90,90,90	0
54	MG	YA	3975	1/1	0.79	0.53	90,90,90,90	0
54	MG	YA	3816	1/1	0.79	0.48	90,90,90,90	0
54	MG	XP	101	1/1	0.80	0.15	208,208,208,208	0
54	MG	XA	1602	1/1	0.80	0.31	162,162,162,162	0
54	MG	XA	1603	1/1	0.80	0.21	90,90,90,90	0
54	MG	RA	3174	1/1	0.80	0.13	103,103,103,103	0
54	MG	RA	3453	1/1	0.80	0.21	90,90,90,90	0
54	MG	YA	3837	1/1	0.80	0.34	90,90,90,90	0
54	MG	XA	1616	1/1	0.80	0.26	90,90,90,90	0
54	MG	XA	1680	1/1	0.80	0.13	159,159,159,159	0
54	MG	XA	1681	1/1	0.80	0.12	128,128,128,128	0
54	MG	XA	1682	1/1	0.80	0.25	90,90,90,90	0
54	MG	RA	3536	1/1	0.80	0.27	114,114,114,114	0
54	MG	YA	3979	1/1	0.80	0.12	119,119,119,119	0
54	MG	YA	3840	1/1	0.80	0.26	102,102,102,102	0
54	MG	RA	3537	1/1	0.80	0.23	117,117,117,117	0
54	MG	YA	3950	1/1	0.80	0.16	93,93,93,93	0
54	MG	QA	1718	1/1	0.80	0.20	205,205,205,205	0
54	MG	YA	3807	1/1	0.80	0.16	90,90,90,90	0
54	MG	QA	1720	1/1	0.80	0.14	137,137,137,137	0
54	MG	RA	3118	1/1	0.80	0.19	90,90,90,90	0
54	MG	YA	3872	1/1	0.80	0.15	90,90,90,90	0
54	MG	XA	1637	1/1	0.80	0.09	137,137,137,137	0
54	MG	RA	3463	1/1	0.80	0.12	91,91,91,91	0
54	MG	YD	301	1/1	0.80	0.24	90,90,90,90	0
54	MG	XA	1641	1/1	0.80	0.10	90,90,90,90	0
54	MG	RB	210	1/1	0.80	0.23	217,217,217,217	0
54	MG	YA	3642	1/1	0.80	0.30	96,96,96,96	0
54	MG	YA	3727	1/1	0.80	0.20	91,91,91,91	0
54	MG	QA	1731	1/1	0.80	0.25	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	YA	3823	1/1	0.80	0.46	90,90,90,90	0
54	MG	RA	3321	1/1	0.80	0.10	102,102,102,102	0
54	MG	RA	3051	1/1	0.80	0.14	145,145,145,145	0
54	MG	XA	1663	1/1	0.80	0.16	90,90,90,90	0
54	MG	YA	3791	1/1	0.80	0.20	132,132,132,132	0
54	MG	RA	3505	1/1	0.81	0.11	92,92,92,92	0
54	MG	XA	1658	1/1	0.81	0.14	117,117,117,117	0
54	MG	YA	3620	1/1	0.81	0.15	95,95,95,95	0
54	MG	YA	3833	1/1	0.81	0.22	137,137,137,137	0
54	MG	RA	3527	1/1	0.81	0.20	90,90,90,90	0
54	MG	YA	3873	1/1	0.81	0.29	91,91,91,91	0
54	MG	YA	3963	1/1	0.81	0.13	91,91,91,91	0
54	MG	RA	3534	1/1	0.81	0.32	119,119,119,119	0
54	MG	RA	3387	1/1	0.81	0.10	143,143,143,143	0
54	MG	YA	3634	1/1	0.81	0.15	93,93,93,93	0
54	MG	YA	3877	1/1	0.81	0.11	92,92,92,92	0
54	MG	RA	3034	1/1	0.81	0.24	99,99,99,99	0
54	MG	RA	3003	1/1	0.81	0.18	208,208,208,208	0
54	MG	RA	3088	1/1	0.81	0.13	95,95,95,95	0
54	MG	RA	3136	1/1	0.81	0.20	139,139,139,139	0
54	MG	QA	1650	1/1	0.81	0.10	141,141,141,141	0
54	MG	YA	3756	1/1	0.81	0.39	90,90,90,90	0
54	MG	XA	1622	1/1	0.81	0.15	189,189,189,189	0
54	MG	RA	3544	1/1	0.81	0.10	90,90,90,90	0
54	MG	YA	3641	1/1	0.81	0.09	93,93,93,93	0
54	MG	RA	3179	1/1	0.81	0.26	172,172,172,172	0
54	MG	RA	3302	1/1	0.81	0.19	98,98,98,98	0
54	MG	RA	3060	1/1	0.81	0.17	157,157,157,157	0
54	MG	YA	3938	1/1	0.81	0.18	97,97,97,97	0
54	MG	YA	3893	1/1	0.81	0.21	101,101,101,101	0
54	MG	RA	3478	1/1	0.81	0.34	90,90,90,90	0
54	MG	XA	1635	1/1	0.81	0.09	102,102,102,102	0
54	MG	YA	3855	1/1	0.81	0.40	90,90,90,90	0
54	MG	RT	202	1/1	0.81	0.19	141,141,141,141	0
54	MG	QA	1667	1/1	0.81	0.11	115,115,115,115	0
54	MG	XA	1708	1/1	0.81	0.08	133,133,133,133	0
54	MG	RY	201	1/1	0.81	0.19	100,100,100,100	0
54	MG	RA	3369	1/1	0.81	0.15	113,113,113,113	0
54	MG	YA	3818	1/1	0.81	0.30	128,128,128,128	0
54	MG	QA	1722	1/1	0.81	0.12	151,151,151,151	0
54	MG	XA	1647	1/1	0.81	0.20	143,143,143,143	0
54	MG	YA	3771	1/1	0.81	0.18	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3439	1/1	0.81	0.13	100,100,100,100	0
54	MG	XA	1721	1/1	0.81	0.30	143,143,143,143	0
54	MG	YA	3906	1/1	0.81	0.29	90,90,90,90	0
54	MG	RA	3028	1/1	0.82	0.27	97,97,97,97	0
54	MG	RA	3177	1/1	0.82	0.14	91,91,91,91	0
54	MG	RA	3446	1/1	0.82	0.70	177,177,177,177	0
54	MG	YA	3713	1/1	0.82	0.12	90,90,90,90	0
54	MG	RA	3007	1/1	0.82	0.17	93,93,93,93	0
54	MG	YA	3859	1/1	0.82	0.31	92,92,92,92	0
54	MG	YA	3719	1/1	0.82	0.24	90,90,90,90	0
