



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 07:38 PM EST

PDB ID : 6BZ8  
Title : Thermus thermophilus 70S containing 16S G347U point mutation and near-cognate ASL Leucine in A site  
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.  
Deposited on : 2017-12-22  
Resolution : 3.74 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

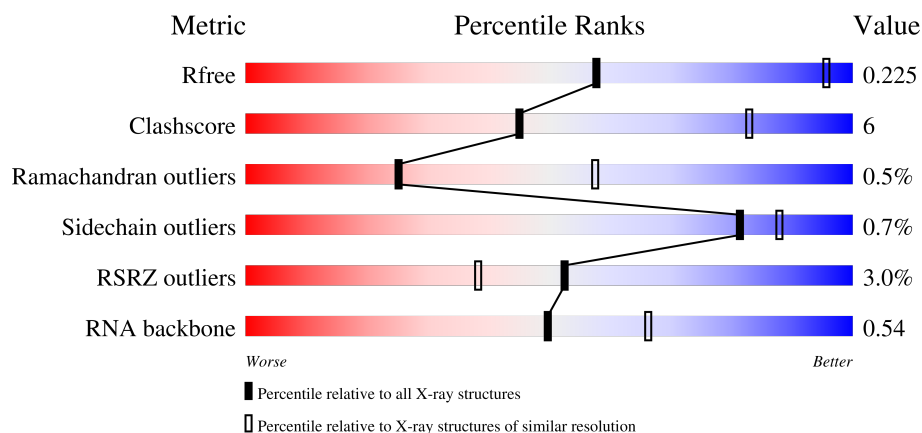
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.74 Å.

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







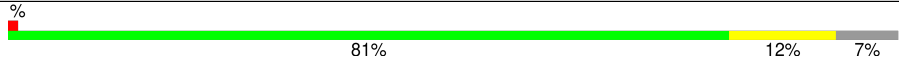
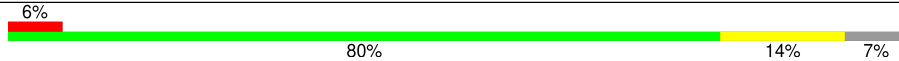
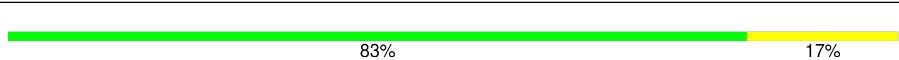
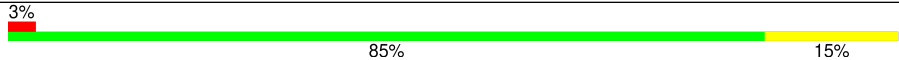
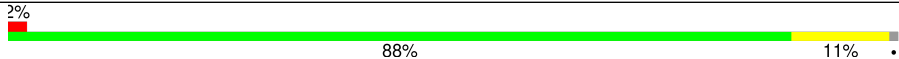
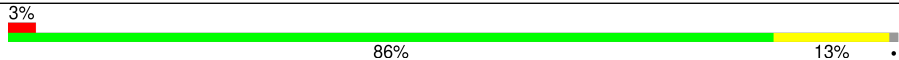
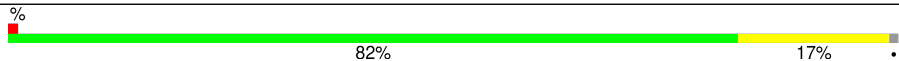
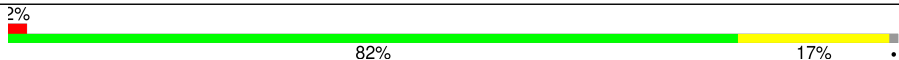


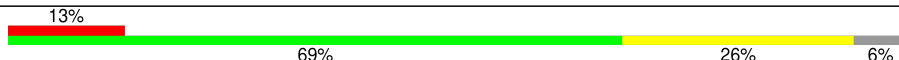
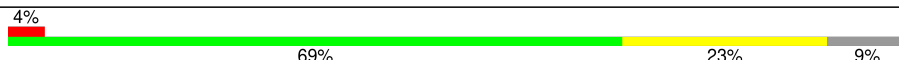
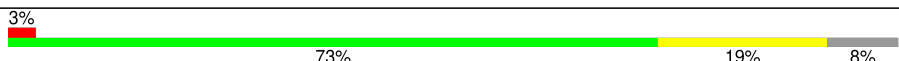
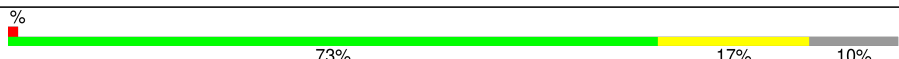
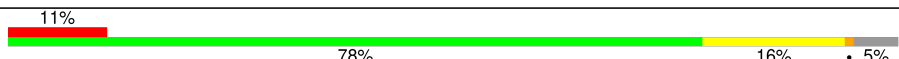

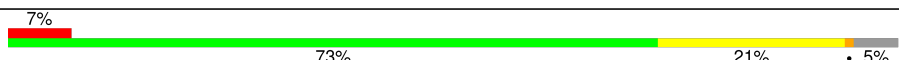
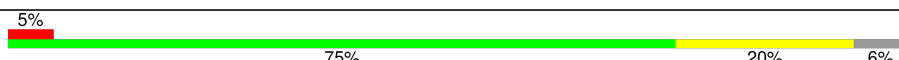
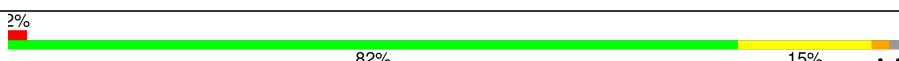
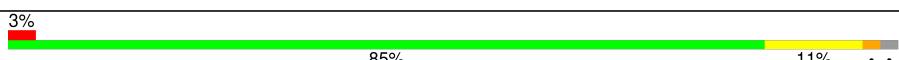
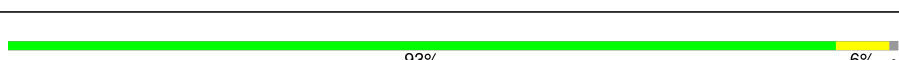
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1104 (3.88-3.60)
Clashscore	180529	1161 (3.88-3.60)
Ramachandran outliers	177936	1139 (3.88-3.60)
Sidechain outliers	177891	1134 (3.88-3.60)
RSRZ outliers	164620	1104 (3.88-3.60)
RNA backbone	3690	1123 (4.46-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1508	<div> <div>2%</div> <div>54%</div> <div>36%</div> <div>8%</div> <div>..</div> </div>
1	XA	1508	<div> <div>2%</div> <div>54%</div> <div>35%</div> <div>8%</div> <div>..</div> </div>
2	QB	256	<div> <div>2%</div> <div>70%</div> <div>21%</div> <div>8%</div> </div>
2	XB	256	<div> <div>2%</div> <div>74%</div> <div>18%</div> <div>8%</div> </div>

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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	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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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	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	QW	77	
22	XV	77	
22	XW	77	
23	QX	25	
23	XX	25	
24	QY	17	
24	XY	17	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	

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Mol	Chain	Length	Quality of chain
27	RD	276	
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	

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Mol	Chain	Length	Quality of chain
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	

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Mol	Chain	Length	Quality of chain
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3213	-	-	-	X
56	MG	RA	3409	-	-	-	X
56	MG	YA	3520	-	-	-	X

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 295646 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
			32244	14352	5978	10415	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32246	14353	5981	10413	1499			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	347	U	G	engineered mutation	GB 55771382
XA	347	U	G	engineered mutation	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	126	Total	C	N	O		0	0	0
			998	633	193	172				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	27	57	8			
23	XX	11	Total	C	N	O	P	0	0	0
			230	105	42	73	10			

- Molecule 24 is a RNA chain called ASL Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	17	Total	C	N	O	P	0	0	0
			362	162	65	118	17			
24	XY	17	Total	C	N	O	P	0	0	0
			362	162	65	118	17			

- Molecule 25 is a RNA chain called 23S rRNA.

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

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
31	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	72	Total	Mg	0	0
			72	72		
56	QC	1	Total	Mg	0	0
			1	1		
56	QF	1	Total	Mg	0	0
			1	1		
56	QH	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QV	6	Total 6	Mg 6	0	0
56	QX	1	Total 1	Mg 1	0	0
56	QY	1	Total 1	Mg 1	0	0
56	RA	513	Total 513	Mg 513	0	0
56	RB	11	Total 11	Mg 11	0	0
56	RE	3	Total 3	Mg 3	0	0
56	RN	1	Total 1	Mg 1	0	0
56	RO	1	Total 1	Mg 1	0	0
56	RP	2	Total 2	Mg 2	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	RR	2	Total 2	Mg 2	0	0
56	RT	1	Total 1	Mg 1	0	0
56	RY	1	Total 1	Mg 1	0	0
56	R0	3	Total 3	Mg 3	0	0
56	R8	1	Total 1	Mg 1	0	0
56	XA	80	Total 80	Mg 80	0	0
56	XC	1	Total 1	Mg 1	0	0
56	XE	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	XQ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XS	1	Total 1	Mg 1	0	0
56	XV	8	Total 8	Mg 8	0	0
56	XX	1	Total 1	Mg 1	0	0
56	YA	541	Total 541	Mg 541	0	0
56	YB	12	Total 12	Mg 12	0	0
56	YD	1	Total 1	Mg 1	0	0
56	YE	3	Total 3	Mg 3	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	4	Total 4	Mg 4	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	YX	2	Total 2	Mg 2	0	0
56	YY	1	Total 1	Mg 1	0	0
56	Y0	2	Total 2	Mg 2	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	Y8	1	Total 1	Mg 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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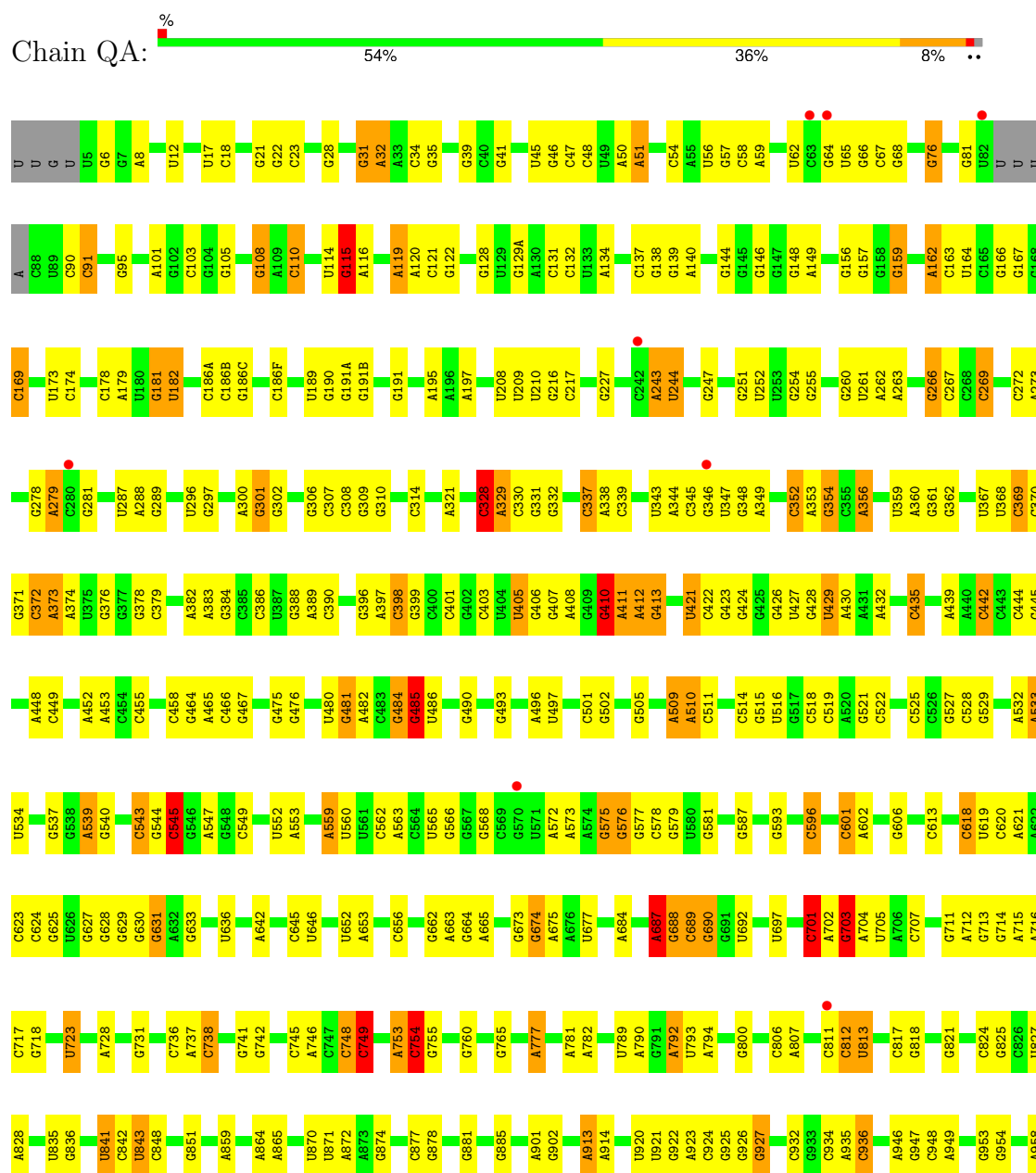
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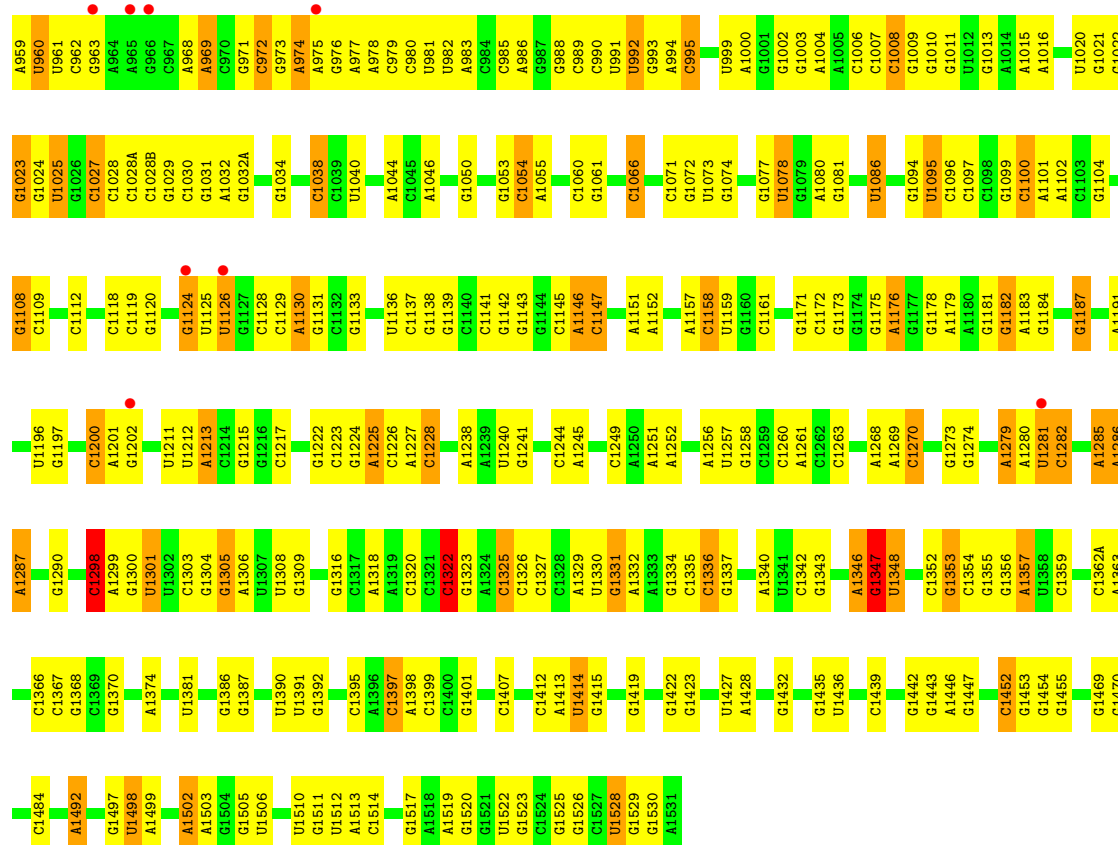
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y6	1	Total 1	Zn 1	0	0
58	Y9	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

