wwPDB X-ray Structure Validation Summary Report (i)

Mar 14, 2026 – 12:39 PM UTC

PDB ID	:	6ORD / pdb_00006ord
Title	:	Crystal structure of tRNA^ Ala(GGC) U32-A38 bound to cognate 70S A site
Authors	:	Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on	:	2019-04-30
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

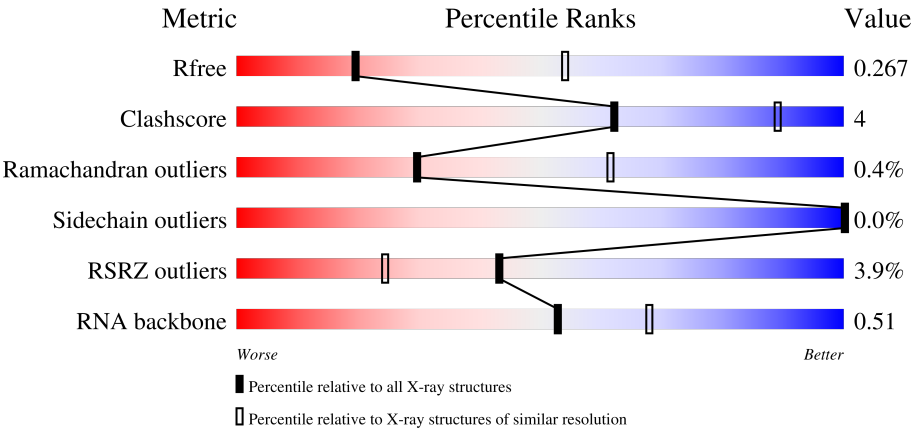
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1522	70% 25%
1	XA	1522	70% 26%
2	QB	256	5% 68% 20% 10%
2	XB	256	3% 73% 17% 10%

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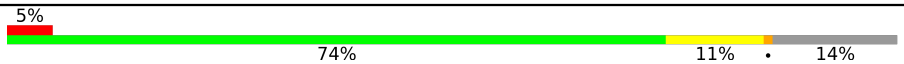
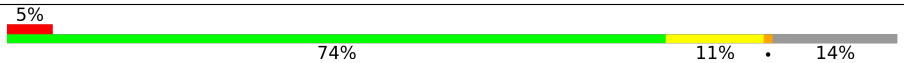
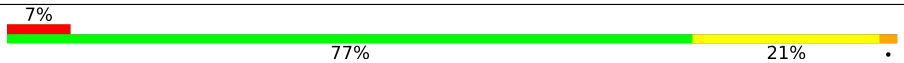
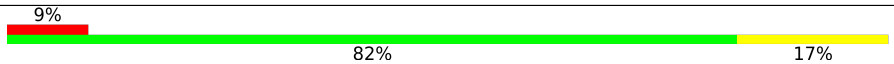
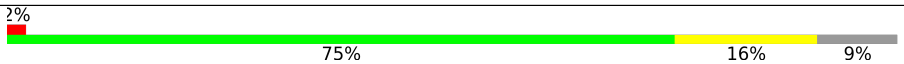
Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
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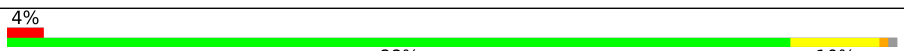
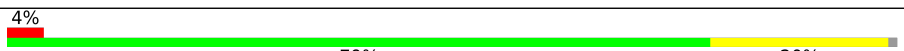
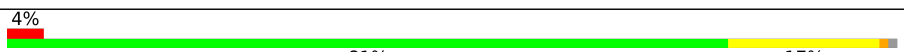
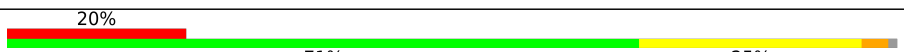
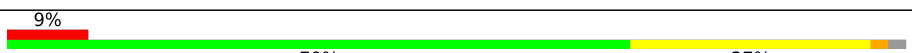
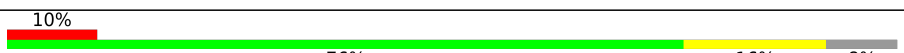
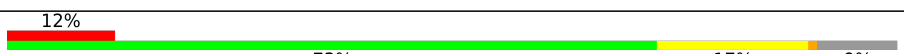
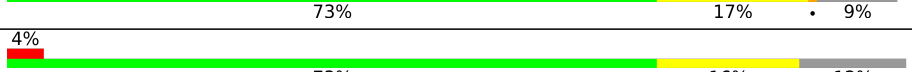
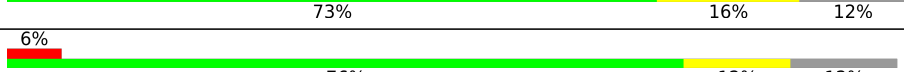
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
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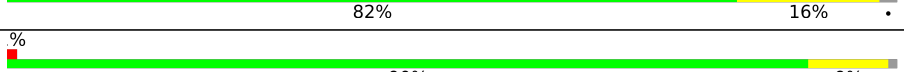
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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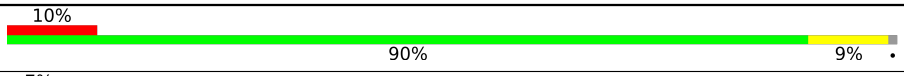
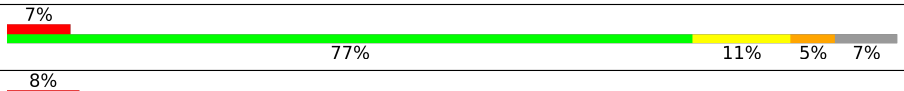
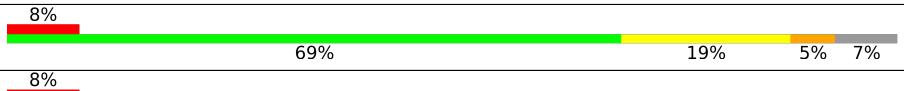
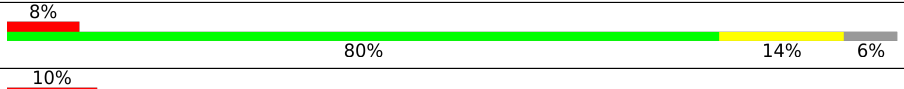
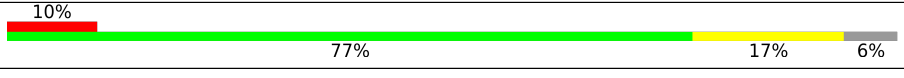
Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
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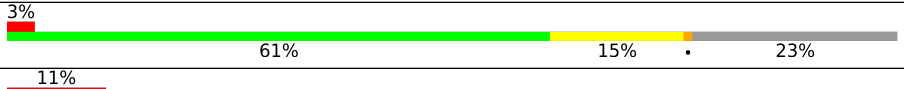
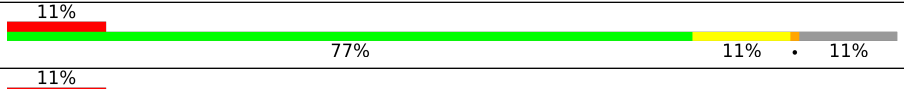
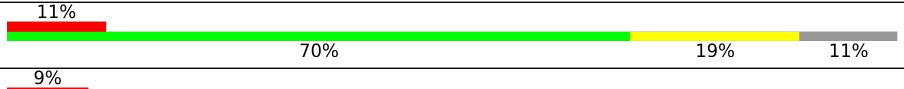
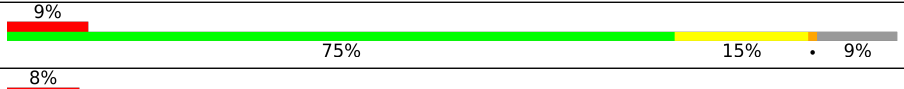
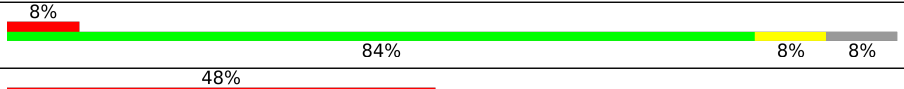
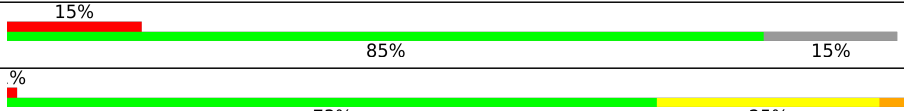
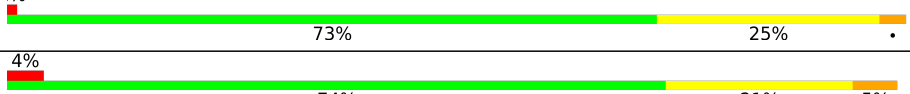
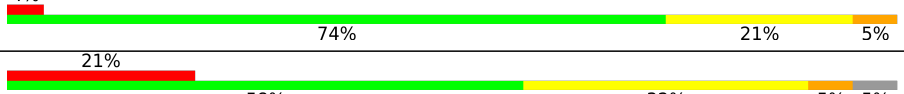
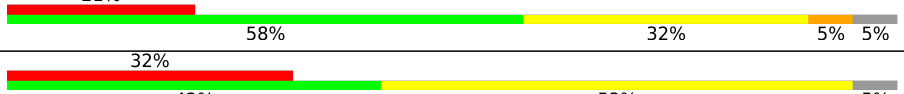
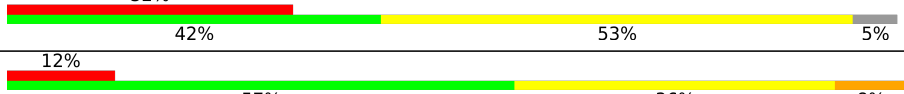
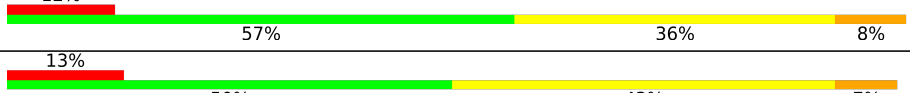
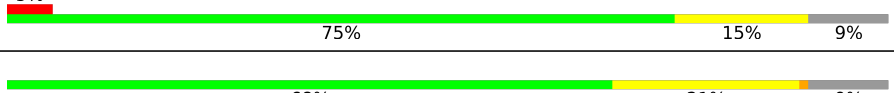
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	QY	76	
24	XY	76	
25	R0	85	
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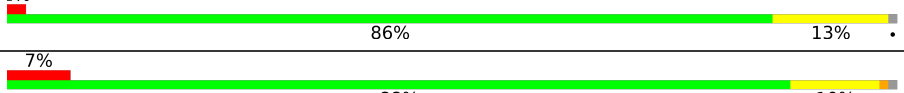
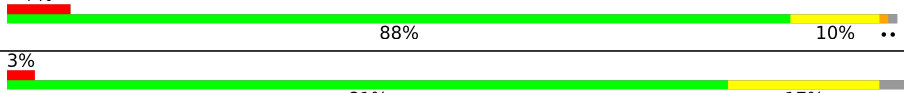
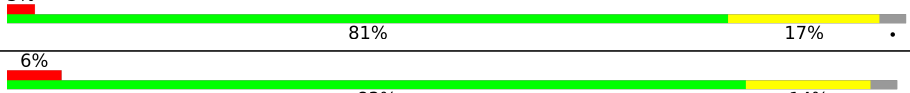
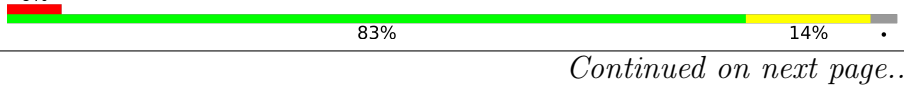
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	

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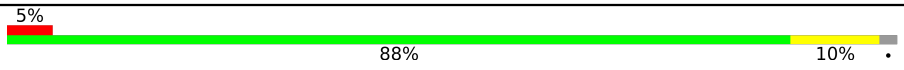
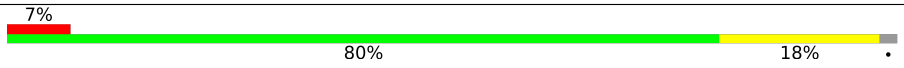
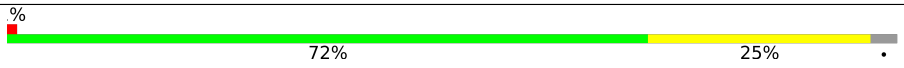
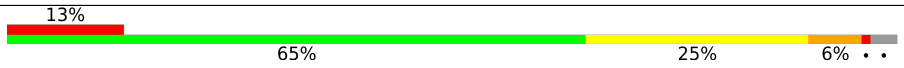
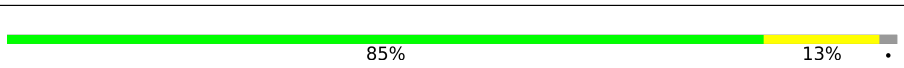
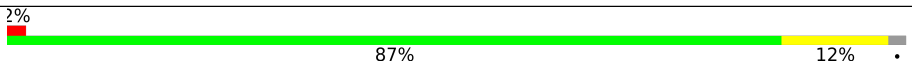
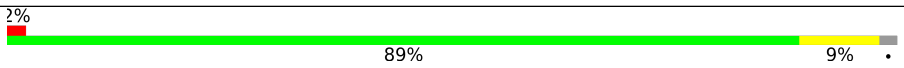
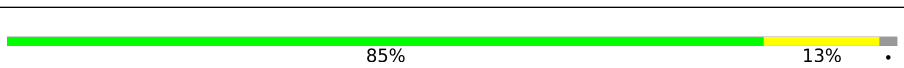
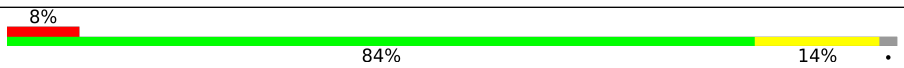
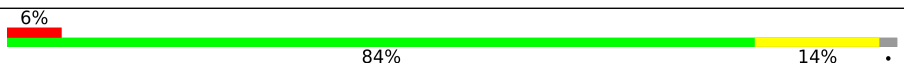
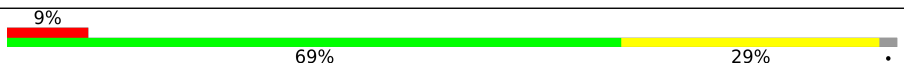
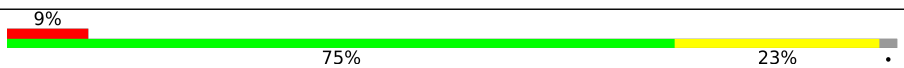
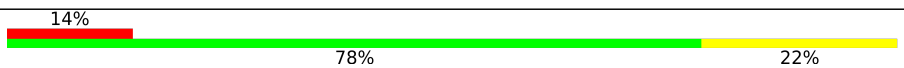
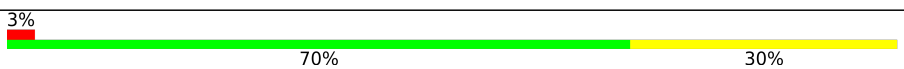
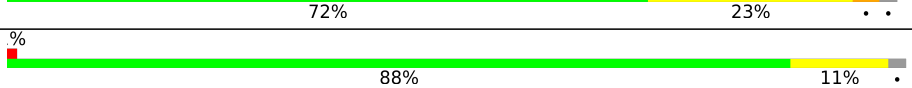
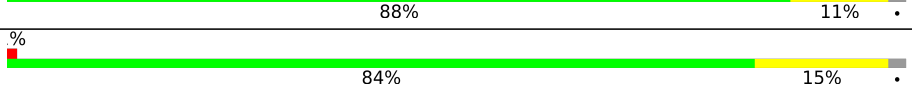
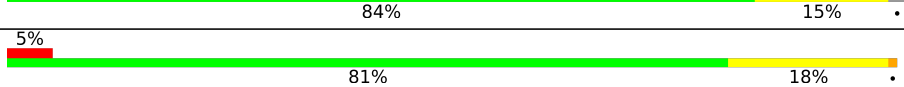
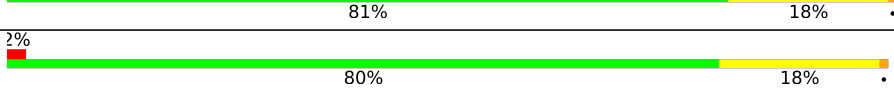
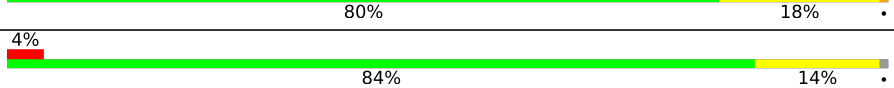
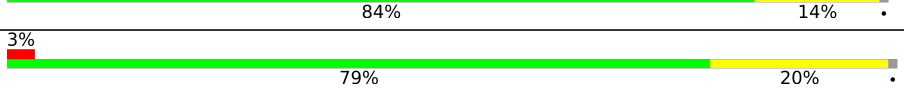
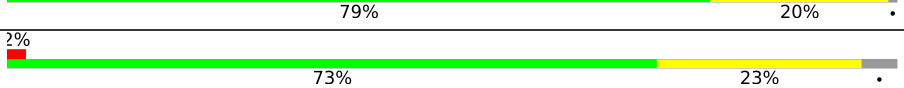
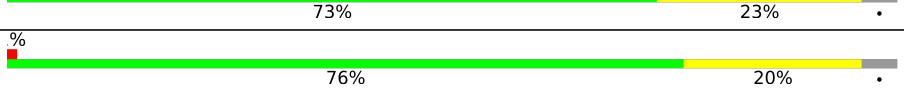
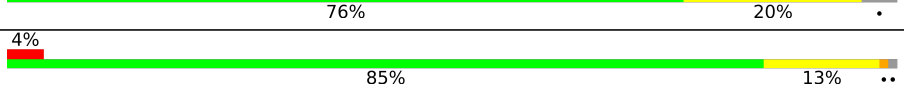
Mol	Chain	Length	Quality of chain
28	R3	60	
28	Y3	60	
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	122	
36	YB	122	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	
40	RG	182	

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Mol	Chain	Length	Quality of chain
40	YG	182	2% 79% 20%
41	RH	180	2% 84% 12%
41	YH	180	2% 82% 13%
42	RI	148	2% 89% 10%
42	YI	148	2% 93% 5%
43	RN	140	4% 84% 16%
43	YN	140	2% 89% 11%
44	RO	122	2% 77% 22%
44	YO	122	2% 80% 20%
45	RP	150	5% 81% 17%
45	YP	150	5% 77% 21%
46	RQ	141	11% 82% 18%
46	YQ	141	3% 87% 13%
47	RR	118	4% 89% 11%
47	YR	118	% 86% 14%
48	RS	112	4% 81% 16%
48	YS	112	4% 88% 11%
49	RT	146	2% 72% 17% 10%
49	YT	146	3% 74% 15% 10%
50	RU	118	3% 82% 15%
50	YU	118	% 86% 11%
51	RV	101	4% 78% 19%
51	YV	101	% 93% 6%
52	RW	113	2% 86% 13%
52	YW	113	2% 87% 12%

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Mol	Chain	Length	Quality of chain
53	RX	96	5% 85% 14%
53	YX	96	4% 90% 9%
54	RY	110	6% 84% 14%
54	YY	110	4% 80% 17%
55	RZ	206	9% 72% 13% 14%
55	YZ	206	13% 72% 12% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1703	-	-	-	X
56	MG	QA	1795	-	-	-	X
56	MG	QO	101	-	-	-	X
56	MG	RA	3011	-	-	-	X
56	MG	RA	3027	-	-	-	X
56	MG	RA	3053	-	-	-	X
56	MG	RA	3063	-	-	-	X
56	MG	RA	3069	-	-	-	X
56	MG	RA	3072	-	-	-	X
56	MG	RA	3080	-	-	-	X
56	MG	RA	3104	-	-	-	X
56	MG	RA	3152	-	-	-	X
56	MG	RA	3153	-	-	-	X
56	MG	RA	3159	-	-	-	X
56	MG	RA	3173	-	-	-	X
56	MG	RA	3175	-	-	-	X
56	MG	RA	3192	-	-	-	X
56	MG	RA	3201	-	-	-	X
56	MG	RA	3205	-	-	-	X
56	MG	RA	3221	-	-	-	X
56	MG	RA	3256	-	-	-	X
56	MG	RA	3269	-	-	-	X
56	MG	RA	3311	-	-	-	X
56	MG	RA	3322	-	-	-	X
56	MG	RA	3350	-	-	-	X
56	MG	RA	3363	-	-	-	X
56	MG	RA	3381	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3383	-	-	-	X
56	MG	RA	3395	-	-	-	X
56	MG	RA	3401	-	-	-	X
56	MG	RA	3416	-	-	-	X
56	MG	RA	3417	-	-	-	X
56	MG	RA	3424	-	-	-	X
56	MG	RA	3450	-	-	-	X
56	MG	RA	3460	-	-	-	X
56	MG	RA	3469	-	-	-	X
56	MG	RA	3482	-	-	-	X
56	MG	RA	3499	-	-	-	X
56	MG	RA	3511	-	-	-	X
56	MG	RA	3514	-	-	-	X
56	MG	RA	3526	-	-	-	X
56	MG	RA	3591	-	-	-	X
56	MG	RA	3641	-	-	-	X
56	MG	RA	3647	-	-	-	X
56	MG	RA	3654	-	-	-	X
56	MG	RA	3673	-	-	-	X
56	MG	XA	1718	-	-	-	X
56	MG	XA	1778	-	-	-	X
56	MG	YA	3066	-	-	-	X
56	MG	YA	3119	-	-	-	X
56	MG	YA	3201	-	-	-	X
56	MG	YA	3400	-	-	-	X
56	MG	YA	3412	-	-	-	X
56	MG	YA	3478	-	-	-	X
56	MG	YA	3499	-	-	-	X
56	MG	YA	3512	-	-	-	X
56	MG	YA	3547	-	-	-	X
56	MG	YA	3697	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 293819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
1	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
2	XB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
3	XC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
5	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
6	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O	0	0	0
			986	625	193	168			
9	XI	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	QJ	97	Total	C	N	O	0	0	0
			719	446	142	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	XJ	96	Total 710	C 442	N 137	O 131	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	114	Total 834	C 520	N 156	O 155	S 3	0	0	0
11	XK	114	Total 833	C 519	N 156	O 155	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	122	Total 932	C 586	N 185	O 159	S 2	0	0	0
12	XL	122	Total 932	C 586	N 185	O 159	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	116	Total 914	C 564	N 189	O 159	S 2	0	0	0
13	XM	114	Total 895	C 550	N 186	O 157	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total 728	C 456	N 144	O 126	S 2	0	0	0
15	XO	88	Total 728	C 456	N 144	O 126	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	XP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	XQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	XR	68	Total	C	N	O	0	0	0
			555	355	108	92			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
19	XS	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
20	XT	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	23	Total 199	C 122	N 48	O 29	0	0	0
21	XU	23	Total 199	C 122	N 48	O 29	0	0	0

- Molecule 22 is a RNA chain called P-site tRNAfMet.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total 394	C 176	N 80	O 120	P 18	0	0	0
23	XX	18	Total 394	C 176	N 80	O 120	P 18	0	0	0

- Molecule 24 is a RNA chain called A-site tRNAAla(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	76	Total 1625	C 724	N 293	O 532	P 76	0	0	0
24	XY	76	Total 1625	C 724	N 293	O 532	P 76	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	77	Total 608	C 375	N 129	O 103	S 1	0	0	0
25	Y0	77	Total 608	C 375	N 129	O 103	S 1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total 754	C 475	N 148	O 130	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y1	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
27	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
28	Y3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
31	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
32	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			
35	YA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
36	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RD	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
37	YD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RF	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
39	YF	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RG	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
40	YG	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
41	YH	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
43	YN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
45	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

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

- Molecule 48 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	RS	110	Total	C	N	O	0	0	0
			877	553	175	149			
48	YS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 49 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
49	YT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
50	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 51 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
51	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 52 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
52	YW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 53 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RX	95	Total 750	C 488	N 135	O 126	S 1	0	0	0
53	YX	95	Total 750	C 488	N 135	O 126	S 1	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RY	107	Total 810	C 520	N 153	O 131	S 6	0	0	0
54	YY	107	Total 810	C 519	N 153	O 132	S 6	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	178	Total 1406	C 898	N 253	O 253	S 2	0	0	0
55	YZ	177	Total 1381	C 885	N 246	O 248	S 2	0	0	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	221	Total 221	Mg 221	0	0
56	QB	1	Total 1	Mg 1	0	0
56	QD	4	Total 4	Mg 4	0	0
56	QE	4	Total 4	Mg 4	0	0
56	QF	2	Total 2	Mg 2	0	0
56	QG	2	Total 2	Mg 2	0	0
56	QH	2	Total 2	Mg 2	0	0
56	QI	1	Total 1	Mg 1	0	0
56	QK	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	QL	3	Total Mg 3 3	0	0
56	QN	1	Total Mg 1 1	0	0
56	QO	2	Total Mg 2 2	0	0
56	QP	1	Total Mg 1 1	0	0
56	QT	1	Total Mg 1 1	0	0
56	QV	5	Total Mg 5 5	0	0
56	R0	3	Total Mg 3 3	0	0
56	R1	1	Total Mg 1 1	0	0
56	R3	3	Total Mg 3 3	0	0
56	R5	2	Total Mg 2 2	0	0
56	R6	1	Total Mg 1 1	0	0
56	R7	3	Total Mg 3 3	0	0
56	R9	1	Total Mg 1 1	0	0
56	RA	709	Total Mg 709 709	0	0
56	RB	17	Total Mg 17 17	0	0
56	RD	8	Total Mg 8 8	0	0
56	RE	4	Total Mg 4 4	0	0
56	RF	4	Total Mg 4 4	0	0
56	RG	4	Total Mg 4 4	0	0
56	RH	2	Total Mg 2 2	0	0
56	RN	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RO	1	Total Mg 1 1	0	0
56	RP	3	Total Mg 3 3	0	0
56	RQ	4	Total Mg 4 4	0	0
56	RR	2	Total Mg 2 2	0	0
56	RT	4	Total Mg 4 4	0	0
56	RU	2	Total Mg 2 2	0	0
56	RV	3	Total Mg 3 3	0	0
56	RW	1	Total Mg 1 1	0	0
56	RZ	1	Total Mg 1 1	0	0
56	XA	193	Total Mg 193 193	0	0
56	XE	2	Total Mg 2 2	0	0
56	XF	2	Total Mg 2 2	0	0
56	XJ	1	Total Mg 1 1	0	0
56	XL	2	Total Mg 2 2	0	0
56	XR	1	Total Mg 1 1	0	0
56	XT	1	Total Mg 1 1	0	0
56	XV	3	Total Mg 3 3	0	0
56	XY	1	Total Mg 1 1	0	0
56	Y0	1	Total Mg 1 1	0	0
56	Y1	2	Total Mg 2 2	0	0
56	Y3	1	Total Mg 1 1	0	0

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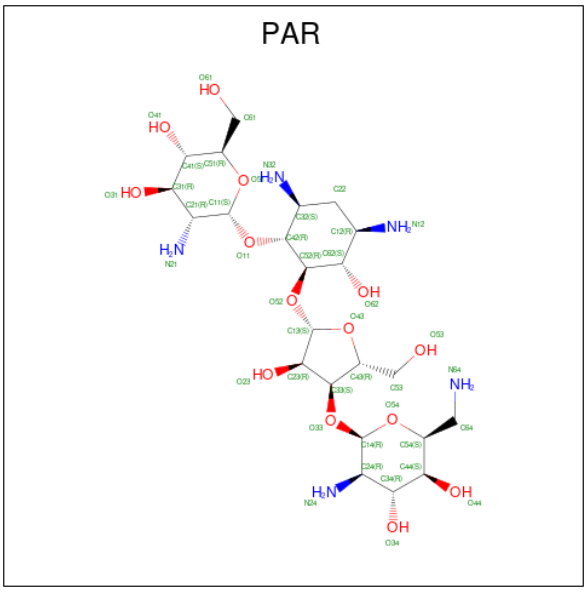
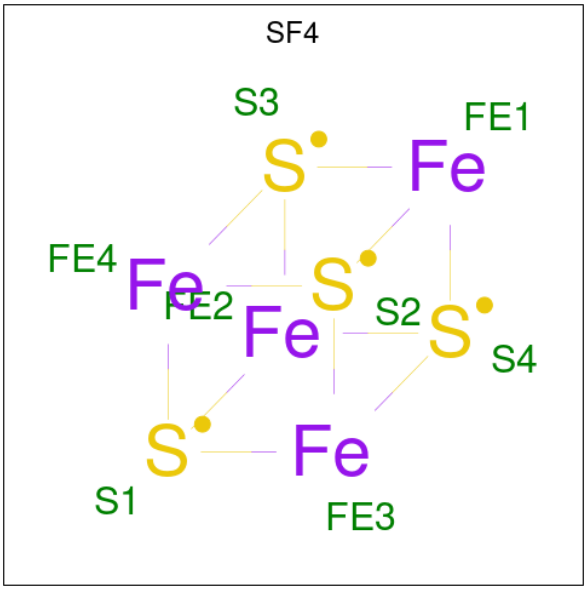
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	Y5	1	Total Mg 1 1	0	0
56	Y6	1	Total Mg 1 1	0	0
56	Y7	2	Total Mg 2 2	0	0
56	Y8	1	Total Mg 1 1	0	0
56	YA	707	Total Mg 707 707	0	0
56	YB	20	Total Mg 20 20	0	0
56	YD	7	Total Mg 7 7	0	0
56	YE	5	Total Mg 5 5	0	0
56	YF	3	Total Mg 3 3	0	0
56	YG	3	Total Mg 3 3	0	0
56	YI	1	Total Mg 1 1	0	0
56	YN	1	Total Mg 1 1	0	0
56	YO	1	Total Mg 1 1	0	0
56	YP	2	Total Mg 2 2	0	0
56	YQ	2	Total Mg 2 2	0	0
56	YR	2	Total Mg 2 2	0	0
56	YT	3	Total Mg 3 3	0	0
56	YV	1	Total Mg 1 1	0	0
56	YW	2	Total Mg 2 2	0	0

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



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

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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

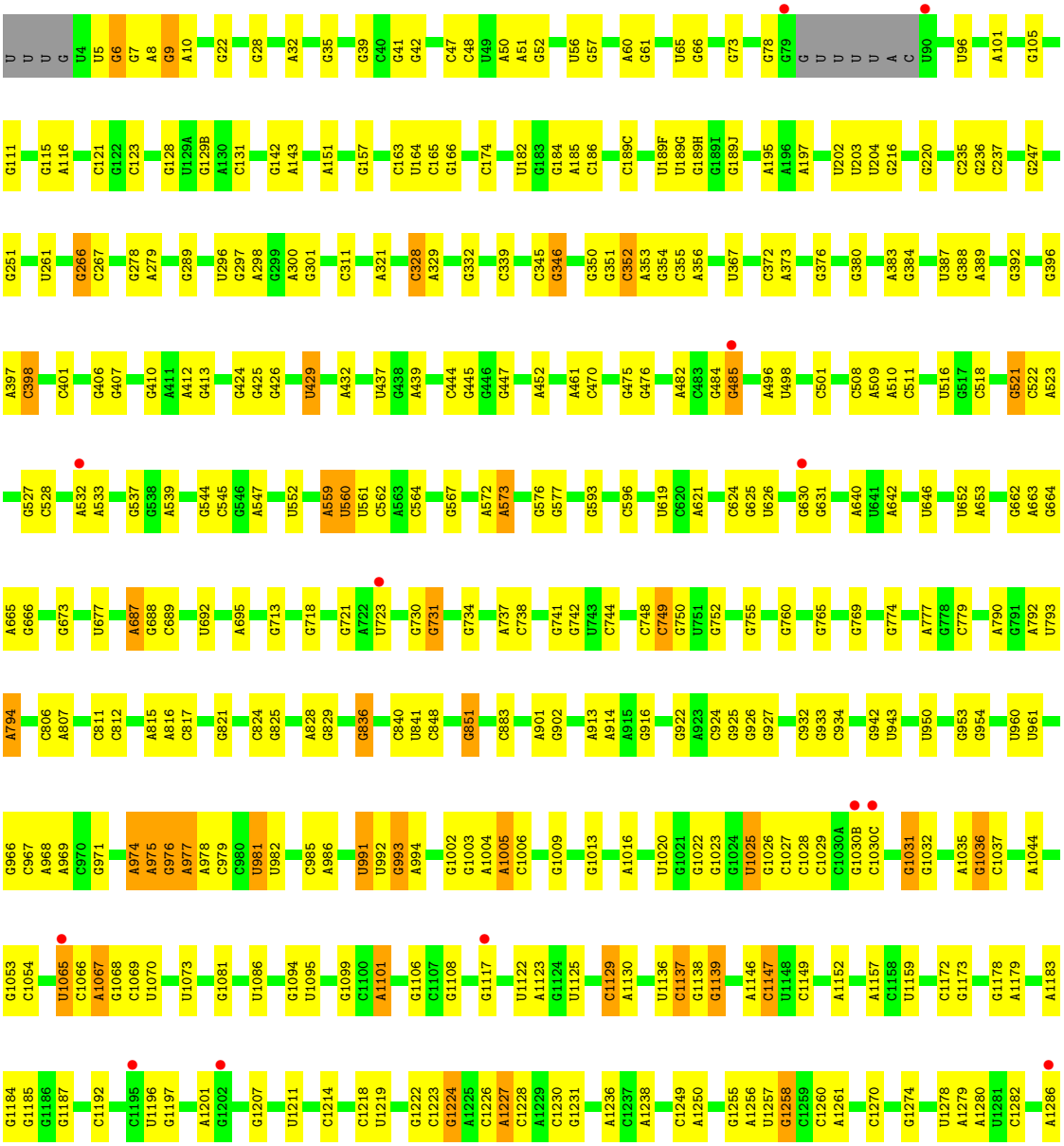
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QN	1	Total Zn 1 1	0	0
59	R4	1	Total Zn 1 1	0	0
59	R5	1	Total Zn 1 1	0	0
59	R6	1	Total Zn 1 1	0	0
59	R9	1	Total Zn 1 1	0	0
59	RY	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0
59	Y4	1	Total Zn 1 1	0	0
59	Y5	1	Total Zn 1 1	0	0
59	Y6	1	Total Zn 1 1	0	0
59	Y9	1	Total Zn 1 1	0	0
59	YY	1	Total Zn 1 1	0	0

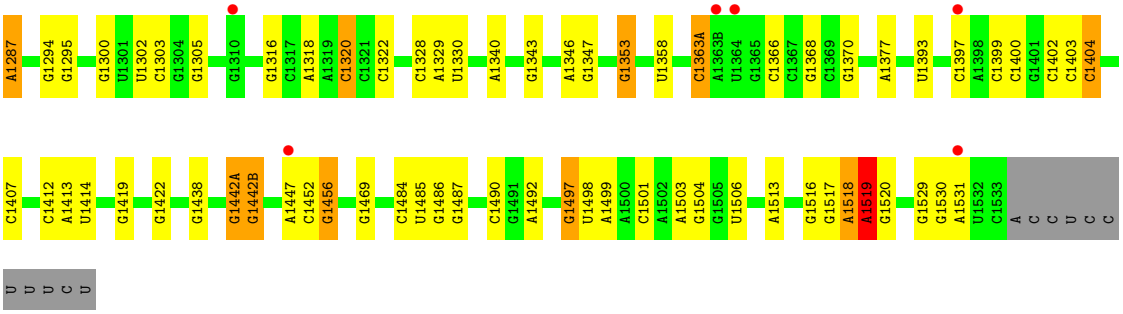
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

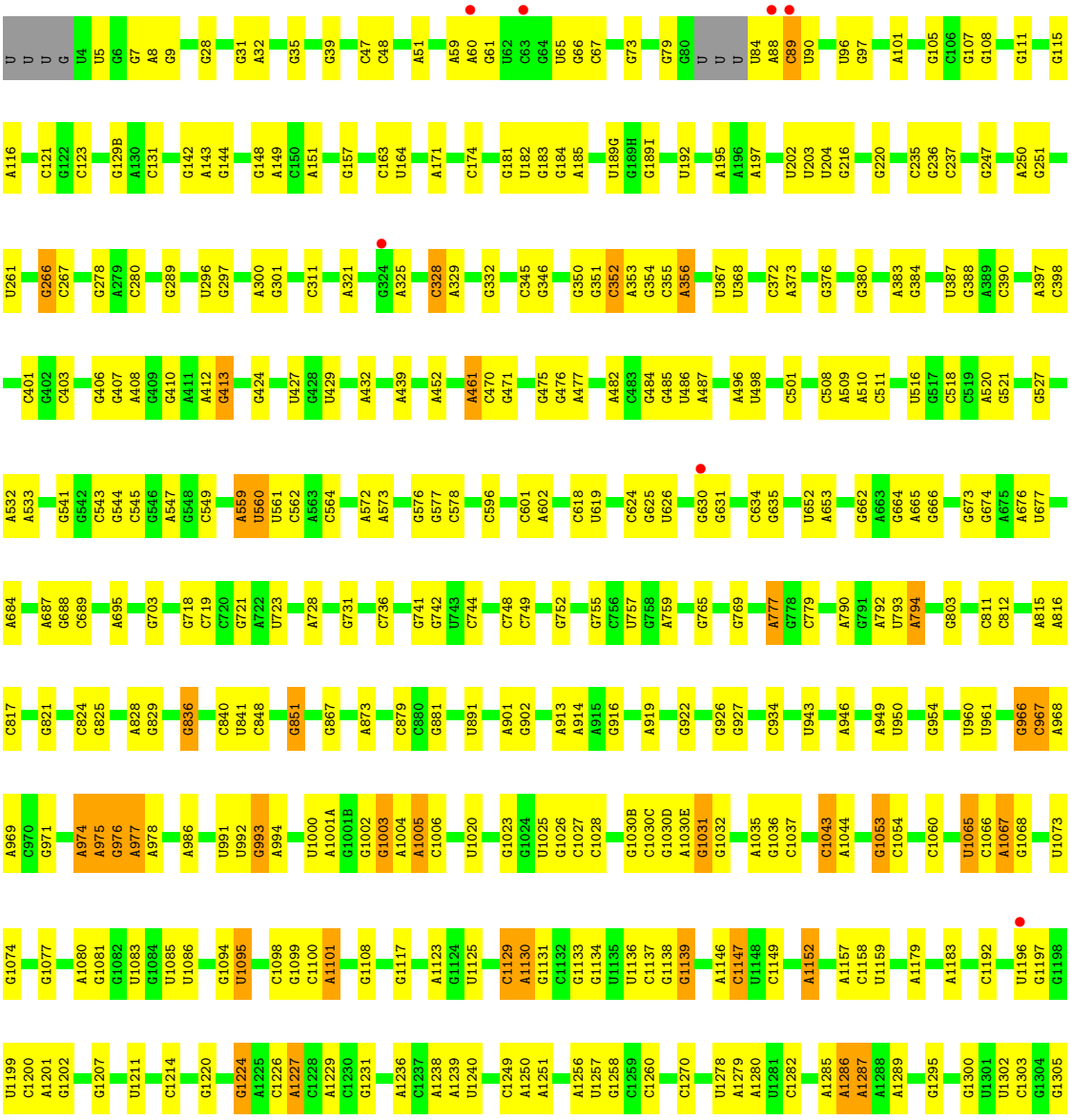
Chain QA:

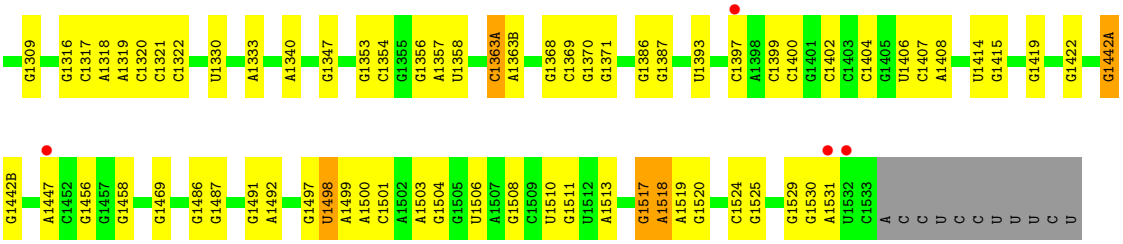




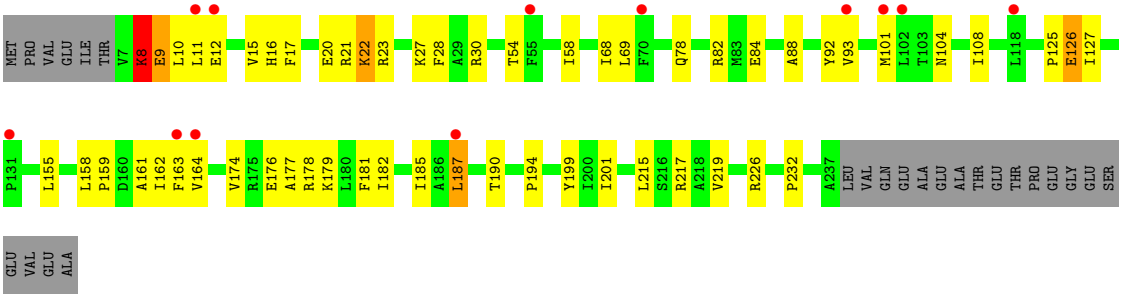
• Molecule 1: 16S rRNA

Chain XA:

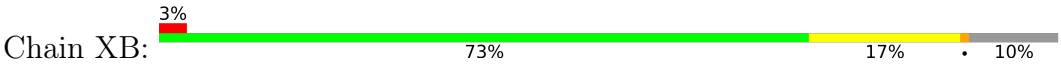


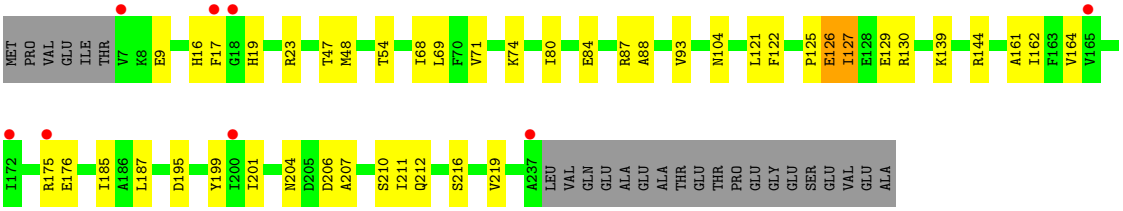


• Molecule 2: 30S ribosomal protein S2

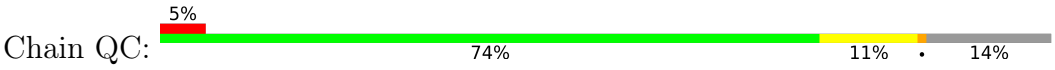


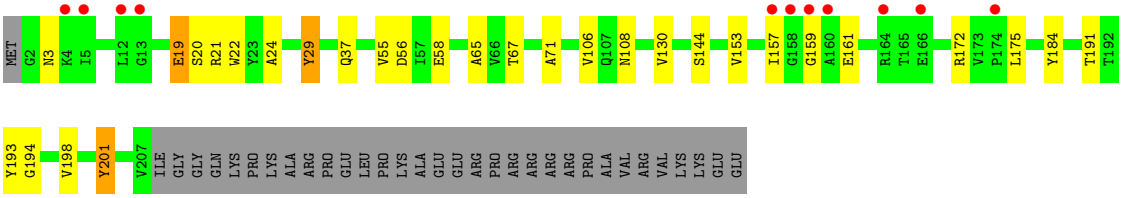
• Molecule 2: 30S ribosomal protein S2



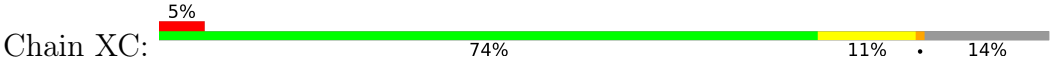


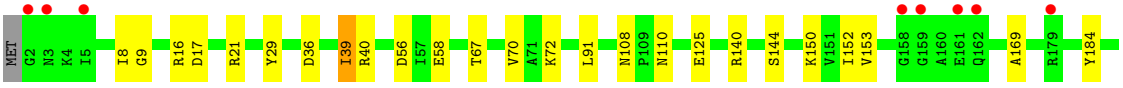
• Molecule 3: 30S ribosomal protein S3

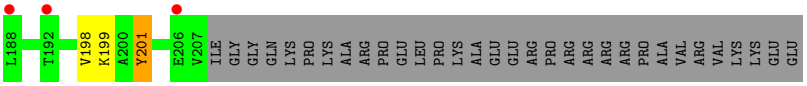




• Molecule 3: 30S ribosomal protein S3

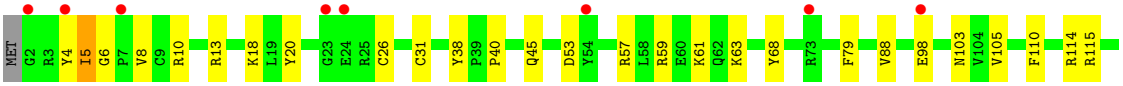


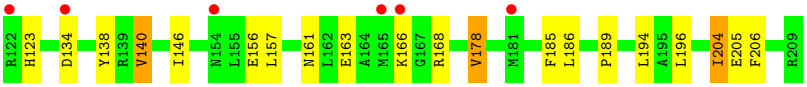




• Molecule 4: 30S ribosomal protein S4

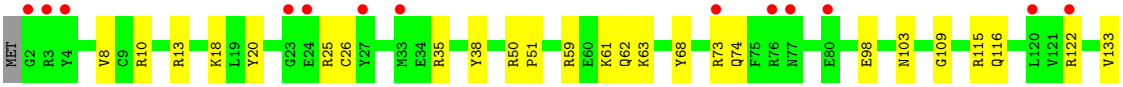
Chain QD:

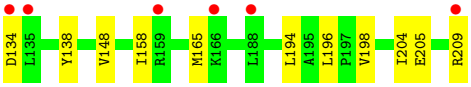




• Molecule 4: 30S ribosomal protein S4

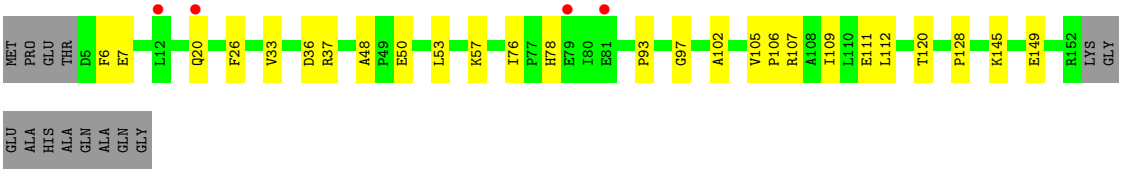
Chain XD:





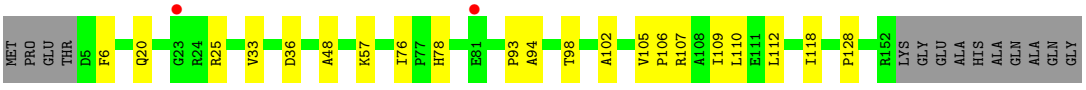
• Molecule 5: 30S ribosomal protein S5

Chain QE:



• Molecule 5: 30S ribosomal protein S5

Chain XE:

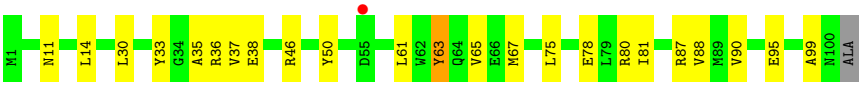


• Molecule 6: 30S ribosomal protein S6

Chain QF:

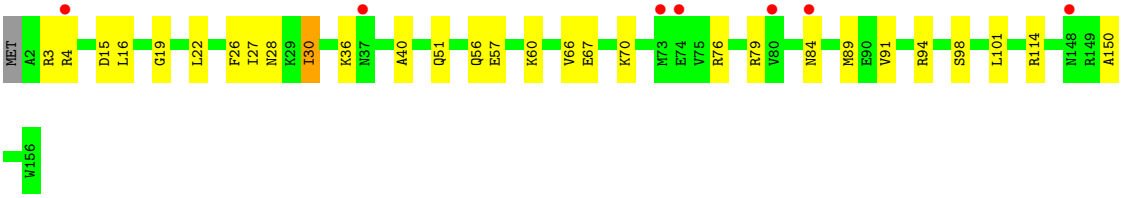
• Molecule 6: 30S ribosomal protein S6

Chain XF:



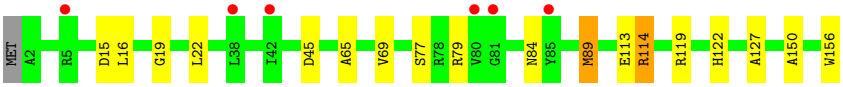
• Molecule 7: 30S ribosomal protein S7

Chain QG:



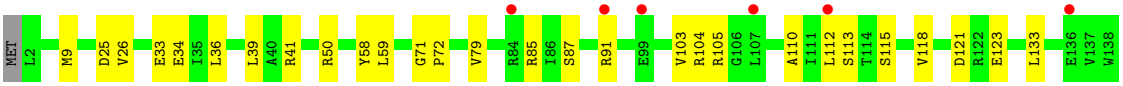
• Molecule 7: 30S ribosomal protein S7

Chain XG:



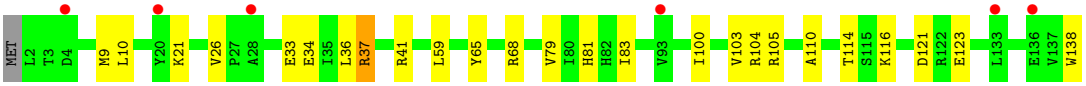
• Molecule 8: 30S ribosomal protein S8

Chain QH:



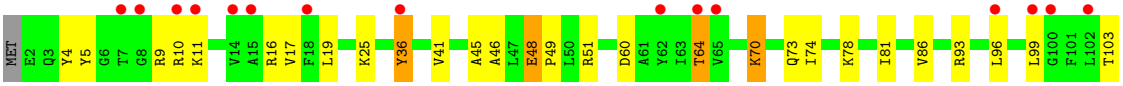
• Molecule 8: 30S ribosomal protein S8

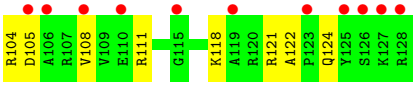
Chain XH:



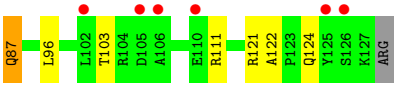
• Molecule 9: 30S ribosomal protein S9

Chain QI:

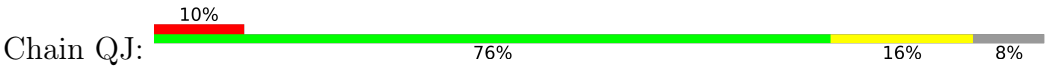


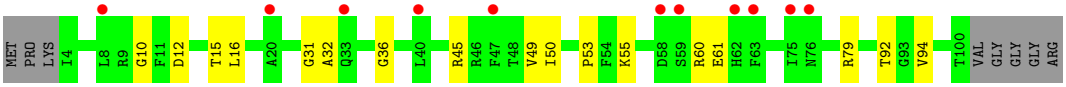


• Molecule 9: 30S ribosomal protein S9

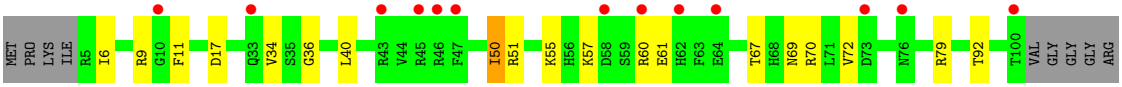


• Molecule 10: 30S ribosomal protein S10

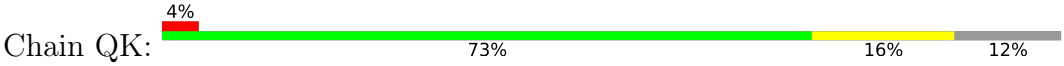




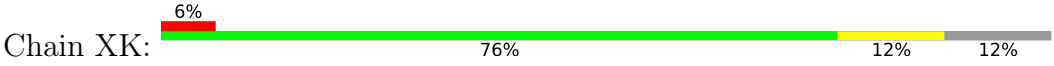
• Molecule 10: 30S ribosomal protein S10

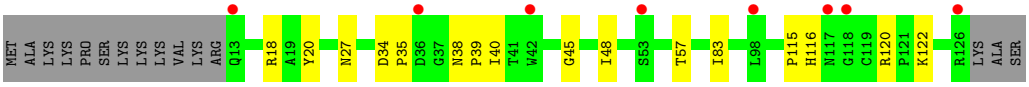


• Molecule 11: 30S ribosomal protein S11

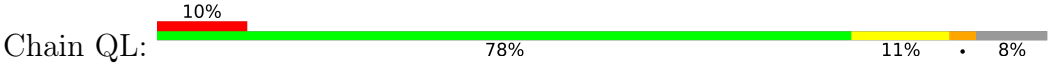


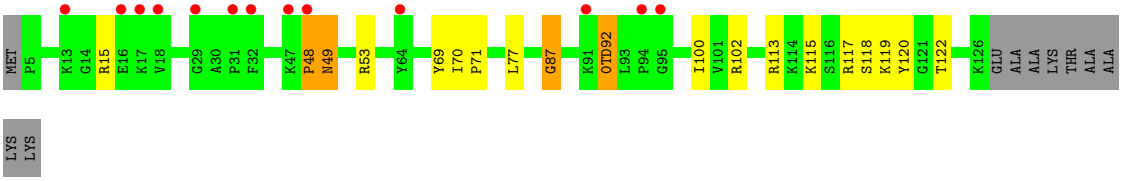
• Molecule 11: 30S ribosomal protein S11



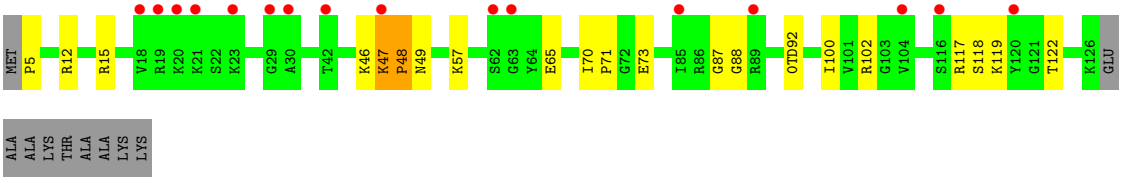


• Molecule 12: 30S ribosomal protein S12

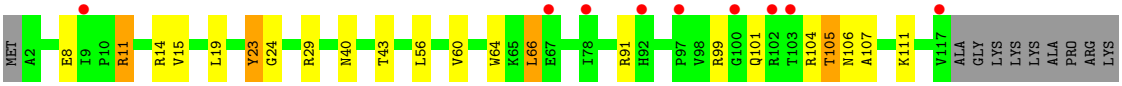




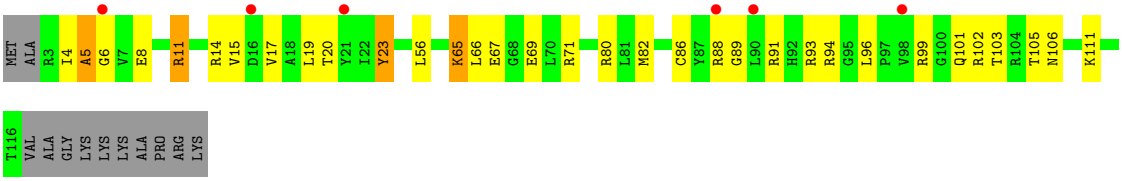
• Molecule 12: 30S ribosomal protein S12



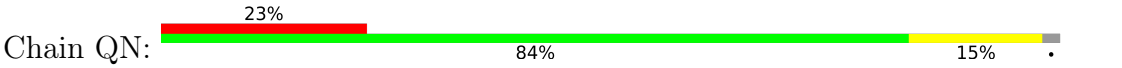
• Molecule 13: 30S ribosomal protein S13

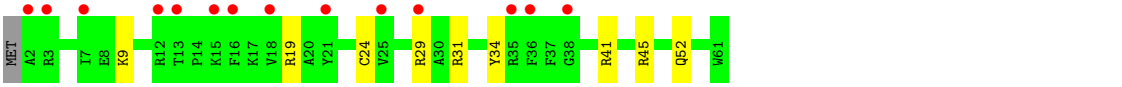


• Molecule 13: 30S ribosomal protein S13

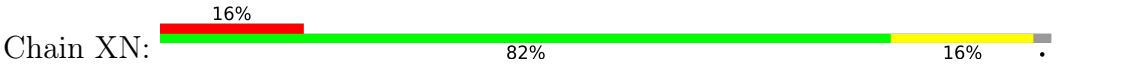


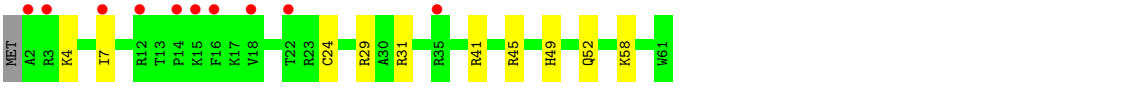
• Molecule 14: 30S ribosomal protein S14 type Z





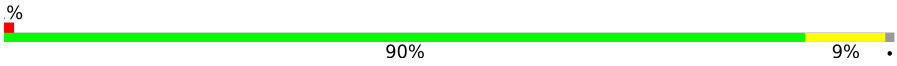
• Molecule 14: 30S ribosomal protein S14 type Z

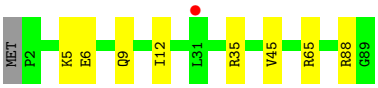




• Molecule 15: 30S ribosomal protein S15

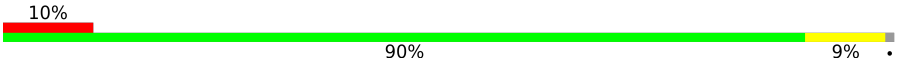
Chain QO:

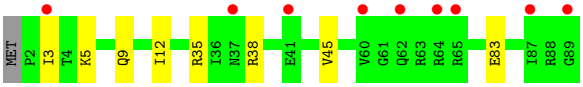




• Molecule 15: 30S ribosomal protein S15

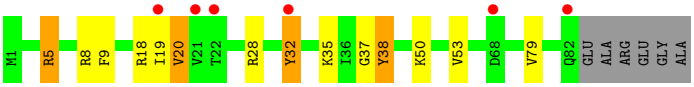
Chain XO:





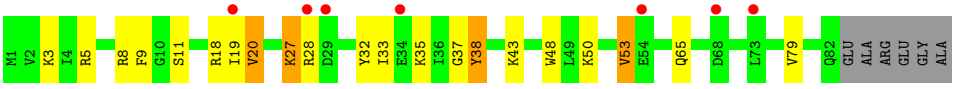
• Molecule 16: 30S ribosomal protein S16

Chain QP:



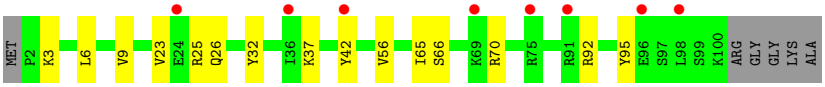
• Molecule 16: 30S ribosomal protein S16

Chain XP:



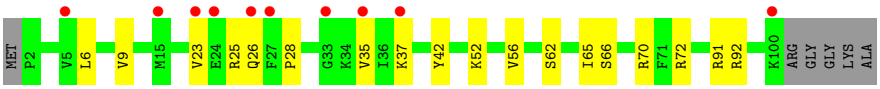
• Molecule 17: 30S ribosomal protein S17

Chain QQ:



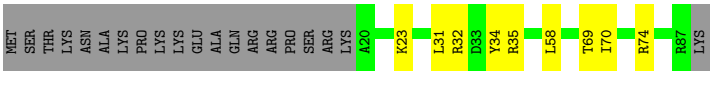
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



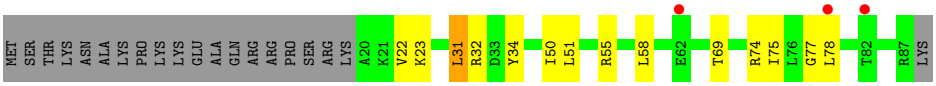
• Molecule 18: 30S ribosomal protein S18

Chain QR:



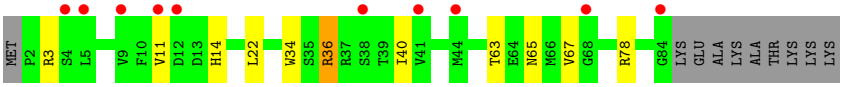
• Molecule 18: 30S ribosomal protein S18

Chain XR:



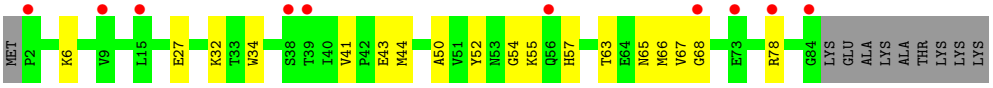
• Molecule 19: 30S ribosomal protein S19

Chain QS:



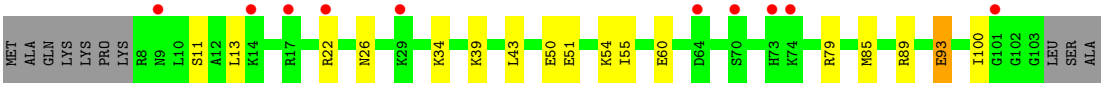
• Molecule 19: 30S ribosomal protein S19

Chain XS:



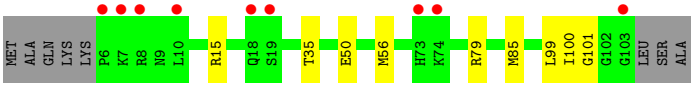
• Molecule 20: 30S ribosomal protein S20

Chain QT:



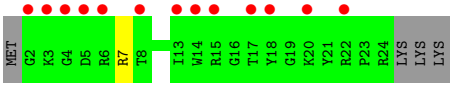
• Molecule 20: 30S ribosomal protein S20

Chain XT:



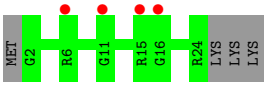
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



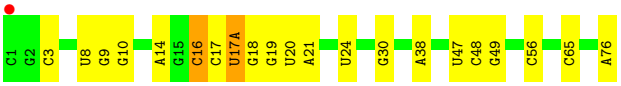
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



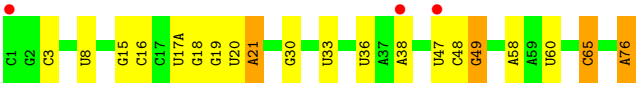
• Molecule 22: P-site tRNAfMet

Chain QV:



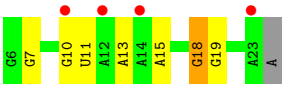
• Molecule 22: P-site tRNAfMet

Chain XV:



• Molecule 23: mRNA

Chain QX:

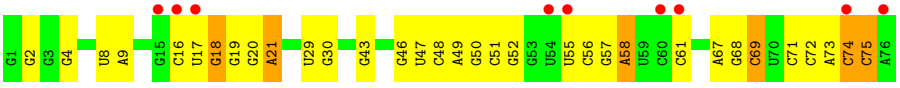


• Molecule 23: mRNA

Chain XX:

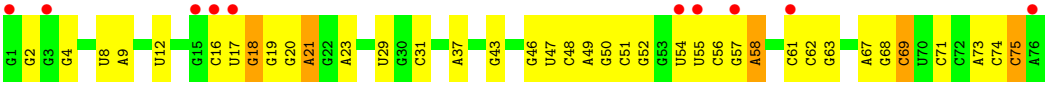
• Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain QY:



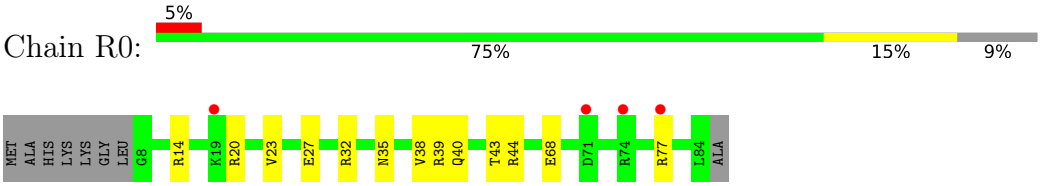
• Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain XY:



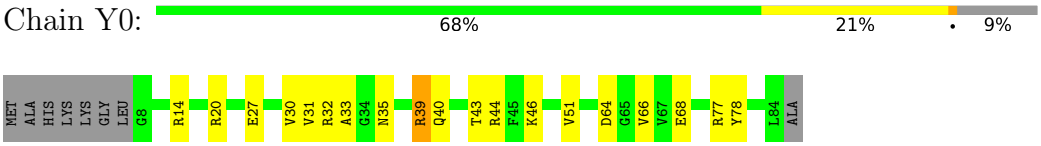
• Molecule 25: 50S ribosomal protein L27

Chain R0:



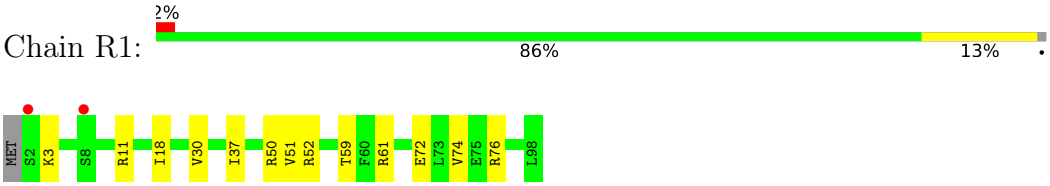
• Molecule 25: 50S ribosomal protein L27

Chain Y0:



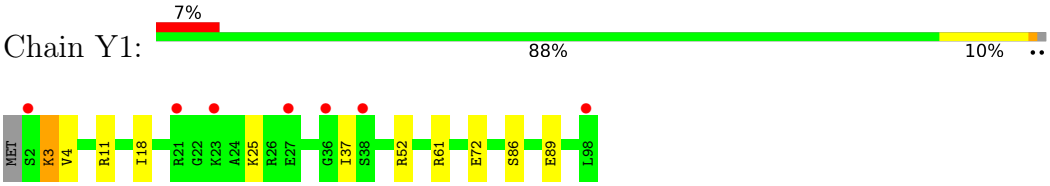
• Molecule 26: 50S ribosomal protein L28

Chain R1:



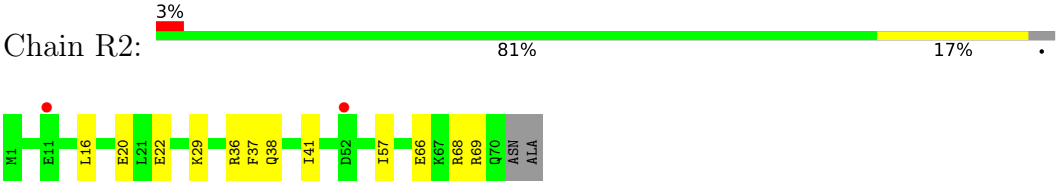
• Molecule 26: 50S ribosomal protein L28

Chain Y1:



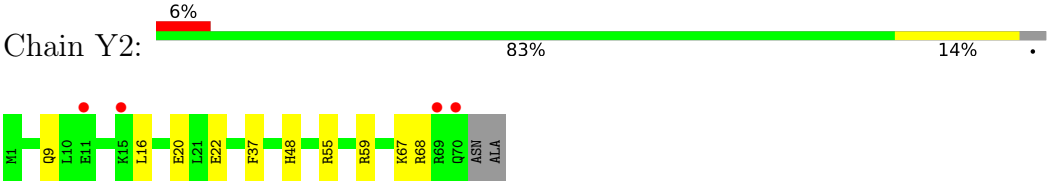
• Molecule 27: 50S ribosomal protein L29

Chain R2:



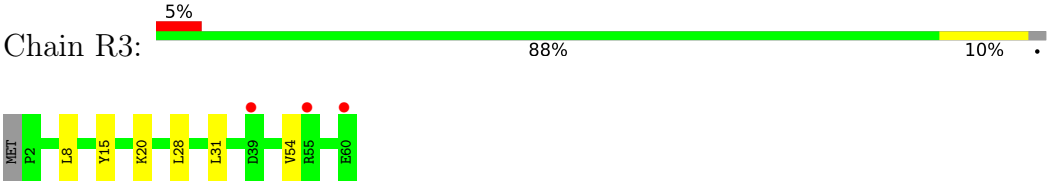
• Molecule 27: 50S ribosomal protein L29

Chain Y2:



• Molecule 28: 50S ribosomal protein L30

Chain R3:

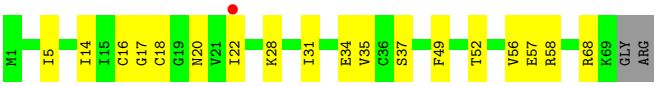


• Molecule 28: 50S ribosomal protein L30

Chain Y3:

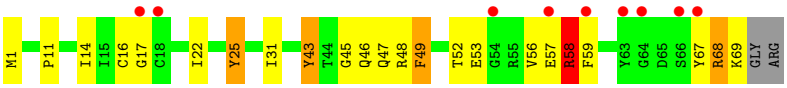
• Molecule 29: 50S ribosomal protein L31

Chain R4:



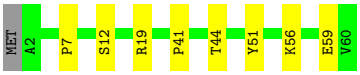
• Molecule 29: 50S ribosomal protein L31

Chain Y4:



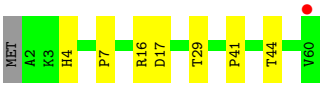
• Molecule 30: 50S ribosomal protein L32

Chain R5:



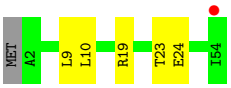
• Molecule 30: 50S ribosomal protein L32

Chain Y5:



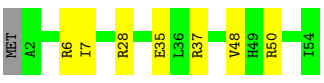
• Molecule 31: 50S ribosomal protein L33

Chain R6:



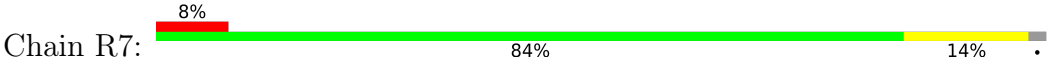
• Molecule 31: 50S ribosomal protein L33

Chain Y6:



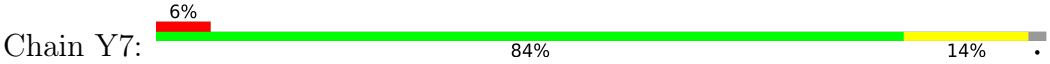
• Molecule 32: 50S ribosomal protein L34

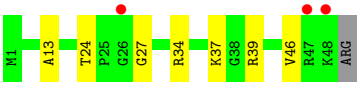
Chain R7:



• Molecule 32: 50S ribosomal protein L34

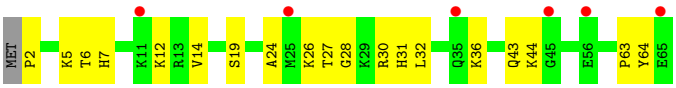
Chain Y7:





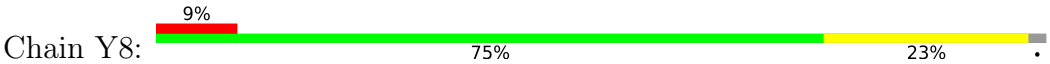
• Molecule 33: 50S ribosomal protein L35

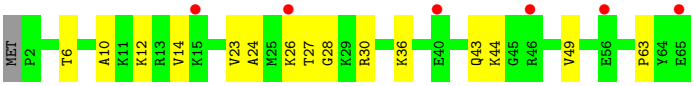
Chain R8:



• Molecule 33: 50S ribosomal protein L35

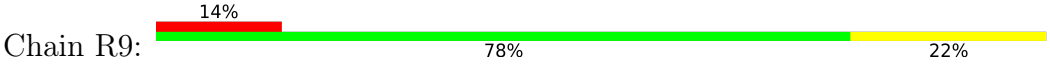
Chain Y8:

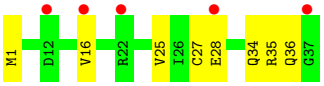




• Molecule 34: 50S ribosomal protein L36

Chain R9:



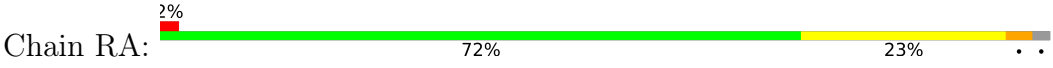


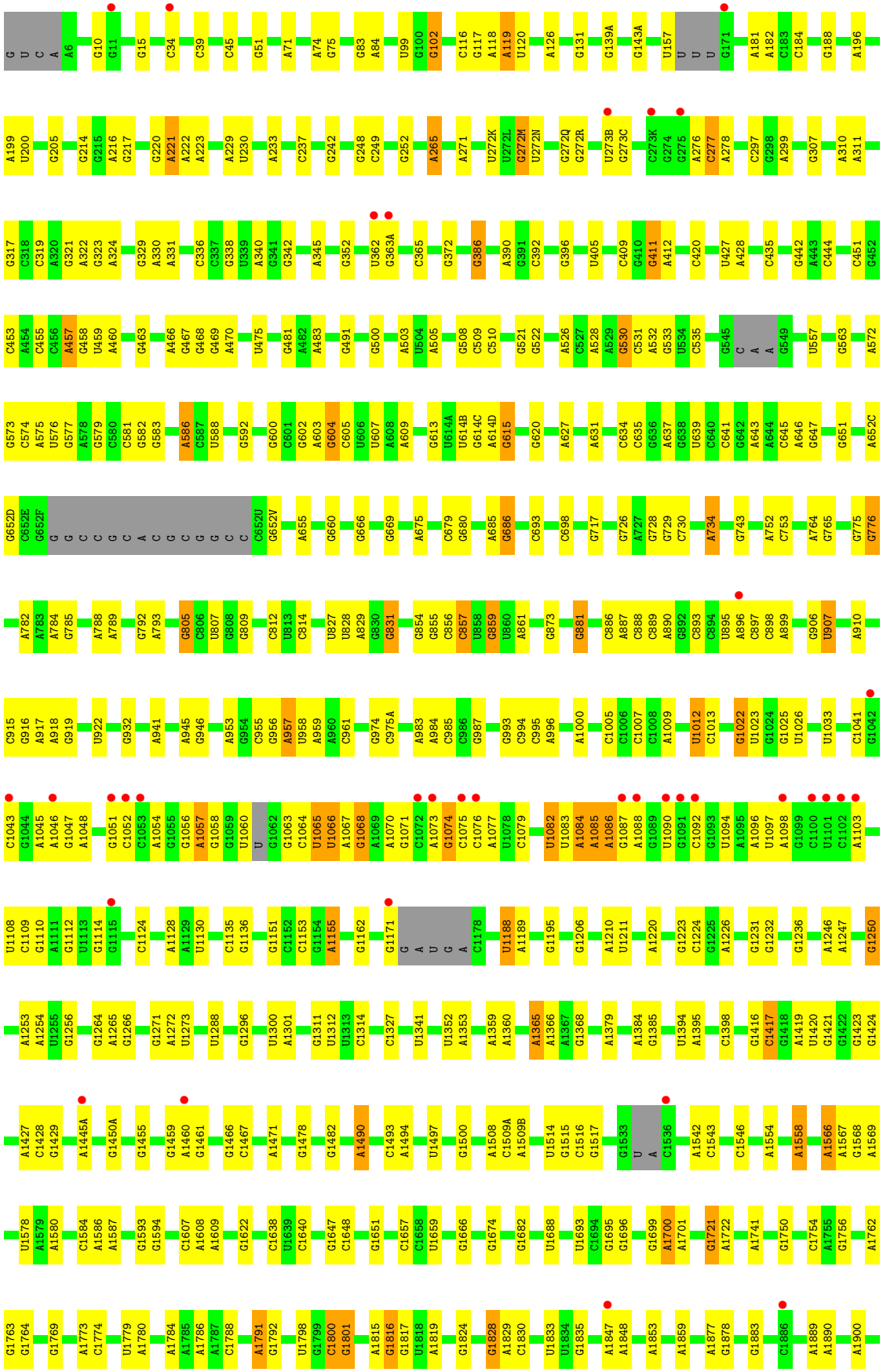
• Molecule 34: 50S ribosomal protein L36

Chain Y9:

• Molecule 35: 23S rRNA

Chain RA:

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A199 U200 G205 G214 G215 A216 G217 G220 A221 A222 A223 A229 U230 A233 C237 G242 G248 C249 G252 A265 A271 U272K U272L G272M U272N G272Q G272R U273B G273C C273K G274 G275 A276 C277 A278 C297 G298 A299 G307 A310 A311
G317 C318 C319 A320 G321 A322 G323 A324 G329 A330 A331 C336 C337 G338 U339 A340 G341 G342 A345 G352 U362 G363A C365 G372 G386 A390 G391 C392 G396 U405 C409 G410 G411 A412 C420 U427 A428 C435 G442 A443 C444 C451 G452
C453 A454 C455 C456 A457 G458 U459 A460 G463 A466 G467 G468 G469 A470 U475 G481 A482 A483 G491 G500 A503 U504 A505 G508 C509 C510 G521 G522 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 G545 C A A G549 U557 G563 A572
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G652D C652E G652F G G C C G C G C G C C C652U G652V A655 G660 G666 G669 A675 C679 G680 A685 G686 C693 C698 G717 G726 A727 G728 G729 C730 A734 G743 A752 C753 A764 G765 G775 G776
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C1043 G1044 A1045 A1046 G1047 A1048 G1051 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103
U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1124 A1128 A1129 U1130 C1135 G1136 G1151 C1152 C1153 G1154 A1155 G1162 G1171 G A U G A C1178 U1188 A1189 G1195 G1206 A1210 U1211 A1220 G1223 C1224 G1225 A1226 G1231 G1232 G1236 A1246 A1247 G1250
A1253 A1254 U1255 G1256 G1264 A1265 G1266 G1271 A1272 U1273 U1288 G1296 U1300 A1301 G1311 U1312 U1313 C1314 C1327 U1341 U1352 A1353 A1359 A1360 A1365 A1366 A1367 G1368 A1379 A1384 G1385 U1394 A1395 C1398 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424
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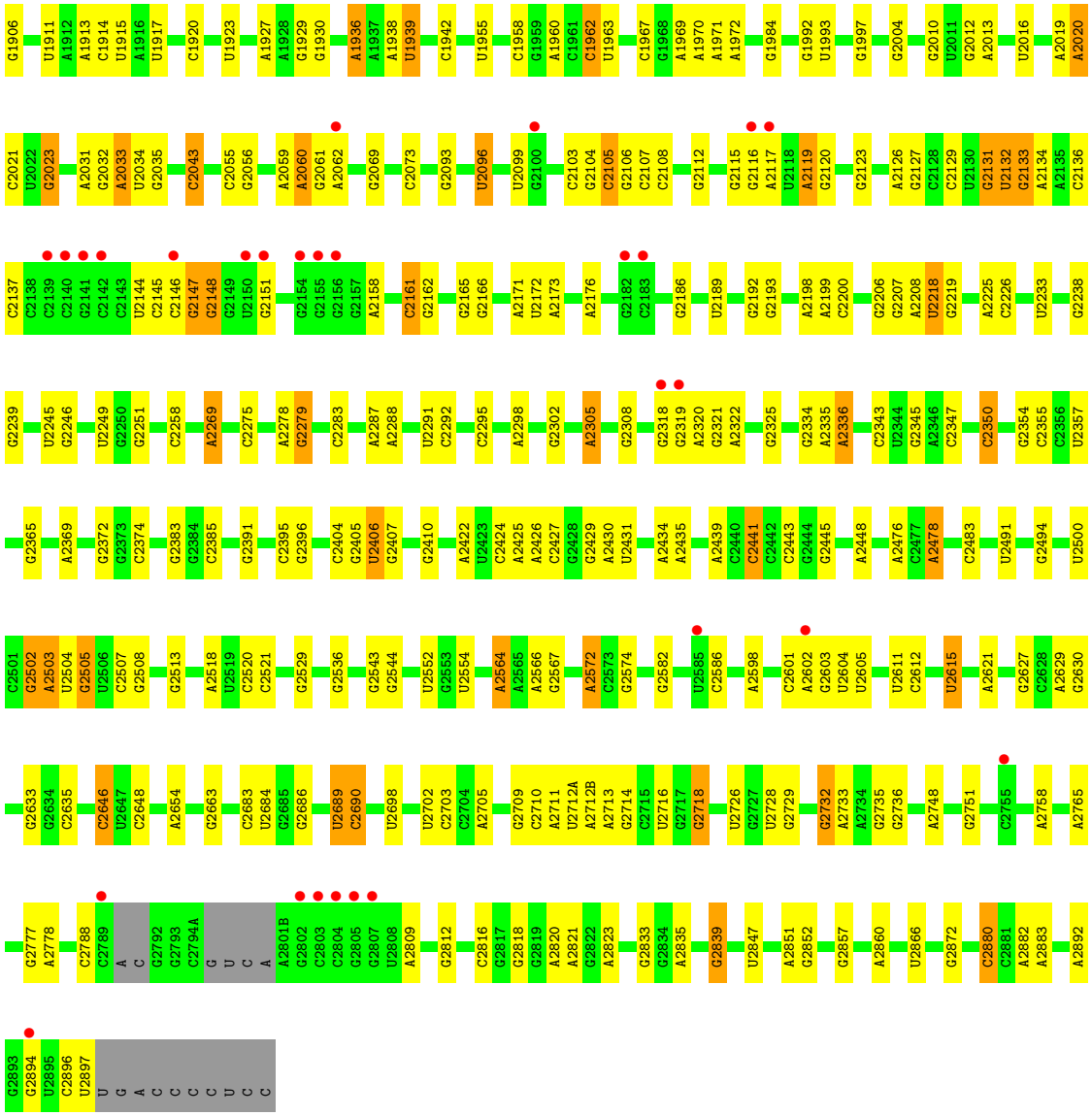
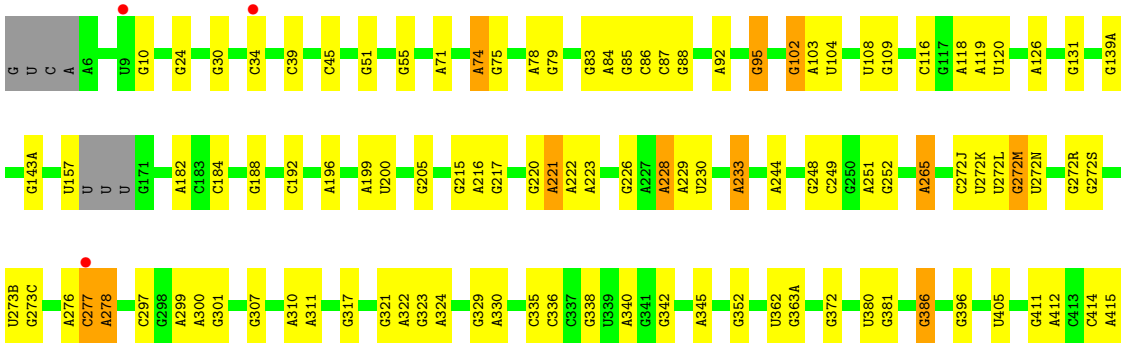
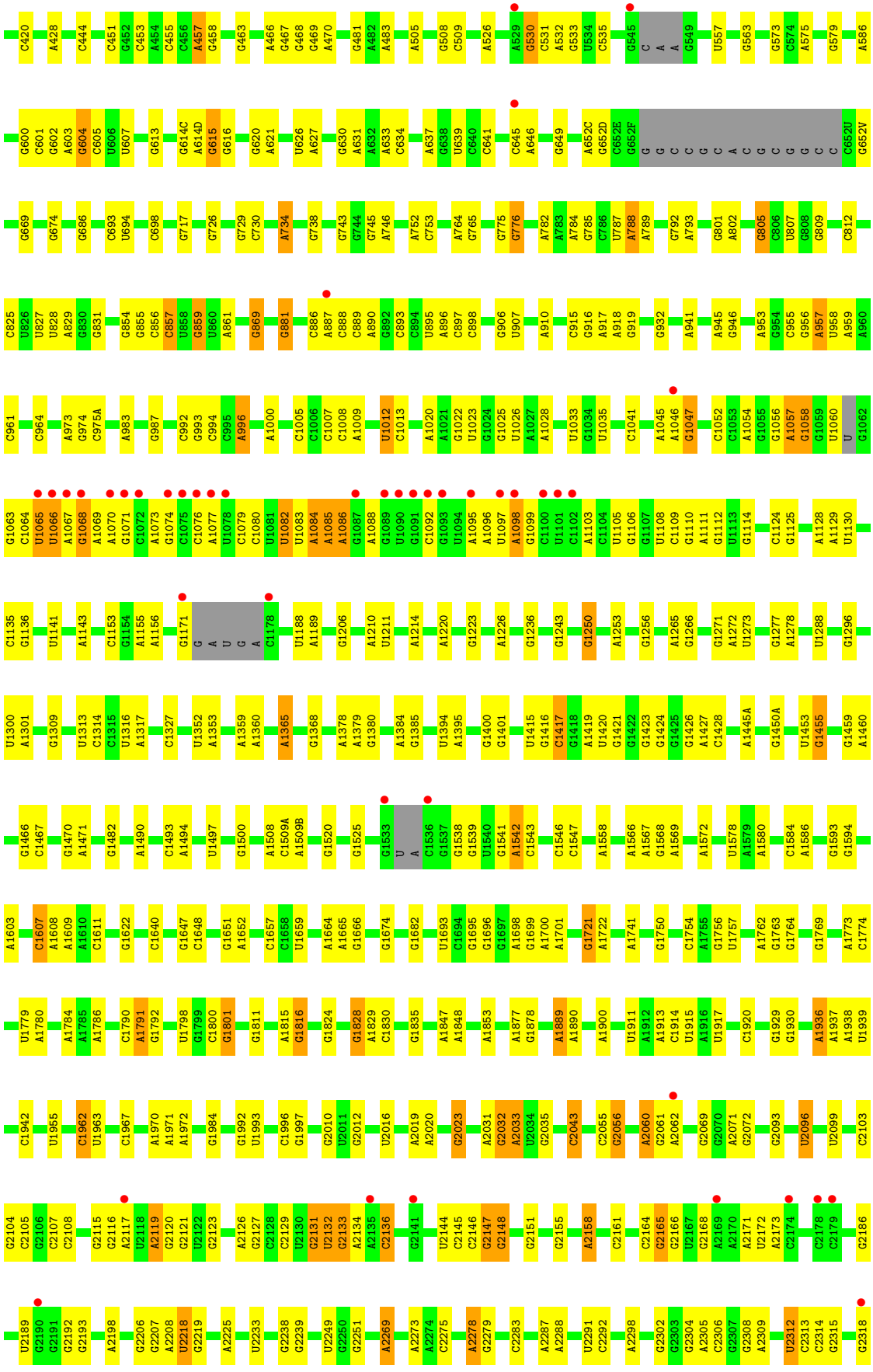
U1578 A1579 A1580 C1584 A1586 A1587 G1593 G1594 C1607 A1608 A1609 G1622 C1638 U1639 C1640 G1647 C1648 G1651 C1657 C1658 U1659 G1666 G1674 G1682 U1688 U1693 C1694 G1695 G1696 G1699 A1700 A1701 G1721 A1722 A1741 G1750 C1754 A1755 G1756 A1762
G1763 G1764 G1769 A1773 C1774 U1779 A1780 A1784 A1785 A1786 A1787 C1788 A1791 G1792 U1798 G1799 C1800 G1801 A1815 G1816 G1817 U1818 A1819 G1824 G1828 A1829 C1830 U1833 U1834 G1835 A1847 A1848 A1853 A1859 A1877 G1878 G1883 C1886 A1889 A1890 A1900