54	MG	YA	3829	1/1	0.82	0.27	90,90,90,90	0
54	MG	XA	1686	1/1	0.82	0.10	158,158,158,158	0
54	MG	RA	3169	1/1	0.82	0.15	91,91,91,91	0
54	MG	RA	3024	1/1	0.82	0.14	156,156,156,156	0
54	MG	XA	1634	1/1	0.82	0.17	91,91,91,91	0
54	MG	RA	3070	1/1	0.82	0.25	90,90,90,90	0
54	MG	RA	3368	1/1	0.82	0.05	93,93,93,93	0
54	MG	QA	1689	1/1	0.82	0.27	93,93,93,93	0
54	MG	QA	1729	1/1	0.82	0.09	94,94,94,94	0
54	MG	RA	3349	1/1	0.82	0.35	127,127,127,127	0
54	MG	RA	3433	1/1	0.82	0.11	101,101,101,101	0
54	MG	YA	3696	1/1	0.82	0.22	93,93,93,93	0
54	MG	RA	3027	1/1	0.82	0.28	98,98,98,98	0
54	MG	XA	1702	1/1	0.82	0.08	144,144,144,144	0
54	MG	RR	201	1/1	0.82	0.27	131,131,131,131	0
54	MG	RA	3436	1/1	0.82	0.12	113,113,113,113	0
54	MG	YA	3844	1/1	0.82	0.23	90,90,90,90	0
54	MG	XA	1601	1/1	0.82	0.17	166,166,166,166	0
54	MG	RA	3073	1/1	0.82	0.33	159,159,159,159	0
54	MG	XA	1656	1/1	0.82	0.18	90,90,90,90	0
54	MG	YA	3811	1/1	0.82	0.17	91,91,91,91	0
54	MG	XA	1606	1/1	0.82	0.09	185,185,185,185	0
54	MG	RA	3438	1/1	0.82	0.16	126,126,126,126	0
54	MG	RA	3278	1/1	0.82	0.20	92,92,92,92	0
54	MG	QA	1671	1/1	0.82	0.22	93,93,93,93	0
54	MG	QT	202	1/1	0.82	0.06	112,112,112,112	0
54	MG	XA	1619	1/1	0.82	0.09	90,90,90,90	0
55	ZN	QD	305	1/1	0.82	0.14	338,338,338,338	0
54	MG	YA	3662	1/1	0.83	0.14	108,108,108,108	0
54	MG	YA	3664	1/1	0.83	0.12	110,110,110,110	0
54	MG	QA	1659	1/1	0.83	0.13	98,98,98,98	0
54	MG	RA	3242	1/1	0.83	0.24	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	YA	3639	1/1	0.83	0.60	90,90,90,90	0
54	MG	RA	3053	1/1	0.83	0.22	90,90,90,90	0
54	MG	RA	3255	1/1	0.83	0.37	90,90,90,90	0
54	MG	YA	3824	1/1	0.83	0.24	160,160,160,160	0
54	MG	RA	3474	1/1	0.83	0.09	103,103,103,103	0
54	MG	RA	3440	1/1	0.83	0.09	170,170,170,170	0
54	MG	YA	3712	1/1	0.83	0.32	90,90,90,90	0
54	MG	RA	3082	1/1	0.83	0.08	140,140,140,140	0
54	MG	XA	1609	1/1	0.83	0.07	100,100,100,100	0
54	MG	RA	3006	1/1	0.83	0.20	90,90,90,90	0
54	MG	YA	3647	1/1	0.83	0.17	115,115,115,115	0
54	MG	RA	3132	1/1	0.83	0.18	136,136,136,136	0
54	MG	YA	3601	1/1	0.83	0.17	111,111,111,111	0
54	MG	YA	3903	1/1	0.83	0.31	90,90,90,90	0
54	MG	RA	3507	1/1	0.83	0.33	90,90,90,90	0
54	MG	XA	1665	1/1	0.83	0.18	92,92,92,92	0
54	MG	RA	3050	1/1	0.83	0.27	93,93,93,93	0
54	MG	RA	3110	1/1	0.83	0.24	90,90,90,90	0
54	MG	YA	3799	1/1	0.83	0.21	91,91,91,91	0
54	MG	XA	1713	1/1	0.83	0.23	91,91,91,91	0
54	MG	RA	3182	1/1	0.83	0.10	139,139,139,139	0
54	MG	RA	3495	1/1	0.83	0.20	97,97,97,97	0
54	MG	YA	3915	1/1	0.83	0.16	92,92,92,92	0
54	MG	XA	1720	1/1	0.83	0.13	169,169,169,169	0
54	MG	RU	201	1/1	0.83	0.21	123,123,123,123	0
54	MG	YA	3810	1/1	0.83	0.41	90,90,90,90	0
54	MG	YA	3735	1/1	0.83	0.23	90,90,90,90	0
54	MG	RA	3364	1/1	0.84	0.16	144,144,144,144	0
54	MG	QA	1637	1/1	0.84	0.08	91,91,91,91	0
54	MG	RA	3488	1/1	0.84	0.19	91,91,91,91	0
54	MG	RA	3263	1/1	0.84	0.16	90,90,90,90	0
54	MG	YA	3961	1/1	0.84	0.22	93,93,93,93	0
54	MG	RR	203	1/1	0.84	0.44	90,90,90,90	0
54	MG	XA	1614	1/1	0.84	0.18	126,126,126,126	0
54	MG	RA	3524	1/1	0.84	0.12	138,138,138,138	0
54	MG	XA	1617	1/1	0.84	0.11	97,97,97,97	0
54	MG	YA	3965	1/1	0.84	0.18	90,90,90,90	0
54	MG	YA	3870	1/1	0.84	0.41	90,90,90,90	0
54	MG	RA	3205	1/1	0.84	0.19	96,96,96,96	0
54	MG	RA	3460	1/1	0.84	0.42	146,146,146,146	0
54	MG	RA	3322	1/1	0.84	0.47	90,90,90,90	0
54	MG	YA	3726	1/1	0.84	0.17	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3104	1/1	0.84	0.10	113,113,113,113	0
54	MG	YA	3675	1/1	0.84	0.21	100,100,100,100	0
54	MG	RA	3251	1/1	0.84	0.20	90,90,90,90	0
54	MG	RA	3348	1/1	0.84	0.17	140,140,140,140	0
54	MG	RA	3030	1/1	0.84	0.35	90,90,90,90	0
54	MG	RA	3153	1/1	0.84	0.20	177,177,177,177	0
54	MG	RA	3309	1/1	0.84	0.18	182,182,182,182	0
54	MG	RA	3543	1/1	0.84	0.21	139,139,139,139	0