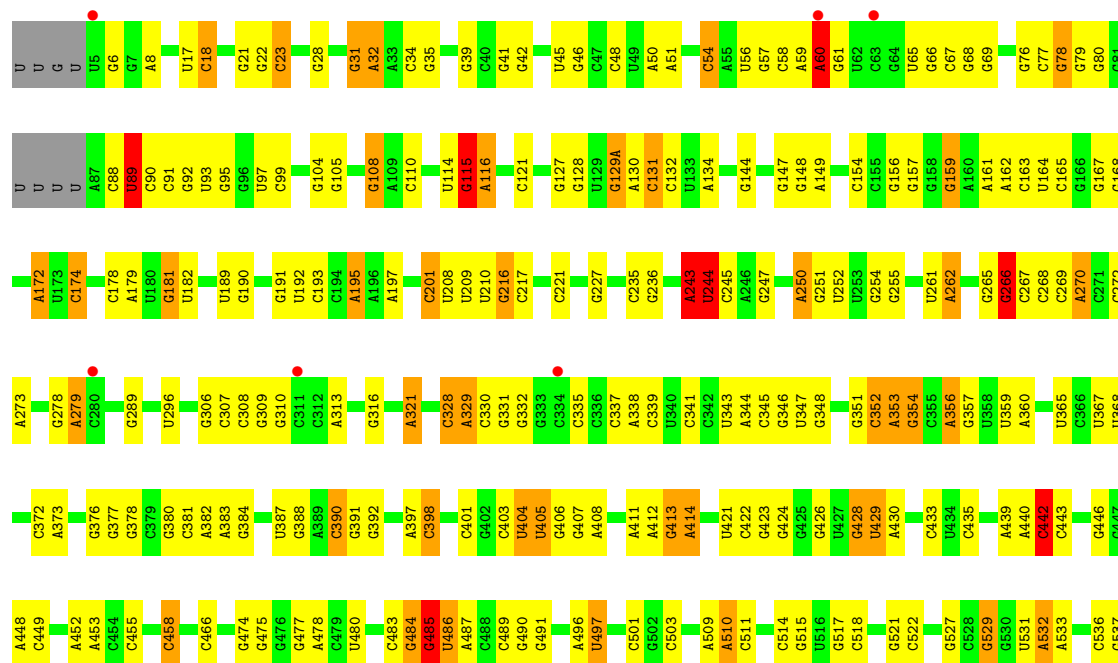
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 16S rRNA

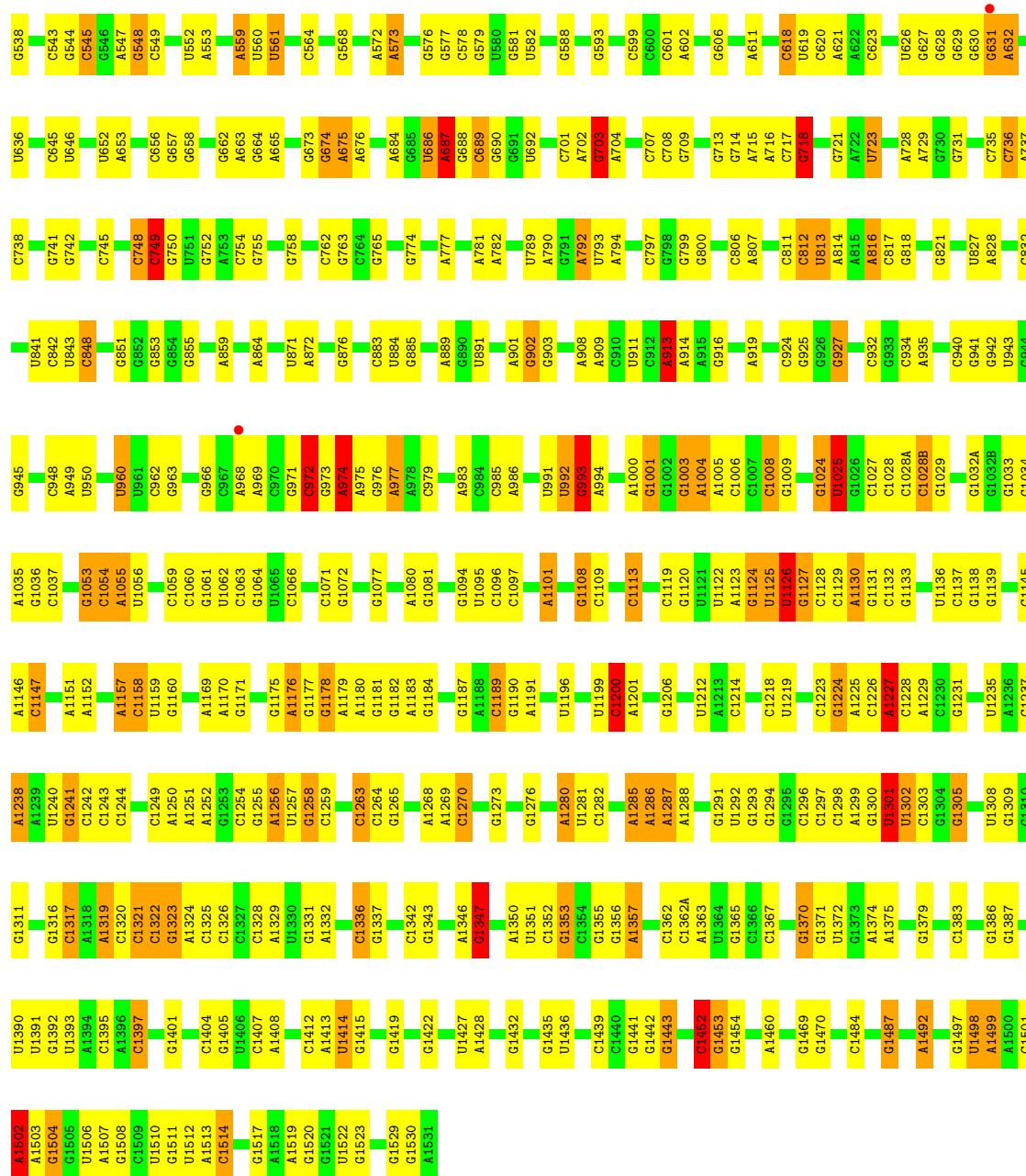




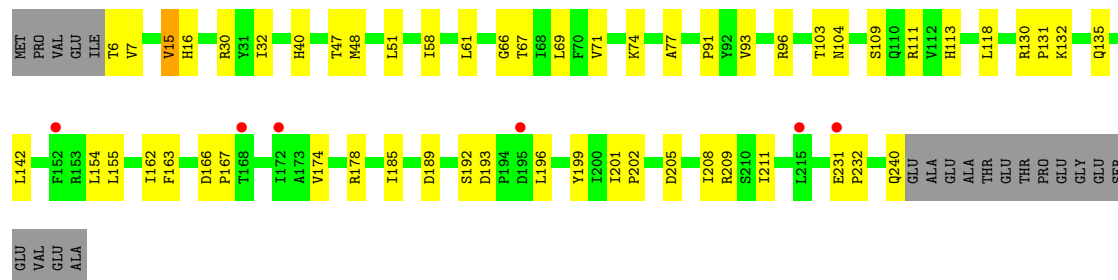
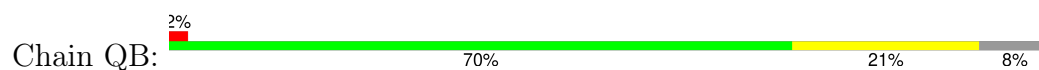
• Molecule 1: 16S rRNA