• Molecule 35: 23S rRNA

Chain YA:

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G600 C601 G602 A603 G604 C605 U606 U607 G613 G614C A614D G615 G616 G620 A621 U626 A627 G630 A631 A632 A633 C634 A637 G638 U639 C640 C641 C645 A646 G649 A652C G652D C652E G652F G G C C G C A C G G C G G C C6520U G652V
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C961 C964 A973 G974 C975A A983 G987 C992 G993 C994 C995 A996 A1000 C1005 C1006 C1007 C1008 A1009 U1012 C1013 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 U1033 G1034 U1035 C1041 A1045 A1046 G1047 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U G1062
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C1135 G1136 U1141 A1143 C1153 G1154 A1155 A1156 G1171 G A A U G A C1178 U1188 A1189 G1206 A1210 U1211 A1214 A1220 G1223 A1226 G1236 G1243 G1250 A1253 G1256 A1265 G1266 G1271 A1272 U1273 G1277 A1278 U1288 G1296
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G1466 C1467 G1470 A1471 G1482 A1490 C1493 A1494 U1497 G1500 A1508 C1509A A1509B G1520 G1525 G1533 U A C1536 G1537 G1538 G1539 U1540 G1541 A1542 C1543 C1546 C1547 A1558 A1566 A1567 G1568 A1569 A1572 U1578 A1579 A1580 C1584 A1586 G1593 G1594
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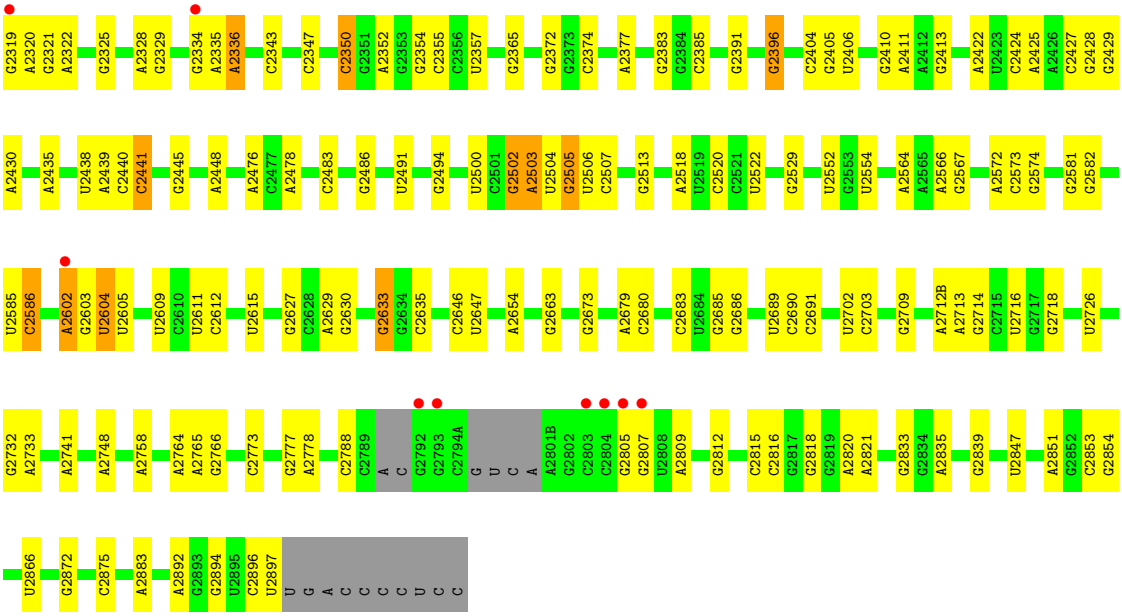
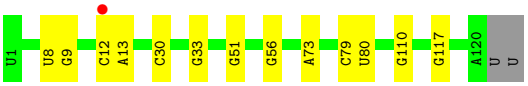
G2104 C2105 G2106 C2107 C2108 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 G2141 U2144 C2145 C2146 G2147 G2148 G2151 G2155 A2158 C2161 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2178 C2179 G2186
U2189 G2190 G2191 G2192 G2193 A2198 G2206 G2207 A2208 U2218 G2219 A2225 U2233 G2238 G2239 U2249 G2250 G2251 A2269 A2273 A2274 C2275 A2278 G2279 C2283 A2287 A2288 U2291 C2292 A2298 G2302 G2303 G2304 A2305 C2306 G2307 G2308 A2309 U2312 C2313 C2314 C2315 G2318



• Molecule 36: 5S rRNA

Chain RB:

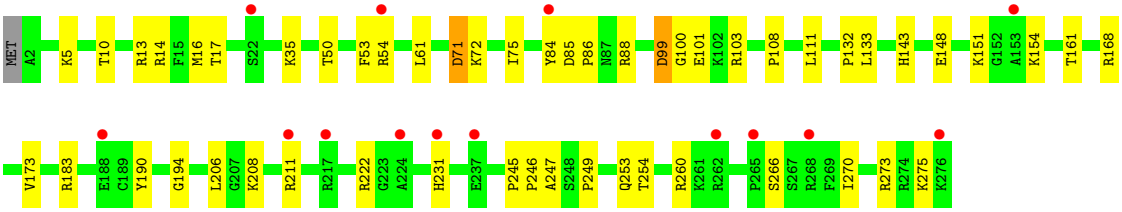


• Molecule 36: 5S rRNA

Chain YB:

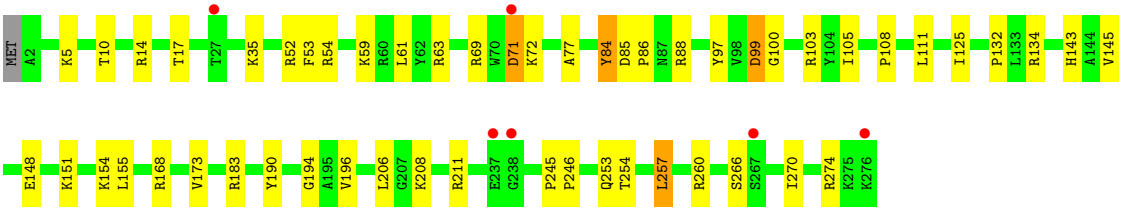
• Molecule 37: 50S ribosomal protein L2

Chain RD:

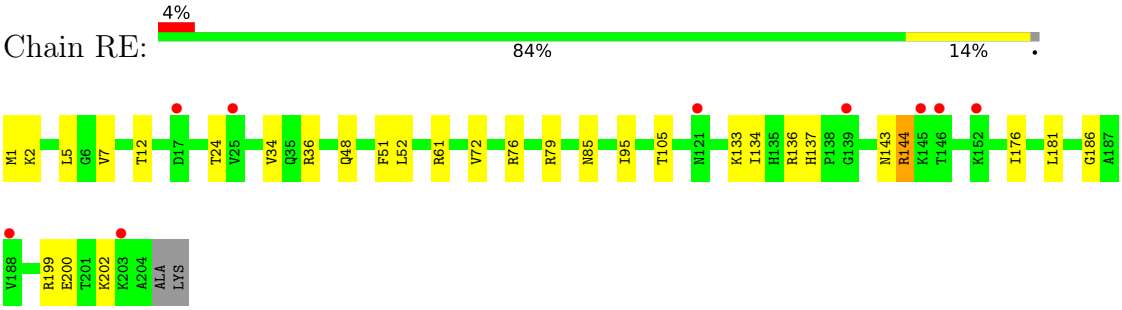


• Molecule 37: 50S ribosomal protein L2

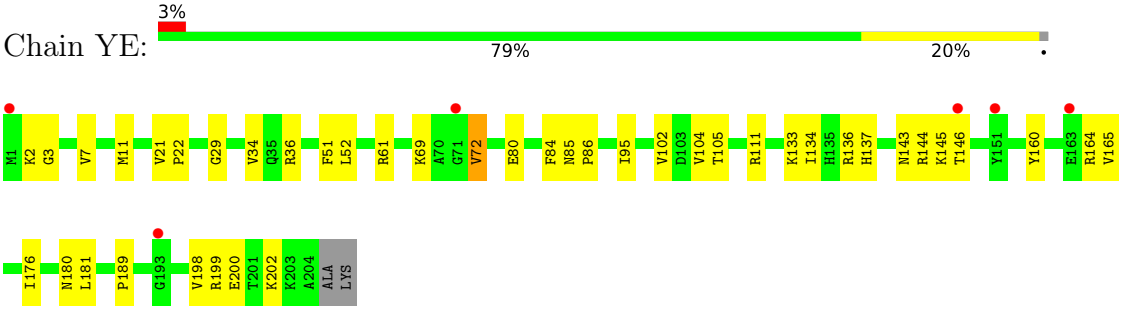
Chain YD:



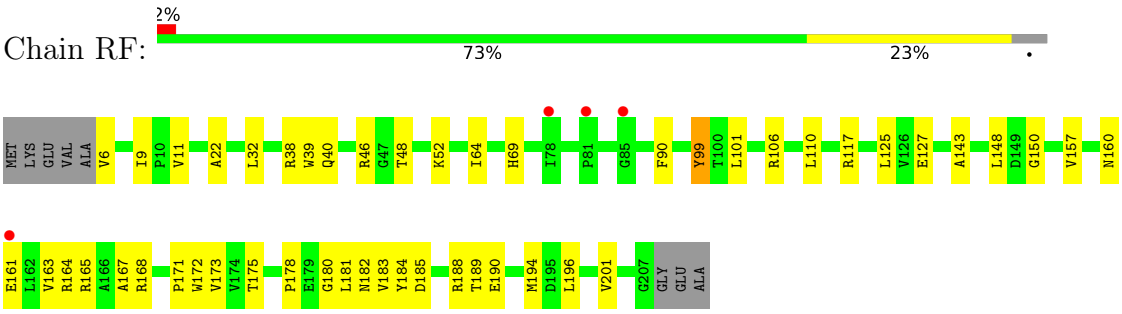
• Molecule 38: 50S ribosomal protein L3



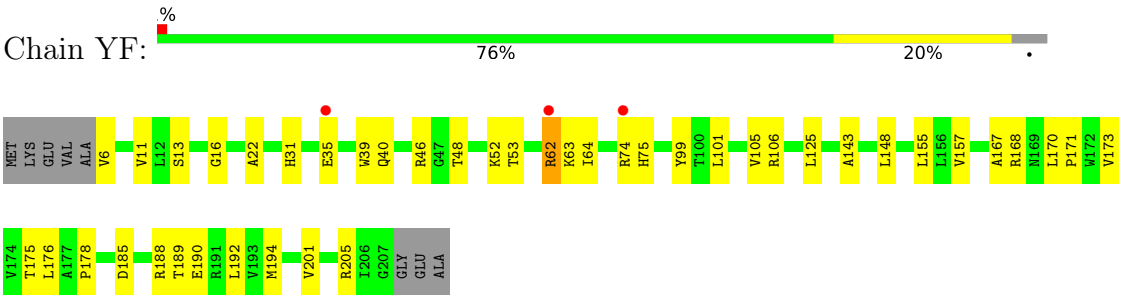
• Molecule 38: 50S ribosomal protein L3



• Molecule 39: 50S ribosomal protein L4

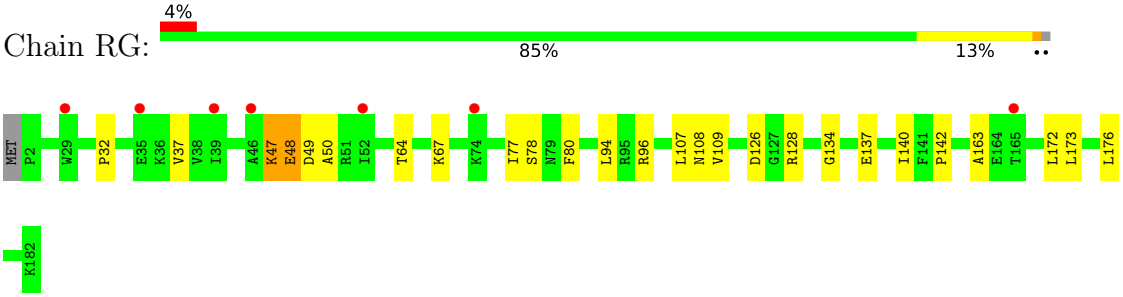


• Molecule 39: 50S ribosomal protein L4



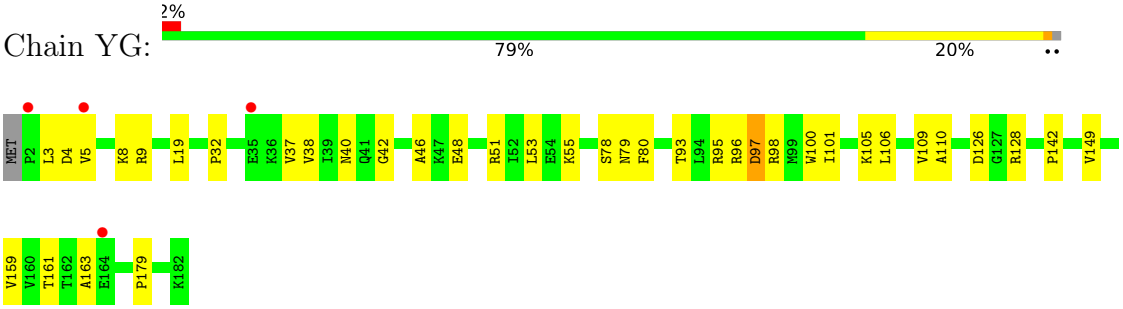
• Molecule 40: 50S ribosomal protein L5

Chain RG:



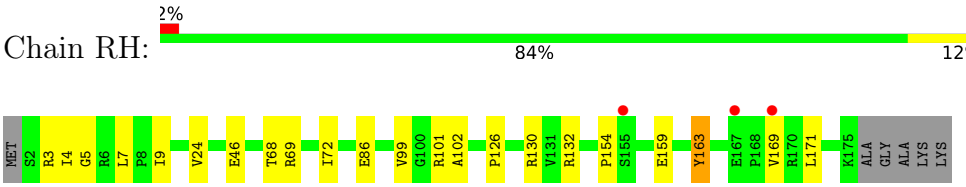
• Molecule 40: 50S ribosomal protein L5

Chain YG:



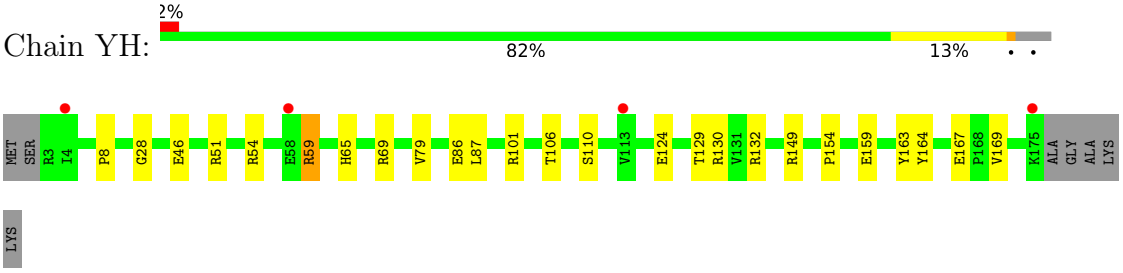
• Molecule 41: 50S ribosomal protein L6

Chain RH:



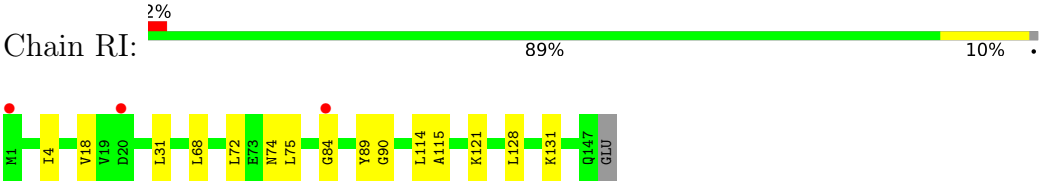
• Molecule 41: 50S ribosomal protein L6

Chain YH:



• Molecule 42: 50S ribosomal protein L9

Chain RI:

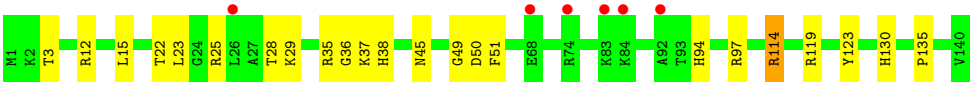


• Molecule 42: 50S ribosomal protein L9

Chain YI:

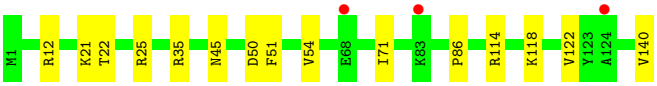
• Molecule 43: 50S ribosomal protein L13

Chain RN:



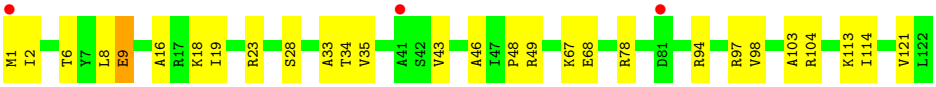
• Molecule 43: 50S ribosomal protein L13

Chain YN:



• Molecule 44: 50S ribosomal protein L14

Chain RO:

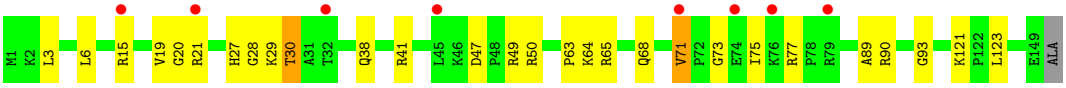


• Molecule 44: 50S ribosomal protein L14

Chain YO:

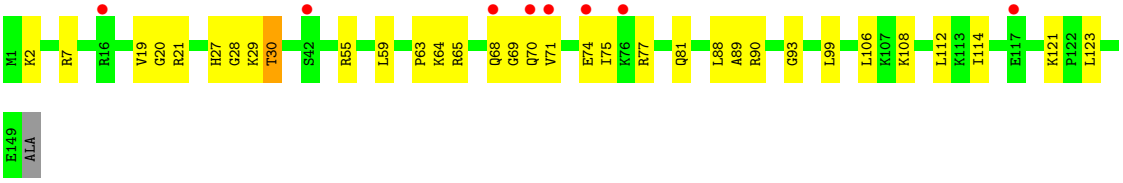
• Molecule 45: 50S ribosomal protein L15

Chain RP:



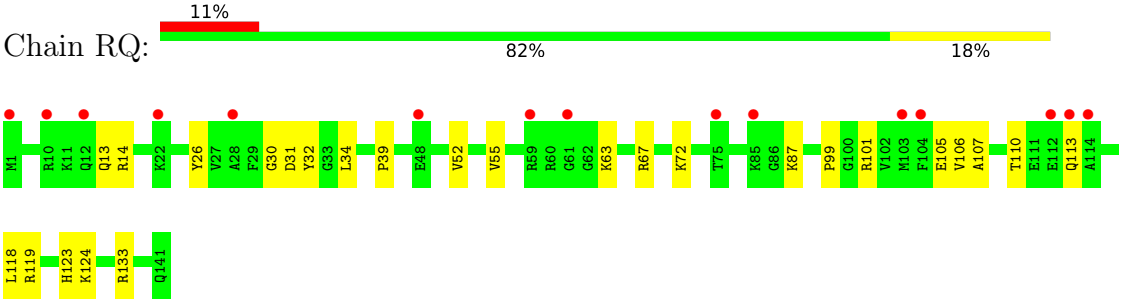
• Molecule 45: 50S ribosomal protein L15

Chain YP:



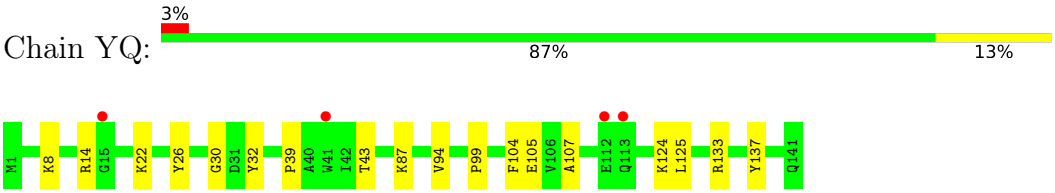
• Molecule 46: 50S ribosomal protein L16

Chain RQ:



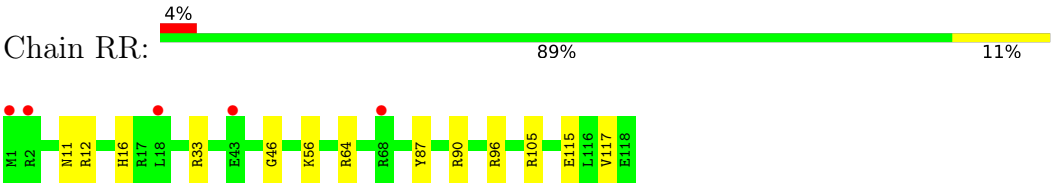
• Molecule 46: 50S ribosomal protein L16

Chain YQ:



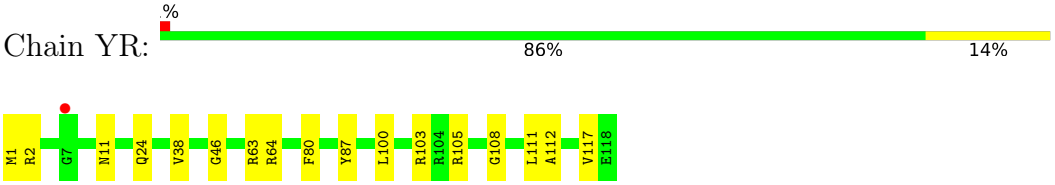
• Molecule 47: 50S ribosomal protein L17

Chain RR:



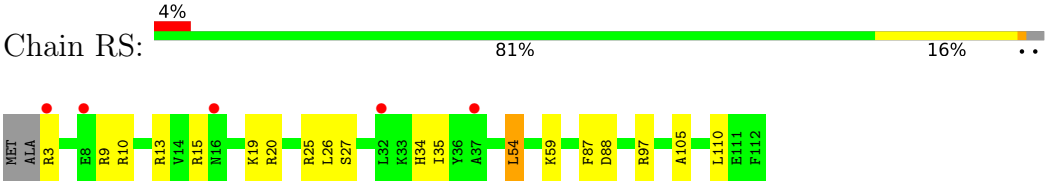
• Molecule 47: 50S ribosomal protein L17

Chain YR:



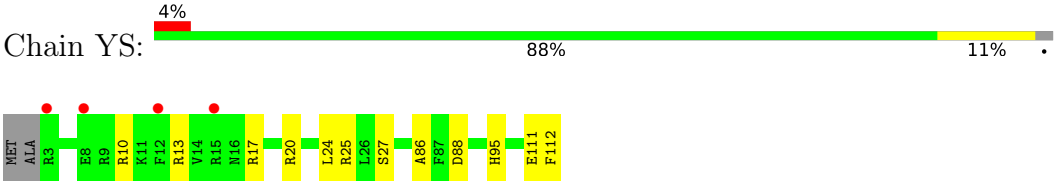
• Molecule 48: 50S ribosomal protein L18

Chain RS:



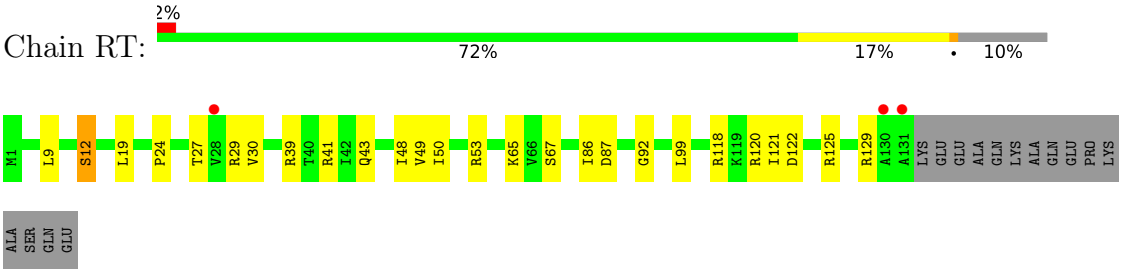
• Molecule 48: 50S ribosomal protein L18

Chain YS:



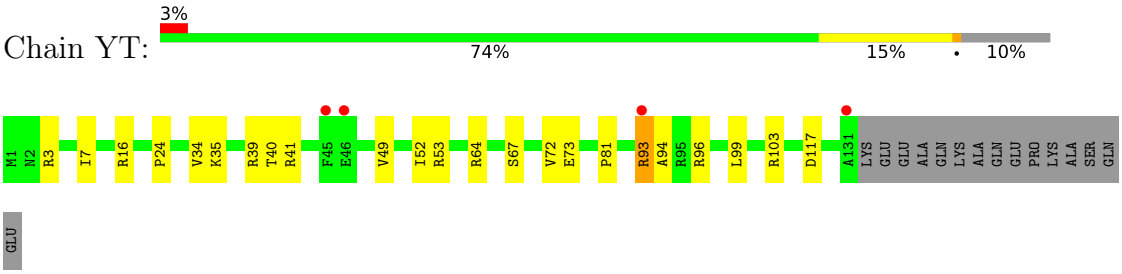
• Molecule 49: 50S ribosomal protein L19

Chain RT:



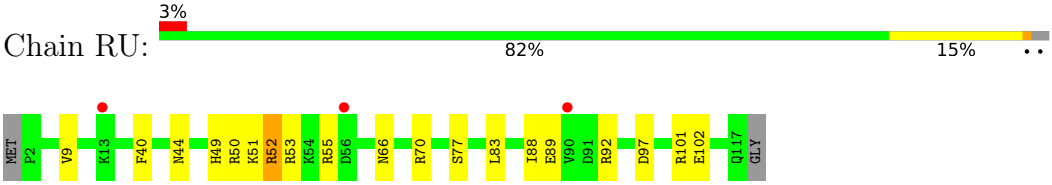
• Molecule 49: 50S ribosomal protein L19

Chain YT:



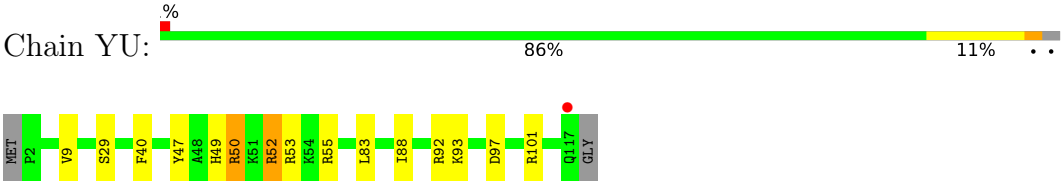
• Molecule 50: 50S ribosomal protein L20

Chain RU:



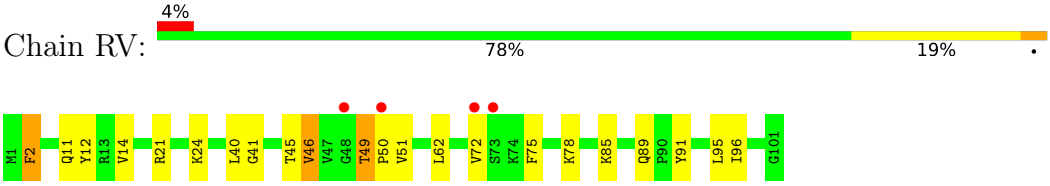
• Molecule 50: 50S ribosomal protein L20

Chain YU:



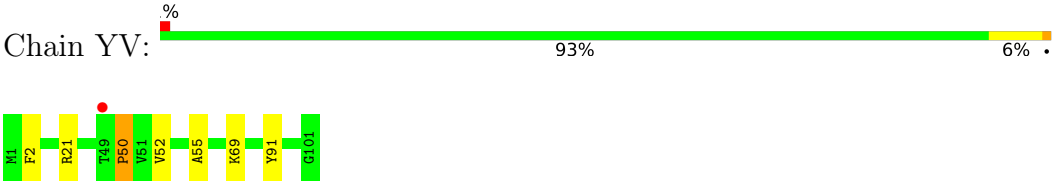
• Molecule 51: 50S ribosomal protein L21

Chain RV:



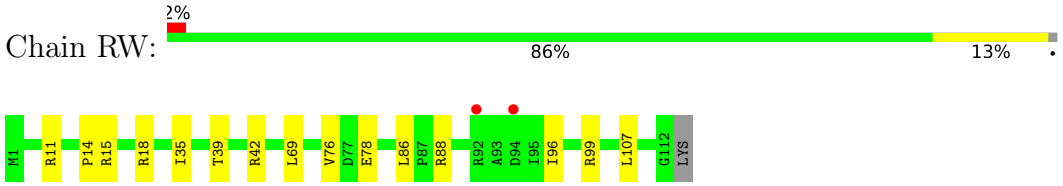
• Molecule 51: 50S ribosomal protein L21

Chain YV:



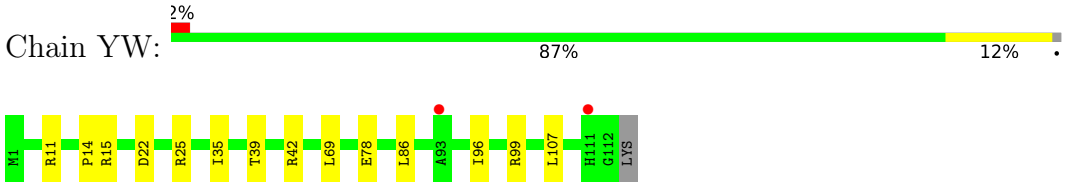
• Molecule 52: 50S ribosomal protein L22

Chain RW:



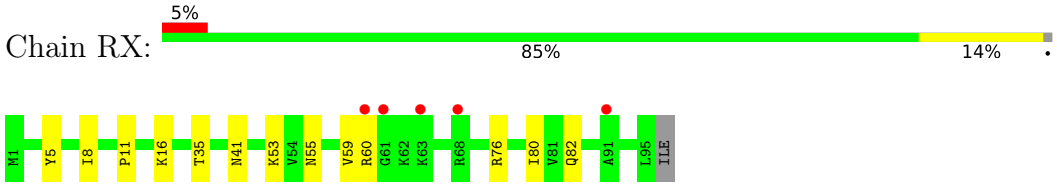
• Molecule 52: 50S ribosomal protein L22

Chain YW:



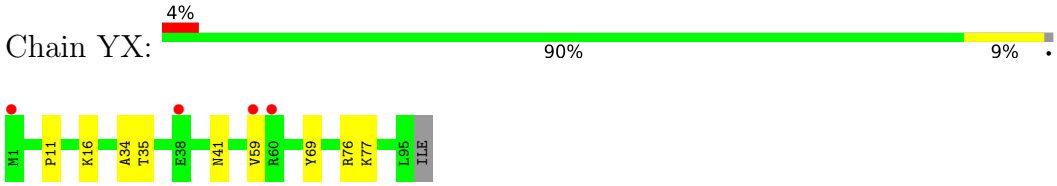
• Molecule 53: 50S ribosomal protein L23

Chain RX:



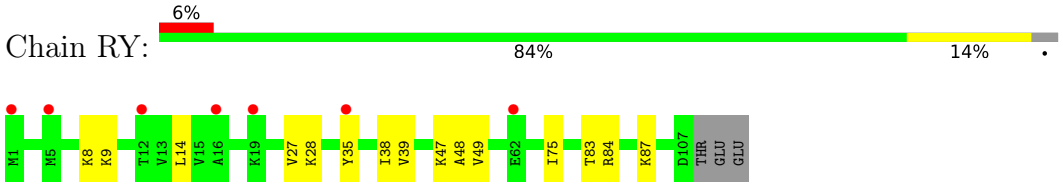
• Molecule 53: 50S ribosomal protein L23

Chain YX:



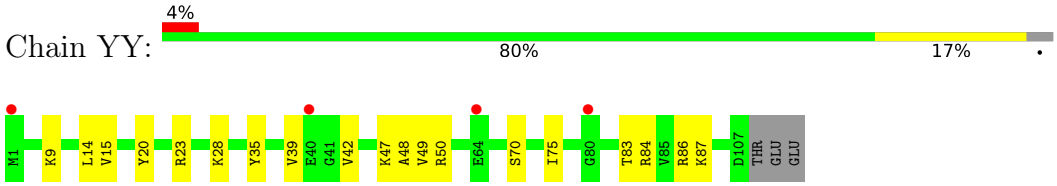
• Molecule 54: 50S ribosomal protein L24

Chain RY:



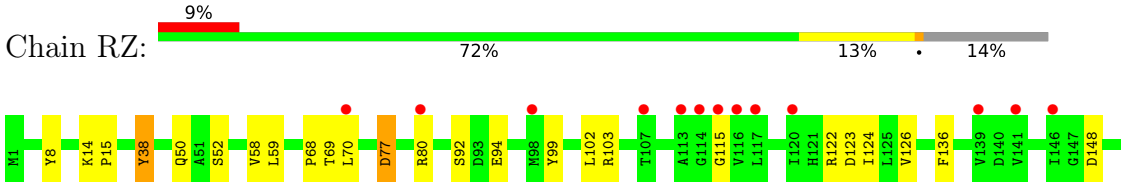
• Molecule 54: 50S ribosomal protein L24

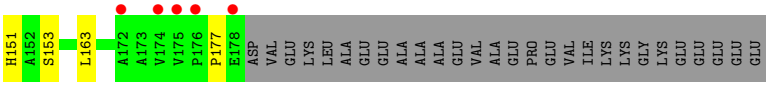
Chain YY:



• Molecule 55: 50S ribosomal protein L25

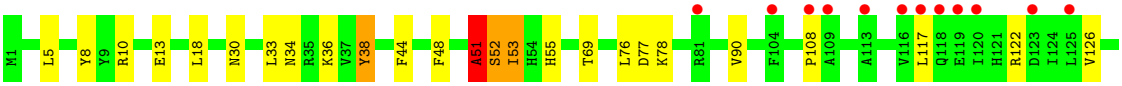
Chain RZ:

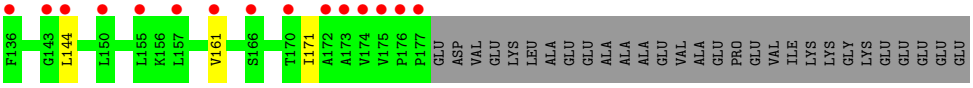




• Molecule 55: 50S ribosomal protein L25

Chain YZ:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.38Å 445.83Å 616.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-3.10) 95.2 (50.00-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.231 , 0.268 0.231 , 0.267	Depositor DCC
R_{free} test set	48817 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	293819	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, PAR, 4OC, UR3, 2MA, G7M, OMG, OMC, PSU, M2G, 5MC, 5MU, OMU, ZN, 2MG, 0TD, MG, MA6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	QA	0.37	0/35795	0.38	7/55864 (0.0%)
1	XA	0.39	0/35890	0.39	5/56012 (0.0%)
2	QB	0.41	0/1876	1.14	20/2533 (0.8%)
2	XB	0.40	0/1860	1.03	11/2518 (0.4%)
3	QC	0.35	0/1582	0.81	4/2137 (0.2%)
3	XC	0.42	0/1566	0.89	7/2119 (0.3%)
4	QD	0.48	0/1695	1.01	13/2274 (0.6%)
4	XD	0.43	0/1698	0.89	4/2277 (0.2%)
5	QE	0.36	0/1149	0.76	2/1548 (0.1%)
5	XE	0.38	0/1149	0.77	0/1548
6	QF	0.45	0/827	0.80	2/1120 (0.2%)
6	XF	0.45	0/829	0.80	1/1123 (0.1%)
7	QG	0.37	0/1254	0.86	3/1683 (0.2%)
7	XG	0.42	0/1248	0.87	6/1676 (0.4%)
8	QH	0.40	0/1118	0.85	2/1506 (0.1%)
8	XH	0.40	0/1108	0.84	4/1494 (0.3%)
9	QI	0.36	0/1005	0.97	7/1351 (0.5%)
9	XI	0.36	0/985	0.93	4/1329 (0.3%)
10	QJ	0.40	0/732	0.96	3/993 (0.3%)
10	XJ	0.43	0/723	0.85	2/984 (0.2%)
11	QK	0.38	0/849	0.79	2/1150 (0.2%)
11	XK	0.38	0/848	0.80	3/1149 (0.3%)
12	QL	0.49	0/937	1.03	4/1260 (0.3%)
12	XL	0.52	0/937	1.02	3/1260 (0.2%)
13	QM	0.38	0/924	1.03	9/1242 (0.7%)
13	XM	0.42	0/905	1.05	7/1217 (0.6%)
14	QN	0.37	0/501	0.80	0/664
14	XN	0.39	0/501	0.79	0/664
15	QO	0.41	0/739	0.91	4/985 (0.4%)
15	XO	0.40	0/739	0.90	3/985 (0.3%)
16	QP	0.41	0/697	0.99	5/939 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	XP	0.43	0/693	0.97	6/935 (0.6%)
17	QQ	0.42	0/836	0.82	1/1117 (0.1%)
17	XQ	0.40	0/836	0.85	2/1117 (0.2%)
18	QR	0.38	0/560	0.78	2/746 (0.3%)
18	XR	0.42	0/560	0.79	2/746 (0.3%)
19	QS	0.40	0/663	0.97	4/895 (0.4%)
19	XS	0.38	0/660	0.97	4/893 (0.4%)
20	QT	0.36	0/734	0.84	4/969 (0.4%)
20	XT	0.36	0/736	0.75	0/976
21	QU	0.32	0/203	0.67	0/266
21	XU	0.36	0/203	0.73	0/266
22	QV	0.33	0/1832	0.35	0/2855
22	XV	0.38	0/1832	0.38	0/2855
23	QX	0.31	0/443	0.51	0/690
23	XX	0.31	0/443	0.53	0/690
24	QY	0.28	0/1816	0.39	0/2830
24	XY	0.33	0/1816	0.42	0/2830
25	R0	0.44	0/616	0.93	2/821 (0.2%)
25	Y0	0.48	0/616	0.97	3/821 (0.4%)
26	R1	0.44	0/761	0.76	0/1013
26	Y1	0.47	0/766	0.78	2/1018 (0.2%)
27	R2	0.43	0/590	0.81	0/781
27	Y2	0.48	0/594	0.95	2/785 (0.3%)
28	R3	0.43	0/474	0.91	2/635 (0.3%)
28	Y3	0.48	0/469	0.90	1/630 (0.2%)
29	R4	0.46	0/559	1.22	6/754 (0.8%)
29	Y4	0.48	0/549	1.28	13/741 (1.8%)
30	R5	0.48	0/473	0.86	1/639 (0.2%)
30	Y5	0.48	0/469	0.78	0/635
31	R6	0.48	0/460	0.91	1/613 (0.2%)
31	Y6	0.50	0/456	0.89	2/608 (0.3%)
32	R7	0.49	0/426	0.92	1/561 (0.2%)
32	Y7	0.49	0/426	0.90	0/561
33	R8	0.46	0/525	0.76	0/691
33	Y8	0.50	0/525	0.75	0/691
34	R9	0.45	0/310	0.79	0/407
34	Y9	0.52	0/310	0.79	0/407
35	RA	0.42	0/68903	0.40	3/107552 (0.0%)
35	YA	0.47	0/68903	0.41	3/107552 (0.0%)
36	RB	0.37	0/2876	0.36	0/4486
36	YB	0.43	0/2878	0.38	0/4490
37	RD	0.49	0/2181	0.87	6/2940 (0.2%)
37	YD	0.52	0/2186	0.85	6/2944 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	RE	0.44	0/1592	0.89	3/2149 (0.1%)
38	YE	0.51	0/1592	0.91	5/2149 (0.2%)
39	RF	0.50	0/1618	0.94	8/2191 (0.4%)
39	YF	0.49	0/1614	0.91	3/2186 (0.1%)
40	RG	0.41	0/1451	0.92	8/1961 (0.4%)
40	YG	0.44	0/1449	0.87	5/1957 (0.3%)
41	RH	0.40	0/1356	0.86	4/1834 (0.2%)
41	YH	0.45	0/1350	0.78	4/1826 (0.2%)
42	RI	0.39	0/1109	0.90	6/1512 (0.4%)
42	YI	0.42	0/1091	0.80	1/1490 (0.1%)
43	RN	0.44	0/1148	0.78	3/1547 (0.2%)
43	YN	0.48	0/1144	0.80	1/1543 (0.1%)
44	RO	0.47	0/943	0.84	3/1269 (0.2%)
44	YO	0.51	0/943	0.82	0/1269
45	RP	0.45	0/1152	0.88	3/1533 (0.2%)
45	YP	0.51	0/1152	0.88	4/1533 (0.3%)
46	RQ	0.39	0/1143	0.77	0/1527
46	YQ	0.45	0/1143	0.80	0/1527
47	RR	0.45	0/982	0.84	0/1312
47	YR	0.48	0/982	0.85	1/1312 (0.1%)
48	RS	0.40	0/887	0.91	4/1180 (0.3%)
48	YS	0.44	0/880	0.84	1/1172 (0.1%)
49	RT	0.42	0/1105	0.81	2/1477 (0.1%)
49	YT	0.43	0/1097	0.83	2/1468 (0.1%)
50	RU	0.44	0/977	0.88	5/1301 (0.4%)
50	YU	0.49	0/977	0.92	7/1301 (0.5%)
51	RV	0.50	0/786	1.02	4/1053 (0.4%)
51	YV	0.49	0/782	0.88	3/1049 (0.3%)
52	RW	0.43	0/897	0.77	1/1205 (0.1%)
52	YW	0.47	0/897	0.75	1/1205 (0.1%)
53	RX	0.43	0/764	0.81	0/1025
53	YX	0.45	0/764	0.81	1/1025 (0.1%)
54	RY	0.41	0/823	0.85	0/1099
54	YY	0.48	0/823	0.89	0/1100
55	RZ	0.39	0/1438	0.95	6/1955 (0.3%)
55	YZ	0.43	0/1413	1.00	8/1924 (0.4%)
All	All	0.43	0/316097	0.57	333/473222 (0.1%)

There are no bond length outliers.