54	MG	RA	3186	1/1	0.84	0.14	140,140,140,140	0
54	MG	RD	309	1/1	0.84	0.54	189,189,189,189	0
54	MG	RE	301	1/1	0.84	0.16	121,121,121,121	0
54	MG	RA	3189	1/1	0.84	0.08	118,118,118,118	0
54	MG	YB	210	1/1	0.84	0.22	91,91,91,91	0
54	MG	RA	3258	1/1	0.84	0.24	90,90,90,90	0
54	MG	YA	3797	1/1	0.84	0.21	92,92,92,92	0
54	MG	QA	1623	1/1	0.84	0.10	118,118,118,118	0
54	MG	RA	3475	1/1	0.84	0.33	133,133,133,133	0
54	MG	RA	3360	1/1	0.84	0.23	91,91,91,91	0
54	MG	RA	3072	1/1	0.84	0.45	110,110,110,110	0
54	MG	RA	3093	1/1	0.84	0.17	100,100,100,100	0
54	MG	YA	3856	1/1	0.84	0.42	90,90,90,90	0
54	MG	RA	3484	1/1	0.84	0.18	91,91,91,91	0
54	MG	RA	3232	1/1	0.84	0.37	90,90,90,90	0
54	MG	YA	3616	1/1	0.84	0.25	139,139,139,139	0
54	MG	XA	1727	1/1	0.84	0.16	168,168,168,168	0
54	MG	YA	3657	1/1	0.84	0.22	137,137,137,137	0
54	MG	YA	3853	1/1	0.85	0.19	105,105,105,105	0
54	MG	RA	3285	1/1	0.85	0.16	90,90,90,90	0
54	MG	XA	1654	1/1	0.85	0.12	97,97,97,97	0
54	MG	RA	3157	1/1	0.85	0.20	90,90,90,90	0
54	MG	RA	3506	1/1	0.85	0.11	122,122,122,122	0
54	MG	RA	3137	1/1	0.85	0.11	170,170,170,170	0
54	MG	QA	1728	1/1	0.85	0.12	92,92,92,92	0
54	MG	RA	3224	1/1	0.85	0.09	96,96,96,96	0
54	MG	YA	3801	1/1	0.85	0.34	94,94,94,94	0
54	MG	RA	3161	1/1	0.85	0.34	102,102,102,102	0
54	MG	YA	3716	1/1	0.85	0.24	90,90,90,90	0
54	MG	YA	3717	1/1	0.85	0.28	90,90,90,90	0
54	MG	RA	3203	1/1	0.85	0.77	105,105,105,105	0
54	MG	RA	3204	1/1	0.85	0.19	93,93,93,93	0
54	MG	RA	3424	1/1	0.85	0.15	130,130,130,130	0
54	MG	QA	1651	1/1	0.85	0.18	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3220	1/1	0.85	0.08	97,97,97,97	0
54	MG	RA	3256	1/1	0.85	0.32	126,126,126,126	0
54	MG	RA	3282	1/1	0.85	0.25	97,97,97,97	0
54	MG	XA	1716	1/1	0.85	0.16	99,99,99,99	0
54	MG	QA	1716	1/1	0.85	0.32	158,158,158,158	0
54	MG	YA	3621	1/1	0.85	0.24	90,90,90,90	0
54	MG	YA	3606	1/1	0.85	0.33	201,201,201,201	0
54	MG	RA	3221	1/1	0.85	0.13	118,118,118,118	0
54	MG	YA	3630	1/1	0.85	0.15	130,130,130,130	0
54	MG	YA	3964	1/1	0.85	0.36	90,90,90,90	0
54	MG	YA	3659	1/1	0.86	0.27	90,90,90,90	0
54	MG	RA	3542	1/1	0.86	0.10	194,194,194,194	0
54	MG	YA	3746	1/1	0.86	0.24	90,90,90,90	0
54	MG	XA	1683	1/1	0.86	0.17	109,109,109,109	0
54	MG	XA	1633	1/1	0.86	0.09	109,109,109,109	0
54	MG	YA	3722	1/1	0.86	0.56	90,90,90,90	0
54	MG	YA	3849	1/1	0.86	0.16	90,90,90,90	0
54	MG	YA	3782	1/1	0.86	0.09	101,101,101,101	0
54	MG	RA	3406	1/1	0.86	0.21	131,131,131,131	0
54	MG	QA	1699	1/1	0.86	0.11	90,90,90,90	0
54	MG	XL	202	1/1	0.86	0.07	109,109,109,109	0
54	MG	XA	1694	1/1	0.86	0.09	104,104,104,104	0
54	MG	RA	3409	1/1	0.86	0.46	156,156,156,156	0
54	MG	QA	1703	1/1	0.86	0.12	95,95,95,95	0
54	MG	RA	3330	1/1	0.86	0.09	92,92,92,92	0
54	MG	RB	203	1/1	0.86	0.17	165,165,165,165	0
54	MG	RD	310	1/1	0.86	0.08	150,150,150,150	0
54	MG	XA	1650	1/1	0.86	0.18	138,138,138,138	0
54	MG	QA	1707	1/1	0.86	0.08	137,137,137,137	0
54	MG	XA	1608	1/1	0.86	0.11	136,136,136,136	0
54	MG	XA	1704	1/1	0.86	0.15	96,96,96,96	0
54	MG	RA	3064	1/1	0.86	0.09	142,142,142,142	0
54	MG	RA	3152	1/1	0.86	0.16	109,109,109,109	0
54	MG	YA	3673	1/1	0.86	0.21	255,255,255,255	0
54	MG	RA	3308	1/1	0.86	0.15	129,129,129,129	0
54	MG	XA	1659	1/1	0.86	0.44	93,93,93,93	0
54	MG	YA	3960	1/1	0.86	0.07	90,90,90,90	0
54	MG	RA	3212	1/1	0.86	0.17	121,121,121,121	0
54	MG	RB	208	1/1	0.86	0.14	178,178,178,178	0
54	MG	YA	3839	1/1	0.86	0.14	90,90,90,90	0
54	MG	XA	1666	1/1	0.86	0.53	95,95,95,95	0
54	MG	YA	3681	1/1	0.86	0.16	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	XA	1717	1/1	0.86	0.11	145,145,145,145	0
54	MG	RA	3328	1/1	0.86	0.07	110,110,110,110	0
54	MG	RF	303	1/1	0.86	0.28	141,141,141,141	0
54	MG	YT	202	1/1	0.86	0.13	143,143,143,143	0
54	MG	RA	3461	1/1	0.86	0.46	90,90,90,90	0
54	MG	YA	3934	1/1	0.86	0.29	90,90,90,90	0