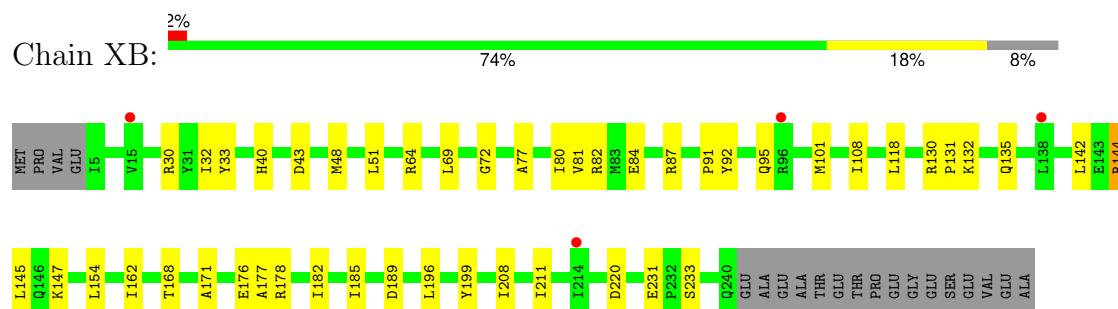




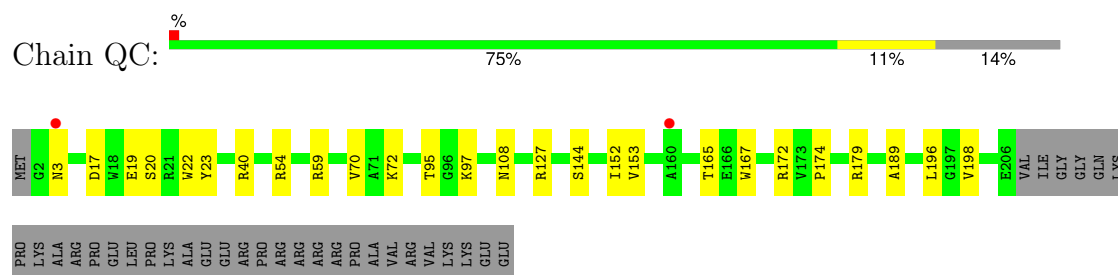
• Molecule 2: 30S ribosomal protein S2



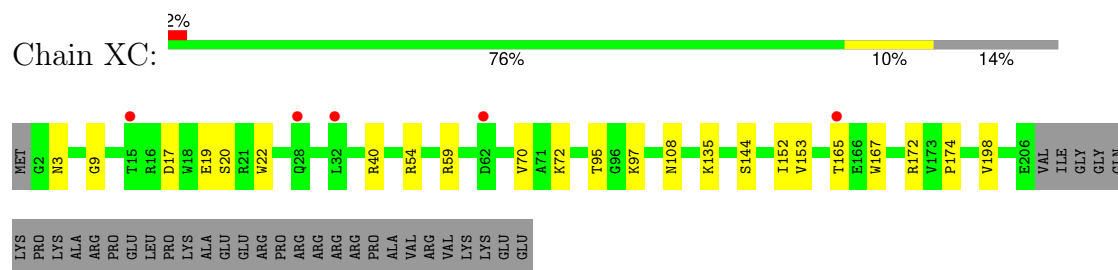
- Molecule 2: 30S ribosomal protein S2



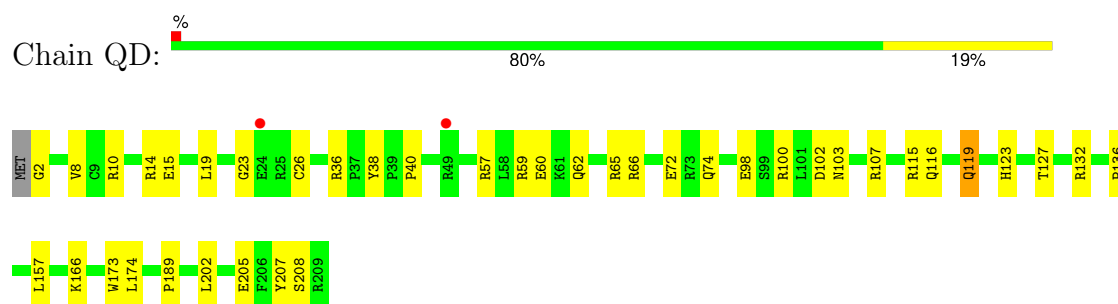
- Molecule 3: 30S ribosomal protein S3



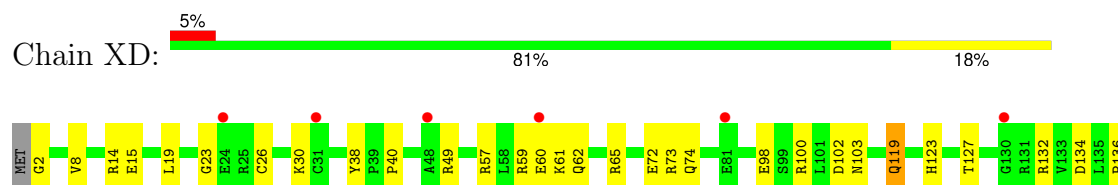
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

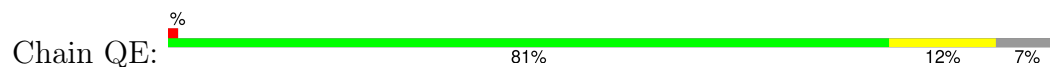


- Molecule 4: 30S ribosomal protein S4

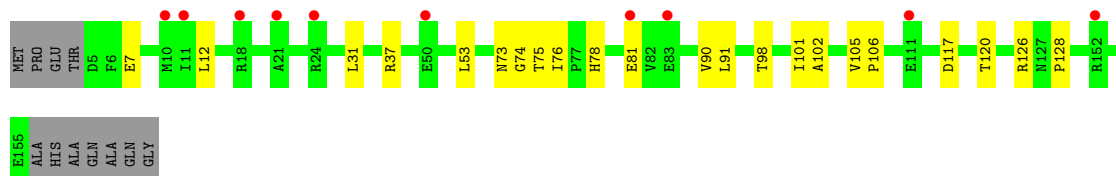
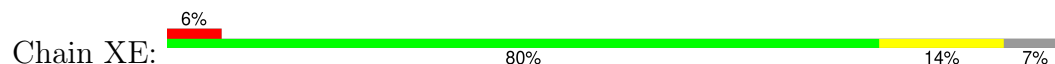




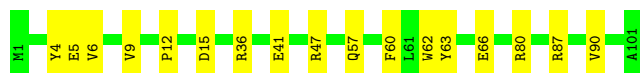
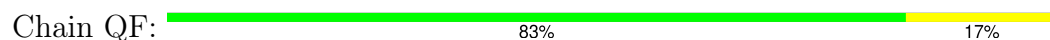
- Molecule 5: 30S ribosomal protein S5



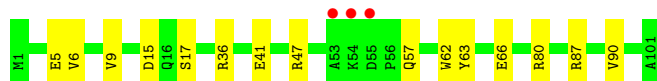
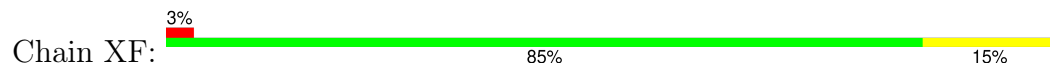
- Molecule 5: 30S ribosomal protein S5



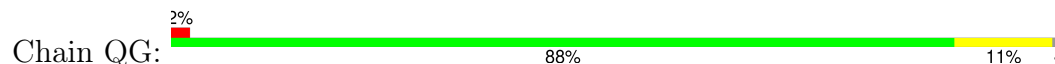
- Molecule 6: 30S ribosomal protein S6



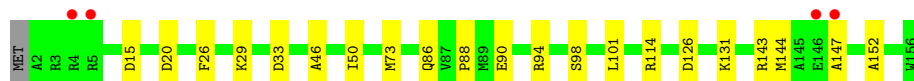
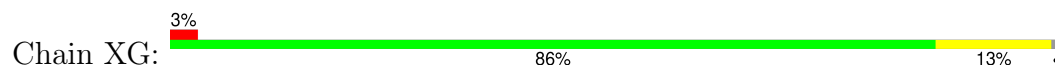
- Molecule 6: 30S ribosomal protein S6



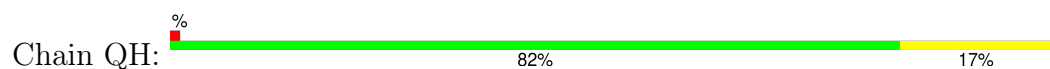
- Molecule 7: 30S ribosomal protein S7



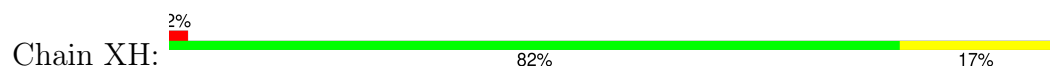
- Molecule 7: 30S ribosomal protein S7



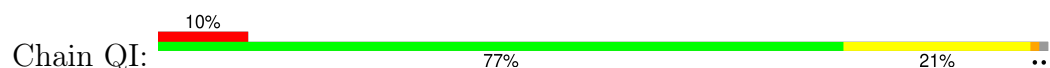
- Molecule 8: 30S ribosomal protein S8



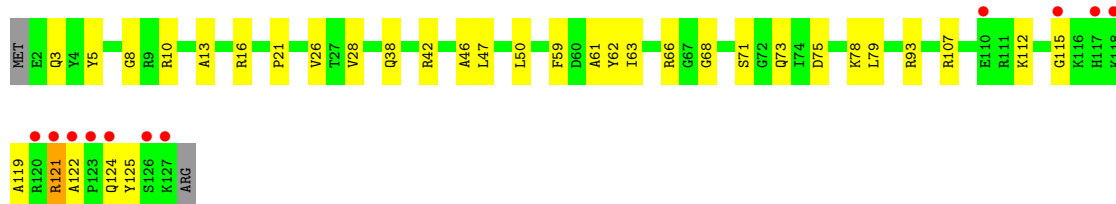
- Molecule 8: 30S ribosomal protein S8



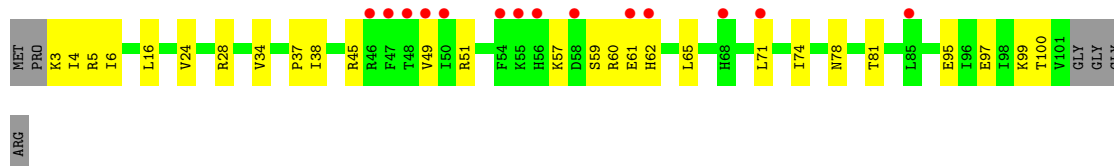
- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10




- Molecule 10: 30S ribosomal protein S10




VAL  
GLY  
GLY  
GLY  
ARG

- Molecule 11: 30S ribosomal protein S11

Chain QK: 


MET ALA LYS LYS PRO SER LYS LYS LYS VAL K11 R18 R19 Y20 Y21 H22 N26 N27 T28 T29 V30 D34 N38 P39 R54 T57 P58 Q62 D81 V82 I83 V84 R85 G86 R91 E92 Q93 A97 L103 V109 K127 A128 S129

- Molecule 11: 30S ribosomal protein S11

Chain XK: 

MET ALA LYS LYS PRO SER LYS LYS VAL K11 Y20 I21 V30 D34 G37 N38 P39 W42 R54 R55 G56 T57 P58 Y59 I83 V84 R85 G86 T87 R91 V109 T112 P115 H116 N117 K124 F125 R126 LYS ALA SER


- Molecule 12: 30S ribosomal protein S12

Chain QL: 

MET P5 R12 K13 G14 R15 E16 K17 V18 R19 K20 K21 S22 A26 L27 K28 F32 R33 R34 K47 K48 R53 V58 R59 L60 T61 S62 G63 Y64 E65 Y66 T67 T85 R86 D92 G95 V104 Y105 R113 R117 S118 T122 A129 LYS THR ALA

ALA  
LYS  
LYS


- Molecule 12: 30S ribosomal protein S12

Chain XL: 

MET P5 T6 I7 R8 K13 G14 R15 E16 K17 V18 R19 A26 L27 K28 F32 R33 T44 P45 K46 K47 P48 N49 R53 A56 L60 T61 S62 Y69 L70 F71 L84 D92 R97 T100 V101 R102 T103 R104 T105 G106 A107 Y105 K114 R117 S118 K126 GLU

ALA  
ALA  
LYS  
THR  
ALA  
LYS  
LYS

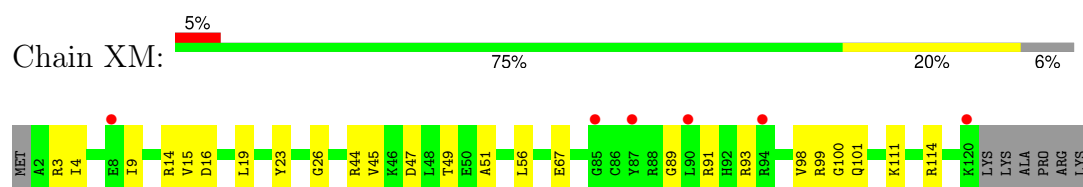
- Molecule 13: 30S ribosomal protein S13

Chain QM: 

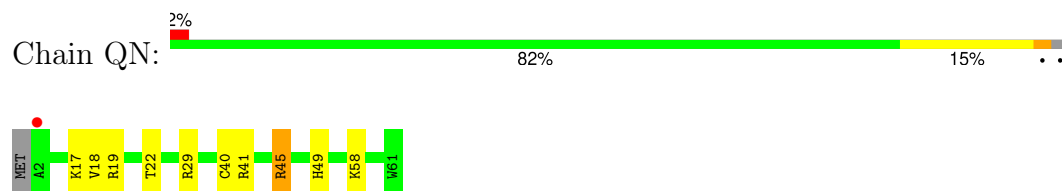
MET A2 R3 I9 K13 R14 V15 D16 G26 M40 T43 R44 V45 K46 D47 L48 T49 E50 A51 R57 E58 N61 N62 L66 I84 G85 C86 Y87 R88 R93 R94 R99 G100 Q101 R102 T103 R104 T105 N106 A107 R108 T116 V117 K120 K121 LYS ALA

PRO  
ARG  
LYS

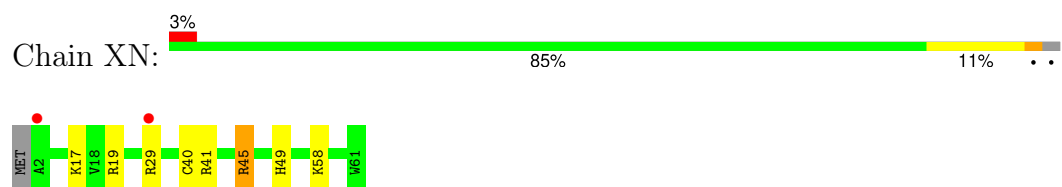
- Molecule 13: 30S ribosomal protein S13