The worst 5 of 333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	RV	49	THR	N-CA-C	-13.80	90.09	110.24
55	RZ	38	TYR	CA-CB-CG	11.45	134.50	113.90
2	QB	232	PRO	CA-C-N	11.02	152.25	120.97
2	QB	232	PRO	C-N-CA	11.02	152.25	120.97
13	XM	80	ARG	N-CA-C	-10.71	98.52	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32246	0	16295	176	0
1	XA	32331	0	16337	186	0
2	QB	1842	0	1861	27	0
2	XB	1825	0	1828	23	0
3	QC	1558	0	1557	29	0
3	XC	1542	0	1517	16	0
4	QD	1665	0	1691	35	0
4	XD	1668	0	1707	26	0
5	QE	1133	0	1191	16	0
5	XE	1133	0	1191	14	0
6	QF	814	0	808	8	0
6	XF	816	0	808	20	0
7	QG	1235	0	1249	17	0
7	XG	1229	0	1238	11	0
8	QH	1098	0	1143	18	0
8	XH	1088	0	1126	14	0
9	QI	986	0	990	25	0
9	XI	966	0	953	25	0
10	QJ	719	0	672	10	0
10	XJ	710	0	661	15	0
11	QK	834	0	838	12	0
11	XK	833	0	836	12	0
12	QL	932	0	981	17	0
12	XL	932	0	981	11	0
13	QM	914	0	954	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	XM	895	0	920	23	0
14	QN	492	0	529	11	0
14	XN	492	0	529	11	0
15	QO	728	0	760	2	0
15	XO	728	0	760	3	0
16	QP	681	0	697	20	0
16	XP	677	0	686	22	0
17	QQ	823	0	891	10	0
17	XQ	823	0	891	10	0
18	QR	555	0	618	5	0
18	XR	555	0	618	12	0
19	QS	648	0	658	6	0
19	XS	645	0	635	17	0
20	QT	732	0	809	9	0
20	XT	733	0	795	9	0
21	QU	199	0	208	1	0
21	XU	199	0	208	0	0
22	QV	1640	0	837	6	0
22	XV	1640	0	837	7	0
23	QX	394	0	197	1	0
23	XX	394	0	197	1	0
24	QY	1625	0	822	5	0
24	XY	1625	0	822	7	0
25	R0	608	0	622	8	0
25	Y0	608	0	622	12	0
26	R1	754	0	823	10	0
26	Y1	759	0	837	7	0
27	R2	588	0	643	8	0
27	Y2	592	0	654	6	0
28	R3	469	0	518	2	0
28	Y3	464	0	514	8	0
29	R4	546	0	522	9	0
29	Y4	536	0	514	12	0
30	R5	459	0	476	8	0
30	Y5	455	0	465	6	0
31	R6	453	0	473	2	0
31	Y6	449	0	469	3	0
32	R7	418	0	466	5	0
32	Y7	418	0	466	4	0
33	R8	517	0	582	16	0
33	Y8	517	0	582	12	0
34	R9	307	0	335	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Y9	307	0	335	8	0
35	RA	61758	0	31137	286	0
35	YA	61758	0	31138	275	0
36	RB	2572	0	1304	3	0
36	YB	2573	0	1306	7	0
37	RD	2131	0	2205	41	0
37	YD	2136	0	2217	44	0
38	RE	1559	0	1618	21	0
38	YE	1559	0	1618	35	0
39	RF	1583	0	1624	43	0
39	YF	1579	0	1618	29	0
40	RG	1426	0	1445	14	0
40	YG	1424	0	1441	22	0
41	RH	1330	0	1407	16	0
41	YH	1324	0	1402	14	0
42	RI	1094	0	1127	5	0
42	YI	1076	0	1094	4	0
43	RN	1121	0	1195	16	0
43	YN	1117	0	1184	9	0
44	RO	933	0	996	19	0
44	YO	933	0	996	18	0
45	RP	1135	0	1212	22	0
45	YP	1135	0	1212	24	0
46	RQ	1122	0	1179	18	0
46	YQ	1122	0	1179	14	0
47	RR	968	0	1033	10	0
47	YR	968	0	1033	12	0
48	RS	877	0	938	10	0
48	YS	870	0	923	8	0
49	RT	1091	0	1151	17	0
49	YT	1083	0	1136	15	0
50	RU	959	0	1019	15	0
50	YU	959	0	1019	11	0
51	RV	775	0	841	15	0
51	YV	771	0	830	8	0
52	RW	886	0	940	9	0
52	YW	886	0	940	9	0
53	RX	750	0	814	11	0
53	YX	750	0	814	6	0
54	RY	810	0	892	10	0
54	YY	810	0	887	14	0
55	RZ	1406	0	1418	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	YZ	1381	0	1386	15	0
56	QA	221	0	0	0	0
56	QB	1	0	0	0	0
56	QD	4	0	0	0	0
56	QE	4	0	0	0	0
56	QF	2	0	0	0	0
56	QG	2	0	0	0	0
56	QH	2	0	0	0	0
56	QI	1	0	0	0	0
56	QK	1	0	0	0	0
56	QL	3	0	0	0	0
56	QN	1	0	0	0	0
56	QO	2	0	0	0	0
56	QP	1	0	0	0	0
56	QT	1	0	0	0	0
56	QV	5	0	0	0	0
56	R0	3	0	0	0	0
56	R1	1	0	0	0	0
56	R3	3	0	0	0	0
56	R5	2	0	0	0	0
56	R6	1	0	0	0	0
56	R7	3	0	0	0	0
56	R9	1	0	0	0	0
56	RA	709	0	0	0	0
56	RB	17	0	0	0	0
56	RD	8	0	0	0	0
56	RE	4	0	0	0	0
56	RF	4	0	0	0	0
56	RG	4	0	0	0	0
56	RH	2	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	3	0	0	0	0
56	RQ	4	0	0	0	0
56	RR	2	0	0	0	0
56	RT	4	0	0	0	0
56	RU	2	0	0	0	0
56	RV	3	0	0	0	0
56	RW	1	0	0	0	0
56	RZ	1	0	0	0	0
56	XA	193	0	0	0	0
56	XE	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	XF	2	0	0	0	0
56	XJ	1	0	0	0	0
56	XL	2	0	0	0	0
56	XR	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	3	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	2	0	0	0	0
56	Y3	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0
56	Y7	2	0	0	0	0
56	Y8	1	0	0	0	0
56	YA	707	0	0	0	0
56	YB	20	0	0	0	0
56	YD	7	0	0	0	0
56	YE	5	0	0	0	0
56	YF	3	0	0	0	0
56	YG	3	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	2	0	0	0	0
56	YQ	2	0	0	0	0
56	YR	2	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
57	QA	42	0	45	1	0
57	XA	42	0	45	2	0
58	QD	8	0	0	0	0
58	XD	8	0	0	1	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	RY	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	Y6	1	0	0	0	0
59	Y9	1	0	0	0	0
59	YY	1	0	0	0	0
All	All	293819	0	196213	1818	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 4.

The worst 5 of 1818 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)
55:RZ:8:TYR:HB2	55:RZ:38:TYR:CE1	1.78	1.17
16:QP:20:VAL:HG21	16:QP:32:TYR:HD2	1.09	1.13
55:RZ:8:TYR:HB2	55:RZ:38:TYR:CD1	1.90	1.07
35:RA:660:G:H5'	39:RF:99:TYR:CE2	1.94	1.03
16:QP:20:VAL:HG21	16:QP:32:TYR:CD2	1.94	1.02

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	QB	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3 16
2	XB	229/256 (90%)	204 (89%)	22 (10%)	3 (1%)	9 35
3	QC	204/239 (85%)	197 (97%)	7 (3%)	0	100 100
3	XC	204/239 (85%)	195 (96%)	9 (4%)	0	100 100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	24 57
4	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100 100
5	QE	146/162 (90%)	140 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	XE	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
6	QF	98/101 (97%)	98 (100%)	0	0	100	100
6	XF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
9	QI	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	XI	124/128 (97%)	111 (90%)	13 (10%)	0	100	100
10	QJ	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	18
10	XJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	5	25
11	QK	112/129 (87%)	107 (96%)	5 (4%)	0	100	100
11	XK	112/129 (87%)	108 (96%)	4 (4%)	0	100	100
12	QL	119/132 (90%)	105 (88%)	12 (10%)	2 (2%)	7	30
12	XL	119/132 (90%)	109 (92%)	6 (5%)	4 (3%)	3	16
13	QM	114/126 (90%)	107 (94%)	4 (4%)	3 (3%)	4	21
13	XM	112/126 (89%)	106 (95%)	6 (5%)	0	100	100
14	QN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	XN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	QO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	37
15	XO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	QP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	QQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	XQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	QR	66/88 (75%)	66 (100%)	0	0	100	100
18	XR	66/88 (75%)	66 (100%)	0	0	100	100
19	QS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
19	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
20	QT	94/106 (89%)	91 (97%)	3 (3%)	0	100	100
20	XT	96/106 (91%)	92 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	QU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	XU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
25	R0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
25	Y0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
26	R1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	Y1	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
27	R2	68/72 (94%)	68 (100%)	0	0	100	100
27	Y2	68/72 (94%)	68 (100%)	0	0	100	100
28	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	Y3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	R4	67/71 (94%)	59 (88%)	7 (10%)	1 (2%)	8	32
29	Y4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	4
30	R5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
31	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
32	R7	46/49 (94%)	46 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	Y8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
37	YD	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
38	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	57
38	YE	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	57
39	RF	200/210 (95%)	196 (98%)	4 (2%)	0	100	100
39	YF	200/210 (95%)	198 (99%)	2 (1%)	0	100	100
40	RG	179/182 (98%)	163 (91%)	13 (7%)	3 (2%)	7	30
40	YG	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	11	39
41	RH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	YH	171/180 (95%)	165 (96%)	6 (4%)	0	100	100
42	RI	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
42	YI	144/148 (97%)	140 (97%)	4 (3%)	0	100	100
43	RN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
43	YN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
44	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
45	RP	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
45	YP	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
46	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
46	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
47	RR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
47	YR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
48	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
48	YS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
49	RT	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
49	YT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
50	RU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
50	YU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
51	RV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	41
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	41
52	RW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
52	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
53	RX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
53	YX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
54	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
54	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
55	RZ	176/206 (85%)	164 (93%)	11 (6%)	1 (1%)	21	52
55	YZ	175/206 (85%)	165 (94%)	8 (5%)	2 (1%)	11	39
All	All	11389/12128 (94%)	10866 (95%)	478 (4%)	45 (0%)	30	61

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	17	PHE
2	QB	127	ILE
4	QD	5	ILE
10	QJ	32	ALA
10	QJ	79	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	191/220 (87%)	191 (100%)	0	100	100
2	XB	187/220 (85%)	187 (100%)	0	100	100
3	QC	144/188 (77%)	144 (100%)	0	100	100
3	XC	140/188 (74%)	140 (100%)	0	100	100
4	QD	171/181 (94%)	171 (100%)	0	100	100
4	XD	172/181 (95%)	172 (100%)	0	100	100
5	QE	114/123 (93%)	114 (100%)	0	100	100
5	XE	114/123 (93%)	114 (100%)	0	100	100
6	QF	85/90 (94%)	85 (100%)	0	100	100
6	XF	85/90 (94%)	85 (100%)	0	100	100
7	QG	120/127 (94%)	120 (100%)	0	100	100
7	XG	119/127 (94%)	119 (100%)	0	100	100
8	QH	116/119 (98%)	116 (100%)	0	100	100
8	XH	114/119 (96%)	114 (100%)	0	100	100
9	QI	91/99 (92%)	91 (100%)	0	100	100
9	XI	88/99 (89%)	88 (100%)	0	100	100
10	QJ	68/92 (74%)	68 (100%)	0	100	100
10	XJ	68/92 (74%)	68 (100%)	0	100	100
11	QK	83/99 (84%)	83 (100%)	0	100	100
11	XK	83/99 (84%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	QL	96/108 (89%)	96 (100%)	0	100	100
12	XL	96/108 (89%)	96 (100%)	0	100	100
13	QM	90/101 (89%)	90 (100%)	0	100	100
13	XM	87/101 (86%)	87 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	78/80 (98%)	78 (100%)	0	100	100
15	XO	78/80 (98%)	78 (100%)	0	100	100
16	QP	69/74 (93%)	69 (100%)	0	100	100
16	XP	68/74 (92%)	68 (100%)	0	100	100
17	QQ	94/97 (97%)	94 (100%)	0	100	100
17	XQ	94/97 (97%)	94 (100%)	0	100	100
18	QR	59/77 (77%)	59 (100%)	0	100	100
18	XR	59/77 (77%)	59 (100%)	0	100	100
19	QS	68/80 (85%)	68 (100%)	0	100	100
19	XS	67/80 (84%)	67 (100%)	0	100	100
20	QT	71/82 (87%)	70 (99%)	1 (1%)	59	76
20	XT	70/82 (85%)	70 (100%)	0	100	100
21	QU	18/22 (82%)	18 (100%)	0	100	100
21	XU	18/22 (82%)	18 (100%)	0	100	100
25	R0	61/67 (91%)	61 (100%)	0	100	100
25	Y0	61/67 (91%)	61 (100%)	0	100	100
26	R1	79/83 (95%)	79 (100%)	0	100	100
26	Y1	81/83 (98%)	81 (100%)	0	100	100
27	R2	65/67 (97%)	65 (100%)	0	100	100
27	Y2	66/67 (98%)	66 (100%)	0	100	100
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	50/52 (96%)	50 (100%)	0	100	100
29	R4	58/63 (92%)	58 (100%)	0	100	100
29	Y4	54/63 (86%)	54 (100%)	0	100	100
30	R5	51/52 (98%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Y5	50/52 (96%)	50 (100%)	0	100	100
31	R6	51/52 (98%)	51 (100%)	0	100	100
31	Y6	50/52 (96%)	50 (100%)	0	100	100
32	R7	41/42 (98%)	41 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100
33	Y8	54/55 (98%)	54 (100%)	0	100	100
34	R9	34/34 (100%)	34 (100%)	0	100	100
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	214 (100%)	0	100	100
37	YD	215/218 (99%)	215 (100%)	0	100	100
38	RE	164/166 (99%)	164 (100%)	0	100	100
38	YE	164/166 (99%)	164 (100%)	0	100	100
39	RF	160/166 (96%)	160 (100%)	0	100	100
39	YF	159/166 (96%)	159 (100%)	0	100	100
40	RG	144/156 (92%)	144 (100%)	0	100	100
40	YG	142/156 (91%)	142 (100%)	0	100	100
41	RH	144/148 (97%)	144 (100%)	0	100	100
41	YH	143/148 (97%)	143 (100%)	0	100	100
42	RI	111/124 (90%)	111 (100%)	0	100	100
42	YI	108/124 (87%)	108 (100%)	0	100	100
43	RN	119/119 (100%)	119 (100%)	0	100	100
43	YN	118/119 (99%)	118 (100%)	0	100	100
44	RO	100/100 (100%)	100 (100%)	0	100	100
44	YO	100/100 (100%)	100 (100%)	0	100	100
45	RP	115/116 (99%)	115 (100%)	0	100	100
45	YP	115/116 (99%)	115 (100%)	0	100	100
46	RQ	111/111 (100%)	111 (100%)	0	100	100
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	RS	87/88 (99%)	87 (100%)	0	100	100
48	YS	85/88 (97%)	85 (100%)	0	100	100
49	RT	115/127 (91%)	115 (100%)	0	100	100
49	YT	113/127 (89%)	113 (100%)	0	100	100
50	RU	93/94 (99%)	93 (100%)	0	100	100
50	YU	93/94 (99%)	93 (100%)	0	100	100
51	RV	81/82 (99%)	81 (100%)	0	100	100
51	YV	80/82 (98%)	80 (100%)	0	100	100
52	RW	90/92 (98%)	90 (100%)	0	100	100
52	YW	90/92 (98%)	90 (100%)	0	100	100
53	RX	77/78 (99%)	77 (100%)	0	100	100
53	YX	77/78 (99%)	77 (100%)	0	100	100
54	RY	86/91 (94%)	86 (100%)	0	100	100
54	YY	86/91 (94%)	86 (100%)	0	100	100
55	RZ	152/179 (85%)	152 (100%)	0	100	100
55	YZ	148/179 (83%)	148 (100%)	0	100	100
All	All	9329/10064 (93%)	9328 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	QT	60	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
15	XO	62	GLN
55	YZ	55	HIS
20	XT	16	HIS
45	YP	70	GLN
39	RF	8	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1497/1522 (98%)	239 (15%)	15 (1%)
1	XA	1501/1522 (98%)	230 (15%)	15 (0%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	13 (17%)	0
23	QX	17/19 (89%)	6 (35%)	1 (5%)
23	XX	17/19 (89%)	8 (47%)	1 (5%)
24	QY	75/76 (98%)	31 (41%)	0
24	XY	75/76 (98%)	33 (44%)	0
35	RA	2858/2915 (98%)	453 (15%)	16 (0%)
35	YA	2858/2915 (98%)	454 (15%)	15 (0%)
36	RB	119/122 (97%)	10 (8%)	0
36	YB	119/122 (97%)	11 (9%)	0
All	All	9288/9462 (98%)	1503 (16%)	63 (0%)

5 of 1503 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A

5 of 63 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	RA	2172	U
35	YA	1073	A
1	XA	266	G
35	YA	1065	U
35	YA	2171	A

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

48 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	$\#\|Z\|>2$
12	0TD	XL	92	12	8,9,10	3.41	3 (37%)	6,11,13	1.49	1 (16%)
1	MA6	QA	1519	1	23,26,27	1.51	5 (21%)	33,38,41	2.41	13 (39%)
1	2MG	QA	1207	1	23,26,27	1.27	4 (17%)	33,38,41	2.26	10 (30%)
1	2MG	XA	1207	1	23,26,27	1.27	3 (13%)	33,38,41	2.29	10 (30%)
1	5MC	QA	967	1	19,22,23	1.56	3 (15%)	26,32,35	1.18	3 (11%)
35	2MA	RA	2503	35,56	22,25,26	1.44	5 (22%)	32,37,40	2.44	8 (25%)
35	OMC	RA	1920	35	19,22,23	0.83	1 (5%)	25,31,34	1.17	3 (12%)
35	5MU	RA	1939	35	19,22,23	1.42	4 (21%)	27,32,35	2.30	6 (22%)
35	OMC	YA	1920	35	19,22,23	0.86	2 (10%)	25,31,34	1.19	3 (12%)
1	MA6	QA	1518	1	23,26,27	1.60	6 (26%)	33,38,41	2.35	10 (30%)
1	MA6	XA	1518	1	23,26,27	1.60	6 (26%)	33,38,41	2.41	12 (36%)
1	5MC	XA	1404	1	19,22,23	1.28	2 (10%)	26,32,35	1.18	3 (11%)
35	2MA	YA	2503	35,56	22,25,26	1.43	5 (22%)	32,37,40	2.31	8 (25%)
35	5MU	YA	1939	35	19,22,23	1.39	4 (21%)	27,32,35	2.26	6 (22%)
35	5MU	YA	1915	35	19,22,23	1.48	5 (26%)	27,32,35	2.66	9 (33%)
12	0TD	QL	92	12	8,9,10	3.79	1 (12%)	6,11,13	2.26	3 (50%)
35	PSU	RA	1911	35	18,21,22	1.42	4 (22%)	21,30,33	2.09	4 (19%)
1	PSU	XA	516	1	18,21,22	1.44	4 (22%)	21,30,33	2.06	5 (23%)
1	M2G	XA	966	1	24,27,28	1.29	5 (20%)	33,40,43	1.82	5 (15%)
1	5MC	XA	967	1	19,22,23	1.24	2 (10%)	26,32,35	1.18	3 (11%)
1	MA6	XA	1519	1	23,26,27	1.51	6 (26%)	33,38,41	2.40	13 (39%)
1	5MC	XA	1400	1	19,22,23	1.44	3 (15%)	26,32,35	1.21	2 (7%)
1	G7M	XA	527	56,1	23,26,27	2.27	5 (21%)	34,39,42	3.28	10 (29%)
1	4OC	XA	1402	1	20,23,24	0.81	1 (5%)	25,32,35	1.03	1 (4%)
1	5MC	QA	1407	1	19,22,23	1.33	3 (15%)	26,32,35	1.45	2 (7%)
1	UR3	XA	1498	1	19,22,23	0.98	2 (10%)	26,32,35	1.71	3 (11%)
35	PSU	RA	2605	35	18,21,22	1.47	4 (22%)	21,30,33	2.03	4 (19%)
35	PSU	YA	2605	35	18,21,22	1.51	4 (22%)	21,30,33	2.11	4 (19%)
35	5MU	RA	1915	35	19,22,23	1.54	5 (26%)	27,32,35	2.68	9 (33%)
35	5MC	RA	1942	35	19,22,23	1.50	3 (15%)	26,32,35	1.22	3 (11%)
35	OMG	RA	2251	22,35,56	23,26,27	1.25	3 (13%)	32,38,41	1.98	6 (18%)
35	OMG	YA	2251	22,35,56	23,26,27	1.27	3 (13%)	32,38,41	2.08	6 (18%)
1	G7M	QA	527	56,1	23,26,27	2.32	5 (21%)	34,39,42	3.15	11 (32%)
35	PSU	YA	1917	35,56	18,21,22	1.45	4 (22%)	21,30,33	2.01	3 (14%)
1	5MC	QA	1400	1	19,22,23	1.41	3 (15%)	26,32,35	1.17	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	5MC	RA	1962	35,56	19,22,23	1.30	3 (15%)	26,32,35	1.23	2 (7%)
35	5MC	YA	1942	35	19,22,23	1.41	2 (10%)	26,32,35	1.31	4 (15%)
1	4OC	QA	1402	1	20,23,24	0.79	0	25,32,35	1.13	2 (8%)
1	UR3	QA	1498	1	19,22,23	0.93	1 (5%)	26,32,35	1.70	2 (7%)
1	5MC	QA	1404	1	19,22,23	1.35	3 (15%)	26,32,35	1.12	3 (11%)
35	5MC	YA	1962	35,56	19,22,23	1.34	3 (15%)	26,32,35	1.17	2 (7%)
1	5MC	XA	1407	1	19,22,23	1.15	2 (10%)	26,32,35	1.30	2 (7%)
35	PSU	RA	1917	35,56	18,21,22	1.43	4 (22%)	21,30,33	1.96	4 (19%)
35	OMU	RA	2552	35,56	19,22,23	1.31	2 (10%)	25,31,34	1.87	5 (20%)
1	M2G	QA	966	1	24,27,28	1.30	5 (20%)	33,40,43	1.78	5 (15%)
35	OMU	YA	2552	35,56	19,22,23	1.35	3 (15%)	25,31,34	1.89	5 (20%)
1	PSU	QA	516	1	18,21,22	1.40	5 (27%)	21,30,33	1.88	3 (14%)
35	PSU	YA	1911	35	18,21,22	1.44	4 (22%)	21,30,33	2.03	4 (19%)

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
12	0TD	XL	92	12	-	3/7/12/14	-
1	MA6	QA	1519	1	-	3/11/29/30	0/3/3/3
1	2MG	QA	1207	1	-	0/9/27/28	0/3/3/3
1	2MG	XA	1207	1	-	0/9/27/28	0/3/3/3
1	5MC	QA	967	1	-	0/7/25/26	0/2/2/2
35	2MA	RA	2503	35,56	-	0/7/25/26	0/3/3/3
35	OMC	RA	1920	35	-	0/9/27/28	0/2/2/2
35	5MU	RA	1939	35	-	0/7/25/26	0/2/2/2
35	OMC	YA	1920	35	-	0/9/27/28	0/2/2/2
1	MA6	QA	1518	1	-	3/11/29/30	0/3/3/3
1	MA6	XA	1518	1	-	3/11/29/30	0/3/3/3
1	5MC	XA	1404	1	-	0/7/25/26	0/2/2/2
35	2MA	YA	2503	35,56	-	0/7/25/26	0/3/3/3
35	5MU	YA	1939	35	-	0/7/25/26	0/2/2/2
35	5MU	YA	1915	35	-	2/7/25/26	0/2/2/2
12	0TD	QL	92	12	-	1/7/12/14	-
35	PSU	RA	1911	35	-	0/7/25/26	0/2/2/2
1	PSU	XA	516	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M2G	XA	966	1	-	0/11/29/30	0/3/3/3
1	5MC	XA	967	1	-	0/7/25/26	0/2/2/2
1	MA6	XA	1519	1	-	4/11/29/30	0/3/3/3
1	5MC	XA	1400	1	-	2/7/25/26	0/2/2/2
1	G7M	XA	527	56,1	-	3/7/25/26	0/3/3/3
1	4OC	XA	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	QA	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	XA	1498	1	-	0/7/25/26	0/2/2/2
35	PSU	RA	2605	35	-	0/7/25/26	0/2/2/2
35	PSU	YA	2605	35	-	0/7/25/26	0/2/2/2
35	5MU	RA	1915	35	-	2/7/25/26	0/2/2/2
35	5MC	RA	1942	35	-	0/7/25/26	0/2/2/2
35	OMG	RA	2251	22,35,56	-	0/9/27/28	0/3/3/3
35	OMG	YA	2251	22,35,56	-	0/9/27/28	0/3/3/3
1	G7M	QA	527	56,1	-	2/7/25/26	0/3/3/3
35	PSU	YA	1917	35,56	-	0/7/25/26	0/2/2/2
1	5MC	QA	1400	1	-	2/7/25/26	0/2/2/2
35	5MC	RA	1962	35,56	-	0/7/25/26	0/2/2/2
35	5MC	YA	1942	35	-	0/7/25/26	0/2/2/2
1	4OC	QA	1402	1	-	2/9/29/30	0/2/2/2
1	UR3	QA	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	QA	1404	1	-	2/7/25/26	0/2/2/2
35	5MC	YA	1962	35,56	-	1/7/25/26	0/2/2/2
1	5MC	XA	1407	1	-	0/7/25/26	0/2/2/2
35	PSU	RA	1917	35,56	-	0/7/25/26	0/2/2/2
35	OMU	RA	2552	35,56	-	1/9/27/28	0/2/2/2
1	M2G	QA	966	1	-	0/11/29/30	0/3/3/3
35	OMU	YA	2552	35,56	-	0/9/27/28	0/2/2/2
1	PSU	QA	516	1	-	0/7/25/26	0/2/2/2
35	PSU	YA	1911	35	-	0/7/25/26	0/2/2/2

The worst 5 of 165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	QL	92	0TD	CB-CA	-10.41	1.51	1.54
12	XL	92	0TD	CB-CA	-8.91	1.51	1.54
1	QA	527	G7M	C8-N7	7.07	1.45	1.33
1	XA	527	G7M	C8-N7	6.77	1.44	1.33
1	QA	967	5MC	C5-C4	5.55	1.48	1.44

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	527	G7M	CN7-N7-C8	-10.02	109.61	124.79
35	RA	2503	2MA	C5-C4-N3	-9.19	117.50	127.18
1	QA	527	G7M	CN7-N7-C8	-8.85	111.39	124.79
35	YA	2503	2MA	C5-C4-N3	-8.42	118.31	127.18
1	XA	1207	2MG	C2-N3-C4	7.36	121.20	112.00

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	QA	1518	MA6	C5-C6-N6-C9
1	XA	1518	MA6	C5-C6-N6-C9
1	QA	1519	MA6	O4'-C4'-C5'-O5'
1	XA	1519	MA6	O4'-C4'-C5'-O5'
35	RA	1915	5MU	O4'-C1'-N1-C2

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	QA	1519	MA6	1	0
35	RA	2503	2MA	2	0
35	RA	1939	5MU	1	0
1	QA	1518	MA6	1	0
1	XA	1518	MA6	1	0
35	YA	2503	2MA	2	0
12	QL	92	0TD	1	0
1	XA	966	M2G	1	0
1	XA	967	5MC	1	0
1	XA	1498	UR3	1	0
35	RA	1962	5MC	1	0
35	YA	1962	5MC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2027 ligands modelled in this entry, 2023 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	QD	302	-	0,12,12	-	-	-		
57	PAR	XA	1794	-	44,45,45	0.65	0	63,67,67	1.22	7 (11%)
57	PAR	QA	1821	-	44,45,45	0.68	0	63,67,67	1.47	10 (15%)
58	SF4	XD	301	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	302	-	-	-	0/6/5/5
57	PAR	XA	1794	-	-	3/18/94/94	0/4/4/4
57	PAR	QA	1821	-	-	4/18/94/94	0/4/4/4
58	SF4	XD	301	-	-	-	0/6/5/5

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	QA	1821	PAR	C44-C34-C24	5.00	119.30	110.99
57	XA	1794	PAR	C13-O52-C52	-3.49	109.70	117.98
57	QA	1821	PAR	C13-O52-C52	-3.48	109.73	117.98
57	XA	1794	PAR	C14-O33-C33	-3.03	110.79	117.98
57	XA	1794	PAR	C11-O51-C51	2.74	119.07	113.72

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1821	PAR	O51-C51-C61-O61
57	QA	1821	PAR	C41-C51-C61-O61
57	XA	1794	PAR	O54-C14-O33-C33
57	QA	1821	PAR	C23-C33-O33-C14
57	QA	1821	PAR	C52-C42-O11-C11

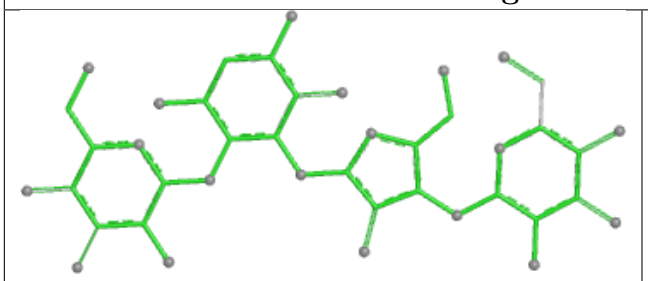
There are no ring outliers.

3 monomers are involved in 4 short contacts:

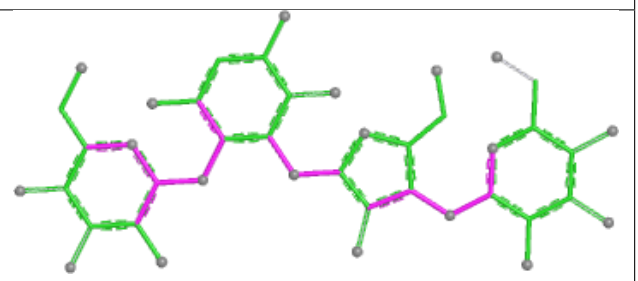
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1794	PAR	2	0
57	QA	1821	PAR	1	0
58	XD	301	SF4	1	0

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

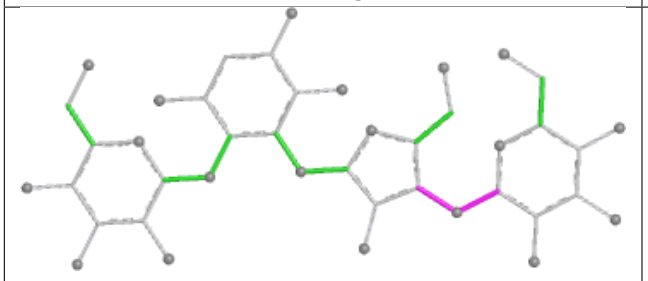
Ligand PAR XA 1794



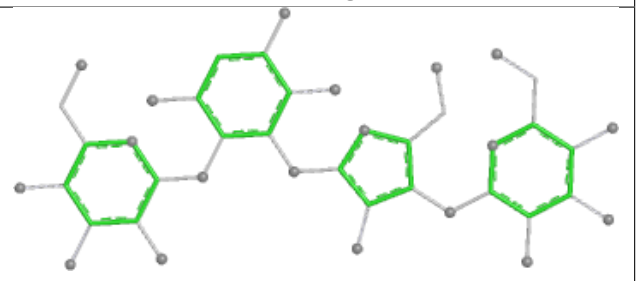
Bond lengths



Bond angles

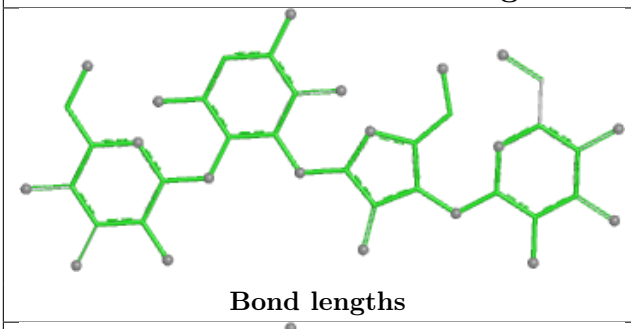


Torsions

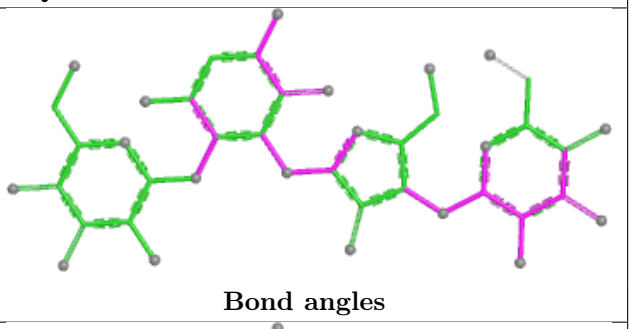


Rings

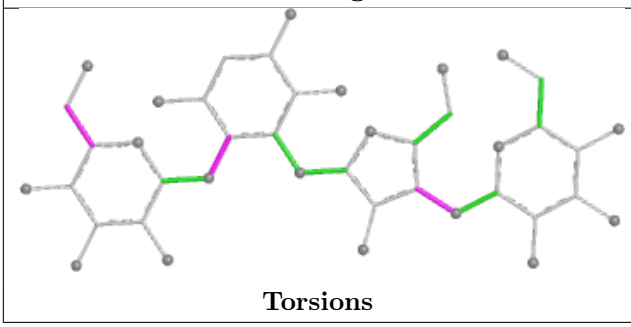
Ligand PAR QA 1821



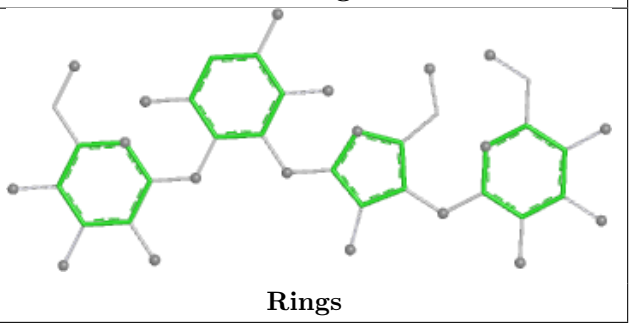
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	QA	1488/1522 (97%)	0.05	19 (1%) 75 56	59, 101, 188, 338	0
1	XA	1492/1522 (98%)	-0.12	11 (0%) 84 68	47, 90, 177, 328	0
2	QB	231/256 (90%)	0.54	12 (5%) 33 17	76, 130, 166, 190	0
2	XB	231/256 (90%)	0.45	8 (3%) 47 27	65, 117, 160, 194	0
3	QC	206/239 (86%)	0.42	11 (5%) 32 17	100, 135, 171, 196	0
3	XC	206/239 (86%)	0.33	11 (5%) 32 17	51, 105, 146, 163	0
4	QD	208/209 (99%)	0.59	14 (6%) 24 13	58, 102, 144, 164	0
4	XD	208/209 (99%)	0.70	19 (9%) 15 8	63, 99, 137, 171	0
5	QE	148/162 (91%)	0.38	4 (2%) 56 35	70, 104, 141, 172	0
5	XE	148/162 (91%)	0.30	2 (1%) 73 53	56, 91, 122, 138	0
6	QF	100/101 (99%)	0.12	0 100 100	63, 92, 129, 145	0
6	XF	100/101 (99%)	0.08	1 (1%) 79 61	64, 96, 127, 158	0
7	QG	155/156 (99%)	0.46	7 (4%) 38 20	88, 124, 155, 209	0
7	XG	155/156 (99%)	0.48	6 (3%) 43 24	75, 107, 147, 184	0
8	QH	137/138 (99%)	0.53	6 (4%) 39 21	67, 104, 135, 156	0
8	XH	137/138 (99%)	0.41	6 (4%) 39 21	59, 92, 127, 154	0
9	QI	127/128 (99%)	1.16	26 (20%) 2 1	94, 141, 174, 200	0
9	XI	126/128 (98%)	0.78	12 (9%) 14 7	70, 113, 147, 186	0
10	QJ	97/105 (92%)	1.00	11 (11%) 10 5	94, 140, 188, 200	0
10	XJ	96/105 (91%)	1.06	13 (13%) 7 4	87, 123, 160, 175	0
11	QK	114/129 (88%)	0.32	5 (4%) 39 21	70, 100, 132, 154	0
11	XK	114/129 (88%)	0.50	8 (7%) 22 12	58, 96, 141, 167	0
12	QL	121/132 (91%)	0.81	13 (10%) 11 6	55, 92, 120, 149	0
12	XL	121/132 (91%)	0.75	16 (13%) 7 4	52, 75, 112, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	QM	116/126 (92%)	0.72	9 (7%) 19 10	88, 127, 162, 177	0
13	XM	114/126 (90%)	0.65	6 (5%) 32 17	75, 111, 156, 195	0
14	QN	60/61 (98%)	1.45	14 (23%) 2 1	81, 135, 179, 194	0
14	XN	60/61 (98%)	1.01	10 (16%) 4 2	76, 101, 135, 139	0
15	QO	88/89 (98%)	0.49	1 (1%) 78 59	64, 94, 137, 167	0
15	XO	88/89 (98%)	0.65	9 (10%) 12 6	58, 88, 136, 145	0
16	QP	82/88 (93%)	0.89	6 (7%) 21 11	53, 94, 123, 156	0
16	XP	82/88 (93%)	0.86	7 (8%) 16 9	65, 94, 138, 174	0
17	QQ	99/105 (94%)	0.84	8 (8%) 18 10	71, 99, 140, 152	0
17	XQ	99/105 (94%)	0.86	10 (10%) 12 6	63, 93, 128, 153	0
18	QR	68/88 (77%)	0.25	0 100 100	75, 97, 130, 163	0
18	XR	68/88 (77%)	0.48	3 (4%) 39 21	62, 93, 139, 161	0
19	QS	83/93 (89%)	0.86	10 (12%) 9 5	101, 136, 184, 192	0
19	XS	83/93 (89%)	0.74	10 (12%) 9 5	75, 118, 155, 172	0
20	QT	96/106 (90%)	1.02	10 (10%) 11 6	65, 95, 144, 161	0
20	XT	98/106 (92%)	0.82	9 (9%) 14 8	75, 97, 152, 165	0
21	QU	23/27 (85%)	2.40	13 (56%) 0 0	91, 122, 147, 158	0
21	XU	23/27 (85%)	1.33	4 (17%) 4 2	90, 108, 124, 144	0
22	QV	77/77 (100%)	0.10	1 (1%) 75 56	86, 122, 172, 240	0
22	XV	77/77 (100%)	0.05	3 (3%) 43 24	58, 105, 164, 210	0
23	QX	18/19 (94%)	1.03	4 (22%) 2 1	71, 163, 230, 231	0
23	XX	18/19 (94%)	1.00	6 (33%) 1 0	64, 153, 241, 253	0
24	QY	76/76 (100%)	0.80	9 (11%) 9 5	105, 192, 252, 287	0
24	XY	76/76 (100%)	0.89	10 (13%) 7 4	85, 162, 243, 269	0
25	R0	77/85 (90%)	0.58	4 (5%) 33 17	54, 81, 100, 143	0
25	Y0	77/85 (90%)	0.17	0 100 100	21, 55, 85, 93	0
26	R1	97/98 (98%)	0.57	2 (2%) 63 42	52, 76, 116, 133	0
26	Y1	97/98 (98%)	0.56	7 (7%) 21 11	30, 63, 106, 133	0
27	R2	70/72 (97%)	0.42	2 (2%) 53 32	61, 93, 137, 159	0
27	Y2	70/72 (97%)	0.36	4 (5%) 29 16	38, 69, 100, 154	0
28	R3	59/60 (98%)	0.37	3 (5%) 33 18	50, 81, 129, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	Y3	59/60 (98%)	0.25	4 (6%) 23 12	28, 51, 104, 137	0
29	R4	69/71 (97%)	0.57	1 (1%) 73 53	104, 149, 191, 208	0
29	Y4	69/71 (97%)	0.60	9 (13%) 7 4	85, 126, 184, 223	0
30	R5	59/60 (98%)	0.14	0 100 100	39, 73, 97, 152	0
30	Y5	59/60 (98%)	0.13	1 (1%) 69 48	32, 57, 102, 184	0
31	R6	53/54 (98%)	0.27	1 (1%) 66 45	60, 82, 120, 148	0
31	Y6	53/54 (98%)	-0.05	0 100 100	45, 65, 89, 92	0
32	R7	48/49 (97%)	0.43	4 (8%) 17 9	32, 58, 82, 117	0
32	Y7	48/49 (97%)	0.30	3 (6%) 26 14	34, 49, 74, 131	0
33	R8	64/65 (98%)	0.81	6 (9%) 14 8	46, 70, 96, 129	0
33	Y8	64/65 (98%)	0.48	6 (9%) 14 8	37, 51, 86, 111	0
34	R9	37/37 (100%)	1.11	5 (13%) 7 4	68, 96, 127, 185	0
34	Y9	37/37 (100%)	0.58	1 (2%) 56 35	46, 60, 78, 101	0
35	RA	2856/2915 (97%)	-0.01	64 (2%) 62 41	45, 74, 216, 308	0
35	YA	2856/2915 (97%)	-0.32	55 (1%) 66 45	31, 53, 205, 329	0
36	RB	120/122 (98%)	-0.08	1 (0%) 82 65	79, 108, 141, 171	0
36	YB	120/122 (98%)	-0.25	1 (0%) 82 65	54, 75, 101, 137	0
37	RD	275/276 (99%)	0.49	14 (5%) 33 18	40, 64, 104, 121	0
37	YD	275/276 (99%)	0.23	6 (2%) 62 41	33, 55, 86, 155	0
38	RE	204/206 (99%)	0.40	9 (4%) 39 21	46, 76, 113, 157	0
38	YE	204/206 (99%)	0.24	6 (2%) 53 32	35, 58, 96, 128	0
39	RF	202/210 (96%)	0.29	4 (1%) 65 44	39, 81, 129, 184	0
39	YF	202/210 (96%)	0.12	3 (1%) 72 52	27, 58, 111, 141	0
40	RG	181/182 (99%)	0.48	7 (3%) 43 24	84, 121, 157, 203	0
40	YG	181/182 (99%)	0.38	4 (2%) 62 41	63, 91, 139, 182	0
41	RH	174/180 (96%)	0.54	3 (1%) 69 48	80, 124, 159, 185	0
41	YH	173/180 (96%)	0.18	4 (2%) 61 39	38, 72, 108, 145	0
42	RI	147/148 (99%)	0.31	3 (2%) 65 44	57, 106, 145, 165	0
42	YI	146/148 (98%)	0.16	3 (2%) 63 42	55, 96, 141, 167	0
43	RN	140/140 (100%)	0.45	6 (4%) 40 22	48, 83, 128, 153	0
43	YN	140/140 (100%)	0.23	3 (2%) 63 42	35, 59, 97, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	RO	122/122 (100%)	0.31	3 (2%) 58 37	43, 76, 104, 123	0
44	YO	122/122 (100%)	0.21	2 (1%) 70 49	27, 57, 93, 108	0
45	RP	149/150 (99%)	0.59	8 (5%) 31 17	38, 90, 138, 163	0
45	YP	149/150 (99%)	0.45	8 (5%) 31 17	33, 65, 104, 133	0
46	RQ	141/141 (100%)	0.76	15 (10%) 11 6	57, 89, 128, 180	0
46	YQ	141/141 (100%)	0.42	4 (2%) 55 34	31, 60, 94, 157	0
47	RR	118/118 (100%)	0.54	5 (4%) 40 22	45, 69, 103, 116	0
47	YR	118/118 (100%)	0.35	1 (0%) 82 65	37, 53, 89, 129	0
48	RS	110/112 (98%)	0.56	5 (4%) 38 20	61, 98, 132, 151	0
48	YS	110/112 (98%)	0.26	4 (3%) 46 26	40, 72, 106, 130	0
49	RT	131/146 (89%)	0.29	3 (2%) 61 39	49, 78, 130, 166	0
49	YT	131/146 (89%)	0.25	4 (3%) 51 30	42, 70, 116, 148	0
50	RU	116/118 (98%)	0.59	3 (2%) 57 36	44, 81, 123, 134	0
50	YU	116/118 (98%)	0.16	1 (0%) 81 63	29, 49, 79, 115	0
51	RV	101/101 (100%)	0.29	4 (3%) 42 23	55, 91, 130, 172	0
51	YV	101/101 (100%)	0.03	1 (0%) 79 61	37, 62, 101, 168	0
52	RW	112/113 (99%)	0.39	2 (1%) 67 47	36, 64, 105, 138	0
52	YW	112/113 (99%)	0.16	2 (1%) 67 47	32, 50, 89, 184	0
53	RX	95/96 (98%)	0.54	5 (5%) 32 17	42, 75, 116, 140	0
53	YX	95/96 (98%)	0.24	4 (4%) 40 22	28, 56, 104, 134	0
54	RY	107/110 (97%)	0.81	7 (6%) 25 13	59, 98, 129, 162	0
54	YY	107/110 (97%)	0.35	4 (3%) 45 25	41, 73, 109, 157	0
55	RZ	178/206 (86%)	0.86	18 (10%) 12 6	82, 136, 202, 263	0
55	YZ	177/206 (85%)	0.77	27 (15%) 5 3	53, 108, 209, 266	0
All	All	20859/21590 (96%)	0.23	812 (3%) 43 24	21, 84, 164, 338	0