54	MG	RA	3057	1/1	0.86	0.09	105,105,105,105	0
54	MG	YA	3715	1/1	0.87	0.37	90,90,90,90	0
54	MG	YA	3680	1/1	0.87	0.16	90,90,90,90	0
54	MG	RA	3442	1/1	0.87	0.13	94,94,94,94	0
54	MG	RA	3521	1/1	0.87	0.09	158,158,158,158	0
54	MG	YA	3683	1/1	0.87	0.49	90,90,90,90	0
54	MG	YA	3622	1/1	0.87	0.33	90,90,90,90	0
54	MG	QA	1626	1/1	0.87	0.13	121,121,121,121	0
54	MG	R8	102	1/1	0.87	0.06	118,118,118,118	0
54	MG	RA	3112	1/1	0.87	0.12	143,143,143,143	0
54	MG	YA	3937	1/1	0.87	0.17	90,90,90,90	0
54	MG	RA	3482	1/1	0.87	0.23	92,92,92,92	0
54	MG	RA	3063	1/1	0.87	0.18	158,158,158,158	0
54	MG	RA	3099	1/1	0.87	0.24	97,97,97,97	0
54	MG	RA	3183	1/1	0.87	0.25	95,95,95,95	0
54	MG	YA	3907	1/1	0.87	0.34	92,92,92,92	0
54	MG	RA	3531	1/1	0.87	0.16	113,113,113,113	0
54	MG	YA	3609	1/1	0.87	0.49	90,90,90,90	0
54	MG	RD	306	1/1	0.87	0.21	142,142,142,142	0
54	MG	RA	3557	1/1	0.87	0.18	154,154,154,154	0
54	MG	RA	3115	1/1	0.87	0.14	173,173,173,173	0
54	MG	QA	1641	1/1	0.87	0.06	118,118,118,118	0
54	MG	RA	3469	1/1	0.87	0.10	96,96,96,96	0
54	MG	RA	3141	1/1	0.87	0.20	267,267,267,267	0
54	MG	XA	1673	1/1	0.87	0.48	90,90,90,90	0
54	MG	QA	1608	1/1	0.87	0.26	91,91,91,91	0
54	MG	YA	3955	1/1	0.87	0.09	110,110,110,110	0
54	MG	RA	3367	1/1	0.87	0.08	160,160,160,160	0
54	MG	RA	3061	1/1	0.87	0.20	90,90,90,90	0
54	MG	XA	1718	1/1	0.87	0.33	90,90,90,90	0
54	MG	XA	1679	1/1	0.87	0.16	123,123,123,123	0
54	MG	RA	3388	1/1	0.87	0.17	95,95,95,95	0
54	MG	YA	3826	1/1	0.87	0.13	120,120,120,120	0
54	MG	RA	3280	1/1	0.87	0.07	129,129,129,129	0
54	MG	RA	3241	1/1	0.87	0.28	90,90,90,90	0
54	MG	XK	201	1/1	0.87	0.10	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	QA	1643	1/1	0.88	0.26	123,123,123,123	0
54	MG	RA	3551	1/1	0.88	0.21	118,118,118,118	0
54	MG	RA	3117	1/1	0.88	0.43	90,90,90,90	0
54	MG	R8	103	1/1	0.88	0.26	97,97,97,97	0
54	MG	YA	3968	1/1	0.88	0.07	90,90,90,90	0
54	MG	RA	3010	1/1	0.88	0.48	92,92,92,92	0
54	MG	RE	302	1/1	0.88	0.05	141,141,141,141	0
54	MG	YA	3973	1/1	0.88	0.33	101,101,101,101	0
54	MG	RA	3187	1/1	0.88	0.10	143,143,143,143	0
54	MG	YA	3605	1/1	0.88	0.38	245,245,245,245	0
54	MG	RE	304	1/1	0.88	0.42	157,157,157,157	0
54	MG	RA	3029	1/1	0.88	0.11	97,97,97,97	0
54	MG	RA	3352	1/1	0.88	0.13	98,98,98,98	0
54	MG	YA	3883	1/1	0.88	0.09	92,92,92,92	0
54	MG	QA	1662	1/1	0.88	0.07	137,137,137,137	0
54	MG	RA	3353	1/1	0.88	0.14	90,90,90,90	0
54	MG	XA	1692	1/1	0.88	0.14	156,156,156,156	0
54	MG	QA	1717	1/1	0.88	0.12	152,152,152,152	0
54	MG	RA	3144	1/1	0.88	0.21	150,150,150,150	0
54	MG	RF	302	1/1	0.88	0.12	232,232,232,232	0
54	MG	RA	3528	1/1	0.88	0.08	90,90,90,90	0
54	MG	RA	3016	1/1	0.88	0.10	93,93,93,93	0
54	MG	RA	3217	1/1	0.88	0.24	138,138,138,138	0
54	MG	RA	3359	1/1	0.88	0.29	142,142,142,142	0
54	MG	YA	3753	1/1	0.88	0.27	90,90,90,90	0
54	MG	YA	3852	1/1	0.88	0.32	90,90,90,90	0
54	MG	RA	3097	1/1	0.88	0.10	90,90,90,90	0
54	MG	YD	304	1/1	0.88	0.22	121,121,121,121	0
54	MG	RA	3318	1/1	0.88	0.34	91,91,91,91	0
54	MG	RA	3538	1/1	0.88	0.22	93,93,93,93	0
54	MG	RA	3098	1/1	0.88	0.35	90,90,90,90	0
54	MG	RA	3252	1/1	0.88	0.15	90,90,90,90	0
54	MG	RB	211	1/1	0.88	0.37	176,176,176,176	0
54	MG	RA	3239	1/1	0.88	0.18	93,93,93,93	0
54	MG	RX	101	1/1	0.88	0.16	93,93,93,93	0
54	MG	YX	101	1/1	0.88	0.10	90,90,90,90	0
54	MG	QA	1685	1/1	0.88	0.08	178,178,178,178	0
54	MG	RA	3304	1/1	0.88	0.24	136,136,136,136	0
54	MG	YA	3864	1/1	0.88	0.15	114,114,114,114	0
54	MG	RA	3454	1/1	0.88	0.25	90,90,90,90	0
54	MG	RA	3345	1/1	0.88	0.17	90,90,90,90	0
54	MG	RD	305	1/1	0.88	0.65	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	QA	1692	1/1	0.88	0.09	151,151,151,151	0
54	MG	RA	3083	1/1	0.88	0.11	92,92,92,92	0
54	MG	XA	1725	1/1	0.88	0.08	137,137,137,137	0
54	MG	XA	1726	1/1	0.88	0.33	93,93,93,93	0