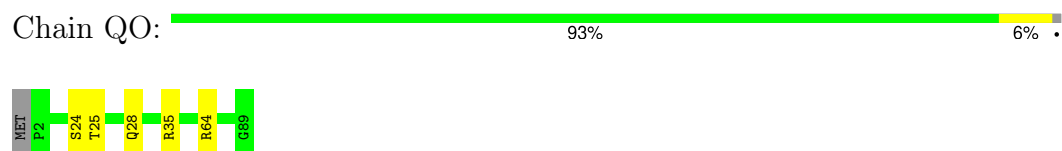
- Molecule 14: 30S ribosomal protein S14 type Z



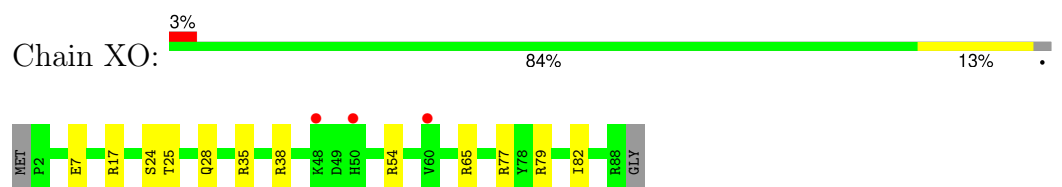
- Molecule 14: 30S ribosomal protein S14 type Z



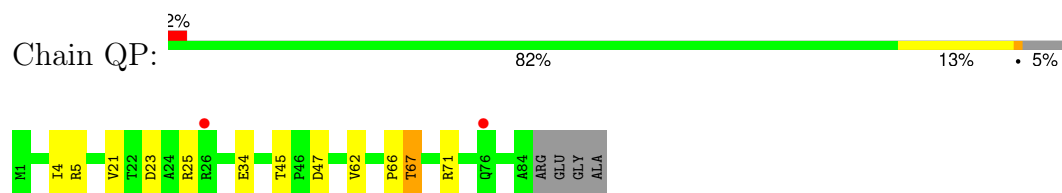
- Molecule 15: 30S ribosomal protein S15



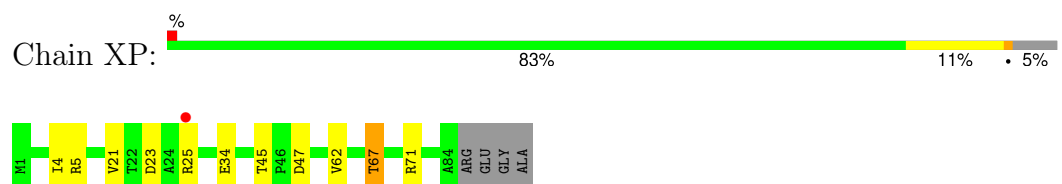
- Molecule 15: 30S ribosomal protein S15



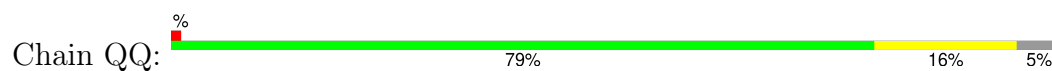
- Molecule 16: 30S ribosomal protein S16



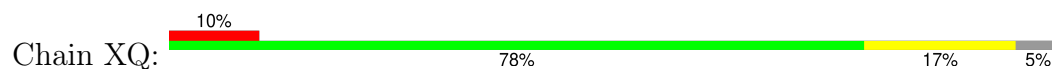
- Molecule 16: 30S ribosomal protein S16



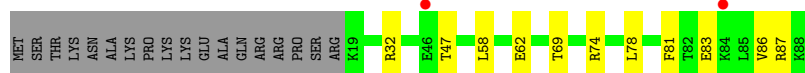
## • Molecule 17: 30S ribosomal protein S17



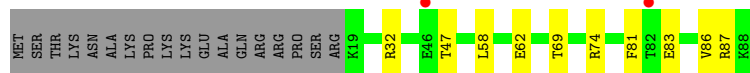
## • Molecule 17: 30S ribosomal protein S17



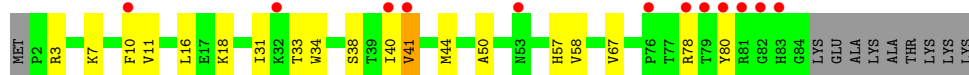
## • Molecule 18: 30S ribosomal protein S18



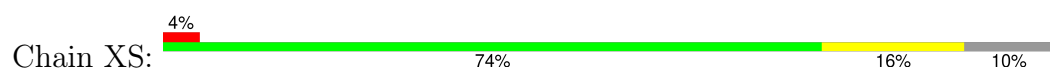
## • Molecule 18: 30S ribosomal protein S18



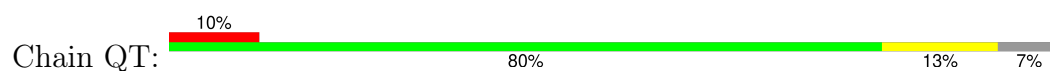
## • Molecule 19: 30S ribosomal protein S19

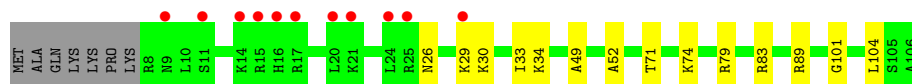


## • Molecule 19: 30S ribosomal protein S19

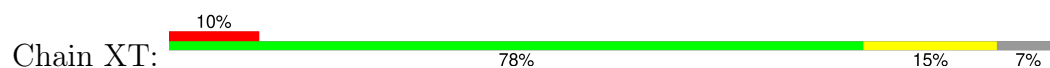


## • Molecule 20: 30S ribosomal protein S20

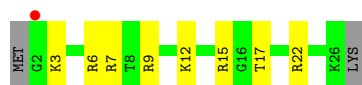




- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



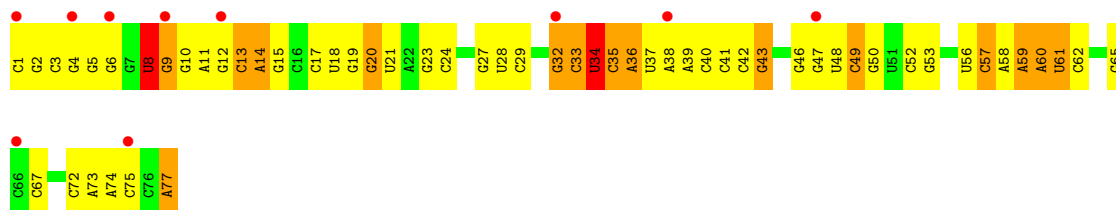
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA fMet