The worst 5 of 812 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	RA	2602	A	8.1
20	QT	9	ASN	7.8
35	YA	1091	G	7.2
20	XT	6	PRO	6.6
9	QI	126	SER	6.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
35	5MU	RA	1915	21/22	0.86	0.10	86,101,109,111	0
1	PSU	QA	516	20/21	0.87	0.10	94,102,120,123	0
1	PSU	XA	516	20/21	0.87	0.10	78,89,96,97	0
1	2MG	QA	1207	24/25	0.87	0.11	126,135,147,148	0
12	0TD	XL	92	10/11	0.87	0.14	65,73,88,113	0
1	5MC	QA	967	21/22	0.89	0.12	97,98,105,116	0
1	2MG	XA	1207	24/25	0.90	0.11	91,102,107,114	0
1	G7M	XA	527	24/25	0.90	0.12	64,72,87,114	0
35	PSU	RA	1911	20/21	0.91	0.09	72,85,93,99	0
1	M2G	QA	966	25/26	0.91	0.13	96,100,111,116	0
35	5MU	YA	1915	21/22	0.91	0.09	60,70,89,93	0
35	OMC	RA	1920	21/22	0.91	0.10	67,70,77,83	0
12	0TD	QL	92	10/11	0.92	0.21	131,143,166,185	0
35	PSU	RA	1917	20/21	0.92	0.08	84,91,97,106	0
1	5MC	XA	1404	21/22	0.92	0.12	51,52,66,72	0
35	PSU	YA	1917	20/21	0.93	0.08	59,70,97,100	0
1	G7M	QA	527	24/25	0.93	0.12	79,88,104,109	0
35	5MC	RA	1962	21/22	0.93	0.10	57,64,94,105	0
35	OMU	RA	2552	21/22	0.93	0.11	48,49,71,96	0
35	PSU	YA	1911	20/21	0.94	0.08	58,71,82,84	0
1	5MC	XA	967	21/22	0.94	0.11	86,94,104,108	0
35	5MU	YA	1939	21/22	0.94	0.10	37,44,55,61	0
35	5MC	RA	1942	21/22	0.94	0.08	61,74,92,94	0
1	5MC	QA	1407	21/22	0.94	0.10	68,70,78,81	0
1	4OC	QA	1402	22/23	0.94	0.10	77,82,90,101	0
1	UR3	QA	1498	21/22	0.95	0.10	68,69,75,86	0
1	UR3	XA	1498	21/22	0.95	0.10	55,57,75,88	0
1	MA6	XA	1518	24/25	0.95	0.11	52,59,86,88	0
35	5MU	RA	1939	21/22	0.95	0.10	53,61,75,83	0
1	5MC	QA	1404	21/22	0.95	0.09	67,68,69,70	0
1	5MC	XA	1400	21/22	0.95	0.09	65,75,89,94	0
1	5MC	QA	1400	21/22	0.95	0.09	78,79,92,100	0
35	2MA	RA	2503	23/24	0.95	0.12	45,46,50,65	0
1	5MC	XA	1407	21/22	0.95	0.09	50,51,62,70	0
35	OMU	YA	2552	21/22	0.95	0.09	35,43,55,65	0
35	PSU	RA	2605	20/21	0.95	0.10	47,48,65,66	0
35	PSU	YA	2605	20/21	0.95	0.09	35,38,53,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	M2G	XA	966	25/26	0.96	0.11	73,82,100,102	0
35	5MC	YA	1962	21/22	0.96	0.08	37,38,52,72	0
35	OMG	RA	2251	24/25	0.96	0.09	47,49,65,68	0
35	OMG	YA	2251	24/25	0.96	0.09	34,35,41,43	0
35	OMC	YA	1920	21/22	0.96	0.08	59,67,75,79	0
1	MA6	XA	1519	24/25	0.96	0.10	55,60,73,80	0
1	4OC	XA	1402	22/23	0.96	0.10	62,72,90,95	0
1	MA6	QA	1518	24/25	0.96	0.09	64,65,71,75	0
35	5MC	YA	1942	21/22	0.96	0.07	43,53,69,74	0
1	MA6	QA	1519	24/25	0.97	0.11	65,66,70,80	0
35	2MA	YA	2503	23/24	0.97	0.08	36,39,50,79	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3424	1/1	-0.12	0.53	121,121,121,121	0
56	MG	RA	3256	1/1	-0.02	0.52	96,96,96,96	0
56	MG	RA	3301	1/1	0.10	0.30	98,98,98,98	0
56	MG	RA	3189	1/1	0.11	0.24	86,86,86,86	0
56	MG	RA	3309	1/1	0.13	0.20	99,99,99,99	0
56	MG	RA	3205	1/1	0.19	0.43	136,136,136,136	0
56	MG	QA	1737	1/1	0.24	0.36	78,78,78,78	0
56	MG	RA	3666	1/1	0.25	0.28	116,116,116,116	0
56	MG	RA	3579	1/1	0.26	0.19	87,87,87,87	0
56	MG	RA	3369	1/1	0.26	0.34	119,119,119,119	0
56	MG	RA	3536	1/1	0.33	0.22	114,114,114,114	0
56	MG	RA	3450	1/1	0.34	0.55	94,94,94,94	0
56	MG	RB	205	1/1	0.34	0.17	75,75,75,75	0
56	MG	QA	1607	1/1	0.35	0.37	73,73,73,73	0
56	MG	QA	1658	1/1	0.36	0.24	91,91,91,91	0
56	MG	QA	1796	1/1	0.36	0.34	111,111,111,111	0
56	MG	XR	101	1/1	0.36	0.27	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3607	1/1	0.36	0.31	105,105,105,105	0
56	MG	RA	3159	1/1	0.37	0.63	97,97,97,97	0
56	MG	QE	201	1/1	0.37	0.39	114,114,114,114	0
56	MG	RA	3058	1/1	0.37	0.23	83,83,83,83	0
56	MG	RA	3400	1/1	0.37	0.36	88,88,88,88	0
56	MG	RA	3083	1/1	0.37	0.16	72,72,72,72	0
56	MG	RA	3272	1/1	0.37	0.19	51,51,51,51	0
56	MG	RA	3221	1/1	0.39	0.41	89,89,89,89	0
56	MG	RA	3381	1/1	0.40	0.43	87,87,87,87	0
56	MG	RA	3513	1/1	0.40	0.27	73,73,73,73	0
56	MG	RA	3053	1/1	0.40	0.51	108,108,108,108	0
56	MG	RA	3213	1/1	0.40	0.30	105,105,105,105	0
56	MG	RA	3214	1/1	0.41	0.36	105,105,105,105	0
56	MG	RA	3155	1/1	0.41	0.18	72,72,72,72	0
56	MG	RA	3153	1/1	0.42	0.61	127,127,127,127	0
56	MG	XA	1671	1/1	0.42	0.17	96,96,96,96	0
56	MG	QO	101	1/1	0.42	0.63	113,113,113,113	0
56	MG	YA	3024	1/1	0.42	0.23	102,102,102,102	0
56	MG	RA	3322	1/1	0.42	0.42	79,79,79,79	0
56	MG	RA	3069	1/1	0.43	0.71	144,144,144,144	0
56	MG	QA	1705	1/1	0.43	0.21	103,103,103,103	0
56	MG	RA	3096	1/1	0.43	0.28	102,102,102,102	0
56	MG	RA	3350	1/1	0.44	0.56	127,127,127,127	0
56	MG	RA	3591	1/1	0.47	0.42	74,74,74,74	0
56	MG	RA	3163	1/1	0.47	0.28	80,80,80,80	0
56	MG	XA	1718	1/1	0.47	0.42	116,116,116,116	0
56	MG	RA	3460	1/1	0.48	0.47	89,89,89,89	0
56	MG	XA	1723	1/1	0.48	0.26	72,72,72,72	0
56	MG	RA	3152	1/1	0.48	0.78	92,92,92,92	0
56	MG	RA	3011	1/1	0.48	0.41	106,106,106,106	0
56	MG	YA	3480	1/1	0.48	0.32	74,74,74,74	0
56	MG	QG	202	1/1	0.48	0.17	133,133,133,133	0
56	MG	XA	1781	1/1	0.49	0.36	92,92,92,92	0
56	MG	RA	3507	1/1	0.49	0.33	76,76,76,76	0
56	MG	RA	3100	1/1	0.49	0.25	144,144,144,144	0
56	MG	RA	3484	1/1	0.49	0.26	71,71,71,71	0
56	MG	RA	3673	1/1	0.49	0.49	91,91,91,91	0
56	MG	QA	1695	1/1	0.50	0.23	65,65,65,65	0
56	MG	RA	3138	1/1	0.50	0.27	96,96,96,96	0
56	MG	RA	3382	1/1	0.50	0.21	57,57,57,57	0
56	MG	XA	1670	1/1	0.51	0.22	90,90,90,90	0
56	MG	QA	1762	1/1	0.52	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3482	1/1	0.52	0.76	127,127,127,127	0
56	MG	RA	3103	1/1	0.52	0.19	59,59,59,59	0
56	MG	YA	3097	1/1	0.52	0.20	72,72,72,72	0
56	MG	RA	3182	1/1	0.52	0.23	94,94,94,94	0
56	MG	QV	102	1/1	0.52	0.19	92,92,92,92	0
56	MG	RA	3093	1/1	0.53	0.29	92,92,92,92	0
56	MG	RA	3326	1/1	0.53	0.22	67,67,67,67	0
56	MG	RA	3175	1/1	0.53	0.45	79,79,79,79	0
56	MG	QA	1618	1/1	0.53	0.28	86,86,86,86	0
56	MG	RA	3049	1/1	0.53	0.24	61,61,61,61	0
56	MG	RA	3405	1/1	0.54	0.16	71,71,71,71	0
56	MG	Y1	101	1/1	0.54	0.19	76,76,76,76	0
56	MG	RA	3682	1/1	0.54	0.27	84,84,84,84	0
56	MG	RA	3376	1/1	0.54	0.21	98,98,98,98	0
56	MG	RA	3104	1/1	0.54	0.46	89,89,89,89	0
56	MG	XJ	201	1/1	0.54	0.20	81,81,81,81	0
56	MG	RA	3178	1/1	0.55	0.20	97,97,97,97	0
56	MG	RB	204	1/1	0.55	0.17	140,140,140,140	0
56	MG	QA	1813	1/1	0.55	0.14	86,86,86,86	0
56	MG	RA	3458	1/1	0.55	0.23	97,97,97,97	0
56	MG	RA	3571	1/1	0.55	0.15	89,89,89,89	0
56	MG	RB	202	1/1	0.56	0.14	107,107,107,107	0
56	MG	RA	3110	1/1	0.56	0.12	83,83,83,83	0
56	MG	RA	3347	1/1	0.56	0.26	99,99,99,99	0
56	MG	RA	3403	1/1	0.57	0.36	84,84,84,84	0
56	MG	XA	1778	1/1	0.57	0.74	127,127,127,127	0
56	MG	QA	1676	1/1	0.57	0.31	81,81,81,81	0
56	MG	RA	3123	1/1	0.57	0.31	71,71,71,71	0
56	MG	RA	3080	1/1	0.57	0.48	108,108,108,108	0
56	MG	RA	3140	1/1	0.57	0.19	67,67,67,67	0
56	MG	QA	1659	1/1	0.57	0.17	95,95,95,95	0
56	MG	QA	1660	1/1	0.57	0.18	120,120,120,120	0
56	MG	RA	3631	1/1	0.57	0.35	69,69,69,69	0
56	MG	RA	3654	1/1	0.57	0.55	90,90,90,90	0
56	MG	YA	3668	1/1	0.57	0.29	109,109,109,109	0
56	MG	RA	3219	1/1	0.58	0.37	101,101,101,101	0
56	MG	RA	3072	1/1	0.58	0.82	109,109,109,109	0
56	MG	RA	3323	1/1	0.58	0.11	76,76,76,76	0
56	MG	QA	1728	1/1	0.58	0.19	90,90,90,90	0
56	MG	RA	3397	1/1	0.58	0.35	96,96,96,96	0
56	MG	RA	3589	1/1	0.58	0.33	117,117,117,117	0
56	MG	RA	3469	1/1	0.58	0.74	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3412	1/1	0.58	0.60	82,82,82,82	0
56	MG	YA	3426	1/1	0.58	0.14	67,67,67,67	0
56	MG	RA	3045	1/1	0.58	0.23	79,79,79,79	0
56	MG	RA	3647	1/1	0.58	0.70	121,121,121,121	0
56	MG	YA	3652	1/1	0.58	0.16	67,67,67,67	0
56	MG	QA	1787	1/1	0.58	0.18	140,140,140,140	0
56	MG	RA	3009	1/1	0.59	0.34	98,98,98,98	0
56	MG	QN	102	1/1	0.59	0.39	82,82,82,82	0
56	MG	YA	3253	1/1	0.59	0.26	41,41,41,41	0
56	MG	YG	201	1/1	0.59	0.15	111,111,111,111	0
56	MG	RA	3201	1/1	0.60	0.50	83,83,83,83	0
56	MG	QA	1646	1/1	0.60	0.11	80,80,80,80	0
56	MG	RA	3039	1/1	0.60	0.35	85,85,85,85	0
56	MG	RA	3392	1/1	0.60	0.18	103,103,103,103	0
56	MG	RA	3091	1/1	0.60	0.14	78,78,78,78	0
56	MG	RA	3134	1/1	0.61	0.21	63,63,63,63	0
56	MG	RA	3374	1/1	0.61	0.12	55,55,55,55	0
56	MG	QA	1770	1/1	0.61	0.21	68,68,68,68	0
56	MG	RA	3606	1/1	0.61	0.22	77,77,77,77	0
56	MG	RA	3060	1/1	0.61	0.23	84,84,84,84	0
56	MG	RA	3161	1/1	0.61	0.16	72,72,72,72	0
56	MG	RA	3143	1/1	0.61	0.20	94,94,94,94	0
56	MG	RA	3064	1/1	0.61	0.27	80,80,80,80	0
56	MG	RA	3481	1/1	0.62	0.38	102,102,102,102	0
56	MG	RA	3363	1/1	0.62	0.41	74,74,74,74	0
56	MG	RA	3313	1/1	0.62	0.16	84,84,84,84	0
56	MG	RA	3037	1/1	0.62	0.25	52,52,52,52	0
56	MG	RA	3029	1/1	0.62	0.19	99,99,99,99	0
56	MG	XA	1624	1/1	0.62	0.23	101,101,101,101	0
56	MG	YA	3387	1/1	0.62	0.38	90,90,90,90	0
56	MG	RA	3461	1/1	0.63	0.39	104,104,104,104	0
56	MG	RA	3462	1/1	0.63	0.23	44,44,44,44	0
56	MG	RA	3173	1/1	0.63	0.52	142,142,142,142	0
56	MG	RA	3477	1/1	0.63	0.33	100,100,100,100	0
56	MG	RA	3059	1/1	0.63	0.15	61,61,61,61	0
56	MG	QA	1633	1/1	0.63	0.19	104,104,104,104	0
56	MG	QA	1601	1/1	0.63	0.25	94,94,94,94	0
56	MG	RA	3055	1/1	0.63	0.14	91,91,91,91	0
56	MG	RA	3224	1/1	0.63	0.16	111,111,111,111	0
56	MG	XA	1782	1/1	0.63	0.16	73,73,73,73	0
56	MG	RA	3250	1/1	0.63	0.37	97,97,97,97	0
56	MG	QA	1718	1/1	0.63	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3454	1/1	0.64	0.11	51,51,51,51	0
56	MG	RA	3479	1/1	0.64	0.23	75,75,75,75	0
56	MG	XA	1700	1/1	0.64	0.26	90,90,90,90	0
56	MG	RA	3209	1/1	0.64	0.23	103,103,103,103	0
56	MG	QA	1694	1/1	0.64	0.23	87,87,87,87	0
56	MG	QA	1643	1/1	0.64	0.31	86,86,86,86	0
56	MG	RA	3497	1/1	0.64	0.13	56,56,56,56	0
56	MG	RA	3129	1/1	0.64	0.18	58,58,58,58	0
56	MG	RP	202	1/1	0.64	0.27	73,73,73,73	0
56	MG	RA	3015	1/1	0.64	0.28	70,70,70,70	0
56	MG	YB	207	1/1	0.64	0.34	77,77,77,77	0
56	MG	XA	1657	1/1	0.64	0.20	102,102,102,102	0
56	MG	QA	1662	1/1	0.65	0.15	42,42,42,42	0
56	MG	RA	3416	1/1	0.65	0.41	63,63,63,63	0
56	MG	RA	3330	1/1	0.65	0.16	57,57,57,57	0
56	MG	XA	1701	1/1	0.65	0.12	53,53,53,53	0
56	MG	QA	1688	1/1	0.65	0.30	98,98,98,98	0
56	MG	QA	1746	1/1	0.65	0.18	54,54,54,54	0
56	MG	RA	3237	1/1	0.65	0.19	111,111,111,111	0
56	MG	YA	3527	1/1	0.65	0.18	75,75,75,75	0
56	MG	QA	1791	1/1	0.65	0.11	83,83,83,83	0
56	MG	YA	3629	1/1	0.65	0.32	50,50,50,50	0
56	MG	XA	1607	1/1	0.65	0.19	95,95,95,95	0
56	MG	XA	1614	1/1	0.65	0.34	85,85,85,85	0
56	MG	RA	3401	1/1	0.65	0.52	124,124,124,124	0
56	MG	RA	3164	1/1	0.65	0.18	65,65,65,65	0
56	MG	RA	3677	1/1	0.66	0.14	47,47,47,47	0
56	MG	RA	3411	1/1	0.66	0.22	60,60,60,60	0
56	MG	QA	1673	1/1	0.66	0.16	95,95,95,95	0
56	MG	RA	3601	1/1	0.66	0.30	88,88,88,88	0
56	MG	RA	3417	1/1	0.66	0.94	125,125,125,125	0
56	MG	RA	3463	1/1	0.66	0.35	104,104,104,104	0
56	MG	QA	1808	1/1	0.66	0.23	65,65,65,65	0
56	MG	RA	3128	1/1	0.66	0.13	69,69,69,69	0
56	MG	YA	3616	1/1	0.66	0.15	84,84,84,84	0
56	MG	RA	3665	1/1	0.66	0.24	63,63,63,63	0
56	MG	YA	3643	1/1	0.66	0.25	67,67,67,67	0
56	MG	XA	1634	1/1	0.66	0.17	40,40,40,40	0
56	MG	RA	3160	1/1	0.66	0.23	51,51,51,51	0
56	MG	RA	3226	1/1	0.66	0.17	72,72,72,72	0
56	MG	YA	3052	1/1	0.66	0.16	48,48,48,48	0
56	MG	RA	3471	1/1	0.67	0.21	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RQ	201	1/1	0.67	0.38	73,73,73,73	0
56	MG	RA	3218	1/1	0.67	0.15	79,79,79,79	0
56	MG	QH	202	1/1	0.67	0.11	82,82,82,82	0
56	MG	RA	3318	1/1	0.67	0.40	73,73,73,73	0
56	MG	YA	3483	1/1	0.67	0.29	83,83,83,83	0
56	MG	RA	3383	1/1	0.67	0.50	88,88,88,88	0
56	MG	RA	3198	1/1	0.67	0.24	97,97,97,97	0
56	MG	XY	101	1/1	0.67	0.25	72,72,72,72	0
56	MG	RA	3066	1/1	0.67	0.37	98,98,98,98	0
56	MG	RA	3421	1/1	0.67	0.26	59,59,59,59	0
56	MG	RA	3204	1/1	0.67	0.38	97,97,97,97	0
56	MG	RB	209	1/1	0.67	0.13	63,63,63,63	0
56	MG	YA	3152	1/1	0.67	0.31	81,81,81,81	0
56	MG	YA	3160	1/1	0.67	0.36	102,102,102,102	0
56	MG	XA	1649	1/1	0.68	0.26	96,96,96,96	0
56	MG	XA	1653	1/1	0.68	0.21	93,93,93,93	0
56	MG	RA	3483	1/1	0.68	0.25	69,69,69,69	0
56	MG	YA	3547	1/1	0.68	0.44	74,74,74,74	0
56	MG	RA	3192	1/1	0.68	0.48	85,85,85,85	0
56	MG	QA	1616	1/1	0.68	0.14	58,58,58,58	0
56	MG	RA	3514	1/1	0.69	0.42	108,108,108,108	0
56	MG	RA	3526	1/1	0.69	0.51	110,110,110,110	0
56	MG	RA	3113	1/1	0.69	0.26	69,69,69,69	0
56	MG	RA	3657	1/1	0.69	0.32	65,65,65,65	0
56	MG	YA	3027	1/1	0.69	0.17	70,70,70,70	0
56	MG	RA	3395	1/1	0.69	0.41	85,85,85,85	0
56	MG	RA	3026	1/1	0.69	0.15	63,63,63,63	0
56	MG	QA	1665	1/1	0.69	0.10	65,65,65,65	0
56	MG	RA	3499	1/1	0.69	0.53	90,90,90,90	0
56	MG	QA	1754	1/1	0.69	0.23	89,89,89,89	0
56	MG	YA	3310	1/1	0.69	0.13	5,5,5,5	0
56	MG	RA	3706	1/1	0.69	0.23	94,94,94,94	0
56	MG	QA	1792	1/1	0.69	0.20	74,74,74,74	0
56	MG	RA	3391	1/1	0.70	0.10	55,55,55,55	0
56	MG	RA	3360	1/1	0.70	0.18	67,67,67,67	0
56	MG	RA	3592	1/1	0.70	0.22	58,58,58,58	0
56	MG	YA	3444	1/1	0.70	0.30	54,54,54,54	0
56	MG	RA	3474	1/1	0.70	0.26	71,71,71,71	0
56	MG	QA	1627	1/1	0.70	0.10	54,54,54,54	0
56	MG	QA	1804	1/1	0.70	0.21	85,85,85,85	0
56	MG	RA	3075	1/1	0.70	0.33	55,55,55,55	0
56	MG	RA	3119	1/1	0.71	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3707	1/1	0.71	0.12	49,49,49,49	0
56	MG	XA	1623	1/1	0.71	0.12	71,71,71,71	0
56	MG	RA	3170	1/1	0.71	0.20	78,78,78,78	0
56	MG	RA	3184	1/1	0.71	0.22	78,78,78,78	0
56	MG	RA	3448	1/1	0.71	0.19	75,75,75,75	0
56	MG	RA	3186	1/1	0.71	0.13	50,50,50,50	0
56	MG	YA	3348	1/1	0.71	0.21	75,75,75,75	0
56	MG	RA	3642	1/1	0.71	0.16	84,84,84,84	0
56	MG	RP	203	1/1	0.71	0.20	60,60,60,60	0
56	MG	RA	3387	1/1	0.71	0.15	43,43,43,43	0
56	MG	RV	201	1/1	0.71	0.13	68,68,68,68	0
56	MG	YA	3186	1/1	0.72	0.14	62,62,62,62	0
56	MG	XA	1673	1/1	0.72	0.22	77,77,77,77	0
56	MG	RA	3057	1/1	0.72	0.23	75,75,75,75	0
56	MG	RA	3051	1/1	0.72	0.10	109,109,109,109	0
56	MG	XA	1706	1/1	0.72	0.32	87,87,87,87	0
56	MG	QA	1715	1/1	0.72	0.35	82,82,82,82	0
56	MG	RA	3639	1/1	0.72	0.21	55,55,55,55	0
56	MG	RA	3509	1/1	0.72	0.33	77,77,77,77	0
56	MG	RA	3426	1/1	0.72	0.19	78,78,78,78	0
56	MG	RA	3441	1/1	0.72	0.29	89,89,89,89	0
56	MG	RA	3139	1/1	0.72	0.20	62,62,62,62	0
56	MG	RA	3662	1/1	0.72	0.36	70,70,70,70	0
56	MG	RA	3087	1/1	0.72	0.25	88,88,88,88	0
56	MG	RA	3545	1/1	0.72	0.34	90,90,90,90	0
56	MG	RA	3566	1/1	0.72	0.20	46,46,46,46	0
56	MG	RA	3408	1/1	0.72	0.34	74,74,74,74	0
56	MG	RA	3455	1/1	0.72	0.31	82,82,82,82	0
56	MG	RA	3457	1/1	0.72	0.13	53,53,53,53	0
56	MG	QA	1689	1/1	0.72	0.20	52,52,52,52	0
56	MG	RA	3380	1/1	0.72	0.20	62,62,62,62	0
56	MG	QA	1630	1/1	0.73	0.13	92,92,92,92	0
56	MG	QA	1812	1/1	0.73	0.09	73,73,73,73	0
56	MG	RA	3126	1/1	0.73	0.12	75,75,75,75	0
56	MG	RA	3106	1/1	0.73	0.11	51,51,51,51	0
56	MG	YA	3017	1/1	0.73	0.14	68,68,68,68	0
56	MG	YA	3365	1/1	0.73	0.24	78,78,78,78	0
56	MG	RA	3151	1/1	0.73	0.12	58,58,58,58	0
56	MG	QA	1703	1/1	0.73	0.73	82,82,82,82	0
56	MG	RA	3644	1/1	0.73	0.20	67,67,67,67	0
56	MG	YA	3697	1/1	0.73	0.42	66,66,66,66	0
56	MG	RA	3007	1/1	0.73	0.37	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3249	1/1	0.73	0.32	84,84,84,84	0
56	MG	RA	3609	1/1	0.74	0.22	69,69,69,69	0
56	MG	QA	1773	1/1	0.74	0.14	51,51,51,51	0
56	MG	RA	3632	1/1	0.74	0.24	48,48,48,48	0
56	MG	RA	3032	1/1	0.74	0.30	95,95,95,95	0
56	MG	XA	1714	1/1	0.74	0.14	45,45,45,45	0
56	MG	YA	3051	1/1	0.74	0.35	58,58,58,58	0
56	MG	XA	1625	1/1	0.74	0.24	79,79,79,79	0
56	MG	YA	3514	1/1	0.74	0.35	85,85,85,85	0
56	MG	YA	3074	1/1	0.74	0.15	39,39,39,39	0
56	MG	QA	1649	1/1	0.74	0.19	115,115,115,115	0
56	MG	YA	3131	1/1	0.74	0.28	87,87,87,87	0
56	MG	XA	1770	1/1	0.74	0.26	87,87,87,87	0
56	MG	YA	3159	1/1	0.74	0.18	75,75,75,75	0
56	MG	RA	3560	1/1	0.74	0.26	72,72,72,72	0
56	MG	YA	3165	1/1	0.74	0.13	54,54,54,54	0
56	MG	RA	3414	1/1	0.74	0.40	91,91,91,91	0
56	MG	YA	3678	1/1	0.74	0.16	70,70,70,70	0
56	MG	RA	3689	1/1	0.74	0.18	66,66,66,66	0
56	MG	RA	3377	1/1	0.74	0.24	73,73,73,73	0
56	MG	YB	215	1/1	0.74	0.12	42,42,42,42	0
56	MG	XA	1604	1/1	0.74	0.19	91,91,91,91	0
56	MG	RA	3542	1/1	0.75	0.13	27,27,27,27	0
56	MG	RA	3242	1/1	0.75	0.15	34,34,34,34	0
56	MG	RA	3246	1/1	0.75	0.38	65,65,65,65	0
56	MG	QA	1655	1/1	0.75	0.22	90,90,90,90	0
56	MG	XE	201	1/1	0.75	0.15	51,51,51,51	0
56	MG	YA	3383	1/1	0.75	0.14	51,51,51,51	0
56	MG	RA	3393	1/1	0.75	0.31	46,46,46,46	0
56	MG	RA	3054	1/1	0.75	0.19	72,72,72,72	0
56	MG	QE	203	1/1	0.75	0.17	71,71,71,71	0
56	MG	YA	3432	1/1	0.75	0.32	79,79,79,79	0
56	MG	QA	1636	1/1	0.75	0.10	70,70,70,70	0
56	MG	YA	3470	1/1	0.75	0.39	93,93,93,93	0
56	MG	YA	3014	1/1	0.75	0.21	48,48,48,48	0
56	MG	RA	3183	1/1	0.75	0.36	99,99,99,99	0
56	MG	RA	3597	1/1	0.75	0.16	46,46,46,46	0
56	MG	QA	1795	1/1	0.75	0.40	84,84,84,84	0
56	MG	RA	3404	1/1	0.75	0.08	47,47,47,47	0
56	MG	RA	3135	1/1	0.75	0.20	98,98,98,98	0
56	MG	YA	3066	1/1	0.75	0.43	103,103,103,103	0
56	MG	QA	1632	1/1	0.75	0.11	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3633	1/1	0.75	0.31	41,41,41,41	0
56	MG	RA	3410	1/1	0.75	0.32	68,68,68,68	0
56	MG	YA	3111	1/1	0.75	0.22	58,58,58,58	0
56	MG	YA	3119	1/1	0.75	0.43	90,90,90,90	0
56	MG	XA	1702	1/1	0.75	0.23	67,67,67,67	0
56	MG	RA	3085	1/1	0.75	0.14	81,81,81,81	0
56	MG	RA	3518	1/1	0.75	0.23	53,53,53,53	0
56	MG	QA	1820	1/1	0.75	0.13	81,81,81,81	0
56	MG	RA	3027	1/1	0.75	0.68	92,92,92,92	0
56	MG	YR	202	1/1	0.75	0.14	44,44,44,44	0
56	MG	XA	1660	1/1	0.76	0.22	96,96,96,96	0
56	MG	XA	1787	1/1	0.76	0.11	94,94,94,94	0
56	MG	QA	1642	1/1	0.76	0.31	68,68,68,68	0
56	MG	YA	3499	1/1	0.76	0.41	78,78,78,78	0
56	MG	RA	3442	1/1	0.76	0.19	67,67,67,67	0
56	MG	XA	1602	1/1	0.76	0.20	66,66,66,66	0
56	MG	R5	103	1/1	0.76	0.13	63,63,63,63	0
56	MG	QE	204	1/1	0.76	0.10	60,60,60,60	0
56	MG	YA	3177	1/1	0.76	0.15	42,42,42,42	0
56	MG	RA	3625	1/1	0.76	0.31	59,59,59,59	0
56	MG	RA	3534	1/1	0.76	0.34	64,64,64,64	0
56	MG	RA	3535	1/1	0.76	0.21	47,47,47,47	0
56	MG	YA	3649	1/1	0.76	0.26	46,46,46,46	0
56	MG	RA	3670	1/1	0.76	0.10	60,60,60,60	0
56	MG	YA	3664	1/1	0.76	0.32	85,85,85,85	0
56	MG	RF	304	1/1	0.76	0.20	55,55,55,55	0
56	MG	XA	1745	1/1	0.76	0.35	74,74,74,74	0
56	MG	RP	201	1/1	0.76	0.28	60,60,60,60	0
56	MG	RA	3094	1/1	0.76	0.17	90,90,90,90	0
56	MG	YB	212	1/1	0.76	0.16	38,38,38,38	0
56	MG	YA	3082	1/1	0.76	0.09	73,73,73,73	0
56	MG	YA	3092	1/1	0.76	0.19	65,65,65,65	0
56	MG	RA	3511	1/1	0.76	0.78	87,87,87,87	0
56	MG	RA	3298	1/1	0.77	0.11	49,49,49,49	0
56	MG	RA	3473	1/1	0.77	0.36	87,87,87,87	0
56	MG	RA	3187	1/1	0.77	0.24	93,93,93,93	0
56	MG	RA	3303	1/1	0.77	0.30	79,79,79,79	0
56	MG	RA	3220	1/1	0.77	0.09	54,54,54,54	0
56	MG	RA	3480	1/1	0.77	0.29	65,65,65,65	0
56	MG	QA	1771	1/1	0.77	0.16	43,43,43,43	0
56	MG	RA	3063	1/1	0.77	0.41	101,101,101,101	0
56	MG	XA	1661	1/1	0.77	0.30	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3029	1/1	0.77	0.20	47,47,47,47	0
56	MG	RA	3052	1/1	0.77	0.11	78,78,78,78	0
56	MG	YA	3490	1/1	0.77	0.25	37,37,37,37	0
56	MG	RA	3227	1/1	0.77	0.16	71,71,71,71	0
56	MG	RA	3228	1/1	0.77	0.18	75,75,75,75	0
56	MG	XA	1696	1/1	0.77	0.12	42,42,42,42	0
56	MG	R9	102	1/1	0.77	0.11	64,64,64,64	0
56	MG	YA	3555	1/1	0.77	0.14	47,47,47,47	0
56	MG	RA	3239	1/1	0.77	0.21	66,66,66,66	0
56	MG	RA	3620	1/1	0.77	0.31	33,33,33,33	0
56	MG	QA	1656	1/1	0.77	0.27	134,134,134,134	0
56	MG	RA	3351	1/1	0.77	0.20	41,41,41,41	0
56	MG	QK	201	1/1	0.77	0.11	73,73,73,73	0
56	MG	YA	3648	1/1	0.77	0.39	80,80,80,80	0
56	MG	YA	3151	1/1	0.77	0.18	70,70,70,70	0
56	MG	QA	1617	1/1	0.77	0.12	73,73,73,73	0
56	MG	RA	3640	1/1	0.77	0.12	50,50,50,50	0
56	MG	XA	1758	1/1	0.77	0.17	52,52,52,52	0
56	MG	RA	3077	1/1	0.77	0.16	50,50,50,50	0
56	MG	RA	3373	1/1	0.77	0.24	73,73,73,73	0
56	MG	QA	1608	1/1	0.77	0.12	87,87,87,87	0
56	MG	YA	3211	1/1	0.77	0.14	66,66,66,66	0
56	MG	YA	3247	1/1	0.77	0.33	77,77,77,77	0
56	MG	RA	3468	1/1	0.77	0.22	39,39,39,39	0
56	MG	QA	1740	1/1	0.77	0.30	100,100,100,100	0
56	MG	RA	3041	1/1	0.78	0.23	85,85,85,85	0
56	MG	YA	3080	1/1	0.78	0.11	65,65,65,65	0
56	MG	RA	3353	1/1	0.78	0.19	38,38,38,38	0
56	MG	RH	202	1/1	0.78	0.13	136,136,136,136	0
56	MG	XA	1772	1/1	0.78	0.20	71,71,71,71	0
56	MG	XA	1656	1/1	0.78	0.13	67,67,67,67	0
56	MG	RN	202	1/1	0.78	0.26	89,89,89,89	0
56	MG	RA	3311	1/1	0.78	0.54	71,71,71,71	0
56	MG	YA	3147	1/1	0.78	0.13	59,59,59,59	0
56	MG	RA	3611	1/1	0.78	0.31	58,58,58,58	0
56	MG	RA	3208	1/1	0.78	0.12	73,73,73,73	0
56	MG	RA	3472	1/1	0.78	0.16	77,77,77,77	0
56	MG	R0	103	1/1	0.78	0.27	96,96,96,96	0
56	MG	XA	1680	1/1	0.78	0.26	65,65,65,65	0
56	MG	YA	3625	1/1	0.78	0.21	40,40,40,40	0
56	MG	QA	1774	1/1	0.78	0.15	108,108,108,108	0
56	MG	Y7	101	1/1	0.78	0.26	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3201	1/1	0.78	0.44	89,89,89,89	0
56	MG	RA	3259	1/1	0.78	0.11	102,102,102,102	0
56	MG	RA	3181	1/1	0.78	0.11	51,51,51,51	0
56	MG	RA	3012	1/1	0.78	0.14	65,65,65,65	0
56	MG	YA	3288	1/1	0.78	0.13	56,56,56,56	0
56	MG	XA	1618	1/1	0.78	0.09	104,104,104,104	0
56	MG	QP	101	1/1	0.78	0.22	88,88,88,88	0
56	MG	XA	1717	1/1	0.78	0.15	70,70,70,70	0
56	MG	YA	3703	1/1	0.78	0.18	56,56,56,56	0
56	MG	RA	3594	1/1	0.78	0.14	43,43,43,43	0
56	MG	YA	3058	1/1	0.78	0.19	63,63,63,63	0
56	MG	YB	214	1/1	0.78	0.21	51,51,51,51	0
56	MG	YA	3396	1/1	0.78	0.16	74,74,74,74	0
56	MG	YD	301	1/1	0.78	0.12	78,78,78,78	0
56	MG	YA	3400	1/1	0.78	0.44	113,113,113,113	0
56	MG	YQ	201	1/1	0.78	0.40	65,65,65,65	0
56	MG	QA	1631	1/1	0.78	0.08	122,122,122,122	0
56	MG	RA	3390	1/1	0.79	0.21	68,68,68,68	0
56	MG	RA	3690	1/1	0.79	0.20	47,47,47,47	0
56	MG	QA	1641	1/1	0.79	0.11	78,78,78,78	0
56	MG	RA	3359	1/1	0.79	0.14	64,64,64,64	0
56	MG	QA	1644	1/1	0.79	0.30	150,150,150,150	0
56	MG	QA	1698	1/1	0.79	0.21	71,71,71,71	0
56	MG	RA	3365	1/1	0.79	0.13	66,66,66,66	0
56	MG	QA	1805	1/1	0.79	0.23	70,70,70,70	0
56	MG	RB	215	1/1	0.79	0.13	58,58,58,58	0
56	MG	QA	1747	1/1	0.79	0.22	65,65,65,65	0
56	MG	RA	3641	1/1	0.79	0.47	110,110,110,110	0
56	MG	RA	3084	1/1	0.79	0.25	64,64,64,64	0
56	MG	YA	3205	1/1	0.79	0.09	52,52,52,52	0
56	MG	XA	1678	1/1	0.79	0.22	91,91,91,91	0
56	MG	QA	1749	1/1	0.79	0.15	113,113,113,113	0
56	MG	XA	1682	1/1	0.79	0.29	85,85,85,85	0
56	MG	XA	1685	1/1	0.79	0.12	77,77,77,77	0
56	MG	YA	3657	1/1	0.79	0.30	76,76,76,76	0
56	MG	XA	1689	1/1	0.79	0.23	59,59,59,59	0
56	MG	QA	1675	1/1	0.79	0.11	45,45,45,45	0
56	MG	RA	3485	1/1	0.79	0.12	59,59,59,59	0
56	MG	RA	3378	1/1	0.79	0.15	43,43,43,43	0
56	MG	QA	1736	1/1	0.79	0.25	39,39,39,39	0
56	MG	RA	3503	1/1	0.79	0.17	63,63,63,63	0
56	MG	YA	3073	1/1	0.79	0.25	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3222	1/1	0.79	0.12	69,69,69,69	0
56	MG	YA	3414	1/1	0.79	0.13	49,49,49,49	0
56	MG	RA	3596	1/1	0.79	0.21	52,52,52,52	0
56	MG	RA	3269	1/1	0.79	0.50	80,80,80,80	0
56	MG	RA	3120	1/1	0.79	0.10	57,57,57,57	0
56	MG	RA	3070	1/1	0.79	0.12	66,66,66,66	0
56	MG	QA	1640	1/1	0.80	0.19	104,104,104,104	0
56	MG	RA	3697	1/1	0.80	0.34	74,74,74,74	0
56	MG	XA	1750	1/1	0.80	0.27	82,82,82,82	0
56	MG	YA	3103	1/1	0.80	0.12	59,59,59,59	0
56	MG	YA	3478	1/1	0.80	0.41	89,89,89,89	0
56	MG	RA	3528	1/1	0.80	0.18	34,34,34,34	0
56	MG	RA	3533	1/1	0.80	0.16	35,35,35,35	0
56	MG	YA	3128	1/1	0.80	0.23	69,69,69,69	0
56	MG	RA	3628	1/1	0.80	0.19	40,40,40,40	0
56	MG	YA	3512	1/1	0.80	0.44	69,69,69,69	0
56	MG	QA	1776	1/1	0.80	0.22	47,47,47,47	0
56	MG	RA	3197	1/1	0.80	0.15	83,83,83,83	0
56	MG	RB	207	1/1	0.80	0.18	67,67,67,67	0
56	MG	RA	3034	1/1	0.80	0.09	35,35,35,35	0
56	MG	XA	1668	1/1	0.80	0.30	87,87,87,87	0
56	MG	RB	214	1/1	0.80	0.14	63,63,63,63	0
56	MG	RA	3001	1/1	0.80	0.20	43,43,43,43	0
56	MG	YA	3179	1/1	0.80	0.24	47,47,47,47	0
56	MG	RA	3145	1/1	0.80	0.09	68,68,68,68	0
56	MG	YA	3197	1/1	0.80	0.19	58,58,58,58	0
56	MG	RA	3453	1/1	0.80	0.16	50,50,50,50	0
56	MG	RA	3375	1/1	0.80	0.39	71,71,71,71	0
56	MG	RA	3132	1/1	0.80	0.15	56,56,56,56	0
56	MG	YA	3226	1/1	0.80	0.28	79,79,79,79	0
56	MG	RA	3268	1/1	0.80	0.18	80,80,80,80	0
56	MG	YA	3666	1/1	0.80	0.28	86,86,86,86	0
56	MG	RA	3333	1/1	0.80	0.17	32,32,32,32	0
56	MG	YA	3265	1/1	0.80	0.36	58,58,58,58	0
56	MG	RA	3406	1/1	0.80	0.20	35,35,35,35	0
56	MG	RA	3379	1/1	0.80	0.11	44,44,44,44	0
56	MG	RA	3341	1/1	0.80	0.20	39,39,39,39	0
56	MG	RA	3185	1/1	0.80	0.23	70,70,70,70	0
56	MG	QA	1693	1/1	0.80	0.12	59,59,59,59	0
56	MG	RA	3210	1/1	0.80	0.25	115,115,115,115	0
56	MG	YA	3070	1/1	0.80	0.15	67,67,67,67	0
56	MG	YF	301	1/1	0.80	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3229	1/1	0.80	0.19	77,77,77,77	0
56	MG	YI	201	1/1	0.80	0.09	83,83,83,83	0
56	MG	QA	1668	1/1	0.80	0.17	70,70,70,70	0
56	MG	XA	1721	1/1	0.80	0.30	64,64,64,64	0
56	MG	QA	1663	1/1	0.81	0.15	61,61,61,61	0
56	MG	YA	3032	1/1	0.81	0.13	24,24,24,24	0
56	MG	YA	3399	1/1	0.81	0.15	50,50,50,50	0
56	MG	YA	3045	1/1	0.81	0.07	38,38,38,38	0
56	MG	YA	3406	1/1	0.81	0.17	43,43,43,43	0
56	MG	RA	3547	1/1	0.81	0.28	57,57,57,57	0
56	MG	RA	3554	1/1	0.81	0.21	52,52,52,52	0
56	MG	YA	3420	1/1	0.81	0.18	54,54,54,54	0
56	MG	YA	3057	1/1	0.81	0.17	48,48,48,48	0
56	MG	QA	1619	1/1	0.81	0.23	77,77,77,77	0
56	MG	XA	1692	1/1	0.81	0.12	58,58,58,58	0
56	MG	YA	3456	1/1	0.81	0.10	47,47,47,47	0
56	MG	QA	1816	1/1	0.81	0.16	108,108,108,108	0
56	MG	QA	1605	1/1	0.81	0.13	48,48,48,48	0
56	MG	RA	3174	1/1	0.81	0.16	102,102,102,102	0
56	MG	QD	303	1/1	0.81	0.22	90,90,90,90	0
56	MG	RA	3024	1/1	0.81	0.10	44,44,44,44	0
56	MG	YA	3498	1/1	0.81	0.10	23,23,23,23	0
56	MG	RA	3510	1/1	0.81	0.20	80,80,80,80	0
56	MG	XA	1606	1/1	0.81	0.15	50,50,50,50	0
56	MG	RA	3025	1/1	0.81	0.38	109,109,109,109	0
56	MG	RA	3671	1/1	0.81	0.32	79,79,79,79	0
56	MG	QA	1786	1/1	0.81	0.12	45,45,45,45	0
56	MG	XA	1740	1/1	0.81	0.33	69,69,69,69	0
56	MG	XA	1621	1/1	0.81	0.12	41,41,41,41	0
56	MG	XA	1622	1/1	0.81	0.38	88,88,88,88	0
56	MG	RA	3429	1/1	0.81	0.15	39,39,39,39	0
56	MG	RA	3438	1/1	0.81	0.31	91,91,91,91	0
56	MG	RA	3245	1/1	0.81	0.14	57,57,57,57	0
56	MG	YA	3642	1/1	0.81	0.22	54,54,54,54	0
56	MG	XA	1628	1/1	0.81	0.34	111,111,111,111	0
56	MG	XA	1780	1/1	0.81	0.30	57,57,57,57	0
56	MG	QA	1678	1/1	0.81	0.10	70,70,70,70	0
56	MG	XA	1636	1/1	0.81	0.09	53,53,53,53	0
56	MG	RA	3531	1/1	0.81	0.11	35,35,35,35	0
56	MG	YA	3660	1/1	0.81	0.20	52,52,52,52	0
56	MG	RA	3615	1/1	0.81	0.23	125,125,125,125	0
56	MG	XE	202	1/1	0.81	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3532	1/1	0.81	0.41	69,69,69,69	0
56	MG	RA	3622	1/1	0.81	0.18	58,58,58,58	0
56	MG	R3	101	1/1	0.81	0.12	78,78,78,78	0
56	MG	R5	102	1/1	0.81	0.23	80,80,80,80	0
56	MG	QA	1671	1/1	0.81	0.08	48,48,48,48	0
56	MG	YA	3010	1/1	0.81	0.16	54,54,54,54	0
56	MG	YA	3276	1/1	0.81	0.17	45,45,45,45	0
56	MG	YA	3012	1/1	0.81	0.18	47,47,47,47	0
56	MG	YB	219	1/1	0.81	0.21	52,52,52,52	0
56	MG	QG	201	1/1	0.81	0.12	65,65,65,65	0
56	MG	YA	3331	1/1	0.81	0.21	50,50,50,50	0
56	MG	RA	3638	1/1	0.81	0.25	70,70,70,70	0
56	MG	YA	3360	1/1	0.81	0.20	32,32,32,32	0
56	MG	QA	1811	1/1	0.81	0.14	54,54,54,54	0
56	MG	RE	301	1/1	0.81	0.38	95,95,95,95	0
56	MG	YA	3068	1/1	0.82	0.51	98,98,98,98	0
56	MG	XA	1615	1/1	0.82	0.09	56,56,56,56	0
56	MG	QA	1803	1/1	0.82	0.17	75,75,75,75	0
56	MG	RA	3399	1/1	0.82	0.18	51,51,51,51	0
56	MG	QA	1652	1/1	0.82	0.41	115,115,115,115	0
56	MG	XA	1736	1/1	0.82	0.12	52,52,52,52	0
56	MG	YA	3428	1/1	0.82	0.28	87,87,87,87	0
56	MG	YA	3085	1/1	0.82	0.30	56,56,56,56	0
56	MG	QA	1653	1/1	0.82	0.10	99,99,99,99	0
56	MG	QA	1733	1/1	0.82	0.11	41,41,41,41	0
56	MG	RA	3372	1/1	0.82	0.22	40,40,40,40	0
56	MG	XA	1627	1/1	0.82	0.19	61,61,61,61	0
56	MG	QH	201	1/1	0.82	0.30	54,54,54,54	0
56	MG	RA	3223	1/1	0.82	0.18	71,71,71,71	0
56	MG	XA	1773	1/1	0.82	0.27	51,51,51,51	0
56	MG	YA	3496	1/1	0.82	0.10	45,45,45,45	0
56	MG	QA	1750	1/1	0.82	0.08	43,43,43,43	0
56	MG	XA	1638	1/1	0.82	0.07	82,82,82,82	0
56	MG	XA	1643	1/1	0.82	0.21	51,51,51,51	0
56	MG	RA	3225	1/1	0.82	0.10	64,64,64,64	0
56	MG	RA	3188	1/1	0.82	0.28	90,90,90,90	0
56	MG	YA	3531	1/1	0.82	0.11	52,52,52,52	0
56	MG	YA	3164	1/1	0.82	0.16	76,76,76,76	0
56	MG	RA	3038	1/1	0.82	0.36	95,95,95,95	0
56	MG	RA	3415	1/1	0.82	0.41	80,80,80,80	0
56	MG	QA	1691	1/1	0.82	0.11	60,60,60,60	0
56	MG	YA	3623	1/1	0.82	0.29	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3133	1/1	0.82	0.12	58,58,58,58	0
56	MG	YA	3189	1/1	0.82	0.17	74,74,74,74	0
56	MG	RD	306	1/1	0.82	0.15	64,64,64,64	0
56	MG	RA	3420	1/1	0.82	0.40	116,116,116,116	0
56	MG	QA	1789	1/1	0.82	0.20	70,70,70,70	0
56	MG	YA	3006	1/1	0.82	0.26	47,47,47,47	0
56	MG	YA	3215	1/1	0.82	0.16	65,65,65,65	0
56	MG	RA	3165	1/1	0.82	0.24	56,56,56,56	0
56	MG	RN	201	1/1	0.82	0.10	86,86,86,86	0
56	MG	XA	1679	1/1	0.82	0.27	55,55,55,55	0
56	MG	RA	3168	1/1	0.82	0.18	71,71,71,71	0
56	MG	QA	1761	1/1	0.82	0.31	79,79,79,79	0
56	MG	RA	3650	1/1	0.82	0.28	55,55,55,55	0
56	MG	YA	3674	1/1	0.82	0.23	63,63,63,63	0
56	MG	YA	3289	1/1	0.82	0.26	44,44,44,44	0
56	MG	YA	3687	1/1	0.82	0.22	107,107,107,107	0
56	MG	YA	3689	1/1	0.82	0.12	59,59,59,59	0
56	MG	RA	3653	1/1	0.82	0.25	57,57,57,57	0
56	MG	YA	3702	1/1	0.82	0.20	27,27,27,27	0
56	MG	YA	3313	1/1	0.82	0.16	78,78,78,78	0
56	MG	RA	3137	1/1	0.82	0.18	52,52,52,52	0
56	MG	RA	3014	1/1	0.82	0.24	88,88,88,88	0
56	MG	QA	1637	1/1	0.82	0.08	45,45,45,45	0
56	MG	RA	3495	1/1	0.82	0.18	69,69,69,69	0
56	MG	YA	3372	1/1	0.82	0.12	63,63,63,63	0
56	MG	YA	3375	1/1	0.82	0.10	23,23,23,23	0
56	MG	YA	3377	1/1	0.82	0.34	65,65,65,65	0
56	MG	YA	3056	1/1	0.82	0.21	85,85,85,85	0
56	MG	YG	202	1/1	0.82	0.15	78,78,78,78	0
56	MG	QA	1602	1/1	0.82	0.44	84,84,84,84	0
56	MG	QA	1741	1/1	0.82	0.09	36,36,36,36	0
56	MG	RA	3451	1/1	0.82	0.29	54,54,54,54	0
56	MG	RA	3629	1/1	0.83	0.15	33,33,33,33	0
56	MG	RA	3294	1/1	0.83	0.11	54,54,54,54	0
56	MG	RA	3446	1/1	0.83	0.27	62,62,62,62	0
56	MG	YA	3492	1/1	0.83	0.28	42,42,42,42	0
56	MG	RA	3633	1/1	0.83	0.23	32,32,32,32	0
56	MG	RA	3162	1/1	0.83	0.35	67,67,67,67	0
56	MG	R7	103	1/1	0.83	0.15	59,59,59,59	0
56	MG	RA	3056	1/1	0.83	0.11	67,67,67,67	0
56	MG	RA	3452	1/1	0.83	0.29	107,107,107,107	0
56	MG	RA	3238	1/1	0.83	0.27	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3028	1/1	0.83	0.28	119,119,119,119	0
56	MG	YA	3064	1/1	0.83	0.13	64,64,64,64	0
56	MG	RA	3074	1/1	0.83	0.10	54,54,54,54	0
56	MG	RA	3648	1/1	0.83	0.21	55,55,55,55	0
56	MG	RA	3586	1/1	0.83	0.17	64,64,64,64	0
56	MG	RA	3149	1/1	0.83	0.13	40,40,40,40	0
56	MG	RO	201	1/1	0.83	0.13	45,45,45,45	0
56	MG	QA	1625	1/1	0.83	0.08	38,38,38,38	0
56	MG	RA	3459	1/1	0.83	0.13	57,57,57,57	0
56	MG	YA	3634	1/1	0.83	0.14	11,11,11,11	0
56	MG	YA	3084	1/1	0.83	0.28	87,87,87,87	0
56	MG	YA	3354	1/1	0.83	0.30	47,47,47,47	0
56	MG	YA	3358	1/1	0.83	0.19	44,44,44,44	0
56	MG	RA	3195	1/1	0.83	0.17	64,64,64,64	0
56	MG	QA	1685	1/1	0.83	0.22	36,36,36,36	0
56	MG	YA	3656	1/1	0.83	0.22	34,34,34,34	0
56	MG	RA	3251	1/1	0.83	0.15	47,47,47,47	0
56	MG	YA	3373	1/1	0.83	0.26	47,47,47,47	0
56	MG	RA	3254	1/1	0.83	0.26	50,50,50,50	0
56	MG	YA	3104	1/1	0.83	0.21	50,50,50,50	0
56	MG	YA	3106	1/1	0.83	0.09	52,52,52,52	0
56	MG	QA	1677	1/1	0.83	0.19	37,37,37,37	0
56	MG	YA	3388	1/1	0.83	0.27	86,86,86,86	0
56	MG	YA	3684	1/1	0.83	0.28	70,70,70,70	0
56	MG	YA	3115	1/1	0.83	0.11	69,69,69,69	0
56	MG	RA	3061	1/1	0.83	0.14	49,49,49,49	0
56	MG	XT	201	1/1	0.83	0.13	55,55,55,55	0
56	MG	XA	1683	1/1	0.83	0.16	67,67,67,67	0
56	MG	RA	3264	1/1	0.83	0.07	48,48,48,48	0
56	MG	YA	3148	1/1	0.83	0.10	35,35,35,35	0
56	MG	Y6	102	1/1	0.83	0.35	54,54,54,54	0
56	MG	XA	1610	1/1	0.83	0.10	73,73,73,73	0
56	MG	RA	3035	1/1	0.83	0.29	75,75,75,75	0
56	MG	QD	305	1/1	0.83	0.15	67,67,67,67	0
56	MG	YA	3436	1/1	0.83	0.31	59,59,59,59	0
56	MG	YA	3439	1/1	0.83	0.11	64,64,64,64	0
56	MG	QA	1815	1/1	0.83	0.07	75,75,75,75	0
56	MG	RA	3285	1/1	0.83	0.12	70,70,70,70	0
56	MG	YA	3457	1/1	0.83	0.08	47,47,47,47	0
56	MG	YA	3174	1/1	0.83	0.07	64,64,64,64	0
56	MG	RA	3290	1/1	0.83	0.10	59,59,59,59	0
56	MG	RV	202	1/1	0.84	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3604	1/1	0.84	0.13	67,67,67,67	0
56	MG	YA	3185	1/1	0.84	0.14	50,50,50,50	0
56	MG	RA	3669	1/1	0.84	0.26	82,82,82,82	0
56	MG	QA	1766	1/1	0.84	0.06	63,63,63,63	0
56	MG	YA	3488	1/1	0.84	0.23	26,26,26,26	0
56	MG	YA	3192	1/1	0.84	0.10	49,49,49,49	0
56	MG	RA	3608	1/1	0.84	0.13	57,57,57,57	0
56	MG	RA	3130	1/1	0.84	0.12	54,54,54,54	0
56	MG	YA	3043	1/1	0.84	0.20	37,37,37,37	0
56	MG	R3	102	1/1	0.84	0.19	83,83,83,83	0
56	MG	XA	1710	1/1	0.84	0.20	51,51,51,51	0
56	MG	YA	3221	1/1	0.84	0.12	34,34,34,34	0
56	MG	QA	1680	1/1	0.84	0.16	58,58,58,58	0
56	MG	RA	3686	1/1	0.84	0.10	65,65,65,65	0
56	MG	RA	3619	1/1	0.84	0.22	38,38,38,38	0
56	MG	RA	3315	1/1	0.84	0.19	74,74,74,74	0
56	MG	YA	3271	1/1	0.84	0.08	28,28,28,28	0
56	MG	RA	3018	1/1	0.84	0.12	43,43,43,43	0
56	MG	XA	1724	1/1	0.84	0.25	55,55,55,55	0
56	MG	QA	1782	1/1	0.84	0.58	80,80,80,80	0
56	MG	YA	3307	1/1	0.84	0.11	41,41,41,41	0
56	MG	RA	3252	1/1	0.84	0.21	33,33,33,33	0
56	MG	RA	3708	1/1	0.84	0.41	56,56,56,56	0
56	MG	RA	3105	1/1	0.84	0.09	41,41,41,41	0
56	MG	YA	3336	1/1	0.84	0.15	25,25,25,25	0
56	MG	YA	3343	1/1	0.84	0.17	32,32,32,32	0
56	MG	QL	202	1/1	0.84	0.13	54,54,54,54	0
56	MG	RA	3044	1/1	0.84	0.12	55,55,55,55	0
56	MG	RA	3498	1/1	0.84	0.33	69,69,69,69	0
56	MG	RA	3563	1/1	0.84	0.27	43,43,43,43	0
56	MG	XA	1774	1/1	0.84	0.21	51,51,51,51	0
56	MG	QA	1744	1/1	0.84	0.23	68,68,68,68	0
56	MG	QA	1817	1/1	0.84	0.15	52,52,52,52	0
56	MG	RA	3385	1/1	0.84	0.15	42,42,42,42	0
56	MG	RA	3584	1/1	0.84	0.26	107,107,107,107	0
56	MG	QF	202	1/1	0.84	0.24	82,82,82,82	0
56	MG	RG	204	1/1	0.84	0.07	74,74,74,74	0
56	MG	RA	3588	1/1	0.84	0.15	40,40,40,40	0
56	MG	XF	201	1/1	0.84	0.19	80,80,80,80	0
56	MG	QA	1818	1/1	0.84	0.34	71,71,71,71	0
56	MG	YA	3146	1/1	0.84	0.09	18,18,18,18	0
56	MG	RA	3177	1/1	0.84	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3408	1/1	0.84	0.10	35,35,35,35	0
56	MG	XA	1672	1/1	0.84	0.20	108,108,108,108	0
56	MG	RA	3512	1/1	0.84	0.10	38,38,38,38	0
56	MG	RA	3233	1/1	0.84	0.36	83,83,83,83	0
56	MG	RA	3092	1/1	0.84	0.10	76,76,76,76	0
56	MG	RA	3658	1/1	0.84	0.19	49,49,49,49	0
56	MG	RA	3127	1/1	0.84	0.08	53,53,53,53	0
56	MG	RU	202	1/1	0.84	0.53	63,63,63,63	0
56	MG	YA	3169	1/1	0.84	0.22	65,65,65,65	0
56	MG	YA	3170	1/1	0.84	0.14	77,77,77,77	0
56	MG	YA	3451	1/1	0.84	0.14	45,45,45,45	0
56	MG	QA	1614	1/1	0.84	0.09	82,82,82,82	0
56	MG	YA	3244	1/1	0.85	0.24	47,47,47,47	0
56	MG	RH	201	1/1	0.85	0.06	68,68,68,68	0
56	MG	RA	3443	1/1	0.85	0.31	49,49,49,49	0
56	MG	YA	3256	1/1	0.85	0.16	47,47,47,47	0
56	MG	YA	3263	1/1	0.85	0.18	43,43,43,43	0
56	MG	QA	1764	1/1	0.85	0.09	41,41,41,41	0
56	MG	RA	3111	1/1	0.85	0.23	97,97,97,97	0
56	MG	XA	1663	1/1	0.85	0.20	50,50,50,50	0
56	MG	RA	3663	1/1	0.85	0.45	90,90,90,90	0
56	MG	QV	105	1/1	0.85	0.19	80,80,80,80	0
56	MG	YA	3301	1/1	0.85	0.38	58,58,58,58	0
56	MG	RA	3262	1/1	0.85	0.09	54,54,54,54	0
56	MG	YA	3096	1/1	0.85	0.06	40,40,40,40	0
56	MG	XA	1783	1/1	0.85	0.12	46,46,46,46	0
56	MG	YA	3321	1/1	0.85	0.18	66,66,66,66	0
56	MG	RA	3031	1/1	0.85	0.13	53,53,53,53	0
56	MG	RA	3265	1/1	0.85	0.18	56,56,56,56	0
56	MG	XA	1677	1/1	0.85	0.06	41,41,41,41	0
56	MG	QA	1650	1/1	0.85	0.07	60,60,60,60	0
56	MG	QA	1711	1/1	0.85	0.25	49,49,49,49	0
56	MG	RA	3546	1/1	0.85	0.30	81,81,81,81	0
56	MG	YA	3639	1/1	0.85	0.17	45,45,45,45	0
56	MG	XA	1681	1/1	0.85	0.29	43,43,43,43	0
56	MG	XV	101	1/1	0.85	0.17	41,41,41,41	0
56	MG	RA	3680	1/1	0.85	0.22	59,59,59,59	0
56	MG	RA	3335	1/1	0.85	0.31	41,41,41,41	0
56	MG	QA	1634	1/1	0.85	0.13	70,70,70,70	0
56	MG	RA	3278	1/1	0.85	0.08	37,37,37,37	0
56	MG	QA	1696	1/1	0.85	0.20	49,49,49,49	0
56	MG	RA	3505	1/1	0.85	0.34	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3011	1/1	0.85	0.23	75,75,75,75	0
56	MG	RA	3506	1/1	0.85	0.12	39,39,39,39	0
56	MG	RA	3575	1/1	0.85	0.23	51,51,51,51	0
56	MG	YA	3670	1/1	0.85	0.30	101,101,101,101	0
56	MG	XA	1620	1/1	0.85	0.14	46,46,46,46	0
56	MG	RA	3635	1/1	0.85	0.10	45,45,45,45	0
56	MG	YA	3407	1/1	0.85	0.14	44,44,44,44	0
56	MG	YA	3171	1/1	0.85	0.20	61,61,61,61	0
56	MG	RA	3288	1/1	0.85	0.20	74,74,74,74	0
56	MG	RA	3581	1/1	0.85	0.20	54,54,54,54	0
56	MG	YA	3418	1/1	0.85	0.26	55,55,55,55	0
56	MG	RA	3389	1/1	0.85	0.27	72,72,72,72	0
56	MG	YA	3423	1/1	0.85	0.21	29,29,29,29	0
56	MG	RA	3585	1/1	0.85	0.23	53,53,53,53	0
56	MG	RA	3243	1/1	0.85	0.24	51,51,51,51	0
56	MG	RB	212	1/1	0.85	0.08	53,53,53,53	0
56	MG	QA	1692	1/1	0.85	0.21	71,71,71,71	0
56	MG	R7	101	1/1	0.85	0.20	68,68,68,68	0
56	MG	YE	302	1/1	0.85	0.39	82,82,82,82	0
56	MG	QA	1775	1/1	0.85	0.10	82,82,82,82	0
56	MG	QA	1679	1/1	0.85	0.13	35,35,35,35	0
56	MG	YA	3059	1/1	0.85	0.18	42,42,42,42	0
56	MG	QA	1801	1/1	0.85	0.11	66,66,66,66	0
56	MG	YP	201	1/1	0.85	0.14	32,32,32,32	0
56	MG	RA	3108	1/1	0.85	0.11	60,60,60,60	0
56	MG	XA	1759	1/1	0.85	0.11	71,71,71,71	0
56	MG	QA	1667	1/1	0.86	0.13	55,55,55,55	0
56	MG	YA	3429	1/1	0.86	0.11	43,43,43,43	0
56	MG	RA	3434	1/1	0.86	0.12	25,25,25,25	0
56	MG	RA	3437	1/1	0.86	0.30	42,42,42,42	0
56	MG	YA	3193	1/1	0.86	0.12	44,44,44,44	0
56	MG	YA	3443	1/1	0.86	0.14	43,43,43,43	0
56	MG	RA	3260	1/1	0.86	0.13	47,47,47,47	0
56	MG	RA	3386	1/1	0.86	0.12	44,44,44,44	0
56	MG	YA	3046	1/1	0.86	0.28	51,51,51,51	0
56	MG	YA	3210	1/1	0.86	0.15	77,77,77,77	0
56	MG	XA	1603	1/1	0.86	0.16	92,92,92,92	0
56	MG	YA	3474	1/1	0.86	0.23	42,42,42,42	0
56	MG	RA	3043	1/1	0.86	0.17	52,52,52,52	0
56	MG	RA	3082	1/1	0.86	0.42	86,86,86,86	0
56	MG	YA	3225	1/1	0.86	0.15	48,48,48,48	0
56	MG	RA	3444	1/1	0.86	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3235	1/1	0.86	0.15	30,30,30,30	0
56	MG	QD	301	1/1	0.86	0.23	56,56,56,56	0
56	MG	QA	1806	1/1	0.86	0.31	85,85,85,85	0
56	MG	YA	3252	1/1	0.86	0.19	22,22,22,22	0
56	MG	RA	3046	1/1	0.86	0.10	38,38,38,38	0
56	MG	YA	3507	1/1	0.86	0.20	81,81,81,81	0
56	MG	YA	3508	1/1	0.86	0.18	38,38,38,38	0
56	MG	YA	3254	1/1	0.86	0.13	40,40,40,40	0
56	MG	RA	3598	1/1	0.86	0.13	30,30,30,30	0
56	MG	YA	3522	1/1	0.86	0.30	31,31,31,31	0
56	MG	RA	3048	1/1	0.86	0.11	46,46,46,46	0
56	MG	RA	3357	1/1	0.86	0.22	47,47,47,47	0
56	MG	YA	3542	1/1	0.86	0.15	28,28,28,28	0
56	MG	YA	3546	1/1	0.86	0.31	73,73,73,73	0
56	MG	YA	3267	1/1	0.86	0.22	37,37,37,37	0
56	MG	RA	3169	1/1	0.86	0.15	93,93,93,93	0
56	MG	YA	3577	1/1	0.86	0.17	29,29,29,29	0
56	MG	YA	3595	1/1	0.86	0.16	52,52,52,52	0
56	MG	RA	3398	1/1	0.86	0.41	97,97,97,97	0
56	MG	RA	3199	1/1	0.86	0.17	45,45,45,45	0
56	MG	YA	3622	1/1	0.86	0.12	18,18,18,18	0
56	MG	RA	3699	1/1	0.86	0.31	96,96,96,96	0
56	MG	XA	1762	1/1	0.86	0.29	36,36,36,36	0
56	MG	YA	3627	1/1	0.86	0.19	37,37,37,37	0
56	MG	YA	3306	1/1	0.86	0.25	37,37,37,37	0
56	MG	RA	3700	1/1	0.86	0.17	72,72,72,72	0
56	MG	RA	3704	1/1	0.86	0.18	40,40,40,40	0
56	MG	RA	3456	1/1	0.86	0.31	63,63,63,63	0
56	MG	RA	3115	1/1	0.86	0.08	46,46,46,46	0
56	MG	RA	3364	1/1	0.86	0.20	37,37,37,37	0
56	MG	RA	3203	1/1	0.86	0.41	95,95,95,95	0
56	MG	YA	3338	1/1	0.86	0.29	33,33,33,33	0
56	MG	RA	3529	1/1	0.86	0.23	34,34,34,34	0
56	MG	RA	3367	1/1	0.86	0.15	69,69,69,69	0
56	MG	RA	3118	1/1	0.86	0.23	98,98,98,98	0
56	MG	RA	3371	1/1	0.86	0.29	117,117,117,117	0
56	MG	YA	3126	1/1	0.86	0.30	72,72,72,72	0
56	MG	YA	3364	1/1	0.86	0.20	34,34,34,34	0
56	MG	RA	3141	1/1	0.86	0.20	49,49,49,49	0
56	MG	YA	3367	1/1	0.86	0.12	61,61,61,61	0
56	MG	RA	3466	1/1	0.86	0.12	29,29,29,29	0
56	MG	YA	3140	1/1	0.86	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3374	1/1	0.86	0.16	84,84,84,84	0
56	MG	RA	3206	1/1	0.86	0.31	89,89,89,89	0
56	MG	XA	1665	1/1	0.86	0.15	81,81,81,81	0
56	MG	QD	304	1/1	0.86	0.13	73,73,73,73	0
56	MG	RD	307	1/1	0.86	0.08	73,73,73,73	0
56	MG	RD	308	1/1	0.86	0.19	75,75,75,75	0
56	MG	QA	1726	1/1	0.86	0.14	61,61,61,61	0
56	MG	RA	3122	1/1	0.86	0.16	90,90,90,90	0
56	MG	RA	3212	1/1	0.86	0.27	70,70,70,70	0
56	MG	QA	1727	1/1	0.86	0.17	46,46,46,46	0
56	MG	YB	216	1/1	0.86	0.21	46,46,46,46	0
56	MG	RA	3418	1/1	0.86	0.21	56,56,56,56	0
56	MG	RA	3478	1/1	0.86	0.21	32,32,32,32	0
56	MG	RA	3006	1/1	0.86	0.13	72,72,72,72	0
56	MG	RA	3569	1/1	0.86	0.41	72,72,72,72	0
56	MG	YA	3415	1/1	0.86	0.70	84,84,84,84	0
56	MG	YA	3416	1/1	0.86	0.12	43,43,43,43	0
56	MG	QE	202	1/1	0.86	0.21	109,109,109,109	0
56	MG	QA	1638	1/1	0.86	0.39	103,103,103,103	0
56	MG	YA	3181	1/1	0.86	0.15	47,47,47,47	0
56	MG	RA	3040	1/1	0.86	0.10	40,40,40,40	0
59	ZN	R4	101	1/1	0.86	0.11	285,285,285,285	0
56	MG	RA	3236	1/1	0.87	0.26	80,80,80,80	0
56	MG	YA	3100	1/1	0.87	0.09	41,41,41,41	0
56	MG	RA	3270	1/1	0.87	0.26	73,73,73,73	0
56	MG	RA	3530	1/1	0.87	0.12	101,101,101,101	0
56	MG	XA	1792	1/1	0.87	0.16	70,70,70,70	0
56	MG	YA	3280	1/1	0.87	0.20	15,15,15,15	0
56	MG	QA	1710	1/1	0.87	0.12	51,51,51,51	0
56	MG	RA	3432	1/1	0.87	0.22	88,88,88,88	0
56	MG	YA	3500	1/1	0.87	0.23	30,30,30,30	0
56	MG	QA	1735	1/1	0.87	0.17	34,34,34,34	0
56	MG	RA	3354	1/1	0.87	0.23	56,56,56,56	0
56	MG	RR	201	1/1	0.87	0.22	74,74,74,74	0
56	MG	YA	3129	1/1	0.87	0.16	47,47,47,47	0
56	MG	RT	202	1/1	0.87	0.15	82,82,82,82	0
56	MG	QA	1639	1/1	0.87	0.18	57,57,57,57	0
56	MG	YA	3327	1/1	0.87	0.31	39,39,39,39	0
56	MG	YA	3533	1/1	0.87	0.12	40,40,40,40	0
56	MG	YA	3534	1/1	0.87	0.11	18,18,18,18	0
56	MG	QA	1697	1/1	0.87	0.25	58,58,58,58	0
56	MG	RA	3047	1/1	0.87	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	Y3	101	1/1	0.87	0.24	38,38,38,38	0
56	MG	YA	3149	1/1	0.87	0.42	77,77,77,77	0
56	MG	RA	3097	1/1	0.87	0.35	77,77,77,77	0
56	MG	YA	3582	1/1	0.87	0.27	59,59,59,59	0
56	MG	YA	3586	1/1	0.87	0.08	44,44,44,44	0
56	MG	YA	3349	1/1	0.87	0.29	70,70,70,70	0
56	MG	RA	3297	1/1	0.87	0.16	38,38,38,38	0
56	MG	YA	3154	1/1	0.87	0.20	57,57,57,57	0
56	MG	YA	3157	1/1	0.87	0.13	39,39,39,39	0
56	MG	YA	3361	1/1	0.87	0.12	53,53,53,53	0
56	MG	RA	3693	1/1	0.87	0.32	77,77,77,77	0
56	MG	QA	1654	1/1	0.87	0.12	92,92,92,92	0
56	MG	RA	3550	1/1	0.87	0.33	70,70,70,70	0
56	MG	RA	3248	1/1	0.87	0.25	38,38,38,38	0
56	MG	RA	3702	1/1	0.87	0.11	41,41,41,41	0
56	MG	RA	3193	1/1	0.87	0.17	90,90,90,90	0
56	MG	YA	3023	1/1	0.87	0.47	90,90,90,90	0
56	MG	RA	3308	1/1	0.87	0.12	25,25,25,25	0
56	MG	YA	3644	1/1	0.87	0.22	38,38,38,38	0
56	MG	YA	3647	1/1	0.87	0.41	54,54,54,54	0
56	MG	RA	3101	1/1	0.87	0.32	60,60,60,60	0
56	MG	RA	3102	1/1	0.87	0.18	48,48,48,48	0
56	MG	QA	1701	1/1	0.87	0.17	67,67,67,67	0
56	MG	QA	1622	1/1	0.87	0.11	60,60,60,60	0
56	MG	YA	3398	1/1	0.87	0.13	43,43,43,43	0
56	MG	YA	3658	1/1	0.87	0.24	36,36,36,36	0
56	MG	QA	1670	1/1	0.87	0.13	37,37,37,37	0
56	MG	YA	3662	1/1	0.87	0.22	39,39,39,39	0
56	MG	YA	3188	1/1	0.87	0.11	48,48,48,48	0
56	MG	QA	1768	1/1	0.87	0.23	51,51,51,51	0
56	MG	RA	3643	1/1	0.87	0.11	44,44,44,44	0
56	MG	RA	3413	1/1	0.87	0.32	72,72,72,72	0
56	MG	YA	3194	1/1	0.87	0.21	50,50,50,50	0
56	MG	YA	3413	1/1	0.87	0.24	46,46,46,46	0
56	MG	YA	3679	1/1	0.87	0.15	49,49,49,49	0
56	MG	XA	1633	1/1	0.87	0.06	45,45,45,45	0
56	MG	XA	1744	1/1	0.87	0.17	72,72,72,72	0
56	MG	RA	3508	1/1	0.87	0.13	50,50,50,50	0
56	MG	QA	1769	1/1	0.87	0.12	68,68,68,68	0
56	MG	XA	1752	1/1	0.87	0.12	38,38,38,38	0
56	MG	YA	3214	1/1	0.87	0.25	66,66,66,66	0
56	MG	YB	202	1/1	0.87	0.14	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YB	204	1/1	0.87	0.10	46,46,46,46	0
56	MG	YA	3424	1/1	0.87	0.30	70,70,70,70	0
56	MG	YB	210	1/1	0.87	0.20	44,44,44,44	0
56	MG	XA	1755	1/1	0.87	0.14	45,45,45,45	0
56	MG	YA	3216	1/1	0.87	0.07	38,38,38,38	0
56	MG	RA	3156	1/1	0.87	0.14	76,76,76,76	0
56	MG	RA	3328	1/1	0.87	0.25	40,40,40,40	0
56	MG	XA	1646	1/1	0.87	0.21	92,92,92,92	0
56	MG	YA	3234	1/1	0.87	0.12	60,60,60,60	0
56	MG	RA	3158	1/1	0.87	0.05	63,63,63,63	0
56	MG	YA	3243	1/1	0.87	0.15	48,48,48,48	0
56	MG	RA	3231	1/1	0.87	0.30	91,91,91,91	0
56	MG	RA	3464	1/1	0.87	0.35	118,118,118,118	0
56	MG	RG	201	1/1	0.87	0.07	79,79,79,79	0
56	MG	YA	3460	1/1	0.87	0.24	48,48,48,48	0
56	MG	RA	3660	1/1	0.87	0.39	62,62,62,62	0
56	MG	RA	3267	1/1	0.87	0.26	45,45,45,45	0
56	MG	RA	3089	1/1	0.87	0.07	35,35,35,35	0
56	MG	YA	3316	1/1	0.88	0.31	44,44,44,44	0
56	MG	YA	3510	1/1	0.88	0.21	49,49,49,49	0
56	MG	YA	3026	1/1	0.88	0.14	43,43,43,43	0
56	MG	YA	3513	1/1	0.88	0.09	38,38,38,38	0
56	MG	QA	1651	1/1	0.88	0.26	91,91,91,91	0
56	MG	YA	3519	1/1	0.88	0.14	48,48,48,48	0
56	MG	XA	1650	1/1	0.88	0.08	54,54,54,54	0
56	MG	YA	3031	1/1	0.88	0.24	58,58,58,58	0
56	MG	YA	3528	1/1	0.88	0.16	18,18,18,18	0
56	MG	YA	3161	1/1	0.88	0.13	65,65,65,65	0
56	MG	RA	3445	1/1	0.88	0.12	51,51,51,51	0
56	MG	YA	3034	1/1	0.88	0.19	41,41,41,41	0
56	MG	YA	3167	1/1	0.88	0.33	51,51,51,51	0
56	MG	QA	1664	1/1	0.88	0.15	60,60,60,60	0
56	MG	RA	3261	1/1	0.88	0.07	36,36,36,36	0
56	MG	YA	3552	1/1	0.88	0.19	16,16,16,16	0
56	MG	RA	3307	1/1	0.88	0.12	35,35,35,35	0
56	MG	RA	3131	1/1	0.88	0.23	58,58,58,58	0
56	MG	YA	3579	1/1	0.88	0.13	43,43,43,43	0
56	MG	RA	3645	1/1	0.88	0.20	42,42,42,42	0
56	MG	YA	3585	1/1	0.88	0.14	45,45,45,45	0
56	MG	RA	3202	1/1	0.88	0.13	49,49,49,49	0
56	MG	YA	3180	1/1	0.88	0.20	57,57,57,57	0
56	MG	RW	201	1/1	0.88	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3611	1/1	0.88	0.15	49,49,49,49	0
56	MG	RA	3065	1/1	0.88	0.15	66,66,66,66	0
56	MG	RA	3709	1/1	0.88	0.37	120,120,120,120	0
56	MG	QA	1729	1/1	0.88	0.27	36,36,36,36	0
56	MG	QA	1788	1/1	0.88	0.11	51,51,51,51	0
56	MG	YA	3378	1/1	0.88	0.12	95,95,95,95	0
56	MG	QA	1763	1/1	0.88	0.11	41,41,41,41	0
56	MG	XA	1608	1/1	0.88	0.40	71,71,71,71	0
56	MG	RA	3321	1/1	0.88	0.23	54,54,54,54	0
56	MG	YA	3196	1/1	0.88	0.14	70,70,70,70	0
56	MG	RA	3366	1/1	0.88	0.68	98,98,98,98	0
56	MG	YA	3077	1/1	0.88	0.21	69,69,69,69	0
56	MG	RA	3422	1/1	0.88	0.17	46,46,46,46	0
56	MG	YA	3206	1/1	0.88	0.26	77,77,77,77	0
56	MG	QA	1748	1/1	0.88	0.13	38,38,38,38	0
56	MG	RA	3073	1/1	0.88	0.26	104,104,104,104	0
56	MG	R3	103	1/1	0.88	0.41	111,111,111,111	0
56	MG	RA	3327	1/1	0.88	0.29	68,68,68,68	0
56	MG	XA	1691	1/1	0.88	0.32	51,51,51,51	0
56	MG	QA	1730	1/1	0.88	0.30	73,73,73,73	0