54	MG	RA	3487	1/1	0.88	0.13	91,91,91,91	0
54	MG	XA	1728	1/1	0.88	0.57	90,90,90,90	0
54	MG	RA	3198	1/1	0.88	0.14	120,120,120,120	0
54	MG	QA	1713	1/1	0.89	0.09	131,131,131,131	0
54	MG	RA	3172	1/1	0.89	0.15	145,145,145,145	0
54	MG	YA	3697	1/1	0.89	0.34	96,96,96,96	0
54	MG	RA	3276	1/1	0.89	0.32	144,144,144,144	0
54	MG	RA	3508	1/1	0.89	0.12	98,98,98,98	0
54	MG	YA	3908	1/1	0.89	0.20	90,90,90,90	0
54	MG	YA	3795	1/1	0.89	0.10	98,98,98,98	0
54	MG	RA	3382	1/1	0.89	0.28	90,90,90,90	0
54	MG	RA	3106	1/1	0.89	0.47	90,90,90,90	0
54	MG	QA	1627	1/1	0.89	0.06	132,132,132,132	0
54	MG	YA	3913	1/1	0.89	0.26	92,92,92,92	0
54	MG	YA	3798	1/1	0.89	0.41	90,90,90,90	0
54	MG	RA	3237	1/1	0.89	0.13	90,90,90,90	0
54	MG	RA	3403	1/1	0.89	0.22	94,94,94,94	0
54	MG	RA	3448	1/1	0.89	0.27	191,191,191,191	0
54	MG	RA	3365	1/1	0.89	0.17	159,159,159,159	0
54	MG	YA	3808	1/1	0.89	0.20	90,90,90,90	0
54	MG	YA	3628	1/1	0.89	0.52	130,130,130,130	0
54	MG	RA	3149	1/1	0.89	0.10	115,115,115,115	0
54	MG	XA	1649	1/1	0.89	0.05	148,148,148,148	0
54	MG	RA	3344	1/1	0.89	0.34	90,90,90,90	0
54	MG	YA	3882	1/1	0.89	0.15	95,95,95,95	0
54	MG	YA	3812	1/1	0.89	0.28	90,90,90,90	0
54	MG	RA	3519	1/1	0.89	0.12	90,90,90,90	0
54	MG	YA	3775	1/1	0.89	0.53	90,90,90,90	0
54	MG	RA	3122	1/1	0.89	0.15	90,90,90,90	0
54	MG	RA	3084	1/1	0.89	0.19	121,121,121,121	0
54	MG	RA	3324	1/1	0.89	0.34	121,121,121,121	0
54	MG	YA	3718	1/1	0.89	0.44	90,90,90,90	0
54	MG	QA	1649	1/1	0.89	0.18	94,94,94,94	0
54	MG	YA	3857	1/1	0.89	0.21	90,90,90,90	0
54	MG	YA	3936	1/1	0.89	0.12	98,98,98,98	0
54	MG	YA	3688	1/1	0.89	0.24	190,190,190,190	0
54	MG	RA	3391	1/1	0.89	0.18	97,97,97,97	0
54	MG	QA	1654	1/1	0.89	0.08	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3163	1/1	0.89	0.39	90,90,90,90	0
54	MG	QA	1610	1/1	0.89	0.13	145,145,145,145	0
54	MG	YA	3785	1/1	0.89	0.10	99,99,99,99	0
54	MG	RA	3377	1/1	0.89	0.15	103,103,103,103	0
54	MG	QA	1613	1/1	0.89	0.11	147,147,147,147	0
54	MG	YA	3900	1/1	0.89	0.16	90,90,90,90	0
54	MG	YA	3863	1/1	0.89	0.22	90,90,90,90	0
54	MG	YA	3789	1/1	0.89	0.10	129,129,129,129	0
54	MG	QA	1691	1/1	0.90	0.21	179,179,179,179	0
54	MG	YA	3970	1/1	0.90	0.15	90,90,90,90	0
54	MG	XA	1685	1/1	0.90	0.10	115,115,115,115	0
54	MG	RA	3296	1/1	0.90	0.10	96,96,96,96	0
54	MG	RA	3090	1/1	0.90	0.17	144,144,144,144	0
54	MG	RA	3530	1/1	0.90	0.10	90,90,90,90	0
54	MG	RA	3378	1/1	0.90	0.05	107,107,107,107	0
54	MG	RA	3049	1/1	0.90	0.37	92,92,92,92	0
54	MG	YA	3911	1/1	0.90	0.43	90,90,90,90	0
54	MG	RB	213	1/1	0.90	0.10	158,158,158,158	0
54	MG	XA	1646	1/1	0.90	0.15	94,94,94,94	0
54	MG	RA	3081	1/1	0.90	0.23	90,90,90,90	0
54	MG	RA	3355	1/1	0.90	0.24	90,90,90,90	0
54	MG	YA	3831	1/1	0.90	0.34	90,90,90,90	0
54	MG	RA	3395	1/1	0.90	0.27	91,91,91,91	0
54	MG	XA	1604	1/1	0.90	0.07	130,130,130,130	0
54	MG	RA	3417	1/1	0.90	0.17	147,147,147,147	0
54	MG	XA	1607	1/1	0.90	0.27	90,90,90,90	0
54	MG	YA	3800	1/1	0.90	0.17	93,93,93,93	0
54	MG	XA	1655	1/1	0.90	0.04	102,102,102,102	0
54	MG	RA	3231	1/1	0.90	0.11	90,90,90,90	0
54	MG	YA	3805	1/1	0.90	0.10	163,163,163,163	0
54	MG	YB	209	1/1	0.90	0.41	174,174,174,174	0
54	MG	XA	1612	1/1	0.90	0.08	125,125,125,125	0
54	MG	XA	1662	1/1	0.90	0.42	93,93,93,93	0
54	MG	RA	3281	1/1	0.90	0.49	90,90,90,90	0
54	MG	RQ	201	1/1	0.90	0.08	113,113,113,113	0
54	MG	RA	3398	1/1	0.90	0.15	144,144,144,144	0
54	MG	YA	3866	1/1	0.90	0.08	110,110,110,110	0
54	MG	QA	1642	1/1	0.90	0.08	131,131,131,131	0
54	MG	YA	3749	1/1	0.90	0.22	134,134,134,134	0
54	MG	QA	1644	1/1	0.90	0.79	90,90,90,90	0
54	MG	RA	3267	1/1	0.90	0.13	104,104,104,104	0
54	MG	YA	3699	1/1	0.90	0.29	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	QA	1647	1/1	0.90	0.11	99,99,99,99	0
54	MG	RA	3275	1/1	0.90	0.17	128,128,128,128	0
54	MG	XA	1722	1/1	0.90	0.09	91,91,91,91	0