- Molecule 22: tRNA fMet

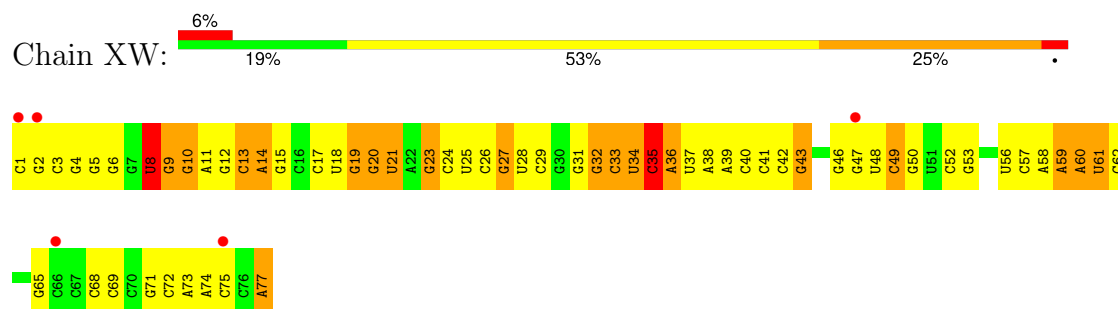


- Molecule 22: tRNA fMet

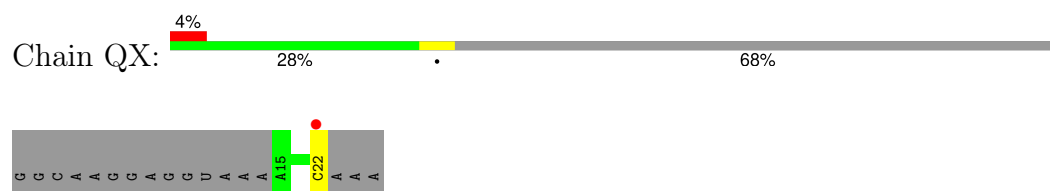




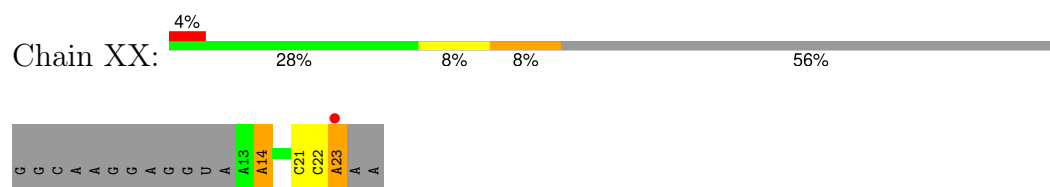
- Molecule 22: tRNA fMet



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



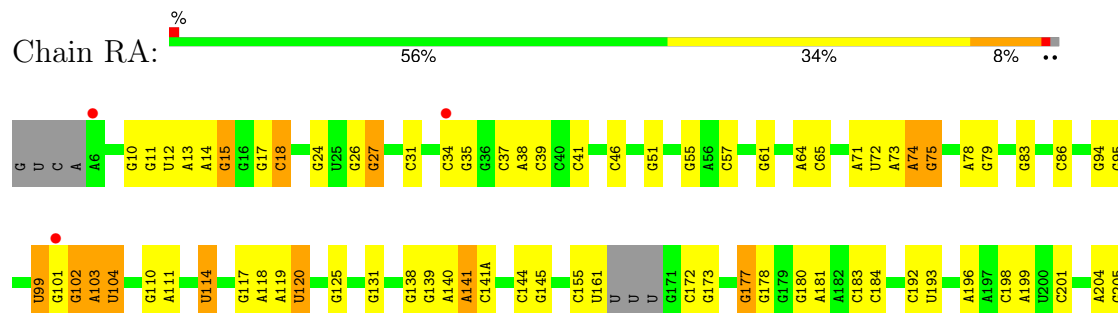
- Molecule 24: ASL Leu



- Molecule 24: ASL Leu

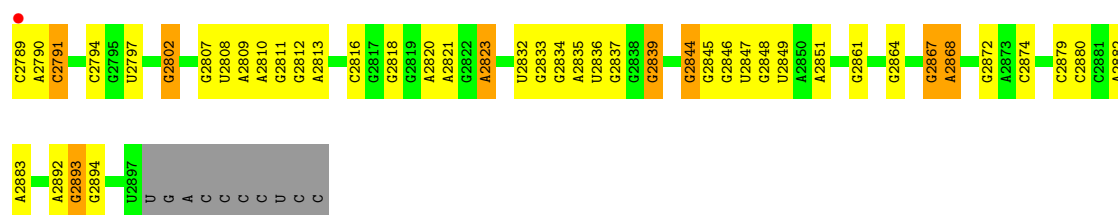


- Molecule 25: 23S rRNA

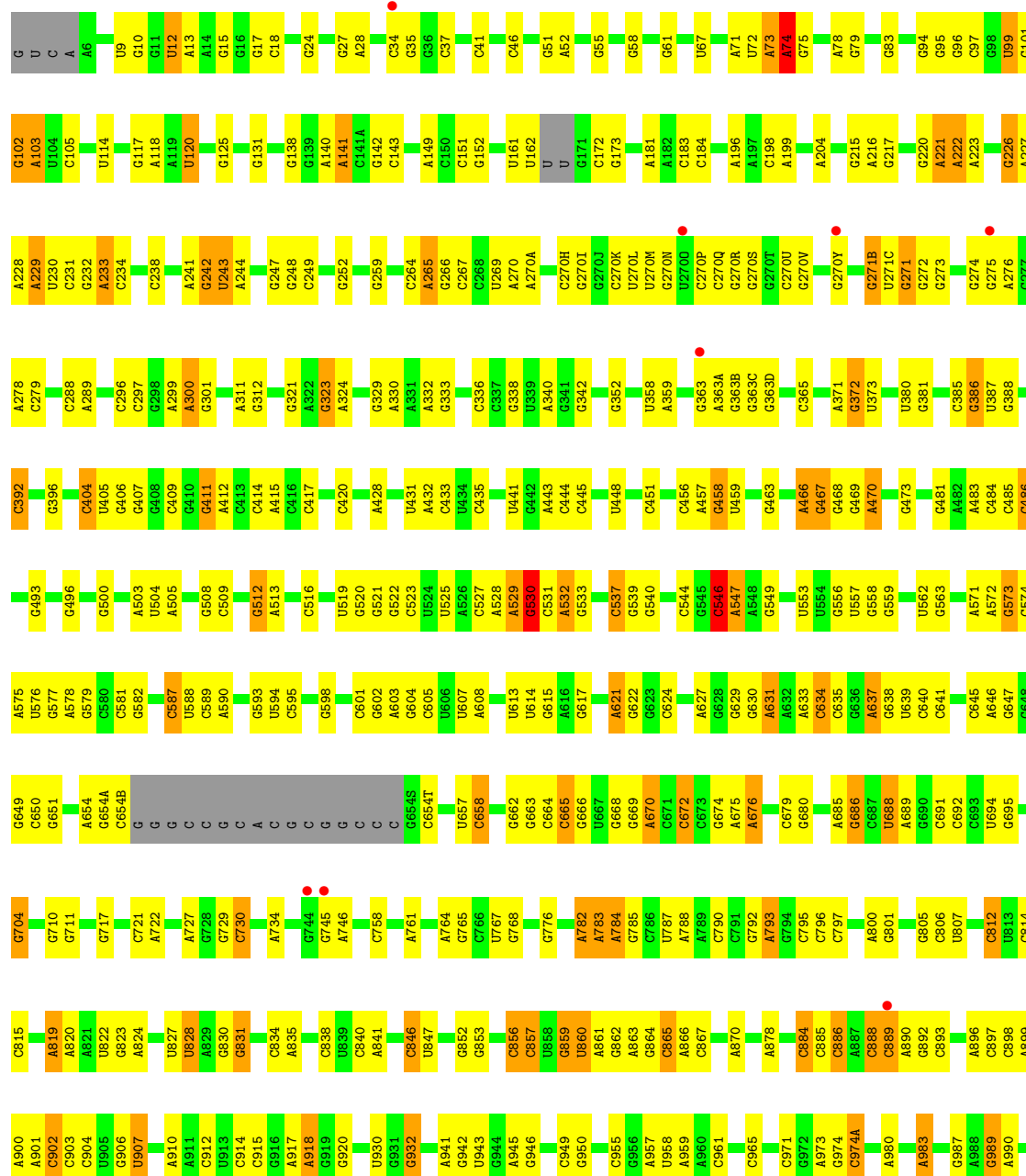




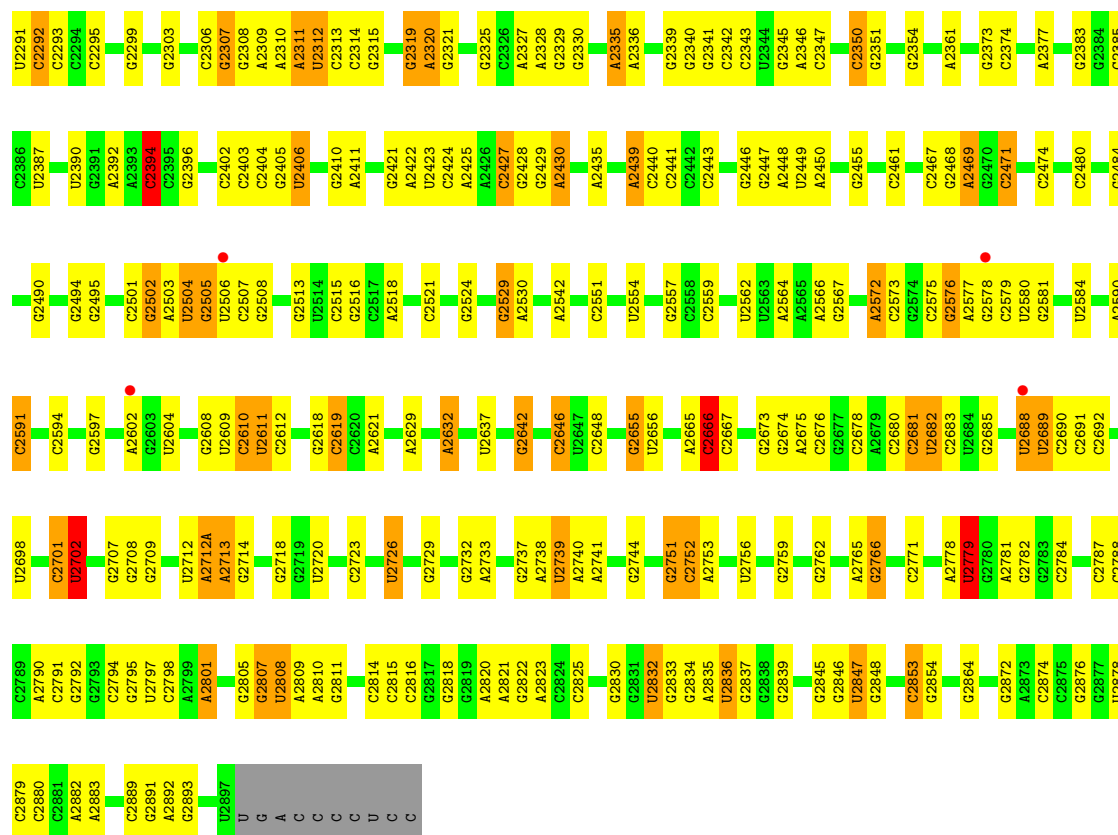
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G2707	U2615	A2518	G2429	G2238	C2140	A2059	U1955	G1845	A1762	C1640	C1544	G1454
G2708	G2615	G2519	A2430	G2239	G2141	A2060	U1956	G1846	G1763	C1644	A1545	G1455
G2709	G2618	G2529	A2435	G2239	C2142	G2061	A1960	A1847	G1764	C1648	C1547	C1458
U2712	G2619	U2537	A2439	U2243	C2145	C2063	C1961	U1851	G1771	G1649	G1548	G1459
A2712A	G2623	C2538	C2440	U2244	G2146	C2064	C1962	C1852	G1772	G1650	C1549	A1460
G2713	C2626	C2539	C2441	U2245	G2147	C2065	C1963	A1853	G1773	G1651	C1549	C1462
G2714	C2627	C2540	A2336	C2246	G2148	C2066	C1964	C1853	C1774	A1652	A1554	
G2715	G2627	A2541	C2443	C2247	G2149	G2067	C1965	G1858	U1775	C1656	A1558	A1471
G2716	C2628	A2542	G2444	C2248	U2150	U2068	A1966	A1859	G1776	C1657	G1559	G1472
A2623	A2623	G2543	G2445	U2249	G2151	G2069	C1967	G1860		C1658	G1560	G1473
G2630	G2630	G2543	G2445	G2250	G2152	G2069	C1967	G1860		C1658	G1560	C1474
G2631	G2631	U2547	A2448	C2254	G2156	C2073	A1969	G1869	U1779	U1659	A1566	
A2632	A2632	G2553	C2456	C2254	G2157	U2074	C1970	C1870	A1780	C1660	A1567	G1479
G2729	C2635	U2554	C2456	C2258	A2158	U2075	A1971	A1871	C1781	G1661	G1480	G1479
G2730	U2636	U2555	C2461	A2266	G2159	A1972	A1972	A1872	C1782	G1662	G1482	G1480
G2731	U2637	C2556	C2467	A2269	C2161	C2081	C1973	G1878	A1783	C1663	G1483	G1482
G2732	U2638	C2559	C2468	A2273	G2162	U2086	C1979	C1881	A1784	A1664	U1578	G1484
A2733	G2642	C2560	A2469	A2274	C2163	G2087	C1990	C1882	A1785	A1665	A1579	G1485
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G2744	G2667	C2570	C2374	G2280	A2170	U2102	C2006	C1893	U1798	U1679	U1590	U1497
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A2748	A2674	A2572	C2379	C2284	C2183	C2105	U2011	C1902	C1800	C1505	C1505	C1505
G2751	A2675	C2573	A2380	C2285	G2184	G2106	G2012	G1903	G1801	C1506	C1506	C1506
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A2757	C2681	U2577	U2387	U2291	G2187	G2110	A2015	G1906	C1804	G1695	C1509	C1509
A2758	C2682	G2578	C2387	C2292	G2190	C2111	A2019	A1913	A1809	A1698	A1510	A1510
G2761	C2683	C2579	C2392	C2293	G2193	G2112	A2020	C1914	A1910	A1698	C1512	C1512
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G2770	U2689	U2500	C2402	G2303	U2197	U2118	A2031	A1928	G1817	A1729	A1603	U1516
A2776	C2690	C2501	C2403	G2307	A2198	G2123	G2032	G1929	U1818	U1730	C1609	U1520
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A2693	A2693	U2504	U2406	G2311	G2210	G2125	G2035	U1931	U1820	G1733	A1615	G1527
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C2695	C2695	C2507	G2410	U2313	A2212	G2127	A2042	A1937	A1825	C1742	C1617	A1528
G2780	U2696	G2508	G2421	C2314	U2213	C2128	C2043	A1938	G1826	G1743	C1533	C1533
G2784	U2697	U2604	A2422	G2315	G2215	C2128	C2043	U1939	C1827	G1743	G1618	G1618
C2785	U2698	C2512	U2423	G2315	G2215	U2132	U2047	U1940	A1829	C1752	U1535	U1535
U2786	C2785	G2513	C2424	G2319	A2226	G2133	G2048	C1947	G1753	G1752	G1622	G1622
G2787	C2786	U2514	A2425	G2320	G2226	G2133	G2048	C1947	G1753	G1752	G1622	G1622
C2788	C2788	A2426	G2426	G2321	G2228	A2134	G2052	G1950	U1833	C1754	C1636	C1636
		G2516	G2427	G2321	G2228	A2135	C2055	U1951	U1834	A1755	A1637	A1637
						C2136			G1835	G1756	C1638	C1638



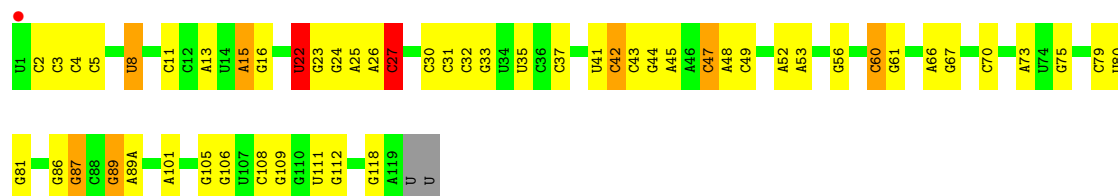
• Molecule 25: 23S rRNA



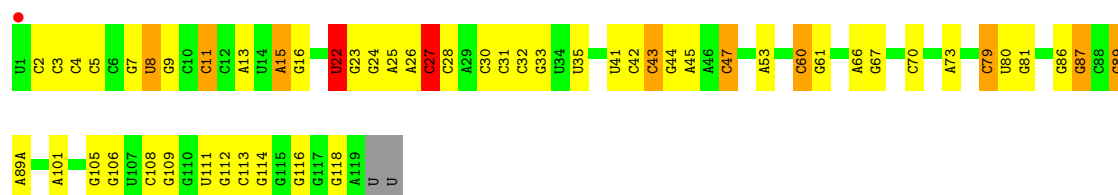




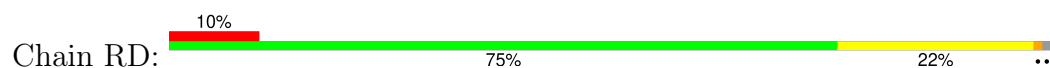
• Molecule 26: 5S rRNA

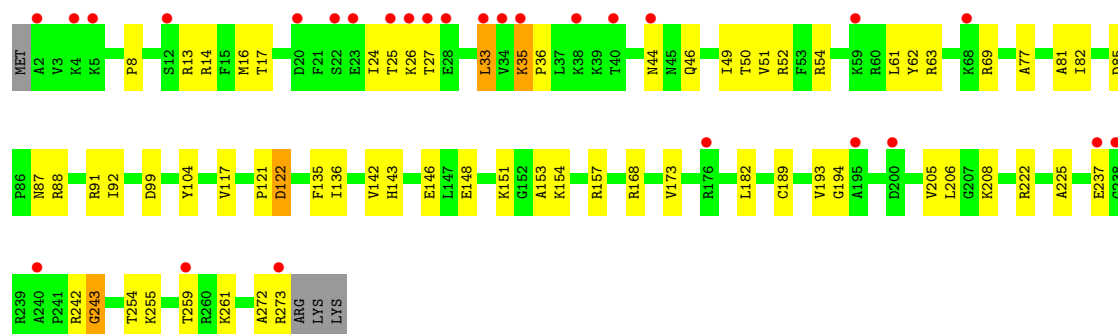


• Molecule 26: 5S rRNA

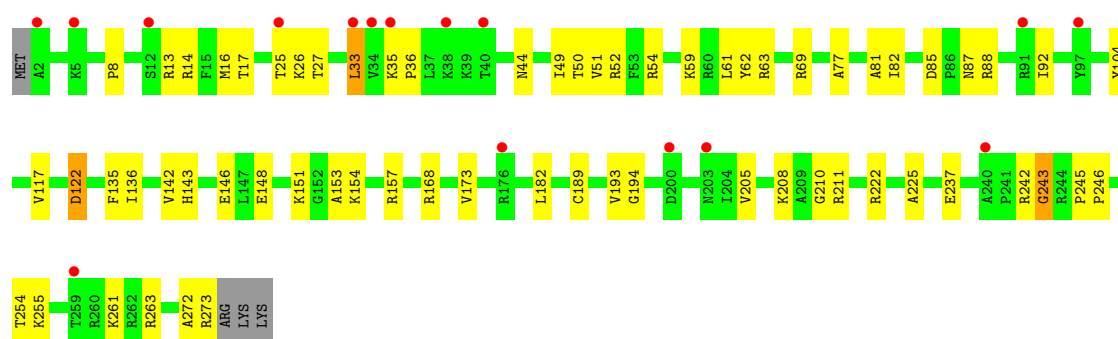
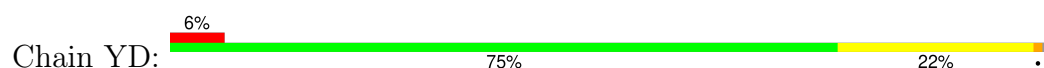