56	MG	YA	3659	1/1	0.88	0.10	39,39,39,39	0
56	MG	RA	3564	1/1	0.88	0.12	41,41,41,41	0
56	MG	RA	3230	1/1	0.88	0.27	41,41,41,41	0
56	MG	YA	3228	1/1	0.88	0.28	63,63,63,63	0
56	MG	RA	3467	1/1	0.88	0.12	55,55,55,55	0
56	MG	QA	1714	1/1	0.88	0.19	76,76,76,76	0
56	MG	YA	3669	1/1	0.88	0.12	56,56,56,56	0
56	MG	YA	3109	1/1	0.88	0.06	54,54,54,54	0
56	MG	YA	3427	1/1	0.88	0.16	44,44,44,44	0
56	MG	XA	1703	1/1	0.88	0.21	55,55,55,55	0
56	MG	XA	1705	1/1	0.88	0.18	50,50,50,50	0
56	MG	YA	3680	1/1	0.88	0.20	133,133,133,133	0
56	MG	YA	3248	1/1	0.88	0.32	52,52,52,52	0
56	MG	YA	3118	1/1	0.88	0.12	34,34,34,34	0
56	MG	YA	3688	1/1	0.88	0.15	51,51,51,51	0
56	MG	XA	1629	1/1	0.88	0.23	71,71,71,71	0
56	MG	YA	3002	1/1	0.88	0.13	45,45,45,45	0
56	MG	RA	3255	1/1	0.88	0.29	35,35,35,35	0
56	MG	YA	3447	1/1	0.88	0.15	42,42,42,42	0
56	MG	YA	3706	1/1	0.88	0.19	82,82,82,82	0
56	MG	YA	3259	1/1	0.88	0.06	24,24,24,24	0
56	MG	YA	3262	1/1	0.88	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3008	1/1	0.88	0.07	67,67,67,67	0
56	MG	YA	3130	1/1	0.88	0.07	28,28,28,28	0
56	MG	RA	3470	1/1	0.88	0.31	88,88,88,88	0
56	MG	YA	3473	1/1	0.88	0.12	66,66,66,66	0
56	MG	RA	3179	1/1	0.88	0.14	51,51,51,51	0
56	MG	YA	3475	1/1	0.88	0.27	47,47,47,47	0
56	MG	YA	3142	1/1	0.88	0.14	39,39,39,39	0
56	MG	RA	3687	1/1	0.88	0.38	148,148,148,148	0
56	MG	YD	307	1/1	0.88	0.19	40,40,40,40	0
56	MG	RA	3583	1/1	0.88	0.07	44,44,44,44	0
56	MG	XA	1645	1/1	0.88	0.16	67,67,67,67	0
56	MG	YA	3296	1/1	0.88	0.08	39,39,39,39	0
56	MG	YA	3019	1/1	0.88	0.19	67,67,67,67	0
56	MG	YA	3150	1/1	0.88	0.11	50,50,50,50	0
56	MG	RA	3344	1/1	0.88	0.24	41,41,41,41	0
56	MG	XA	1648	1/1	0.88	0.08	67,67,67,67	0
56	MG	YA	3311	1/1	0.88	0.22	55,55,55,55	0
56	MG	YA	3153	1/1	0.88	0.10	52,52,52,52	0
59	ZN	Y4	101	1/1	0.88	0.07	284,284,284,284	0
56	MG	YA	3342	1/1	0.89	0.29	23,23,23,23	0
56	MG	QA	1819	1/1	0.89	0.19	46,46,46,46	0
56	MG	RQ	202	1/1	0.89	0.11	45,45,45,45	0
56	MG	XA	1756	1/1	0.89	0.09	35,35,35,35	0
56	MG	RQ	204	1/1	0.89	0.08	49,49,49,49	0
56	MG	XA	1659	1/1	0.89	0.08	40,40,40,40	0
56	MG	YA	3359	1/1	0.89	0.28	31,31,31,31	0
56	MG	YA	3183	1/1	0.89	0.08	39,39,39,39	0
56	MG	RA	3296	1/1	0.89	0.21	45,45,45,45	0
56	MG	QI	201	1/1	0.89	0.11	79,79,79,79	0
56	MG	RT	204	1/1	0.89	0.08	57,57,57,57	0
56	MG	RU	201	1/1	0.89	0.07	43,43,43,43	0
56	MG	YA	3565	1/1	0.89	0.15	45,45,45,45	0
56	MG	YA	3191	1/1	0.89	0.13	38,38,38,38	0
56	MG	XA	1666	1/1	0.89	0.07	59,59,59,59	0
56	MG	RA	3099	1/1	0.89	0.06	40,40,40,40	0
56	MG	RA	3425	1/1	0.89	0.17	53,53,53,53	0
56	MG	QA	1778	1/1	0.89	0.08	50,50,50,50	0
56	MG	YA	3588	1/1	0.89	0.17	45,45,45,45	0
56	MG	RV	203	1/1	0.89	0.18	56,56,56,56	0
56	MG	YA	3596	1/1	0.89	0.24	50,50,50,50	0
56	MG	YA	3605	1/1	0.89	0.23	74,74,74,74	0
56	MG	YA	3198	1/1	0.89	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3385	1/1	0.89	0.35	62,62,62,62	0
56	MG	YA	3199	1/1	0.89	0.19	84,84,84,84	0
56	MG	RA	3427	1/1	0.89	0.16	39,39,39,39	0
56	MG	XA	1784	1/1	0.89	0.20	33,33,33,33	0
56	MG	XA	1785	1/1	0.89	0.20	38,38,38,38	0
56	MG	XA	1674	1/1	0.89	0.15	28,28,28,28	0
56	MG	RA	3346	1/1	0.89	0.20	65,65,65,65	0
56	MG	YA	3401	1/1	0.89	0.16	41,41,41,41	0
56	MG	YA	3403	1/1	0.89	0.09	53,53,53,53	0
56	MG	QA	1780	1/1	0.89	0.08	43,43,43,43	0
56	MG	RA	3537	1/1	0.89	0.10	23,23,23,23	0
56	MG	RA	3539	1/1	0.89	0.13	26,26,26,26	0
56	MG	RA	3541	1/1	0.89	0.16	30,30,30,30	0
56	MG	YA	3223	1/1	0.89	0.17	34,34,34,34	0
56	MG	RB	203	1/1	0.89	0.07	68,68,68,68	0
56	MG	RA	3602	1/1	0.89	0.37	66,66,66,66	0
56	MG	YA	3651	1/1	0.89	0.27	43,43,43,43	0
56	MG	RA	3656	1/1	0.89	0.27	57,57,57,57	0
56	MG	YA	3113	1/1	0.89	0.25	72,72,72,72	0
56	MG	XV	103	1/1	0.89	0.11	40,40,40,40	0
56	MG	QA	1687	1/1	0.89	0.06	40,40,40,40	0
56	MG	RA	3501	1/1	0.89	0.12	41,41,41,41	0
56	MG	RA	3247	1/1	0.89	0.09	46,46,46,46	0
56	MG	RA	3088	1/1	0.89	0.08	77,77,77,77	0
56	MG	QA	1623	1/1	0.89	0.54	86,86,86,86	0
56	MG	RA	3407	1/1	0.89	0.11	59,59,59,59	0
56	MG	RA	3090	1/1	0.89	0.10	52,52,52,52	0
56	MG	YA	3135	1/1	0.89	0.27	56,56,56,56	0
56	MG	YA	3139	1/1	0.89	0.08	38,38,38,38	0
56	MG	YA	3261	1/1	0.89	0.20	67,67,67,67	0
56	MG	RA	3076	1/1	0.89	0.18	72,72,72,72	0
56	MG	YA	3445	1/1	0.89	0.06	67,67,67,67	0
56	MG	YA	3141	1/1	0.89	0.10	58,58,58,58	0
56	MG	RA	3232	1/1	0.89	0.24	69,69,69,69	0
56	MG	RF	301	1/1	0.89	0.23	72,72,72,72	0
56	MG	YA	3268	1/1	0.89	0.25	77,77,77,77	0
56	MG	RA	3282	1/1	0.89	0.24	25,25,25,25	0
56	MG	YA	3691	1/1	0.89	0.20	44,44,44,44	0
56	MG	XA	1711	1/1	0.89	0.16	46,46,46,46	0
56	MG	YA	3472	1/1	0.89	0.13	45,45,45,45	0
56	MG	XA	1632	1/1	0.89	0.14	34,34,34,34	0
56	MG	YA	3705	1/1	0.89	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3284	1/1	0.89	0.25	15,15,15,15	0
56	MG	RA	3672	1/1	0.89	0.18	38,38,38,38	0
56	MG	RA	3283	1/1	0.89	0.21	41,41,41,41	0
56	MG	RA	3676	1/1	0.89	0.41	108,108,108,108	0
56	MG	YA	3298	1/1	0.89	0.20	13,13,13,13	0
56	MG	YA	3484	1/1	0.89	0.11	45,45,45,45	0
56	MG	XA	1722	1/1	0.89	0.32	58,58,58,58	0
56	MG	QA	1669	1/1	0.89	0.19	74,74,74,74	0
56	MG	YA	3491	1/1	0.89	0.20	28,28,28,28	0
56	MG	YB	218	1/1	0.89	0.10	38,38,38,38	0
56	MG	RA	3287	1/1	0.89	0.18	37,37,37,37	0
56	MG	YA	3030	1/1	0.89	0.18	48,48,48,48	0
56	MG	YD	303	1/1	0.89	0.23	44,44,44,44	0
56	MG	QA	1743	1/1	0.89	0.11	66,66,66,66	0
56	MG	RA	3685	1/1	0.89	0.09	58,58,58,58	0
56	MG	XA	1741	1/1	0.89	0.08	23,23,23,23	0
56	MG	YA	3320	1/1	0.89	0.27	54,54,54,54	0
56	MG	YA	3040	1/1	0.89	0.06	33,33,33,33	0
56	MG	YA	3509	1/1	0.89	0.07	3,3,3,3	0
56	MG	YN	201	1/1	0.89	0.07	36,36,36,36	0
56	MG	YA	3042	1/1	0.89	0.21	47,47,47,47	0
56	MG	YA	3511	1/1	0.89	0.08	39,39,39,39	0
56	MG	RA	3524	1/1	0.89	0.21	41,41,41,41	0
56	MG	YW	201	1/1	0.89	0.20	69,69,69,69	0
56	MG	RA	3081	1/1	0.89	0.05	63,63,63,63	0
56	MG	RA	3637	1/1	0.89	0.20	62,62,62,62	0
56	MG	YA	3569	1/1	0.90	0.26	48,48,48,48	0
56	MG	YA	3571	1/1	0.90	0.10	33,33,33,33	0
56	MG	XA	1720	1/1	0.90	0.20	55,55,55,55	0
56	MG	YA	3242	1/1	0.90	0.23	43,43,43,43	0
56	MG	QV	104	1/1	0.90	0.17	71,71,71,71	0
56	MG	RA	3167	1/1	0.90	0.09	53,53,53,53	0
56	MG	RA	3684	1/1	0.90	0.14	44,44,44,44	0
56	MG	RA	3217	1/1	0.90	0.10	86,86,86,86	0
56	MG	YA	3591	1/1	0.90	0.21	37,37,37,37	0
56	MG	YA	3593	1/1	0.90	0.21	30,30,30,30	0
56	MG	YA	3020	1/1	0.90	0.12	44,44,44,44	0
56	MG	XA	1647	1/1	0.90	0.06	68,68,68,68	0
56	MG	RA	3142	1/1	0.90	0.28	59,59,59,59	0
56	MG	YA	3606	1/1	0.90	0.09	9,9,9,9	0
56	MG	QA	1681	1/1	0.90	0.23	34,34,34,34	0
56	MG	YA	3258	1/1	0.90	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3143	1/1	0.90	0.20	51,51,51,51	0
56	MG	QA	1752	1/1	0.90	0.05	51,51,51,51	0
56	MG	RQ	203	1/1	0.90	0.13	67,67,67,67	0
56	MG	YA	3421	1/1	0.90	0.12	28,28,28,28	0
56	MG	YA	3626	1/1	0.90	0.12	27,27,27,27	0
56	MG	RA	3196	1/1	0.90	0.08	42,42,42,42	0
56	MG	QA	1682	1/1	0.90	0.15	66,66,66,66	0
56	MG	RA	3578	1/1	0.90	0.08	45,45,45,45	0
56	MG	RA	3368	1/1	0.90	0.31	52,52,52,52	0
56	MG	YA	3636	1/1	0.90	0.07	48,48,48,48	0
56	MG	YA	3269	1/1	0.90	0.16	54,54,54,54	0
56	MG	YA	3640	1/1	0.90	0.15	37,37,37,37	0
56	MG	YA	3641	1/1	0.90	0.09	46,46,46,46	0
56	MG	RA	3067	1/1	0.90	0.14	66,66,66,66	0
56	MG	RA	3516	1/1	0.90	0.13	35,35,35,35	0
56	MG	YA	3277	1/1	0.90	0.22	22,22,22,22	0
56	MG	RA	3703	1/1	0.90	0.14	55,55,55,55	0
56	MG	XA	1769	1/1	0.90	0.15	28,28,28,28	0
56	MG	QA	1809	1/1	0.90	0.06	43,43,43,43	0
56	MG	RA	3520	1/1	0.90	0.09	40,40,40,40	0
56	MG	QA	1777	1/1	0.90	0.22	46,46,46,46	0
56	MG	RZ	301	1/1	0.90	0.05	44,44,44,44	0
56	MG	YA	3452	1/1	0.90	0.17	42,42,42,42	0
56	MG	RA	3525	1/1	0.90	0.14	83,83,83,83	0
56	MG	RA	3286	1/1	0.90	0.25	25,25,25,25	0
56	MG	QA	1759	1/1	0.90	0.07	49,49,49,49	0
56	MG	YA	3462	1/1	0.90	0.18	44,44,44,44	0
56	MG	YA	3060	1/1	0.90	0.15	60,60,60,60	0
56	MG	RA	3016	1/1	0.90	0.25	65,65,65,65	0
56	MG	QA	1725	1/1	0.90	0.08	51,51,51,51	0
56	MG	RA	3293	1/1	0.90	0.17	15,15,15,15	0
56	MG	QA	1781	1/1	0.90	0.12	48,48,48,48	0
56	MG	XA	1613	1/1	0.90	0.08	41,41,41,41	0
56	MG	YA	3479	1/1	0.90	0.13	53,53,53,53	0
56	MG	YA	3324	1/1	0.90	0.26	48,48,48,48	0
56	MG	YA	3482	1/1	0.90	0.16	72,72,72,72	0
56	MG	YA	3681	1/1	0.90	0.17	35,35,35,35	0
56	MG	XA	1790	1/1	0.90	0.12	56,56,56,56	0
56	MG	YA	3685	1/1	0.90	0.13	58,58,58,58	0
56	MG	XA	1791	1/1	0.90	0.34	67,67,67,67	0
56	MG	RA	3295	1/1	0.90	0.21	68,68,68,68	0
56	MG	RA	3659	1/1	0.90	0.41	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1617	1/1	0.90	0.17	53,53,53,53	0
56	MG	YA	3696	1/1	0.90	0.25	145,145,145,145	0
56	MG	RA	3412	1/1	0.90	0.10	29,29,29,29	0
56	MG	YA	3493	1/1	0.90	0.15	41,41,41,41	0
56	MG	YA	3344	1/1	0.90	0.18	45,45,45,45	0
56	MG	YA	3088	1/1	0.90	0.12	39,39,39,39	0
56	MG	XA	1619	1/1	0.90	0.06	51,51,51,51	0
56	MG	YA	3093	1/1	0.90	0.15	38,38,38,38	0
56	MG	YA	3501	1/1	0.90	0.21	57,57,57,57	0
56	MG	YB	206	1/1	0.90	0.06	52,52,52,52	0
56	MG	YA	3095	1/1	0.90	0.14	33,33,33,33	0
56	MG	RA	3345	1/1	0.90	0.10	27,27,27,27	0
56	MG	RA	3114	1/1	0.90	0.29	50,50,50,50	0
56	MG	RA	3493	1/1	0.90	0.18	43,43,43,43	0
56	MG	R7	102	1/1	0.90	0.32	92,92,92,92	0
56	MG	QA	1657	1/1	0.90	0.09	50,50,50,50	0
56	MG	RA	3384	1/1	0.90	0.07	26,26,26,26	0
56	MG	YA	3369	1/1	0.90	0.10	54,54,54,54	0
56	MG	YA	3108	1/1	0.90	0.11	67,67,67,67	0
56	MG	RF	302	1/1	0.90	0.23	107,107,107,107	0
56	MG	RA	3544	1/1	0.90	0.09	36,36,36,36	0
56	MG	YA	3112	1/1	0.90	0.14	40,40,40,40	0
56	MG	QA	1784	1/1	0.90	0.11	53,53,53,53	0
56	MG	RA	3500	1/1	0.90	0.28	58,58,58,58	0
56	MG	YA	3117	1/1	0.90	0.13	50,50,50,50	0
56	MG	QA	1606	1/1	0.90	0.06	48,48,48,48	0
56	MG	RA	3305	1/1	0.90	0.17	30,30,30,30	0
56	MG	YA	3123	1/1	0.90	0.10	40,40,40,40	0
56	MG	YA	3551	1/1	0.90	0.09	33,33,33,33	0
56	MG	YA	3395	1/1	0.90	0.29	30,30,30,30	0
56	MG	RA	3679	1/1	0.90	0.19	42,42,42,42	0
56	MG	YA	3564	1/1	0.90	0.20	46,46,46,46	0
56	MG	YA	3127	1/1	0.90	0.21	46,46,46,46	0
56	MG	RA	3630	1/1	0.91	0.20	39,39,39,39	0
56	MG	YA	3575	1/1	0.91	0.15	30,30,30,30	0
56	MG	RA	3570	1/1	0.91	0.08	40,40,40,40	0
56	MG	YA	3245	1/1	0.91	0.12	55,55,55,55	0
56	MG	QA	1798	1/1	0.91	0.24	52,52,52,52	0
56	MG	RA	3572	1/1	0.91	0.12	27,27,27,27	0
56	MG	YA	3138	1/1	0.91	0.22	50,50,50,50	0
56	MG	YA	3587	1/1	0.91	0.13	68,68,68,68	0
56	MG	RA	3125	1/1	0.91	0.27	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1654	1/1	0.91	0.12	46,46,46,46	0
56	MG	RA	3692	1/1	0.91	0.29	56,56,56,56	0
56	MG	QA	1717	1/1	0.91	0.33	45,45,45,45	0
56	MG	RT	203	1/1	0.91	0.09	61,61,61,61	0
56	MG	YA	3598	1/1	0.91	0.20	50,50,50,50	0
56	MG	YA	3417	1/1	0.91	0.20	54,54,54,54	0
56	MG	YA	3144	1/1	0.91	0.12	38,38,38,38	0
56	MG	YA	3036	1/1	0.91	0.16	56,56,56,56	0
56	MG	QA	1802	1/1	0.91	0.30	61,61,61,61	0
56	MG	RA	3580	1/1	0.91	0.14	87,87,87,87	0
56	MG	QA	1757	1/1	0.91	0.05	54,54,54,54	0
56	MG	QA	1745	1/1	0.91	0.06	50,50,50,50	0
56	MG	RA	3349	1/1	0.91	0.14	14,14,14,14	0
56	MG	RA	3147	1/1	0.91	0.09	71,71,71,71	0
56	MG	RA	3095	1/1	0.91	0.15	43,43,43,43	0
56	MG	YA	3054	1/1	0.91	0.23	65,65,65,65	0
56	MG	R0	101	1/1	0.91	0.20	56,56,56,56	0
56	MG	YA	3438	1/1	0.91	0.15	32,32,32,32	0
56	MG	RA	3436	1/1	0.91	0.29	60,60,60,60	0
56	MG	RA	3590	1/1	0.91	0.12	22,22,22,22	0
56	MG	RA	3649	1/1	0.91	0.25	98,98,98,98	0
56	MG	YA	3163	1/1	0.91	0.12	63,63,63,63	0
56	MG	QA	1604	1/1	0.91	0.08	60,60,60,60	0
56	MG	YA	3062	1/1	0.91	0.11	43,43,43,43	0
56	MG	RA	3356	1/1	0.91	0.21	39,39,39,39	0
56	MG	QL	203	1/1	0.91	0.12	61,61,61,61	0
56	MG	XA	1609	1/1	0.91	0.28	55,55,55,55	0
56	MG	YA	3069	1/1	0.91	0.37	62,62,62,62	0
56	MG	YA	3173	1/1	0.91	0.10	46,46,46,46	0
56	MG	RA	3358	1/1	0.91	0.32	54,54,54,54	0
56	MG	YA	3471	1/1	0.91	0.24	84,84,84,84	0
56	MG	YA	3319	1/1	0.91	0.12	36,36,36,36	0
56	MG	XA	1789	1/1	0.91	0.16	59,59,59,59	0
56	MG	RA	3154	1/1	0.91	0.06	39,39,39,39	0
56	MG	YA	3322	1/1	0.91	0.12	21,21,21,21	0
56	MG	RA	3289	1/1	0.91	0.19	39,39,39,39	0
56	MG	YA	3663	1/1	0.91	0.26	49,49,49,49	0
56	MG	RA	3599	1/1	0.91	0.25	29,29,29,29	0
56	MG	RA	3086	1/1	0.91	0.11	57,57,57,57	0
56	MG	YA	3481	1/1	0.91	0.29	80,80,80,80	0
56	MG	RB	216	1/1	0.91	0.09	74,74,74,74	0
56	MG	RD	301	1/1	0.91	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1695	1/1	0.91	0.15	34,34,34,34	0
56	MG	RA	3019	1/1	0.91	0.12	37,37,37,37	0
56	MG	RA	3548	1/1	0.91	0.24	41,41,41,41	0
56	MG	YA	3347	1/1	0.91	0.14	8,8,8,8	0
56	MG	RA	3036	1/1	0.91	0.42	80,80,80,80	0
56	MG	RA	3553	1/1	0.91	0.20	22,22,22,22	0
56	MG	RE	302	1/1	0.91	0.16	35,35,35,35	0
56	MG	RA	3475	1/1	0.91	0.13	34,34,34,34	0
56	MG	RA	3449	1/1	0.91	0.08	39,39,39,39	0
56	MG	RA	3612	1/1	0.91	0.25	47,47,47,47	0
56	MG	RA	3562	1/1	0.91	0.15	23,23,23,23	0
56	MG	YA	3107	1/1	0.91	0.26	80,80,80,80	0
56	MG	YA	3202	1/1	0.91	0.24	48,48,48,48	0
56	MG	Y7	102	1/1	0.91	0.08	36,36,36,36	0
56	MG	YA	3368	1/1	0.91	0.14	21,21,21,21	0
56	MG	RA	3263	1/1	0.91	0.10	42,42,42,42	0
56	MG	YA	3370	1/1	0.91	0.20	30,30,30,30	0
56	MG	YB	201	1/1	0.91	0.21	55,55,55,55	0
56	MG	YA	3209	1/1	0.91	0.17	38,38,38,38	0
56	MG	YA	3110	1/1	0.91	0.29	42,42,42,42	0
56	MG	QA	1739	1/1	0.91	0.17	41,41,41,41	0
56	MG	YA	3007	1/1	0.91	0.07	66,66,66,66	0
56	MG	YB	208	1/1	0.91	0.07	44,44,44,44	0
56	MG	YB	209	1/1	0.91	0.15	92,92,92,92	0
56	MG	YA	3525	1/1	0.91	0.18	28,28,28,28	0
56	MG	YA	3376	1/1	0.91	0.11	48,48,48,48	0
56	MG	RA	3565	1/1	0.91	0.10	50,50,50,50	0
56	MG	YA	3530	1/1	0.91	0.16	2,2,2,2	0
56	MG	RA	3678	1/1	0.91	0.27	98,98,98,98	0
56	MG	YA	3380	1/1	0.91	0.33	49,49,49,49	0
56	MG	YA	3116	1/1	0.91	0.11	49,49,49,49	0
56	MG	YA	3537	1/1	0.91	0.20	55,55,55,55	0
56	MG	YD	302	1/1	0.91	0.24	69,69,69,69	0
56	MG	YA	3540	1/1	0.91	0.14	33,33,33,33	0
56	MG	YD	305	1/1	0.91	0.14	42,42,42,42	0
56	MG	YA	3384	1/1	0.91	0.07	18,18,18,18	0
56	MG	YA	3543	1/1	0.91	0.12	16,16,16,16	0
56	MG	YE	303	1/1	0.91	0.27	33,33,33,33	0
56	MG	RA	3623	1/1	0.91	0.28	48,48,48,48	0
56	MG	RA	3180	1/1	0.91	0.11	36,36,36,36	0
56	MG	RA	3568	1/1	0.91	0.10	34,34,34,34	0
56	MG	YA	3393	1/1	0.91	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3016	1/1	0.91	0.15	48,48,48,48	0
56	MG	YA	3557	1/1	0.91	0.09	42,42,42,42	0
56	MG	RA	3419	1/1	0.91	0.24	44,44,44,44	0
56	MG	XA	1728	1/1	0.91	0.26	44,44,44,44	0
56	MG	YA	3566	1/1	0.91	0.10	25,25,25,25	0
57	PAR	QA	1821	42/42	0.91	0.13	52,66,86,95	0
57	PAR	XA	1794	42/42	0.91	0.10	52,63,76,81	0
56	MG	XA	1735	1/1	0.91	0.08	19,19,19,19	0
56	MG	YA	3570	1/1	0.91	0.13	42,42,42,42	0
56	MG	YA	3231	1/1	0.92	0.13	37,37,37,37	0
56	MG	RA	3194	1/1	0.92	0.14	64,64,64,64	0
56	MG	YA	3567	1/1	0.92	0.14	27,27,27,27	0
56	MG	XA	1715	1/1	0.92	0.08	41,41,41,41	0
56	MG	YA	3237	1/1	0.92	0.10	38,38,38,38	0
56	MG	YA	3238	1/1	0.92	0.18	39,39,39,39	0
56	MG	YA	3574	1/1	0.92	0.17	24,24,24,24	0
56	MG	QA	1707	1/1	0.92	0.07	62,62,62,62	0
56	MG	YA	3576	1/1	0.92	0.14	46,46,46,46	0
56	MG	YA	3404	1/1	0.92	0.05	32,32,32,32	0
56	MG	YA	3120	1/1	0.92	0.32	102,102,102,102	0
56	MG	YA	3580	1/1	0.92	0.20	52,52,52,52	0
56	MG	YA	3581	1/1	0.92	0.31	41,41,41,41	0
56	MG	RA	3361	1/1	0.92	0.22	46,46,46,46	0
56	MG	YA	3013	1/1	0.92	0.14	63,63,63,63	0
56	MG	YA	3411	1/1	0.92	0.19	33,33,33,33	0
56	MG	XA	1719	1/1	0.92	0.08	35,35,35,35	0
56	MG	RA	3402	1/1	0.92	0.14	42,42,42,42	0
56	MG	YA	3590	1/1	0.92	0.11	47,47,47,47	0
56	MG	YA	3250	1/1	0.92	0.22	19,19,19,19	0
56	MG	RA	3030	1/1	0.92	0.13	64,64,64,64	0
56	MG	RA	3603	1/1	0.92	0.17	56,56,56,56	0
56	MG	RA	3667	1/1	0.92	0.13	54,54,54,54	0
56	MG	YA	3255	1/1	0.92	0.13	28,28,28,28	0
56	MG	YA	3419	1/1	0.92	0.25	35,35,35,35	0
56	MG	YA	3132	1/1	0.92	0.08	48,48,48,48	0
56	MG	QA	1760	1/1	0.92	0.10	37,37,37,37	0
56	MG	YA	3136	1/1	0.92	0.16	43,43,43,43	0
56	MG	YA	3613	1/1	0.92	0.21	41,41,41,41	0
56	MG	YA	3615	1/1	0.92	0.14	22,22,22,22	0
56	MG	XA	1726	1/1	0.92	0.06	42,42,42,42	0
56	MG	YA	3425	1/1	0.92	0.20	55,55,55,55	0
56	MG	QA	1708	1/1	0.92	0.22	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3624	1/1	0.92	0.14	17,17,17,17	0
56	MG	XA	1642	1/1	0.92	0.05	77,77,77,77	0
56	MG	YA	3264	1/1	0.92	0.15	21,21,21,21	0
56	MG	RG	203	1/1	0.92	0.13	59,59,59,59	0
56	MG	RA	3607	1/1	0.92	0.13	38,38,38,38	0
56	MG	YA	3631	1/1	0.92	0.13	40,40,40,40	0
56	MG	RA	3033	1/1	0.92	0.21	52,52,52,52	0
56	MG	QA	1779	1/1	0.92	0.18	38,38,38,38	0
56	MG	QA	1603	1/1	0.92	0.05	50,50,50,50	0
56	MG	YA	3442	1/1	0.92	0.23	86,86,86,86	0
56	MG	XA	1746	1/1	0.92	0.20	61,61,61,61	0
56	MG	YA	3037	1/1	0.92	0.21	45,45,45,45	0
56	MG	XA	1747	1/1	0.92	0.08	28,28,28,28	0
56	MG	YA	3446	1/1	0.92	0.08	25,25,25,25	0
56	MG	RA	3320	1/1	0.92	0.50	93,93,93,93	0
56	MG	YA	3449	1/1	0.92	0.22	53,53,53,53	0
56	MG	YA	3450	1/1	0.92	0.16	40,40,40,40	0
56	MG	QA	1615	1/1	0.92	0.16	47,47,47,47	0
56	MG	QV	101	1/1	0.92	0.12	52,52,52,52	0
56	MG	YA	3454	1/1	0.92	0.06	31,31,31,31	0
56	MG	YA	3655	1/1	0.92	0.16	43,43,43,43	0
56	MG	QA	1629	1/1	0.92	0.08	75,75,75,75	0
56	MG	YA	3047	1/1	0.92	0.09	60,60,60,60	0
56	MG	RA	3281	1/1	0.92	0.14	26,26,26,26	0
56	MG	RA	3117	1/1	0.92	0.35	69,69,69,69	0
56	MG	YA	3467	1/1	0.92	0.12	51,51,51,51	0
56	MG	YA	3053	1/1	0.92	0.12	35,35,35,35	0
56	MG	YA	3309	1/1	0.92	0.32	54,54,54,54	0
56	MG	RA	3624	1/1	0.92	0.32	77,77,77,77	0
56	MG	XA	1764	1/1	0.92	0.23	25,25,25,25	0
56	MG	XA	1765	1/1	0.92	0.09	31,31,31,31	0
56	MG	QA	1731	1/1	0.92	0.26	46,46,46,46	0
56	MG	YA	3477	1/1	0.92	0.29	98,98,98,98	0
56	MG	YA	3671	1/1	0.92	0.15	55,55,55,55	0
56	MG	YA	3672	1/1	0.92	0.18	68,68,68,68	0
56	MG	RA	3626	1/1	0.92	0.28	47,47,47,47	0
56	MG	YA	3675	1/1	0.92	0.19	40,40,40,40	0
56	MG	YA	3676	1/1	0.92	0.16	48,48,48,48	0
56	MG	YA	3168	1/1	0.92	0.10	41,41,41,41	0
56	MG	RA	3688	1/1	0.92	0.20	35,35,35,35	0
56	MG	RA	3146	1/1	0.92	0.08	44,44,44,44	0
56	MG	RA	3331	1/1	0.92	0.21	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3683	1/1	0.92	0.12	24,24,24,24	0
56	MG	YA	3325	1/1	0.92	0.21	37,37,37,37	0
56	MG	RA	3332	1/1	0.92	0.20	42,42,42,42	0
56	MG	YA	3686	1/1	0.92	0.07	51,51,51,51	0
56	MG	YA	3329	1/1	0.92	0.28	51,51,51,51	0
56	MG	RA	3465	1/1	0.92	0.34	45,45,45,45	0
56	MG	RA	3696	1/1	0.92	0.25	57,57,57,57	0
56	MG	YA	3178	1/1	0.92	0.14	42,42,42,42	0
56	MG	YA	3339	1/1	0.92	0.18	34,34,34,34	0
56	MG	YA	3495	1/1	0.92	0.13	30,30,30,30	0
56	MG	QA	1621	1/1	0.92	0.36	100,100,100,100	0
56	MG	YA	3071	1/1	0.92	0.09	64,64,64,64	0
56	MG	YA	3704	1/1	0.92	0.27	30,30,30,30	0
56	MG	RA	3698	1/1	0.92	0.12	56,56,56,56	0
56	MG	YA	3182	1/1	0.92	0.07	40,40,40,40	0
56	MG	RA	3573	1/1	0.92	0.14	38,38,38,38	0
56	MG	YA	3504	1/1	0.92	0.17	51,51,51,51	0
56	MG	QA	1674	1/1	0.92	0.25	42,42,42,42	0
56	MG	YA	3078	1/1	0.92	0.06	66,66,66,66	0
56	MG	RA	3701	1/1	0.92	0.16	52,52,52,52	0
56	MG	RA	3576	1/1	0.92	0.12	31,31,31,31	0
56	MG	RA	3519	1/1	0.92	0.17	32,32,32,32	0
56	MG	RA	3150	1/1	0.92	0.09	35,35,35,35	0
56	MG	YA	3087	1/1	0.92	0.05	24,24,24,24	0
56	MG	RA	3121	1/1	0.92	0.07	47,47,47,47	0
56	MG	YA	3515	1/1	0.92	0.14	45,45,45,45	0
56	MG	R0	102	1/1	0.92	0.07	65,65,65,65	0
56	MG	RA	3582	1/1	0.92	0.32	49,49,49,49	0
56	MG	RA	3291	1/1	0.92	0.14	26,26,26,26	0
56	MG	RB	201	1/1	0.92	0.25	98,98,98,98	0
56	MG	QA	1609	1/1	0.92	0.09	34,34,34,34	0
56	MG	RA	3348	1/1	0.92	0.10	2,2,2,2	0
56	MG	QA	1719	1/1	0.92	0.06	43,43,43,43	0
56	MG	RA	3022	1/1	0.92	0.11	45,45,45,45	0
56	MG	QA	1720	1/1	0.92	0.08	46,46,46,46	0
56	MG	YA	3536	1/1	0.92	0.14	41,41,41,41	0
56	MG	QA	1814	1/1	0.92	0.32	64,64,64,64	0
56	MG	YF	302	1/1	0.92	0.19	67,67,67,67	0
56	MG	YA	3538	1/1	0.92	0.13	36,36,36,36	0
56	MG	QA	1755	1/1	0.92	0.09	47,47,47,47	0
56	MG	RA	3299	1/1	0.92	0.10	26,26,26,26	0
56	MG	YA	3382	1/1	0.92	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3544	1/1	0.92	0.39	34,34,34,34	0
56	MG	YP	202	1/1	0.92	0.07	41,41,41,41	0
56	MG	RA	3593	1/1	0.92	0.19	52,52,52,52	0
56	MG	XA	1707	1/1	0.92	0.07	49,49,49,49	0
56	MG	XA	1709	1/1	0.92	0.19	42,42,42,42	0
56	MG	YA	3005	1/1	0.92	0.09	49,49,49,49	0
56	MG	YA	3114	1/1	0.92	0.15	60,60,60,60	0
56	MG	QA	1793	1/1	0.92	0.21	64,64,64,64	0
56	MG	QA	1612	1/1	0.92	0.08	43,43,43,43	0
56	MG	YA	3041	1/1	0.93	0.10	41,41,41,41	0
56	MG	YA	3257	1/1	0.93	0.05	38,38,38,38	0
56	MG	QA	1767	1/1	0.93	0.14	52,52,52,52	0
56	MG	XA	1675	1/1	0.93	0.17	39,39,39,39	0
56	MG	RA	3215	1/1	0.93	0.28	69,69,69,69	0
56	MG	RA	3486	1/1	0.93	0.17	50,50,50,50	0
56	MG	RA	3491	1/1	0.93	0.20	40,40,40,40	0
56	MG	XA	1766	1/1	0.93	0.23	53,53,53,53	0
56	MG	RA	3492	1/1	0.93	0.17	36,36,36,36	0
56	MG	YA	3266	1/1	0.93	0.09	37,37,37,37	0
56	MG	RA	3423	1/1	0.93	0.16	31,31,31,31	0
56	MG	RA	3216	1/1	0.93	0.24	52,52,52,52	0
56	MG	YA	3592	1/1	0.93	0.19	16,16,16,16	0
56	MG	RA	3496	1/1	0.93	0.19	43,43,43,43	0
56	MG	YA	3155	1/1	0.93	0.15	35,35,35,35	0
56	MG	YA	3274	1/1	0.93	0.23	67,67,67,67	0
56	MG	RA	3587	1/1	0.93	0.27	72,72,72,72	0
56	MG	YA	3604	1/1	0.93	0.18	43,43,43,43	0
56	MG	XA	1775	1/1	0.93	0.13	39,39,39,39	0
56	MG	YA	3430	1/1	0.93	0.08	42,42,42,42	0
56	MG	YA	3431	1/1	0.93	0.19	10,10,10,10	0
56	MG	XA	1686	1/1	0.93	0.21	55,55,55,55	0
56	MG	YA	3612	1/1	0.93	0.24	41,41,41,41	0
56	MG	YA	3434	1/1	0.93	0.14	22,22,22,22	0
56	MG	YA	3281	1/1	0.93	0.16	23,23,23,23	0
56	MG	YA	3437	1/1	0.93	0.23	29,29,29,29	0
56	MG	XA	1779	1/1	0.93	0.15	42,42,42,42	0
56	MG	YA	3162	1/1	0.93	0.14	34,34,34,34	0
56	MG	XA	1688	1/1	0.93	0.28	55,55,55,55	0
56	MG	YA	3292	1/1	0.93	0.06	42,42,42,42	0
56	MG	RA	3157	1/1	0.93	0.10	59,59,59,59	0
56	MG	XA	1690	1/1	0.93	0.20	31,31,31,31	0
56	MG	YA	3299	1/1	0.93	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3300	1/1	0.93	0.15	28,28,28,28	0
56	MG	RA	3071	1/1	0.93	0.38	102,102,102,102	0
56	MG	QF	201	1/1	0.93	0.07	29,29,29,29	0
56	MG	YA	3635	1/1	0.93	0.14	18,18,18,18	0
56	MG	XA	1694	1/1	0.93	0.08	27,27,27,27	0
56	MG	QA	1753	1/1	0.93	0.21	83,83,83,83	0
56	MG	YA	3072	1/1	0.93	0.12	7,7,7,7	0
56	MG	YA	3455	1/1	0.93	0.07	40,40,40,40	0
56	MG	XA	1788	1/1	0.93	0.05	48,48,48,48	0
56	MG	RA	3543	1/1	0.93	0.14	4,4,4,4	0
56	MG	YA	3175	1/1	0.93	0.13	41,41,41,41	0
56	MG	YA	3317	1/1	0.93	0.10	41,41,41,41	0
56	MG	YA	3464	1/1	0.93	0.10	39,39,39,39	0
56	MG	YA	3176	1/1	0.93	0.10	55,55,55,55	0
56	MG	YA	3468	1/1	0.93	0.10	57,57,57,57	0
56	MG	XA	1699	1/1	0.93	0.09	34,34,34,34	0
56	MG	RA	3694	1/1	0.93	0.35	39,39,39,39	0
56	MG	RA	3302	1/1	0.93	0.14	34,34,34,34	0
56	MG	RA	3502	1/1	0.93	0.10	30,30,30,30	0
56	MG	RA	3433	1/1	0.93	0.13	51,51,51,51	0
56	MG	QA	1684	1/1	0.93	0.33	60,60,60,60	0
56	MG	YA	3328	1/1	0.93	0.13	52,52,52,52	0
56	MG	XA	1641	1/1	0.93	0.17	52,52,52,52	0
56	MG	RA	3435	1/1	0.93	0.16	41,41,41,41	0
56	MG	YA	3335	1/1	0.93	0.05	32,32,32,32	0
56	MG	YA	3089	1/1	0.93	0.07	54,54,54,54	0
56	MG	YA	3667	1/1	0.93	0.19	67,67,67,67	0
56	MG	YA	3091	1/1	0.93	0.18	39,39,39,39	0
56	MG	XA	1708	1/1	0.93	0.24	37,37,37,37	0
56	MG	QA	1635	1/1	0.93	0.10	43,43,43,43	0
56	MG	YA	3487	1/1	0.93	0.25	37,37,37,37	0
56	MG	XA	1644	1/1	0.93	0.10	71,71,71,71	0
56	MG	RA	3273	1/1	0.93	0.14	51,51,51,51	0
56	MG	YA	3345	1/1	0.93	0.07	28,28,28,28	0
56	MG	RA	3651	1/1	0.93	0.06	47,47,47,47	0
56	MG	YA	3195	1/1	0.93	0.09	72,72,72,72	0
56	MG	RA	3275	1/1	0.93	0.11	43,43,43,43	0
56	MG	YA	3350	1/1	0.93	0.12	24,24,24,24	0
56	MG	QA	1756	1/1	0.93	0.05	58,58,58,58	0
56	MG	YA	3682	1/1	0.93	0.21	63,63,63,63	0
56	MG	RA	3017	1/1	0.93	0.07	53,53,53,53	0
56	MG	QA	1772	1/1	0.93	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3001	1/1	0.93	0.13	39,39,39,39	0
56	MG	YA	3502	1/1	0.93	0.24	60,60,60,60	0
56	MG	XA	1651	1/1	0.93	0.05	42,42,42,42	0
56	MG	YA	3505	1/1	0.93	0.10	35,35,35,35	0
56	MG	YA	3203	1/1	0.93	0.14	48,48,48,48	0
56	MG	YA	3003	1/1	0.93	0.13	52,52,52,52	0
56	MG	YA	3693	1/1	0.93	0.39	59,59,59,59	0
56	MG	YA	3694	1/1	0.93	0.30	65,65,65,65	0
56	MG	YA	3366	1/1	0.93	0.17	51,51,51,51	0
56	MG	XA	1652	1/1	0.93	0.06	35,35,35,35	0
56	MG	QA	1713	1/1	0.93	0.15	38,38,38,38	0
56	MG	RA	3317	1/1	0.93	0.13	7,7,7,7	0
56	MG	QA	1645	1/1	0.93	0.12	45,45,45,45	0
56	MG	RA	3610	1/1	0.93	0.10	62,62,62,62	0
56	MG	XA	1727	1/1	0.93	0.12	40,40,40,40	0
56	MG	YA	3516	1/1	0.93	0.13	36,36,36,36	0
56	MG	RA	3517	1/1	0.93	0.06	38,38,38,38	0
56	MG	XA	1730	1/1	0.93	0.08	41,41,41,41	0
56	MG	XA	1733	1/1	0.93	0.16	40,40,40,40	0
56	MG	YA	3224	1/1	0.93	0.16	44,44,44,44	0
56	MG	RA	3253	1/1	0.93	0.23	28,28,28,28	0
56	MG	YA	3379	1/1	0.93	0.19	37,37,37,37	0
56	MG	RB	206	1/1	0.93	0.21	39,39,39,39	0
56	MG	YA	3121	1/1	0.93	0.23	51,51,51,51	0
56	MG	YA	3230	1/1	0.93	0.20	50,50,50,50	0
56	MG	YA	3535	1/1	0.93	0.23	35,35,35,35	0
56	MG	XA	1738	1/1	0.93	0.12	38,38,38,38	0
56	MG	XA	1662	1/1	0.93	0.06	39,39,39,39	0
56	MG	RA	3613	1/1	0.93	0.15	39,39,39,39	0
56	MG	XA	1742	1/1	0.93	0.34	40,40,40,40	0
56	MG	YA	3389	1/1	0.93	0.12	53,53,53,53	0
56	MG	YA	3391	1/1	0.93	0.06	43,43,43,43	0
56	MG	YA	3392	1/1	0.93	0.15	43,43,43,43	0
56	MG	YD	306	1/1	0.93	0.17	84,84,84,84	0
56	MG	XA	1743	1/1	0.93	0.15	33,33,33,33	0
56	MG	YA	3394	1/1	0.93	0.21	46,46,46,46	0
56	MG	YA	3239	1/1	0.93	0.08	14,14,14,14	0
56	MG	RA	3207	1/1	0.93	0.21	107,107,107,107	0
56	MG	YA	3554	1/1	0.93	0.15	7,7,7,7	0
56	MG	QL	201	1/1	0.93	0.16	103,103,103,103	0
56	MG	XA	1667	1/1	0.93	0.14	81,81,81,81	0
56	MG	YA	3134	1/1	0.93	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3523	1/1	0.93	0.15	46,46,46,46	0
56	MG	YO	201	1/1	0.93	0.39	88,88,88,88	0
56	MG	QA	1783	1/1	0.93	0.12	42,42,42,42	0
56	MG	XA	1751	1/1	0.93	0.26	56,56,56,56	0
56	MG	YA	3405	1/1	0.93	0.33	32,32,32,32	0
56	MG	RA	3190	1/1	0.93	0.06	46,46,46,46	0
56	MG	YT	202	1/1	0.93	0.17	85,85,85,85	0
56	MG	YV	201	1/1	0.93	0.07	37,37,37,37	0
56	MG	RA	3068	1/1	0.93	0.09	49,49,49,49	0
56	MG	YA	3572	1/1	0.93	0.15	36,36,36,36	0
56	MG	YA	3573	1/1	0.93	0.10	24,24,24,24	0
56	MG	YA	3039	1/1	0.93	0.11	65,65,65,65	0
56	MG	R1	101	1/1	0.93	0.37	57,57,57,57	0
56	MG	YA	3610	1/1	0.94	0.19	39,39,39,39	0
56	MG	YA	3465	1/1	0.94	0.25	17,17,17,17	0
56	MG	YA	3212	1/1	0.94	0.18	45,45,45,45	0
56	MG	YA	3213	1/1	0.94	0.07	50,50,50,50	0
56	MG	RD	302	1/1	0.94	0.22	82,82,82,82	0
56	MG	YA	3028	1/1	0.94	0.10	40,40,40,40	0
56	MG	YA	3617	1/1	0.94	0.12	19,19,19,19	0
56	MG	YA	3620	1/1	0.94	0.08	33,33,33,33	0
56	MG	RD	303	1/1	0.94	0.23	91,91,91,91	0
56	MG	YA	3352	1/1	0.94	0.21	38,38,38,38	0
56	MG	YA	3219	1/1	0.94	0.07	35,35,35,35	0
56	MG	RA	3675	1/1	0.94	0.07	10,10,10,10	0
56	MG	RA	3021	1/1	0.94	0.14	60,60,60,60	0
56	MG	YA	3125	1/1	0.94	0.10	43,43,43,43	0
56	MG	RA	3487	1/1	0.94	0.09	14,14,14,14	0
56	MG	YA	3363	1/1	0.94	0.12	63,63,63,63	0
56	MG	YA	3632	1/1	0.94	0.12	15,15,15,15	0
56	MG	RA	3003	1/1	0.94	0.18	19,19,19,19	0
56	MG	YA	3035	1/1	0.94	0.13	38,38,38,38	0
56	MG	YA	3229	1/1	0.94	0.20	34,34,34,34	0
56	MG	RA	3171	1/1	0.94	0.09	52,52,52,52	0
56	MG	YA	3486	1/1	0.94	0.09	31,31,31,31	0
56	MG	RA	3023	1/1	0.94	0.20	105,105,105,105	0
56	MG	YA	3233	1/1	0.94	0.11	38,38,38,38	0
56	MG	YA	3489	1/1	0.94	0.17	36,36,36,36	0
56	MG	XA	1626	1/1	0.94	0.06	31,31,31,31	0
56	MG	QA	1610	1/1	0.94	0.06	41,41,41,41	0
56	MG	YA	3645	1/1	0.94	0.09	36,36,36,36	0
56	MG	XA	1771	1/1	0.94	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RF	303	1/1	0.94	0.24	102,102,102,102	0
56	MG	RA	3109	1/1	0.94	0.16	37,37,37,37	0
56	MG	YA	3044	1/1	0.94	0.10	44,44,44,44	0
56	MG	XA	1630	1/1	0.94	0.09	55,55,55,55	0
56	MG	YA	3654	1/1	0.94	0.23	15,15,15,15	0
56	MG	QA	1704	1/1	0.94	0.11	41,41,41,41	0
56	MG	XA	1698	1/1	0.94	0.11	40,40,40,40	0
56	MG	YA	3049	1/1	0.94	0.25	48,48,48,48	0
56	MG	RG	202	1/1	0.94	0.05	56,56,56,56	0
56	MG	RA	3310	1/1	0.94	0.33	77,77,77,77	0
56	MG	XA	1635	1/1	0.94	0.05	55,55,55,55	0
56	MG	YA	3506	1/1	0.94	0.15	17,17,17,17	0
56	MG	RA	3540	1/1	0.94	0.23	29,29,29,29	0
56	MG	YA	3055	1/1	0.94	0.11	40,40,40,40	0
56	MG	XA	1637	1/1	0.94	0.21	78,78,78,78	0
56	MG	QA	1807	1/1	0.94	0.06	63,63,63,63	0
56	MG	QA	1797	1/1	0.94	0.21	51,51,51,51	0
56	MG	RA	3388	1/1	0.94	0.16	38,38,38,38	0
56	MG	RA	3314	1/1	0.94	0.23	51,51,51,51	0
56	MG	YA	3061	1/1	0.94	0.09	40,40,40,40	0
56	MG	QA	1723	1/1	0.94	0.06	39,39,39,39	0
56	MG	RA	3284	1/1	0.94	0.20	21,21,21,21	0
56	MG	YA	3397	1/1	0.94	0.21	59,59,59,59	0
56	MG	YA	3520	1/1	0.94	0.12	10,10,10,10	0
56	MG	YA	3158	1/1	0.94	0.07	44,44,44,44	0
56	MG	RA	3695	1/1	0.94	0.11	47,47,47,47	0
56	MG	YA	3067	1/1	0.94	0.06	33,33,33,33	0
56	MG	XA	1712	1/1	0.94	0.18	44,44,44,44	0
56	MG	RA	3013	1/1	0.94	0.11	87,87,87,87	0
56	MG	RA	3078	1/1	0.94	0.08	55,55,55,55	0
56	MG	RA	3394	1/1	0.94	0.18	35,35,35,35	0
56	MG	RA	3079	1/1	0.94	0.18	56,56,56,56	0
56	MG	YA	3166	1/1	0.94	0.07	60,60,60,60	0
56	MG	XL	202	1/1	0.94	0.09	53,53,53,53	0
56	MG	YA	3409	1/1	0.94	0.13	26,26,26,26	0
56	MG	YA	3279	1/1	0.94	0.21	19,19,19,19	0
56	MG	YA	3690	1/1	0.94	0.24	126,126,126,126	0
56	MG	QA	1799	1/1	0.94	0.05	52,52,52,52	0
56	MG	YA	3075	1/1	0.94	0.15	52,52,52,52	0
56	MG	YA	3283	1/1	0.94	0.17	61,61,61,61	0
56	MG	RA	3555	1/1	0.94	0.37	55,55,55,55	0
56	MG	YA	3286	1/1	0.94	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3699	1/1	0.94	0.17	48,48,48,48	0
56	MG	RA	3557	1/1	0.94	0.11	17,17,17,17	0
56	MG	YA	3550	1/1	0.94	0.20	21,21,21,21	0
56	MG	RA	3098	1/1	0.94	0.09	33,33,33,33	0
56	MG	YA	3081	1/1	0.94	0.21	41,41,41,41	0
56	MG	YA	3293	1/1	0.94	0.21	26,26,26,26	0
56	MG	YA	3707	1/1	0.94	0.25	98,98,98,98	0
56	MG	YA	3295	1/1	0.94	0.12	16,16,16,16	0
56	MG	RA	3605	1/1	0.94	0.16	23,23,23,23	0
56	MG	YA	3562	1/1	0.94	0.18	35,35,35,35	0
56	MG	YA	3563	1/1	0.94	0.22	22,22,22,22	0
56	MG	YA	3083	1/1	0.94	0.08	39,39,39,39	0
56	MG	RA	3705	1/1	0.94	0.17	54,54,54,54	0
56	MG	RA	3258	1/1	0.94	0.11	66,66,66,66	0
56	MG	YA	3086	1/1	0.94	0.13	38,38,38,38	0
56	MG	QA	1800	1/1	0.94	0.13	45,45,45,45	0
56	MG	RA	3292	1/1	0.94	0.22	56,56,56,56	0
56	MG	XA	1729	1/1	0.94	0.07	44,44,44,44	0
56	MG	QA	1790	1/1	0.94	0.06	73,73,73,73	0
56	MG	XA	1731	1/1	0.94	0.19	62,62,62,62	0
56	MG	YA	3312	1/1	0.94	0.22	42,42,42,42	0
56	MG	RA	3440	1/1	0.94	0.14	20,20,20,20	0
56	MG	RA	3661	1/1	0.94	0.28	46,46,46,46	0
56	MG	RA	3370	1/1	0.94	0.27	117,117,117,117	0
56	MG	YD	304	1/1	0.94	0.12	46,46,46,46	0
56	MG	YA	3318	1/1	0.94	0.11	32,32,32,32	0
56	MG	QA	1611	1/1	0.94	0.05	31,31,31,31	0
56	MG	XA	1739	1/1	0.94	0.27	39,39,39,39	0
56	MG	RA	3664	1/1	0.94	0.05	37,37,37,37	0
56	MG	YA	3584	1/1	0.94	0.07	58,58,58,58	0
56	MG	YE	305	1/1	0.94	0.05	53,53,53,53	0
56	MG	RA	3234	1/1	0.94	0.13	60,60,60,60	0
56	MG	YA	3105	1/1	0.94	0.13	48,48,48,48	0
56	MG	RA	3235	1/1	0.94	0.16	18,18,18,18	0
56	MG	RA	3616	1/1	0.94	0.08	39,39,39,39	0
56	MG	RA	3334	1/1	0.94	0.19	24,24,24,24	0
56	MG	YA	3015	1/1	0.94	0.07	34,34,34,34	0
56	MG	RA	3166	1/1	0.94	0.12	68,68,68,68	0
56	MG	YA	3453	1/1	0.94	0.24	56,56,56,56	0
56	MG	YA	3594	1/1	0.94	0.12	30,30,30,30	0
56	MG	RA	3409	1/1	0.94	0.06	30,30,30,30	0
56	MG	XA	1676	1/1	0.94	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YT	201	1/1	0.94	0.12	50,50,50,50	0
56	MG	YA	3597	1/1	0.94	0.14	30,30,30,30	0
56	MG	YT	203	1/1	0.94	0.30	97,97,97,97	0
56	MG	QA	1738	1/1	0.94	0.14	40,40,40,40	0
56	MG	YA	3603	1/1	0.94	0.27	51,51,51,51	0
56	MG	RB	217	1/1	0.94	0.07	62,62,62,62	0
56	MG	QA	1648	1/1	0.94	0.08	69,69,69,69	0
56	MG	YA	3025	1/1	0.94	0.15	49,49,49,49	0
56	MG	XA	1753	1/1	0.94	0.16	38,38,38,38	0
56	MG	XA	1777	1/1	0.95	0.15	28,28,28,28	0
56	MG	RA	3200	1/1	0.95	0.07	45,45,45,45	0
56	MG	RA	3340	1/1	0.95	0.05	31,31,31,31	0
56	MG	XA	1669	1/1	0.95	0.05	55,55,55,55	0
56	MG	YA	3653	1/1	0.95	0.17	29,29,29,29	0
56	MG	RA	3002	1/1	0.95	0.04	55,55,55,55	0
56	MG	YA	3094	1/1	0.95	0.15	36,36,36,36	0
56	MG	RA	3342	1/1	0.95	0.15	19,19,19,19	0
56	MG	QO	102	1/1	0.95	0.14	73,73,73,73	0
56	MG	RA	3004	1/1	0.95	0.14	52,52,52,52	0
56	MG	YA	3440	1/1	0.95	0.17	23,23,23,23	0
56	MG	YA	3441	1/1	0.95	0.08	11,11,11,11	0
56	MG	YA	3098	1/1	0.95	0.26	41,41,41,41	0
56	MG	YA	3548	1/1	0.95	0.28	47,47,47,47	0
56	MG	YA	3351	1/1	0.95	0.15	12,12,12,12	0
56	MG	YA	3099	1/1	0.95	0.21	43,43,43,43	0
56	MG	XA	1725	1/1	0.95	0.16	30,30,30,30	0
56	MG	YA	3355	1/1	0.95	0.19	35,35,35,35	0
56	MG	XA	1786	1/1	0.95	0.11	44,44,44,44	0
56	MG	YA	3556	1/1	0.95	0.28	46,46,46,46	0
56	MG	QA	1686	1/1	0.95	0.14	38,38,38,38	0
56	MG	YA	3561	1/1	0.95	0.09	37,37,37,37	0
56	MG	YA	3038	1/1	0.95	0.07	47,47,47,47	0
56	MG	QA	1702	1/1	0.95	0.05	48,48,48,48	0
56	MG	YA	3362	1/1	0.95	0.19	29,29,29,29	0
56	MG	YA	3677	1/1	0.95	0.08	2,2,2,2	0
56	MG	RA	3244	1/1	0.95	0.06	36,36,36,36	0
56	MG	RA	3428	1/1	0.95	0.15	53,53,53,53	0
56	MG	RA	3668	1/1	0.95	0.12	58,58,58,58	0
56	MG	RA	3551	1/1	0.95	0.14	11,11,11,11	0
56	MG	QA	1628	1/1	0.95	0.09	33,33,33,33	0
56	MG	QA	1613	1/1	0.95	0.05	97,97,97,97	0
56	MG	RA	3490	1/1	0.95	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3556	1/1	0.95	0.05	37,37,37,37	0
56	MG	YA	3048	1/1	0.95	0.05	61,61,61,61	0
56	MG	RA	3319	1/1	0.95	0.12	38,38,38,38	0
56	MG	YA	3050	1/1	0.95	0.05	47,47,47,47	0
56	MG	YA	3469	1/1	0.95	0.18	12,12,12,12	0
56	MG	YA	3578	1/1	0.95	0.20	20,20,20,20	0
56	MG	R6	102	1/1	0.95	0.15	48,48,48,48	0
56	MG	YA	3278	1/1	0.95	0.19	22,22,22,22	0
56	MG	RA	3561	1/1	0.95	0.11	31,31,31,31	0
56	MG	RB	208	1/1	0.95	0.07	44,44,44,44	0
56	MG	YA	3583	1/1	0.95	0.19	39,39,39,39	0
56	MG	XV	102	1/1	0.95	0.06	43,43,43,43	0
56	MG	YA	3700	1/1	0.95	0.06	30,30,30,30	0
56	MG	YA	3282	1/1	0.95	0.12	17,17,17,17	0
56	MG	YA	3476	1/1	0.95	0.28	44,44,44,44	0
56	MG	RA	3124	1/1	0.95	0.18	90,90,90,90	0
56	MG	QA	1810	1/1	0.95	0.21	59,59,59,59	0
56	MG	Y0	101	1/1	0.95	0.07	14,14,14,14	0
56	MG	RB	213	1/1	0.95	0.10	28,28,28,28	0
56	MG	YA	3386	1/1	0.95	0.17	38,38,38,38	0
56	MG	RA	3211	1/1	0.95	0.12	43,43,43,43	0
56	MG	YB	203	1/1	0.95	0.04	48,48,48,48	0
56	MG	YA	3291	1/1	0.95	0.16	2,2,2,2	0
56	MG	YB	205	1/1	0.95	0.12	41,41,41,41	0
56	MG	YA	3200	1/1	0.95	0.08	42,42,42,42	0
56	MG	YA	3390	1/1	0.95	0.09	38,38,38,38	0
56	MG	QA	1721	1/1	0.95	0.09	50,50,50,50	0
56	MG	XA	1748	1/1	0.95	0.07	36,36,36,36	0
56	MG	XA	1749	1/1	0.95	0.08	37,37,37,37	0
56	MG	YB	211	1/1	0.95	0.21	38,38,38,38	0
56	MG	YA	3297	1/1	0.95	0.18	28,28,28,28	0
56	MG	YA	3063	1/1	0.95	0.06	35,35,35,35	0
56	MG	QA	1661	1/1	0.95	0.06	35,35,35,35	0
56	MG	RA	3300	1/1	0.95	0.14	17,17,17,17	0
56	MG	YA	3608	1/1	0.95	0.19	32,32,32,32	0
56	MG	XA	1601	1/1	0.95	0.06	40,40,40,40	0
56	MG	YA	3302	1/1	0.95	0.11	23,23,23,23	0
56	MG	YA	3303	1/1	0.95	0.17	25,25,25,25	0
56	MG	YA	3137	1/1	0.95	0.08	18,18,18,18	0
56	MG	RA	3329	1/1	0.95	0.13	43,43,43,43	0
56	MG	YA	3308	1/1	0.95	0.11	34,34,34,34	0
56	MG	RA	3646	1/1	0.95	0.26	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3112	1/1	0.95	0.11	51,51,51,51	0
56	MG	YA	3621	1/1	0.95	0.18	11,11,11,11	0
56	MG	RD	305	1/1	0.95	0.08	35,35,35,35	0
56	MG	QA	1724	1/1	0.95	0.05	37,37,37,37	0
56	MG	XA	1655	1/1	0.95	0.05	38,38,38,38	0
56	MG	XA	1763	1/1	0.95	0.27	40,40,40,40	0
56	MG	YF	303	1/1	0.95	0.05	38,38,38,38	0
56	MG	YA	3145	1/1	0.95	0.15	28,28,28,28	0
56	MG	QA	1699	1/1	0.95	0.20	41,41,41,41	0
56	MG	YG	203	1/1	0.95	0.05	48,48,48,48	0
56	MG	YA	3628	1/1	0.95	0.10	30,30,30,30	0
56	MG	YA	3076	1/1	0.95	0.22	44,44,44,44	0
56	MG	RA	3691	1/1	0.95	0.22	89,89,89,89	0
56	MG	RA	3504	1/1	0.95	0.08	31,31,31,31	0
56	MG	YA	3079	1/1	0.95	0.23	64,64,64,64	0
56	MG	XA	1611	1/1	0.95	0.08	52,52,52,52	0
56	MG	YQ	202	1/1	0.95	0.08	30,30,30,30	0
56	MG	YR	201	1/1	0.95	0.20	50,50,50,50	0
56	MG	RA	3148	1/1	0.95	0.17	55,55,55,55	0
56	MG	YA	3517	1/1	0.95	0.12	24,24,24,24	0
56	MG	RA	3538	1/1	0.95	0.24	53,53,53,53	0
56	MG	XA	1713	1/1	0.95	0.18	42,42,42,42	0
56	MG	YA	3022	1/1	0.95	0.04	17,17,17,17	0
56	MG	YA	3330	1/1	0.95	0.19	32,32,32,32	0
56	MG	RA	3577	1/1	0.95	0.12	40,40,40,40	0
56	MG	YA	3332	1/1	0.95	0.18	31,31,31,31	0
56	MG	RA	3257	1/1	0.95	0.06	43,43,43,43	0
59	ZN	RY	201	1/1	0.95	0.10	197,197,197,197	0
56	MG	RA	3614	1/1	0.95	0.15	27,27,27,27	0
56	MG	XA	1761	1/1	0.96	0.17	41,41,41,41	0
56	MG	XA	1605	1/1	0.96	0.05	64,64,64,64	0
56	MG	YA	3560	1/1	0.96	0.05	28,28,28,28	0
56	MG	YA	3459	1/1	0.96	0.05	37,37,37,37	0
56	MG	YA	3287	1/1	0.96	0.16	11,11,11,11	0
56	MG	YA	3461	1/1	0.96	0.08	46,46,46,46	0
56	MG	QA	1647	1/1	0.96	0.04	64,64,64,64	0
56	MG	RA	3274	1/1	0.96	0.13	19,19,19,19	0
56	MG	YA	3290	1/1	0.96	0.06	34,34,34,34	0
56	MG	YA	3466	1/1	0.96	0.10	21,21,21,21	0
56	MG	YA	3673	1/1	0.96	0.13	41,41,41,41	0
56	MG	QA	1666	1/1	0.96	0.09	52,52,52,52	0
56	MG	YA	3208	1/1	0.96	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3324	1/1	0.96	0.18	37,37,37,37	0
56	MG	XA	1767	1/1	0.96	0.04	46,46,46,46	0
56	MG	XA	1768	1/1	0.96	0.18	33,33,33,33	0
56	MG	RA	3574	1/1	0.96	0.10	40,40,40,40	0
56	MG	RA	3277	1/1	0.96	0.14	32,32,32,32	0
56	MG	XA	1612	1/1	0.96	0.07	57,57,57,57	0
56	MG	RE	303	1/1	0.96	0.06	50,50,50,50	0
56	MG	RA	3008	1/1	0.96	0.05	45,45,45,45	0
56	MG	YA	3218	1/1	0.96	0.07	39,39,39,39	0
56	MG	XA	1664	1/1	0.96	0.21	64,64,64,64	0
56	MG	YA	3220	1/1	0.96	0.07	51,51,51,51	0
56	MG	XA	1716	1/1	0.96	0.18	52,52,52,52	0
56	MG	YA	3222	1/1	0.96	0.09	64,64,64,64	0
56	MG	RA	3655	1/1	0.96	0.11	18,18,18,18	0
56	MG	RA	3279	1/1	0.96	0.13	31,31,31,31	0
56	MG	QA	1700	1/1	0.96	0.06	47,47,47,47	0
56	MG	YA	3692	1/1	0.96	0.09	44,44,44,44	0
56	MG	RA	3172	1/1	0.96	0.18	72,72,72,72	0
56	MG	RA	3476	1/1	0.96	0.12	63,63,63,63	0
56	MG	YA	3695	1/1	0.96	0.12	39,39,39,39	0
56	MG	YA	3589	1/1	0.96	0.13	30,30,30,30	0
56	MG	RA	3617	1/1	0.96	0.10	15,15,15,15	0
56	MG	YA	3698	1/1	0.96	0.14	40,40,40,40	0
56	MG	YA	3156	1/1	0.96	0.18	39,39,39,39	0
56	MG	YA	3402	1/1	0.96	0.15	42,42,42,42	0
56	MG	RA	3116	1/1	0.96	0.09	57,57,57,57	0
56	MG	RA	3306	1/1	0.96	0.16	11,11,11,11	0
56	MG	RA	3050	1/1	0.96	0.08	49,49,49,49	0
56	MG	YA	3494	1/1	0.96	0.12	38,38,38,38	0
56	MG	RA	3191	1/1	0.96	0.13	30,30,30,30	0
56	MG	RA	3010	1/1	0.96	0.13	58,58,58,58	0
56	MG	RA	3336	1/1	0.96	0.05	15,15,15,15	0
56	MG	RA	3515	1/1	0.96	0.06	38,38,38,38	0
56	MG	RA	3337	1/1	0.96	0.05	39,39,39,39	0
56	MG	YA	3101	1/1	0.96	0.14	49,49,49,49	0
56	MG	YA	3102	1/1	0.96	0.06	19,19,19,19	0
56	MG	YA	3503	1/1	0.96	0.05	13,13,13,13	0
56	MG	RA	3552	1/1	0.96	0.09	38,38,38,38	0
56	MG	RA	3339	1/1	0.96	0.17	38,38,38,38	0
56	MG	RA	3176	1/1	0.96	0.20	69,69,69,69	0
56	MG	YA	3249	1/1	0.96	0.18	31,31,31,31	0
56	MG	YA	3614	1/1	0.96	0.18	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3062	1/1	0.96	0.19	46,46,46,46	0
56	MG	YB	213	1/1	0.96	0.10	34,34,34,34	0
56	MG	YA	3337	1/1	0.96	0.11	7,7,7,7	0
56	MG	XA	1737	1/1	0.96	0.04	38,38,38,38	0
56	MG	YA	3618	1/1	0.96	0.09	7,7,7,7	0
56	MG	RA	3107	1/1	0.96	0.26	83,83,83,83	0
56	MG	YA	3422	1/1	0.96	0.17	29,29,29,29	0
56	MG	XA	1684	1/1	0.96	0.10	35,35,35,35	0
56	MG	RA	3634	1/1	0.96	0.13	30,30,30,30	0
56	MG	RA	3343	1/1	0.96	0.10	34,34,34,34	0
56	MG	XA	1687	1/1	0.96	0.28	57,57,57,57	0
56	MG	RA	3595	1/1	0.96	0.11	39,39,39,39	0
56	MG	XA	1640	1/1	0.96	0.09	53,53,53,53	0
56	MG	RA	3042	1/1	0.96	0.04	45,45,45,45	0
56	MG	RB	210	1/1	0.96	0.17	43,43,43,43	0
56	MG	YA	3630	1/1	0.96	0.24	25,25,25,25	0
56	MG	YA	3523	1/1	0.96	0.17	4,4,4,4	0
56	MG	RA	3430	1/1	0.96	0.05	35,35,35,35	0
56	MG	YA	3526	1/1	0.96	0.12	18,18,18,18	0
56	MG	XA	1693	1/1	0.96	0.24	42,42,42,42	0
56	MG	YA	3433	1/1	0.96	0.09	32,32,32,32	0
56	MG	YA	3353	1/1	0.96	0.17	3,3,3,3	0
56	MG	YA	3184	1/1	0.96	0.10	56,56,56,56	0
56	MG	YA	3532	1/1	0.96	0.10	22,22,22,22	0
56	MG	QA	1716	1/1	0.96	0.05	73,73,73,73	0
56	MG	YA	3356	1/1	0.96	0.15	37,37,37,37	0
56	MG	YA	3357	1/1	0.96	0.12	66,66,66,66	0
56	MG	RA	3527	1/1	0.96	0.30	37,37,37,37	0
56	MG	RA	3683	1/1	0.96	0.06	103,103,103,103	0
56	MG	Y8	101	1/1	0.96	0.17	34,34,34,34	0
56	MG	YA	3270	1/1	0.96	0.06	34,34,34,34	0
56	MG	YA	3124	1/1	0.96	0.13	22,22,22,22	0
56	MG	RA	3494	1/1	0.96	0.14	57,57,57,57	0
56	MG	RA	3136	1/1	0.96	0.03	45,45,45,45	0
56	MG	QV	103	1/1	0.96	0.08	58,58,58,58	0
56	MG	YA	3065	1/1	0.96	0.05	37,37,37,37	0
56	MG	YA	3004	1/1	0.96	0.29	39,39,39,39	0
56	MG	RA	3271	1/1	0.96	0.12	38,38,38,38	0
56	MG	XA	1757	1/1	0.96	0.17	50,50,50,50	0
56	MG	RA	3020	1/1	0.96	0.07	71,71,71,71	0
56	MG	YA	3371	1/1	0.96	0.20	29,29,29,29	0
56	MG	RD	304	1/1	0.96	0.26	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3458	1/1	0.97	0.08	20,20,20,20	0
56	MG	QA	1706	1/1	0.97	0.12	57,57,57,57	0
56	MG	YA	3529	1/1	0.97	0.14	5,5,5,5	0
56	MG	YA	3326	1/1	0.97	0.11	11,11,11,11	0
56	MG	Y5	102	1/1	0.97	0.21	45,45,45,45	0
56	MG	RA	3355	1/1	0.97	0.19	30,30,30,30	0
56	MG	YA	3463	1/1	0.97	0.16	54,54,54,54	0
56	MG	RA	3652	1/1	0.97	0.10	29,29,29,29	0
56	MG	RA	3621	1/1	0.97	0.04	7,7,7,7	0
56	MG	QT	201	1/1	0.97	0.10	51,51,51,51	0
56	MG	RA	3266	1/1	0.97	0.17	31,31,31,31	0
56	MG	QA	1690	1/1	0.97	0.09	48,48,48,48	0
56	MG	YA	3539	1/1	0.97	0.14	32,32,32,32	0
56	MG	XA	1616	1/1	0.97	0.12	31,31,31,31	0
56	MG	RA	3144	1/1	0.97	0.12	38,38,38,38	0
56	MG	RA	3312	1/1	0.97	0.13	7,7,7,7	0
56	MG	YA	3207	1/1	0.97	0.14	23,23,23,23	0
56	MG	YA	3701	1/1	0.97	0.07	20,20,20,20	0
56	MG	RA	3627	1/1	0.97	0.18	44,44,44,44	0
56	MG	XA	1732	1/1	0.97	0.11	35,35,35,35	0
56	MG	QA	1624	1/1	0.97	0.06	63,63,63,63	0
56	MG	YA	3272	1/1	0.97	0.11	6,6,6,6	0
56	MG	YA	3273	1/1	0.97	0.07	16,16,16,16	0
56	MG	YA	3009	1/1	0.97	0.08	8,8,8,8	0
56	MG	XA	1734	1/1	0.97	0.18	46,46,46,46	0
56	MG	QA	1709	1/1	0.97	0.10	33,33,33,33	0
56	MG	XA	1658	1/1	0.97	0.06	47,47,47,47	0
56	MG	QA	1751	1/1	0.97	0.10	45,45,45,45	0
56	MG	XA	1697	1/1	0.97	0.10	41,41,41,41	0
56	MG	YA	3217	1/1	0.97	0.12	37,37,37,37	0
56	MG	YA	3637	1/1	0.97	0.11	24,24,24,24	0
56	MG	YA	3638	1/1	0.97	0.05	32,32,32,32	0
56	MG	RR	202	1/1	0.97	0.05	39,39,39,39	0
56	MG	RT	201	1/1	0.97	0.13	47,47,47,47	0
56	MG	QA	1732	1/1	0.97	0.11	33,33,33,33	0
56	MG	RA	3488	1/1	0.97	0.15	24,24,24,24	0
56	MG	QA	1765	1/1	0.97	0.06	60,60,60,60	0
56	MG	YA	3021	1/1	0.97	0.18	87,87,87,87	0
56	MG	QB	301	1/1	0.97	0.06	69,69,69,69	0
56	MG	YA	3646	1/1	0.97	0.13	10,10,10,10	0
56	MG	XA	1704	1/1	0.97	0.08	59,59,59,59	0
56	MG	YA	3172	1/1	0.97	0.10	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YB	220	1/1	0.97	0.15	38,38,38,38	0
56	MG	YA	3227	1/1	0.97	0.10	16,16,16,16	0
56	MG	YA	3650	1/1	0.97	0.16	40,40,40,40	0
56	MG	QA	1742	1/1	0.97	0.14	10,10,10,10	0
56	MG	YA	3497	1/1	0.97	0.14	17,17,17,17	0
56	MG	QA	1794	1/1	0.97	0.16	43,43,43,43	0
56	MG	XA	1631	1/1	0.97	0.09	37,37,37,37	0
56	MG	XA	1793	1/1	0.97	0.13	57,57,57,57	0
56	MG	QA	1672	1/1	0.97	0.05	54,54,54,54	0
56	MG	QA	1734	1/1	0.97	0.05	46,46,46,46	0
56	MG	YE	304	1/1	0.97	0.07	43,43,43,43	0
56	MG	RA	3521	1/1	0.97	0.24	42,42,42,42	0
56	MG	XF	202	1/1	0.97	0.09	46,46,46,46	0
56	MG	RA	3549	1/1	0.97	0.15	21,21,21,21	0
56	MG	YA	3661	1/1	0.97	0.24	38,38,38,38	0
56	MG	XL	201	1/1	0.97	0.04	22,22,22,22	0
56	MG	YA	3240	1/1	0.97	0.15	2,2,2,2	0
56	MG	YA	3241	1/1	0.97	0.05	18,18,18,18	0
56	MG	YA	3665	1/1	0.97	0.10	26,26,26,26	0
56	MG	RA	3522	1/1	0.97	0.12	19,19,19,19	0
56	MG	RA	3240	1/1	0.97	0.11	2,2,2,2	0
56	MG	RA	3396	1/1	0.97	0.17	48,48,48,48	0
56	MG	XA	1639	1/1	0.97	0.12	34,34,34,34	0
56	MG	YA	3246	1/1	0.97	0.19	18,18,18,18	0
56	MG	YA	3187	1/1	0.97	0.09	19,19,19,19	0
56	MG	YA	3315	1/1	0.97	0.18	3,3,3,3	0
56	MG	RA	3325	1/1	0.97	0.11	9,9,9,9	0
56	MG	RA	3241	1/1	0.97	0.14	26,26,26,26	0
56	MG	YA	3190	1/1	0.97	0.17	45,45,45,45	0
56	MG	YA	3251	1/1	0.97	0.14	16,16,16,16	0
56	MG	QA	1683	1/1	0.97	0.17	37,37,37,37	0
56	MG	QA	1712	1/1	0.97	0.07	44,44,44,44	0
56	MG	YW	202	1/1	0.97	0.04	35,35,35,35	0
56	MG	YA	3599	1/1	0.97	0.32	42,42,42,42	0
56	MG	YA	3600	1/1	0.97	0.19	2,2,2,2	0
58	SF4	QD	302	8/8	0.97	0.08	54,93,149,174	0
56	MG	YA	3524	1/1	0.97	0.08	6,6,6,6	0
56	MG	QA	1758	1/1	0.97	0.06	39,39,39,39	0
56	MG	Y1	102	1/1	0.97	0.07	35,35,35,35	0
59	ZN	YY	201	1/1	0.97	0.05	99,99,99,99	0
56	MG	YA	3260	1/1	0.98	0.06	2,2,2,2	0
56	MG	YA	3553	1/1	0.98	0.07	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3204	1/1	0.98	0.07	49,49,49,49	0
56	MG	YA	3609	1/1	0.98	0.11	28,28,28,28	0
56	MG	YA	3294	1/1	0.98	0.10	13,13,13,13	0
56	MG	YA	3232	1/1	0.98	0.10	2,2,2,2	0
56	MG	YA	3333	1/1	0.98	0.10	4,4,4,4	0
56	MG	YA	3558	1/1	0.98	0.11	9,9,9,9	0
56	MG	YA	3334	1/1	0.98	0.08	14,14,14,14	0
56	MG	RA	3304	1/1	0.98	0.06	16,16,16,16	0
56	MG	RA	3489	1/1	0.98	0.05	4,4,4,4	0
56	MG	YB	217	1/1	0.98	0.10	8,8,8,8	0
56	MG	RA	3280	1/1	0.98	0.10	26,26,26,26	0
56	MG	YA	3236	1/1	0.98	0.15	40,40,40,40	0
56	MG	QA	1620	1/1	0.98	0.03	56,56,56,56	0
56	MG	YA	3340	1/1	0.98	0.10	15,15,15,15	0
56	MG	YA	3341	1/1	0.98	0.09	29,29,29,29	0
56	MG	YA	3568	1/1	0.98	0.09	21,21,21,21	0
56	MG	XA	1776	1/1	0.98	0.25	38,38,38,38	0
56	MG	RA	3439	1/1	0.98	0.12	25,25,25,25	0
56	MG	YA	3033	1/1	0.98	0.11	54,54,54,54	0
56	MG	YA	3305	1/1	0.98	0.06	2,2,2,2	0
56	MG	YA	3346	1/1	0.98	0.08	14,14,14,14	0
56	MG	YA	3521	1/1	0.98	0.10	12,12,12,12	0
56	MG	YA	3133	1/1	0.98	0.10	48,48,48,48	0
56	MG	XA	1754	1/1	0.98	0.11	22,22,22,22	0
56	MG	RA	3338	1/1	0.98	0.08	30,30,30,30	0
56	MG	RA	3276	1/1	0.98	0.16	32,32,32,32	0
56	MG	YA	3435	1/1	0.98	0.08	4,4,4,4	0
56	MG	YA	3275	1/1	0.98	0.09	8,8,8,8	0
56	MG	RA	3600	1/1	0.98	0.12	13,13,13,13	0
56	MG	RA	3674	1/1	0.98	0.06	31,31,31,31	0
56	MG	RA	3636	1/1	0.98	0.14	42,42,42,42	0
56	MG	YA	3314	1/1	0.98	0.14	2,2,2,2	0
56	MG	YA	3485	1/1	0.98	0.12	18,18,18,18	0
56	MG	RA	3618	1/1	0.98	0.10	21,21,21,21	0
56	MG	QA	1722	1/1	0.98	0.14	25,25,25,25	0
56	MG	YA	3090	1/1	0.98	0.15	45,45,45,45	0
56	MG	RA	3431	1/1	0.98	0.25	17,17,17,17	0
56	MG	RA	3316	1/1	0.98	0.18	18,18,18,18	0
56	MG	RA	3005	1/1	0.98	0.21	36,36,36,36	0
56	MG	YA	3285	1/1	0.98	0.09	2,2,2,2	0
56	MG	YA	3448	1/1	0.98	0.13	2,2,2,2	0
56	MG	YA	3541	1/1	0.98	0.12	11,11,11,11	0