54	MG	YP	201	1/1	0.90	0.11	90,90,90,90	0
54	MG	XA	1678	1/1	0.90	0.13	222,222,222,222	0
54	MG	RA	3062	1/1	0.90	0.17	90,90,90,90	0
54	MG	YA	3677	1/1	0.90	0.14	121,121,121,121	0
54	MG	YA	3815	1/1	0.90	0.16	113,113,113,113	0
55	ZN	Y9	101	1/1	0.90	0.07	140,140,140,140	0
54	MG	RA	3373	1/1	0.90	0.14	108,108,108,108	0
54	MG	RA	3416	1/1	0.91	0.16	122,122,122,122	0
54	MG	RA	3272	1/1	0.91	0.26	90,90,90,90	0
54	MG	RA	3300	1/1	0.91	0.16	139,139,139,139	0
54	MG	YA	3894	1/1	0.91	0.15	118,118,118,118	0
54	MG	YA	3780	1/1	0.91	0.39	90,90,90,90	0
54	MG	XA	1705	1/1	0.91	0.07	117,117,117,117	0
54	MG	QA	1684	1/1	0.91	0.44	90,90,90,90	0
54	MG	RA	3018	1/1	0.91	0.13	137,137,137,137	0
54	MG	RA	3216	1/1	0.91	0.22	92,92,92,92	0
54	MG	RA	3134	1/1	0.91	0.14	97,97,97,97	0
54	MG	RA	3483	1/1	0.91	0.08	90,90,90,90	0
54	MG	RA	3077	1/1	0.91	0.14	96,96,96,96	0
54	MG	YY	201	1/1	0.91	0.19	90,90,90,90	0
54	MG	YA	3762	1/1	0.91	0.38	90,90,90,90	0
54	MG	RA	3147	1/1	0.91	0.15	94,94,94,94	0
54	MG	YA	3926	1/1	0.91	0.10	95,95,95,95	0
54	MG	RA	3109	1/1	0.91	0.13	91,91,91,91	0
54	MG	RA	3156	1/1	0.91	0.12	109,109,109,109	0
54	MG	YA	3930	1/1	0.91	0.21	165,165,165,165	0
54	MG	XA	1618	1/1	0.91	0.08	134,134,134,134	0
54	MG	YA	3626	1/1	0.91	0.22	90,90,90,90	0
54	MG	YA	3663	1/1	0.91	0.14	90,90,90,90	0
54	MG	QA	1672	1/1	0.91	0.12	90,90,90,90	0
54	MG	RA	3333	1/1	0.91	0.32	90,90,90,90	0
54	MG	QA	1701	1/1	0.91	0.11	96,96,96,96	0
54	MG	XC	301	1/1	0.91	0.07	138,138,138,138	0
54	MG	YA	3645	1/1	0.91	0.42	90,90,90,90	0
54	MG	YA	3821	1/1	0.91	0.22	90,90,90,90	0
54	MG	YA	3629	1/1	0.91	0.10	100,100,100,100	0
54	MG	YA	3752	1/1	0.91	0.44	138,138,138,138	0
54	MG	YA	3920	1/1	0.92	0.13	92,92,92,92	0
54	MG	RA	3291	1/1	0.92	0.11	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3529	1/1	0.92	0.26	106,106,106,106	0
54	MG	RA	3133	1/1	0.92	0.38	156,156,156,156	0
54	MG	RA	3490	1/1	0.92	0.21	158,158,158,158	0
54	MG	YE	302	1/1	0.92	0.12	96,96,96,96	0
54	MG	RA	3410	1/1	0.92	0.21	97,97,97,97	0
54	MG	YA	3748	1/1	0.92	0.15	90,90,90,90	0
54	MG	RB	215	1/1	0.92	0.07	135,135,135,135	0
54	MG	XA	1657	1/1	0.92	0.13	91,91,91,91	0
54	MG	RA	3001	1/1	0.92	0.16	90,90,90,90	0
54	MG	RA	3124	1/1	0.92	0.20	93,93,93,93	0
54	MG	RA	3477	1/1	0.92	0.09	97,97,97,97	0
54	MG	YA	3669	1/1	0.92	0.10	90,90,90,90	0
54	MG	RA	3443	1/1	0.92	0.05	109,109,109,109	0
54	MG	YA	3904	1/1	0.92	0.11	97,97,97,97	0
54	MG	YA	3786	1/1	0.92	0.14	101,101,101,101	0
54	MG	RA	3462	1/1	0.92	0.15	90,90,90,90	0
54	MG	RA	3075	1/1	0.92	0.32	91,91,91,91	0
54	MG	RA	3372	1/1	0.92	0.12	130,130,130,130	0
54	MG	YA	3940	1/1	0.92	0.17	90,90,90,90	0
54	MG	XA	1671	1/1	0.92	0.10	95,95,95,95	0
54	MG	XA	1672	1/1	0.92	0.09	130,130,130,130	0
54	MG	QD	304	1/1	0.92	0.06	142,142,142,142	0
54	MG	RA	3261	1/1	0.92	0.24	93,93,93,93	0
54	MG	XA	1632	1/1	0.92	0.07	152,152,152,152	0
54	MG	YA	3676	1/1	0.92	0.14	177,177,177,177	0
54	MG	RA	3119	1/1	0.92	0.05	109,109,109,109	0
54	MG	YA	3708	1/1	0.92	0.23	90,90,90,90	0
54	MG	YA	3651	1/1	0.92	0.32	91,91,91,91	0
54	MG	XM	201	1/1	0.92	0.10	180,180,180,180	0
54	MG	YA	3946	1/1	0.92	0.11	97,97,97,97	0
54	MG	RA	3188	1/1	0.92	0.15	95,95,95,95	0
54	MG	RA	3320	1/1	0.92	0.17	119,119,119,119	0
54	MG	XA	1642	1/1	0.92	0.13	161,161,161,161	0
54	MG	YA	3768	1/1	0.92	0.23	147,147,147,147	0
54	MG	RA	3181	1/1	0.92	0.18	90,90,90,90	0
54	MG	RB	209	1/1	0.92	0.32	159,159,159,159	0
55	ZN	QD	301	1/1	0.92	0.07	131,131,131,131	0
54	MG	YA	3890	1/1	0.92	0.20	90,90,90,90	0
54	MG	RA	3540	1/1	0.93	0.05	96,96,96,96	0
54	MG	RA	3234	1/1	0.93	0.38	90,90,90,90	0
54	MG	QA	1601	1/1	0.93	0.14	93,93,93,93	0
54	MG	XA	1639	1/1	0.93	0.11	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3167	1/1	0.93	0.08	98,98,98,98	0
54	MG	YA	3834	1/1	0.93	0.08	97,97,97,97	0