• Molecule 27: 50S ribosomal protein L2

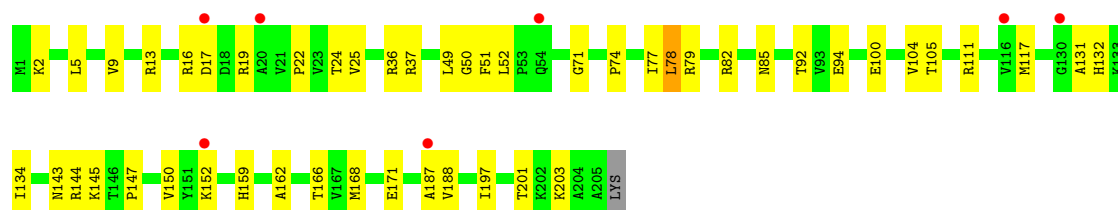
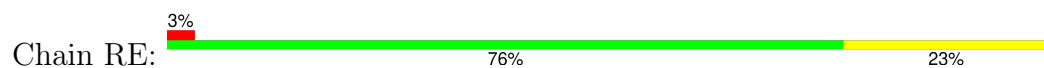




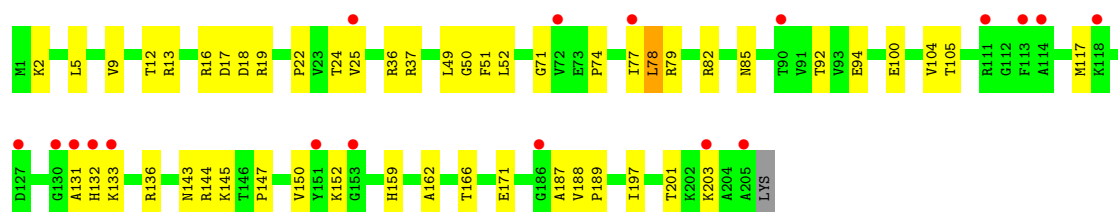
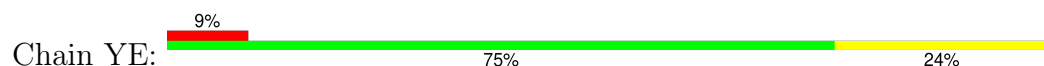
• Molecule 27: 50S ribosomal protein L2



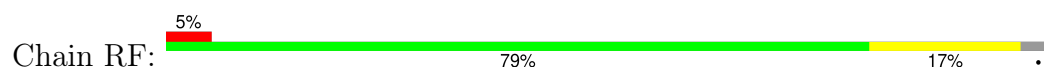
• Molecule 28: 50S ribosomal protein L3

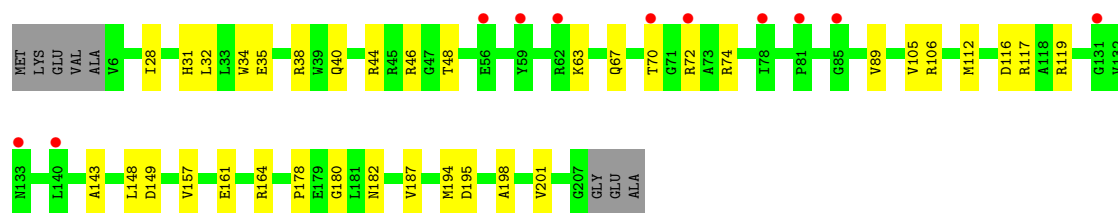


• Molecule 28: 50S ribosomal protein L3

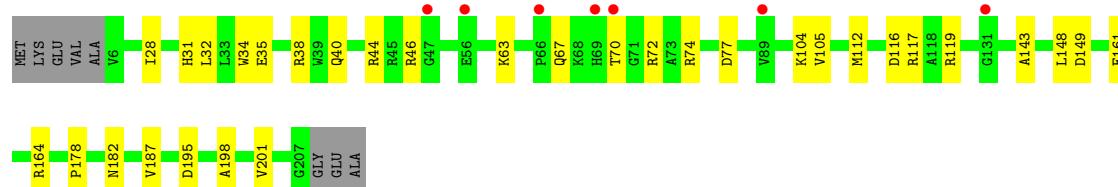
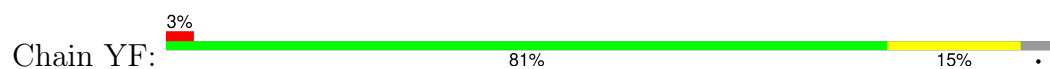


• Molecule 29: 50S ribosomal protein L4

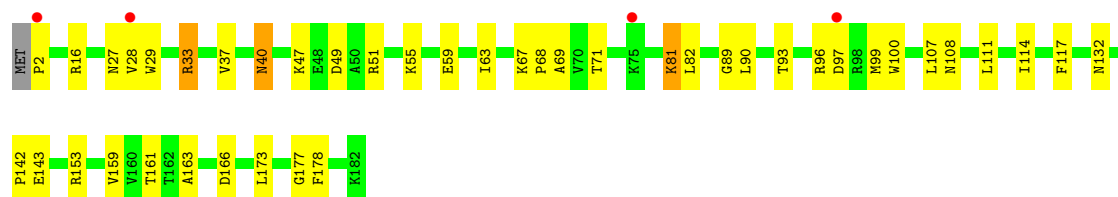
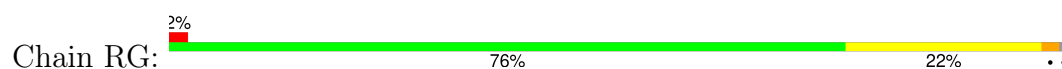




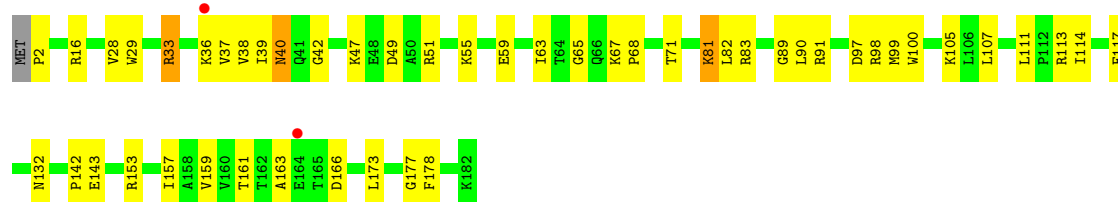
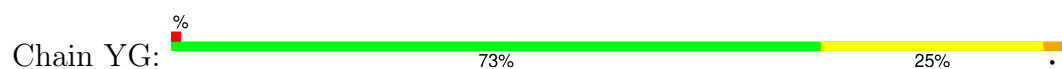
• Molecule 29: 50S ribosomal protein L4



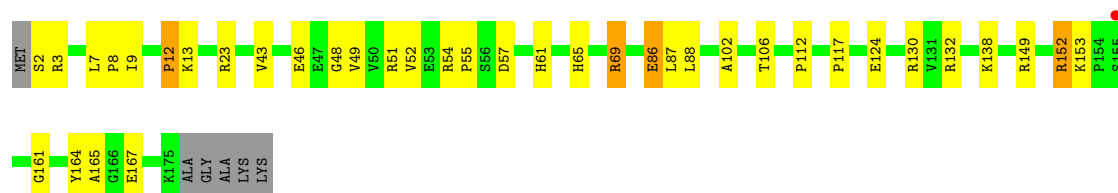
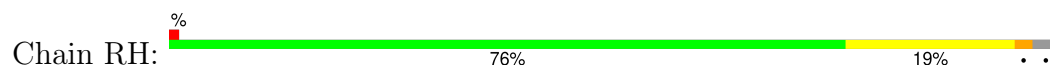
• Molecule 30: 50S ribosomal protein L5



• Molecule 30: 50S ribosomal protein L5

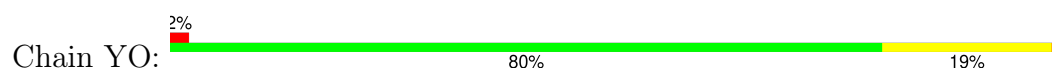


• Molecule 31: 50S ribosomal protein L6

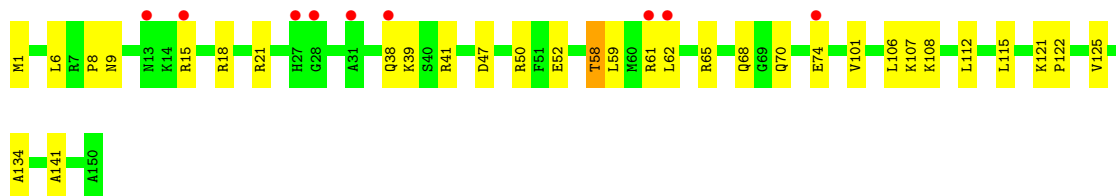
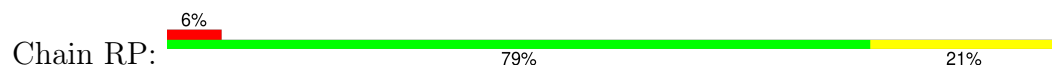




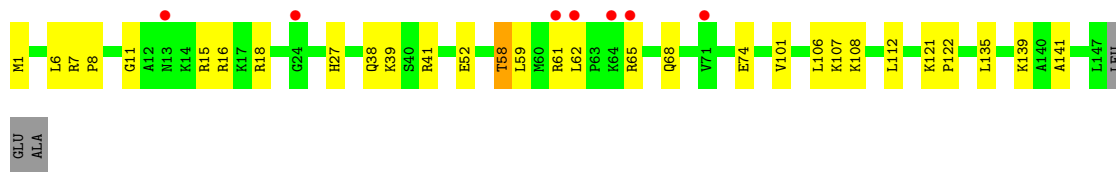
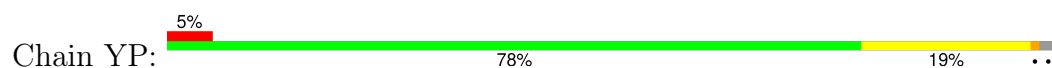
- Molecule 34: 50S ribosomal protein L14



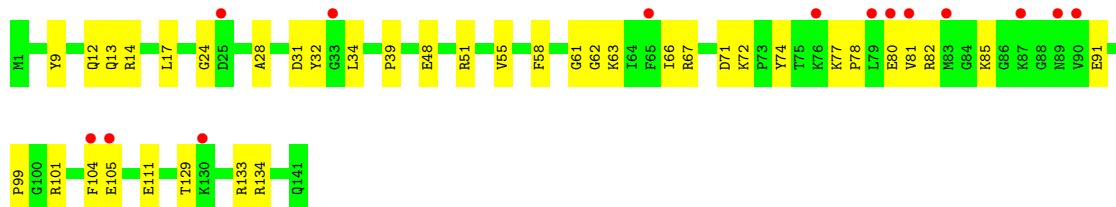
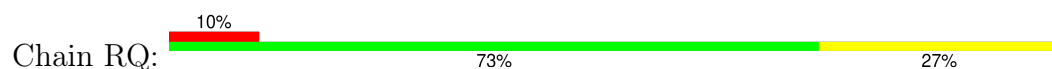
- Molecule 35: 50S ribosomal protein L15



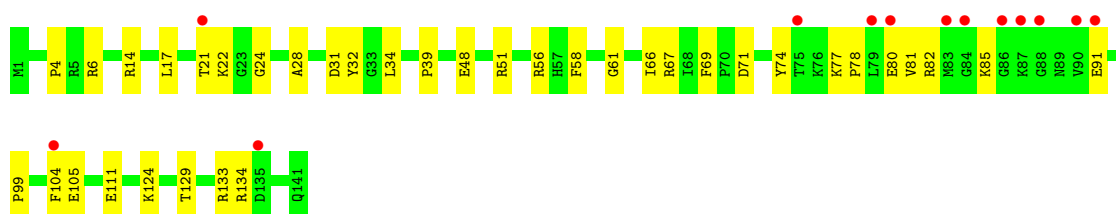
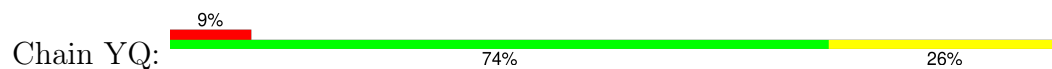
- Molecule 35: 50S ribosomal protein L15