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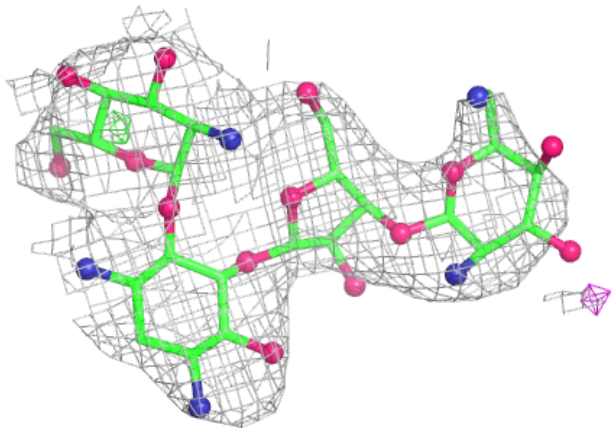
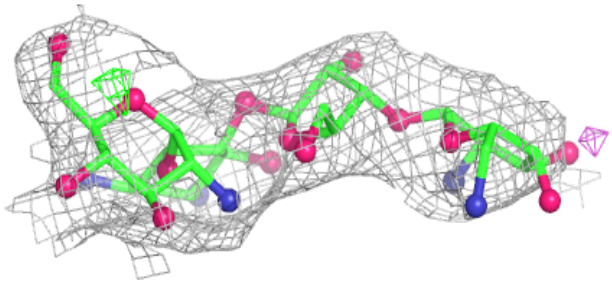
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3681	1/1	0.98	0.05	12,12,12,12	0
56	MG	YA	3323	1/1	0.98	0.12	2,2,2,2	0
56	MG	RA	3352	1/1	0.98	0.04	20,20,20,20	0
56	MG	YA	3545	1/1	0.98	0.04	19,19,19,19	0
56	MG	RA	3447	1/1	0.98	0.13	11,11,11,11	0
56	MG	QA	1785	1/1	0.98	0.06	74,74,74,74	0
58	SF4	XD	301	8/8	0.98	0.07	64,74,104,108	0
59	ZN	QN	101	1/1	0.98	0.07	200,200,200,200	0
56	MG	YA	3602	1/1	0.98	0.26	40,40,40,40	0
56	MG	YA	3410	1/1	0.98	0.08	37,37,37,37	0
59	ZN	XN	101	1/1	0.98	0.06	114,114,114,114	0
56	MG	RA	3558	1/1	0.98	0.06	32,32,32,32	0
59	ZN	Y5	101	1/1	0.98	0.04	88,88,88,88	0
59	ZN	Y9	101	1/1	0.98	0.03	61,61,61,61	0
56	MG	RA	3559	1/1	0.98	0.04	38,38,38,38	0
56	MG	YA	3018	1/1	0.99	0.05	48,48,48,48	0
56	MG	YA	3304	1/1	0.99	0.21	14,14,14,14	0
56	MG	YA	3518	1/1	0.99	0.03	10,10,10,10	0
56	MG	RB	211	1/1	0.99	0.04	39,39,39,39	0
56	MG	QA	1822	1/1	0.99	0.03	62,62,62,62	0
56	MG	QA	1626	1/1	0.99	0.10	34,34,34,34	0
56	MG	YA	3601	1/1	0.99	0.19	12,12,12,12	0
56	MG	YA	3559	1/1	0.99	0.04	9,9,9,9	0
56	MG	RE	304	1/1	0.99	0.07	2,2,2,2	0
56	MG	YA	3619	1/1	0.99	0.05	9,9,9,9	0
56	MG	XA	1760	1/1	0.99	0.25	35,35,35,35	0
59	ZN	R5	101	1/1	0.99	0.05	126,126,126,126	0
59	ZN	R6	101	1/1	0.99	0.03	71,71,71,71	0
56	MG	RA	3362	1/1	0.99	0.06	17,17,17,17	0
56	MG	YA	3549	1/1	0.99	0.31	44,44,44,44	0
56	MG	YE	301	1/1	0.99	0.11	12,12,12,12	0
56	MG	YA	3381	1/1	0.99	0.03	26,26,26,26	0
59	ZN	Y6	101	1/1	0.99	0.03	52,52,52,52	0
56	MG	RA	3567	1/1	0.99	0.10	19,19,19,19	0
56	MG	YA	3122	1/1	0.99	0.04	36,36,36,36	0
59	ZN	R9	101	1/1	1.00	0.02	90,90,90,90	0