54	MG	YA	3602	1/1	0.93	0.17	132,132,132,132	0
54	MG	RA	3493	1/1	0.93	0.08	90,90,90,90	0
54	MG	RA	3307	1/1	0.93	0.17	126,126,126,126	0
54	MG	YA	3633	1/1	0.93	0.08	90,90,90,90	0
54	MG	RA	3154	1/1	0.93	0.19	90,90,90,90	0
54	MG	RA	3473	1/1	0.93	0.08	90,90,90,90	0
54	MG	YD	303	1/1	0.93	0.11	99,99,99,99	0
54	MG	RA	3407	1/1	0.93	0.10	130,130,130,130	0
54	MG	YA	3802	1/1	0.93	0.20	90,90,90,90	0
54	MG	XA	1605	1/1	0.93	0.12	123,123,123,123	0
54	MG	YA	3804	1/1	0.93	0.34	90,90,90,90	0
54	MG	YA	3733	1/1	0.93	0.11	90,90,90,90	0
54	MG	RA	3523	1/1	0.93	0.21	91,91,91,91	0
54	MG	YE	305	1/1	0.93	0.27	90,90,90,90	0
54	MG	RA	3226	1/1	0.93	0.15	90,90,90,90	0
54	MG	YA	3701	1/1	0.93	0.39	90,90,90,90	0
54	MG	YA	3702	1/1	0.93	0.11	98,98,98,98	0
54	MG	YA	3773	1/1	0.93	0.14	90,90,90,90	0
54	MG	YT	201	1/1	0.93	0.11	163,163,163,163	0
54	MG	XA	1615	1/1	0.93	0.14	94,94,94,94	0
54	MG	RD	302	1/1	0.93	0.08	98,98,98,98	0
54	MG	YU	201	1/1	0.93	0.13	122,122,122,122	0
54	MG	RA	3354	1/1	0.93	0.18	138,138,138,138	0
54	MG	RA	3128	1/1	0.93	0.13	131,131,131,131	0
54	MG	RA	3371	1/1	0.93	0.06	144,144,144,144	0
54	MG	XA	1621	1/1	0.93	0.14	184,184,184,184	0
54	MG	RA	3327	1/1	0.93	0.05	94,94,94,94	0
54	MG	RA	3197	1/1	0.93	0.19	95,95,95,95	0
54	MG	YA	3892	1/1	0.93	0.19	90,90,90,90	0
54	MG	RA	3375	1/1	0.93	0.11	136,136,136,136	0
54	MG	RA	3170	1/1	0.93	0.11	116,116,116,116	0
54	MG	YA	3819	1/1	0.93	0.08	90,90,90,90	0
54	MG	RA	3089	1/1	0.93	0.16	94,94,94,94	0
54	MG	RA	3095	1/1	0.93	0.14	91,91,91,91	0
54	MG	RA	3140	1/1	0.93	0.13	183,183,183,183	0
54	MG	RA	3317	1/1	0.93	0.14	92,92,92,92	0
54	MG	RA	3514	1/1	0.93	0.20	125,125,125,125	0
54	MG	RA	3127	1/1	0.93	0.16	153,153,153,153	0
54	MG	YA	3684	1/1	0.93	0.28	90,90,90,90	0
54	MG	QA	1619	1/1	0.94	0.09	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	XA	1695	1/1	0.94	0.37	90,90,90,90	0
54	MG	YA	3631	1/1	0.94	0.46	90,90,90,90	0
54	MG	YA	3729	1/1	0.94	0.13	106,106,106,106	0
54	MG	YB	203	1/1	0.94	0.33	117,117,117,117	0
54	MG	YA	3952	1/1	0.94	0.06	97,97,97,97	0
54	MG	RA	3326	1/1	0.94	0.12	113,113,113,113	0
54	MG	QA	1658	1/1	0.94	0.22	90,90,90,90	0
54	MG	RD	304	1/1	0.94	0.24	125,125,125,125	0
54	MG	RA	3190	1/1	0.94	0.09	148,148,148,148	0
54	MG	RA	3533	1/1	0.94	0.17	95,95,95,95	0
54	MG	YA	3957	1/1	0.94	0.43	112,112,112,112	0
54	MG	RA	3218	1/1	0.94	0.05	90,90,90,90	0
54	MG	XA	1630	1/1	0.94	0.10	127,127,127,127	0
54	MG	RA	3103	1/1	0.94	0.13	169,169,169,169	0
54	MG	RA	3552	1/1	0.94	0.17	160,160,160,160	0
54	MG	RA	3420	1/1	0.94	0.19	126,126,126,126	0
54	MG	YA	3820	1/1	0.94	0.43	90,90,90,90	0
54	MG	RA	3284	1/1	0.94	0.12	91,91,91,91	0
54	MG	QA	1602	1/1	0.94	0.16	90,90,90,90	0
54	MG	YA	3822	1/1	0.94	0.46	90,90,90,90	0
54	MG	RA	3142	1/1	0.94	0.35	140,140,140,140	0
54	MG	RA	3511	1/1	0.94	0.31	121,121,121,121	0
54	MG	YA	3691	1/1	0.94	0.07	94,94,94,94	0
54	MG	RA	3184	1/1	0.94	0.36	90,90,90,90	0
54	MG	RT	203	1/1	0.94	0.07	162,162,162,162	0
54	MG	QA	1712	1/1	0.94	0.05	136,136,136,136	0
54	MG	YA	3624	1/1	0.94	0.22	90,90,90,90	0
54	MG	YA	3830	1/1	0.94	0.11	95,95,95,95	0
54	MG	YA	3720	1/1	0.94	0.12	90,90,90,90	0
54	MG	RA	3067	1/1	0.94	0.13	148,148,148,148	0
54	MG	RA	3374	1/1	0.94	0.35	144,144,144,144	0
54	MG	YA	3627	1/1	0.94	0.42	90,90,90,90	0
54	MG	RX	102	1/1	0.94	0.07	97,97,97,97	0
54	MG	QA	1683	1/1	0.94	0.06	102,102,102,102	0
54	MG	RA	3502	1/1	0.94	0.14	133,133,133,133	0
54	MG	RA	3476	1/1	0.94	0.07	96,96,96,96	0
55	ZN	XD	301	1/1	0.94	0.09	90,90,90,90	0
54	MG	YA	3674	1/1	0.95	0.05	130,130,130,130	0
54	MG	YA	3757	1/1	0.95	0.20	132,132,132,132	0
54	MG	YA	3694	1/1	0.95	0.10	101,101,101,101	0
54	MG	RA	3435	1/1	0.95	0.04	98,98,98,98	0
54	MG	YA	3951	1/1	0.95	0.08	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3108	1/1	0.95	0.05	94,94,94,94	0