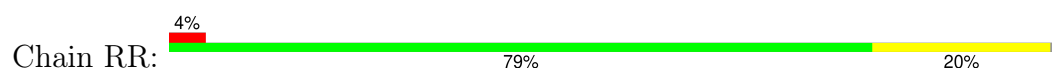
- Molecule 36: 50S ribosomal protein L16



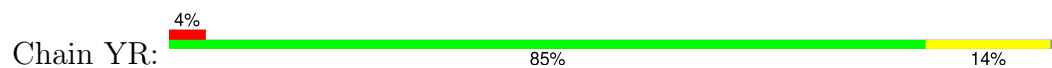
- Molecule 36: 50S ribosomal protein L16



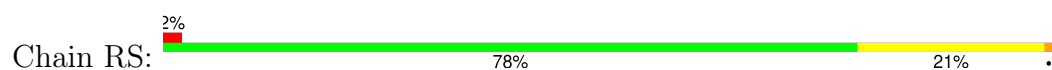
- Molecule 37: 50S ribosomal protein L17



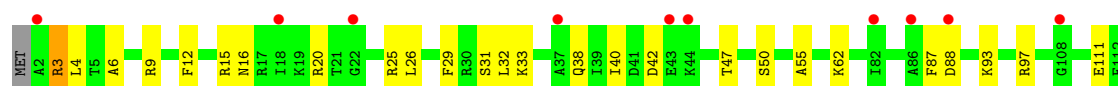
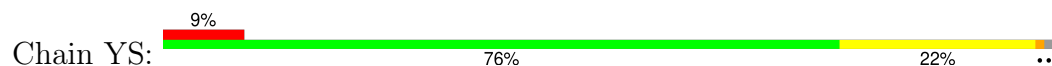
- Molecule 37: 50S ribosomal protein L17



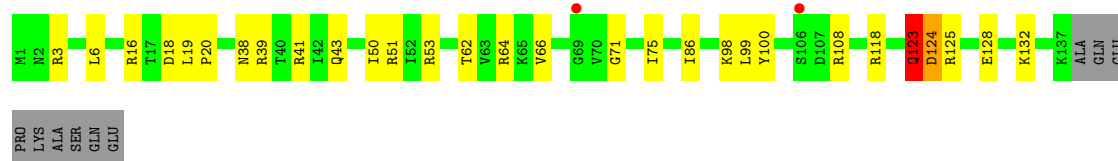
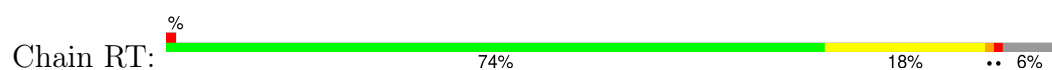
- Molecule 38: 50S ribosomal protein L18



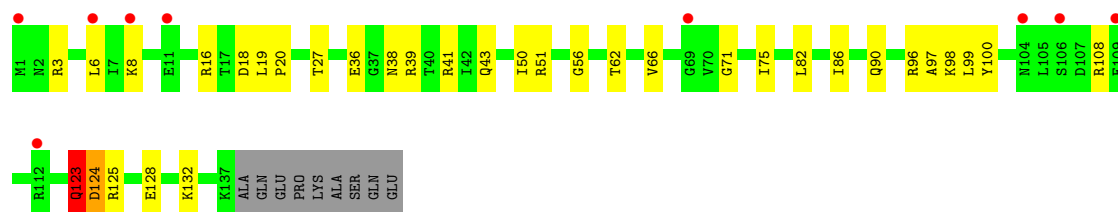
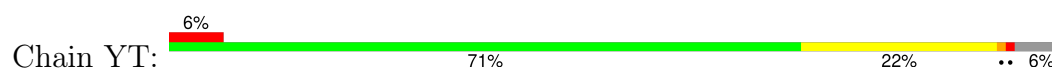
- Molecule 38: 50S ribosomal protein L18



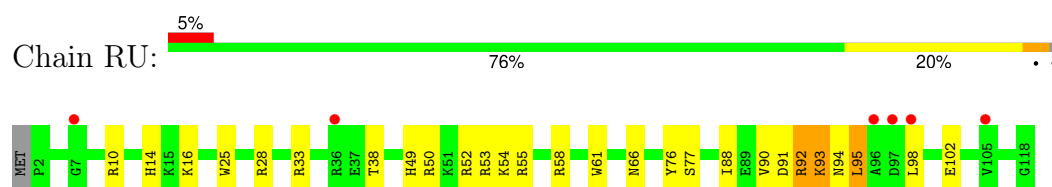
- Molecule 39: 50S ribosomal protein L19



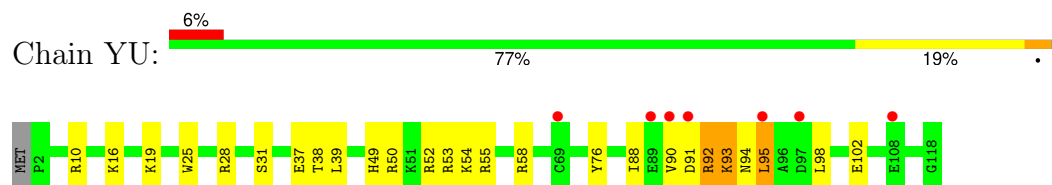
- Molecule 39: 50S ribosomal protein L19



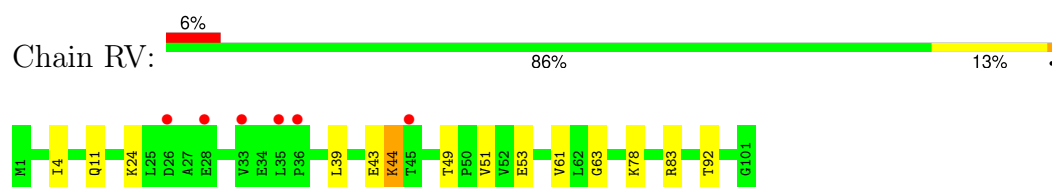
- Molecule 40: 50S ribosomal protein L20



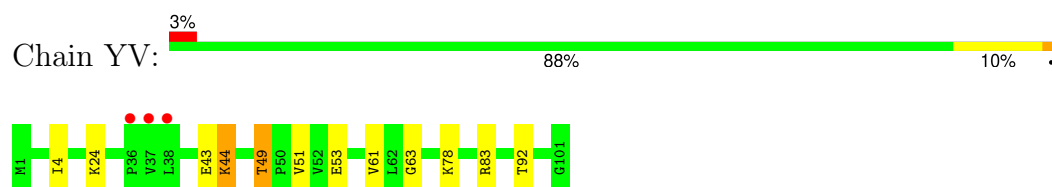
- Molecule 40: 50S ribosomal protein L20



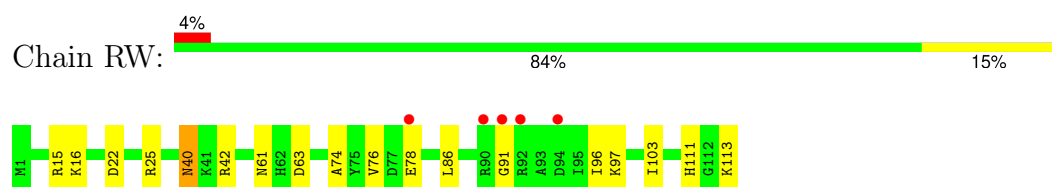
- Molecule 41: 50S ribosomal protein L21



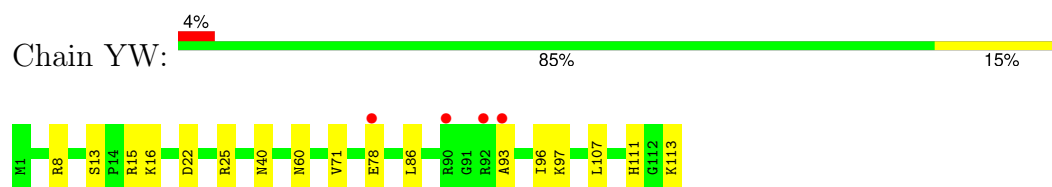
- Molecule 41: 50S ribosomal protein L21



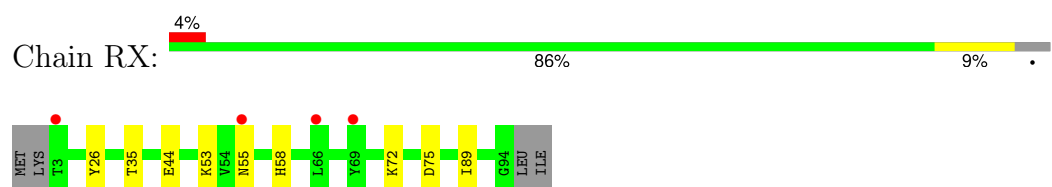
- Molecule 42: 50S ribosomal protein L22




- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23




- Molecule 43: 50S ribosomal protein L23

Chain YX:  85% 10%




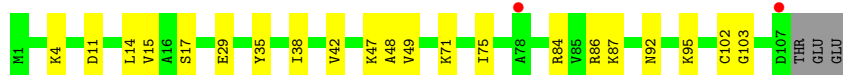
- Molecule 44: 50S ribosomal protein L24

Chain RY:  7% 84% 14%



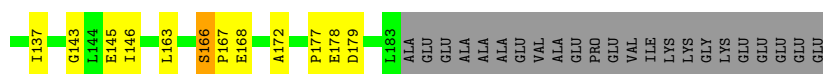
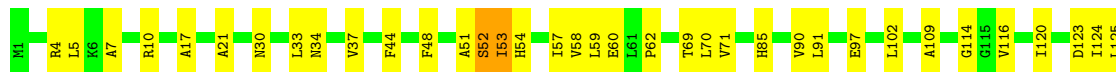
- Molecule 44: 50S ribosomal protein L24

Chain YY:  2% 78% 19%



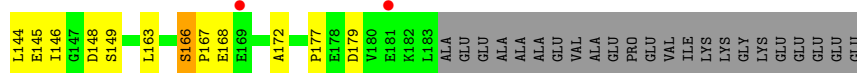
- Molecule 45: 50S ribosomal protein L25

Chain RZ:  66% 22% 11%




- Molecule 45: 50S ribosomal protein L25

Chain YZ:  66% 21% 11%

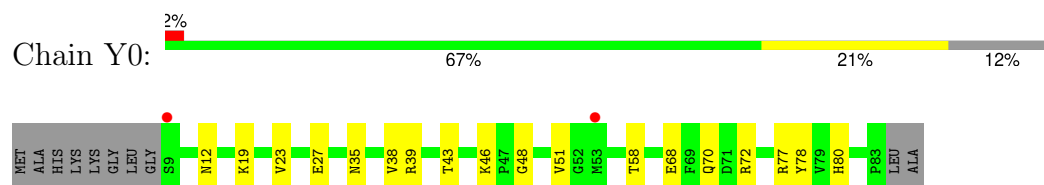


- Molecule 46: 50S ribosomal protein L27

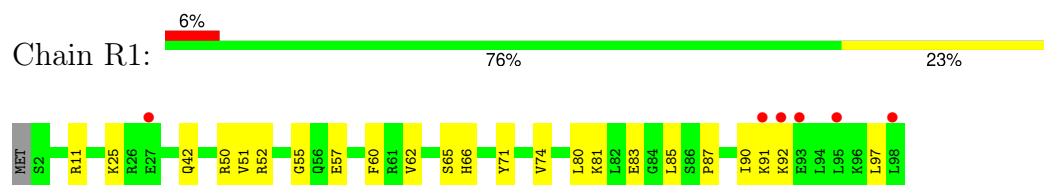
Chain R0:  6% 78% 18% 5%



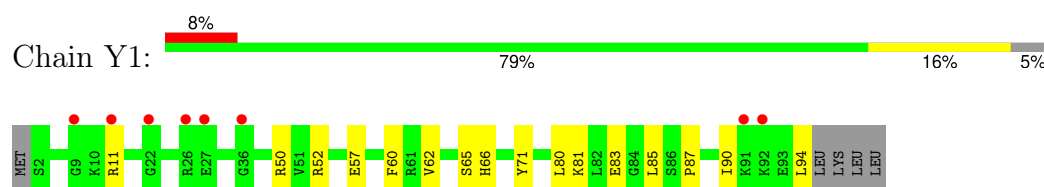
## • Molecule 46: 50S ribosomal protein L27