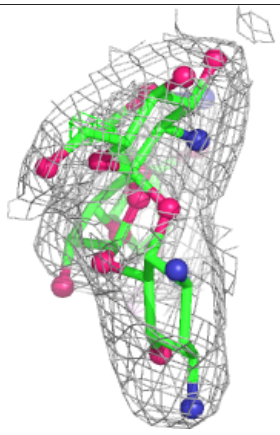
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR QA 1821:

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

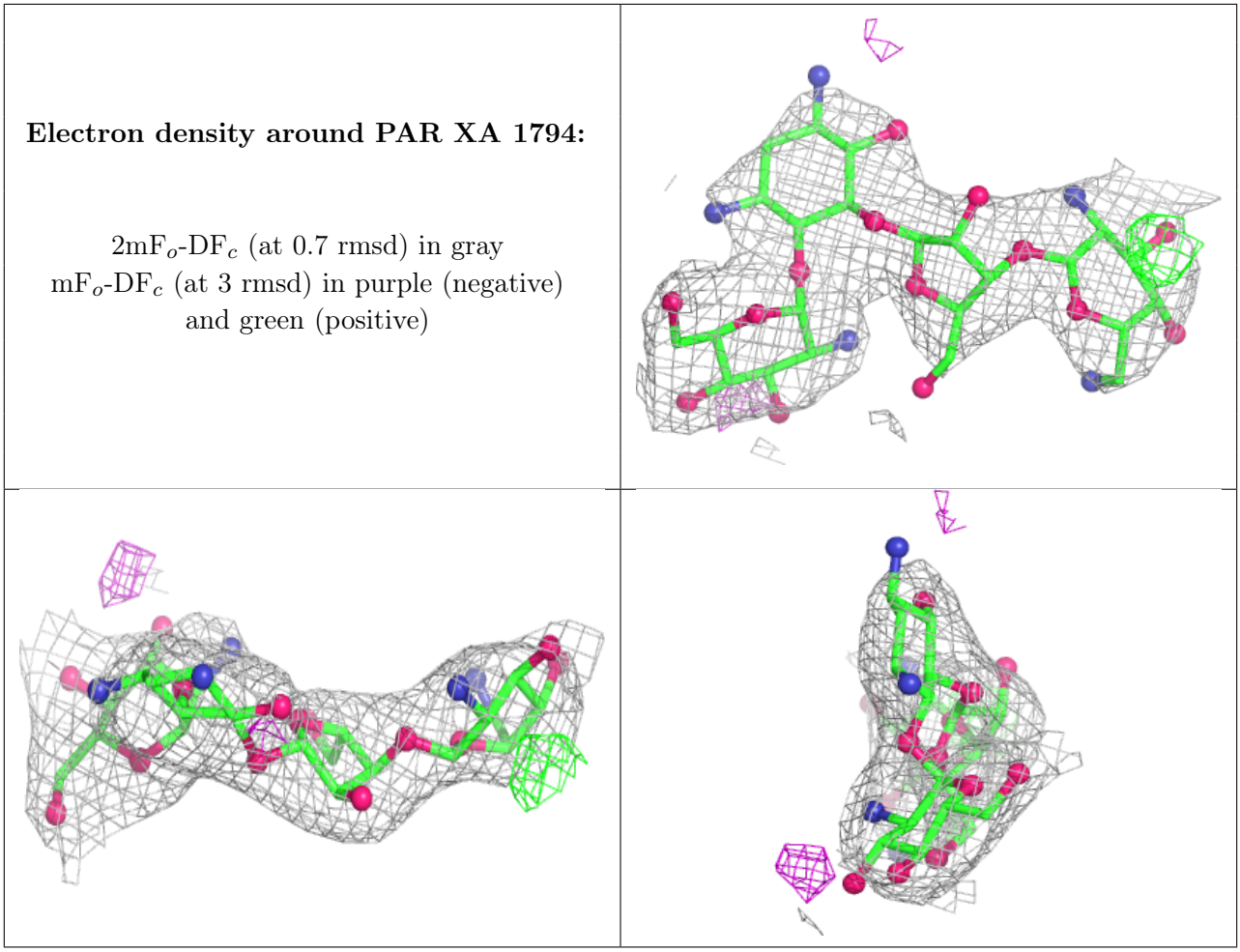






Electron density around PAR XA 1794:

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



6.5 Other polymers (i)

There are no such residues in this entry.