54	MG	RA	3556	1/1	0.95	0.05	96,96,96,96	0
54	MG	YA	3928	1/1	0.95	0.21	90,90,90,90	0
54	MG	RA	3459	1/1	0.95	0.09	125,125,125,125	0
54	MG	RA	3480	1/1	0.95	0.08	94,94,94,94	0
54	MG	YA	3764	1/1	0.95	0.13	90,90,90,90	0
54	MG	YA	3660	1/1	0.95	0.27	90,90,90,90	0
54	MG	XA	1661	1/1	0.95	0.18	136,136,136,136	0
54	MG	RQ	202	1/1	0.95	0.10	134,134,134,134	0
54	MG	RA	3046	1/1	0.95	0.08	120,120,120,120	0
54	MG	RA	3194	1/1	0.95	0.12	90,90,90,90	0
54	MG	R8	101	1/1	0.95	0.05	90,90,90,90	0
54	MG	YA	3770	1/1	0.95	0.14	98,98,98,98	0
54	MG	RA	3532	1/1	0.95	0.07	133,133,133,133	0
54	MG	RA	3496	1/1	0.95	0.11	128,128,128,128	0
54	MG	RA	3325	1/1	0.95	0.12	93,93,93,93	0
54	MG	RA	3092	1/1	0.95	0.52	90,90,90,90	0
54	MG	RA	3208	1/1	0.95	0.08	94,94,94,94	0
54	MG	RA	3165	1/1	0.95	0.09	97,97,97,97	0
54	MG	YA	3777	1/1	0.95	0.09	120,120,120,120	0
54	MG	YA	3971	1/1	0.95	0.04	95,95,95,95	0
54	MG	RA	3008	1/1	0.95	0.13	118,118,118,118	0
54	MG	YA	3656	1/1	0.96	0.07	95,95,95,95	0
54	MG	YA	3939	1/1	0.96	0.13	92,92,92,92	0
54	MG	RA	3421	1/1	0.96	0.29	178,178,178,178	0
54	MG	RA	3559	1/1	0.96	0.59	173,173,173,173	0
54	MG	YA	3751	1/1	0.96	0.11	90,90,90,90	0
54	MG	RA	3456	1/1	0.96	0.05	93,93,93,93	0
54	MG	YA	3689	1/1	0.96	0.17	90,90,90,90	0
54	MG	RA	3422	1/1	0.96	0.11	142,142,142,142	0
54	MG	RA	3054	1/1	0.96	0.15	98,98,98,98	0
54	MG	RA	3139	1/1	0.96	0.06	122,122,122,122	0
54	MG	YA	3887	1/1	0.96	0.11	90,90,90,90	0
54	MG	YA	3728	1/1	0.96	0.10	119,119,119,119	0
54	MG	QA	1624	1/1	0.96	0.13	147,147,147,147	0
54	MG	RA	3013	1/1	0.96	0.05	144,144,144,144	0
54	MG	YA	3705	1/1	0.96	0.22	123,123,123,123	0
54	MG	RA	3401	1/1	0.96	0.07	157,157,157,157	0
54	MG	YA	3695	1/1	0.96	0.10	91,91,91,91	0
54	MG	YA	3803	1/1	0.97	0.12	90,90,90,90	0
54	MG	RA	3102	1/1	0.97	0.07	148,148,148,148	0
54	MG	RA	3408	1/1	0.97	0.19	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	RA	3455	1/1	0.97	0.12	90,90,90,90	0
54	MG	YA	3825	1/1	0.97	0.09	117,117,117,117	0
54	MG	RB	201	1/1	0.97	0.15	127,127,127,127	0
54	MG	XA	1643	1/1	0.97	0.05	133,133,133,133	0
54	MG	RA	3012	1/1	0.97	0.14	112,112,112,112	0
54	MG	RA	3094	1/1	0.97	0.10	95,95,95,95	0
54	MG	XA	1693	1/1	0.97	0.08	90,90,90,90	0
54	MG	RA	3432	1/1	0.97	0.03	134,134,134,134	0
54	MG	RA	3445	1/1	0.97	0.13	175,175,175,175	0
54	MG	RA	3068	1/1	0.97	0.08	145,145,145,145	0
54	MG	RA	3243	1/1	0.97	0.11	100,100,100,100	0
54	MG	RA	3423	1/1	0.97	0.18	152,152,152,152	0
54	MG	QA	1702	1/1	0.97	0.08	141,141,141,141	0
54	MG	XA	1724	1/1	0.97	0.07	114,114,114,114	0
54	MG	RA	3402	1/1	0.97	0.22	101,101,101,101	0
54	MG	RA	3494	1/1	0.97	0.05	90,90,90,90	0
54	MG	RA	3150	1/1	0.97	0.09	94,94,94,94	0
54	MG	RA	3379	1/1	0.97	0.06	149,149,149,149	0
54	MG	YA	3730	1/1	0.97	0.32	188,188,188,188	0
54	MG	Y8	101	1/1	0.97	0.04	102,102,102,102	0
54	MG	RA	3287	1/1	0.97	0.06	150,150,150,150	0
54	MG	QA	1710	1/1	0.97	0.07	120,120,120,120	0
54	MG	YA	3740	1/1	0.98	0.06	101,101,101,101	0
54	MG	YA	3792	1/1	0.98	0.08	124,124,124,124	0
54	MG	RA	3404	1/1	0.98	0.04	124,124,124,124	0
54	MG	RA	3311	1/1	0.98	0.04	99,99,99,99	0
54	MG	YA	3661	1/1	0.98	0.27	135,135,135,135	0
54	MG	RA	3458	1/1	0.98	0.11	160,160,160,160	0
54	MG	RA	3225	1/1	0.98	0.07	142,142,142,142	0
54	MG	RA	3065	1/1	0.98	0.16	121,121,121,121	0
54	MG	RA	3547	1/1	0.98	0.04	99,99,99,99	0
54	MG	YA	3788	1/1	0.98	0.23	110,110,110,110	0
54	MG	RA	3548	1/1	0.98	0.05	103,103,103,103	0
54	MG	YA	3667	1/1	0.98	0.06	96,96,96,96	0
54	MG	QA	1607	1/1	0.99	0.05	115,115,115,115	0
54	MG	RA	3236	1/1	0.99	0.04	98,98,98,98	0
54	MG	RA	3491	1/1	0.99	0.03	97,97,97,97	0
54	MG	RA	3235	1/1	0.99	0.04	104,104,104,104	0
54	MG	XA	1667	1/1	0.99	0.04	159,159,159,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.