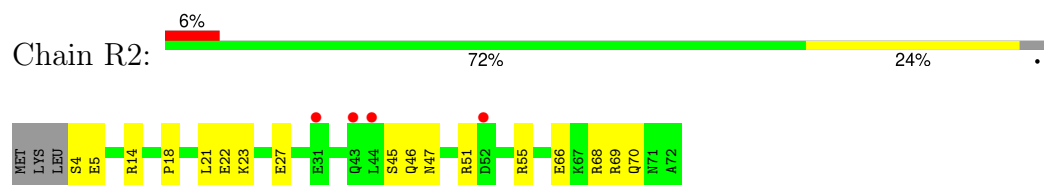
## • Molecule 47: 50S ribosomal protein L28



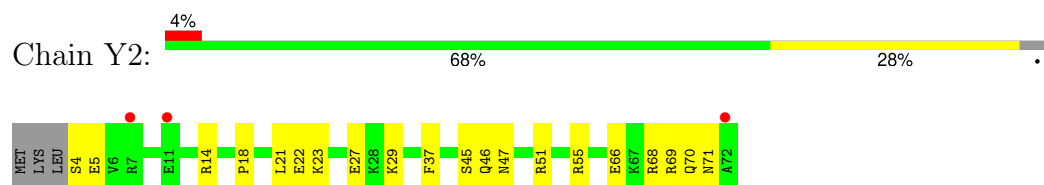
## • Molecule 47: 50S ribosomal protein L28



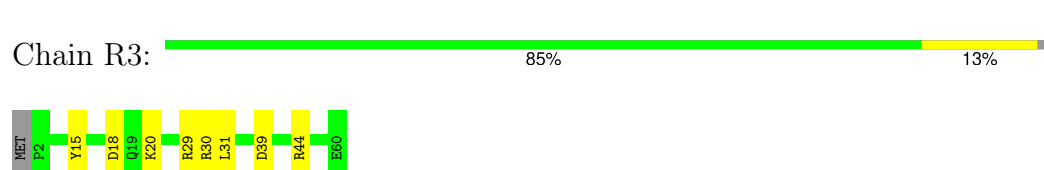
## • Molecule 48: 50S ribosomal protein L29



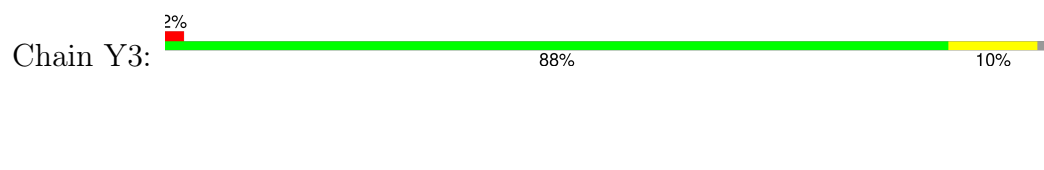
## • Molecule 48: 50S ribosomal protein L29



## • Molecule 49: 50S ribosomal protein L30

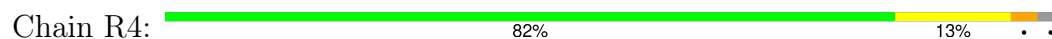


## • Molecule 49: 50S ribosomal protein L30

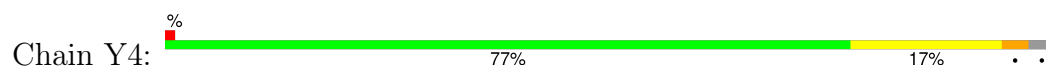




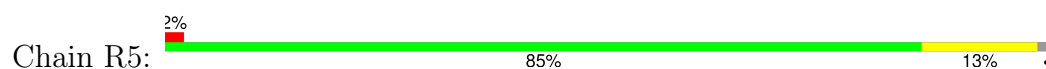
- Molecule 50: 50S ribosomal protein L31



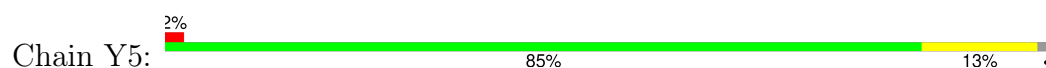
- Molecule 50: 50S ribosomal protein L31



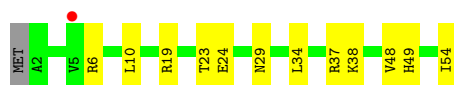
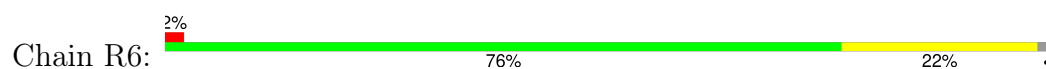
- Molecule 51: 50S ribosomal protein L32



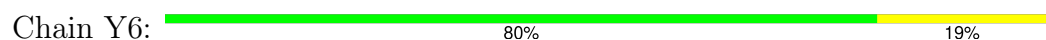
- Molecule 51: 50S ribosomal protein L32



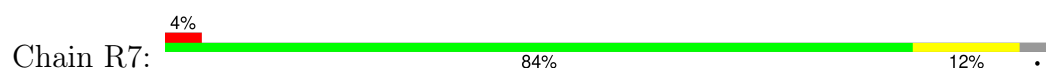
- Molecule 52: 50S ribosomal protein L33



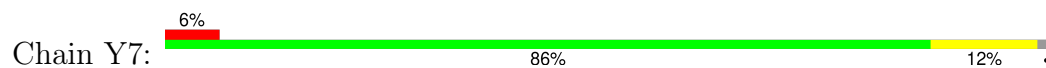
- Molecule 52: 50S ribosomal protein L33



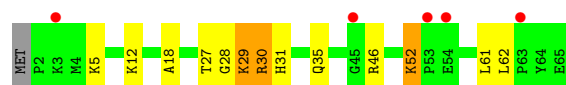
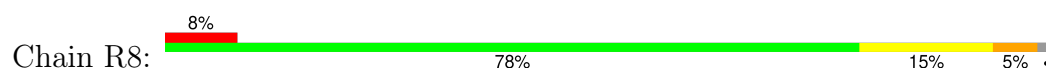
- Molecule 53: 50S ribosomal protein L34



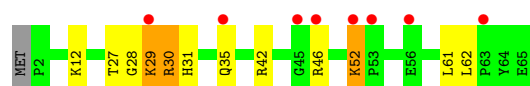
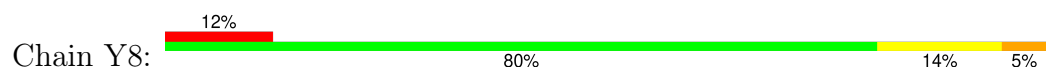
- Molecule 53: 50S ribosomal protein L34



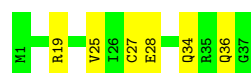
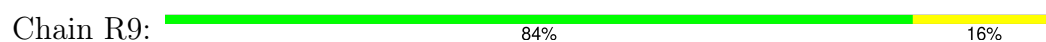
- Molecule 54: 50S ribosomal protein L35



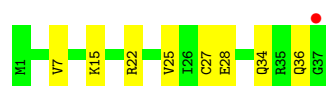
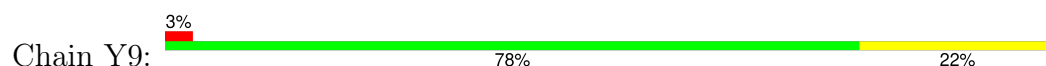
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.81Å 448.83Å 618.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.68 – 3.74 134.68 – 3.74	Depositor EDS
% Data completeness (in resolution range)	100.0 (134.68-3.74) 100.0 (134.68-3.74)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.204 , 0.225 0.205 , 0.225	Depositor DCC
$R_{free}$ test set	569907 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.7	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 139.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	295646	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	QA	0.96	0/36094	1.18	226/56334 (0.4%)
1	XA	0.96	0/36097	1.18	214/56339 (0.4%)
2	QB	0.40	0/1942	0.62	0/2619
2	XB	0.40	0/1950	0.59	0/2630
3	QC	0.39	0/1629	0.56	0/2195
3	XC	0.39	0/1629	0.56	0/2195
4	QD	0.45	0/1733	0.57	0/2318
4	XD	0.45	0/1733	0.57	0/2318
5	QE	0.42	0/1171	0.58	0/1576
5	XE	0.42	0/1171	0.58	0/1576
6	QF	0.44	0/856	0.58	0/1154
6	XF	0.44	0/856	0.58	0/1154
7	QG	0.36	0/1276	0.51	0/1709
7	XG	0.36	0/1276	0.51	0/1709
8	QH	0.44	0/1128	0.57	0/1517
8	XH	0.44	0/1128	0.56	0/1517
9	QI	0.44	0/1029	0.64	0/1379
9	XI	0.43	1/1017 (0.1%)	0.61	0/1365
10	QJ	0.42	0/814	0.62	1/1095 (0.1%)
10	XJ	0.40	0/790	0.61	1/1063 (0.1%)
11	QK	0.45	0/900	0.55	0/1213
11	XK	0.42	0/879	0.54	0/1187
12	QL	0.50	0/991	0.66	0/1327
12	XL	0.57	1/972 (0.1%)	0.68	0/1301
13	QM	0.41	0/965	0.62	0/1292
13	XM	0.39	0/956	0.61	0/1281
14	QN	0.51	0/501	0.60	0/664
14	XN	0.51	0/501	0.60	0/664
15	QO	0.40	0/745	0.55	0/992
15	XO	0.39	0/740	0.53	0/987
16	QP	0.49	0/721	0.58	0/970
16	XP	0.49	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.45	0/847	0.58	0/1131
17	XQ	0.45	0/847	0.58	0/1131
18	QR	0.39	0/579	0.62	0/768
18	XR	0.39	0/579	0.63	0/768
19	QS	0.38	0/680	0.71	1/915 (0.1%)
19	XS	0.40	0/689	0.66	0/926
20	QT	0.35	0/765	0.61	0/1007
20	XT	0.35	0/765	0.61	0/1007
21	QU	0.46	0/221	0.74	0/288
21	XU	0.46	0/221	0.74	0/288
22	QV	0.94	1/1836 (0.1%)	1.22	21/2859 (0.7%)
22	QW	0.31	0/1832	0.96	2/2855 (0.1%)
22	XV	0.94	1/1836 (0.1%)	1.22	21/2859 (0.7%)
22	XW	0.29	0/1832	0.94	2/2855 (0.1%)
23	QX	0.99	0/185	0.85	0/285
23	XX	1.03	1/257 (0.4%)	0.85	0/398
24	QY	0.78	0/404	1.11	0/627
24	XY	0.78	0/404	1.11	0/627
25	RA	1.12	5/69521 (0.0%)	1.24	583/108529 (0.5%)
25	YA	1.16	13/69543 (0.0%)	1.25	546/108563 (0.5%)
26	RB	0.81	0/2878	1.23	25/4490 (0.6%)
26	YB	0.81	0/2878	1.22	25/4490 (0.6%)
27	RD	0.60	0/2165	0.71	1/2919 (0.0%)
27	YD	0.60	0/2165	0.71	1/2919 (0.0%)
28	RE	0.52	0/1601	0.71	2/2160 (0.1%)
28	YE	0.52	0/1601	0.71	2/2160 (0.1%)
29	RF	0.58	0/1620	0.62	0/2194
29	YF	0.58	0/1620	0.62	0/2194
30	RG	0.40	0/1499	0.66	1/2016 (0.0%)
30	YG	0.40	0/1499	0.66	1/2016 (0.0%)
31	RH	0.41	0/1362	0.64	0/1841
31	YH	0.41	0/1362	0.64	0/1841
32	RI	0.37	0/1151	0.65	0/1558
32	YI	0.37	0/1151	0.65	0/1558
33	RN	0.50	0/1131	0.64	0/1525
33	YN	0.50	0/1131	0.64	0/1525
34	RO	0.55	0/943	0.61	0/1269
34	YO	0.55	0/943	0.61	0/1269
35	RP	0.47	0/1162	0.76	1/1544 (0.1%)
35	YP	0.49	0/1139	0.76	1/1514 (0.1%)
36	RQ	0.48	0/1143	0.66	0/1527
36	YQ	0.48	0/1143	0.66	0/1527
37	RR	0.49	0/974	0.69	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	YR	0.50	0/974	0.66	1/1302 (0.1%)
38	RS	0.38	0/892	0.70	0/1187
38	YS	0.38	0/892	0.70	0/1187
39	RT	0.46	0/1155	0.66	0/1542
39	YT	0.46	0/1155	0.66	0/1542
40	RU	0.52	0/982	0.61	0/1306
40	YU	0.52	0/982	0.61	0/1306
41	RV	0.47	0/790	0.67	0/1057
41	YV	0.46	0/790	0.67	0/1057
42	RW	0.54	0/911	0.61	0/1220
42	YW	0.55	0/911	0.61	0/1220
43	RX	0.56	0/739	0.58	0/993
43	YX	0.56	0/739	0.58	0/993
44	RY	0.53	0/831	0.56	0/1108
44	YY	0.53	0/831	0.56	0/1108
45	RZ	0.39	0/1493	0.71	0/2026
45	YZ	0.39	0/1493	0.71	0/2026
46	R0	0.51	0/652	0.57	0/867
46	Y0	0.47	0/607	0.56	0/809
47	R1	0.58	1/770 (0.1%)	0.64	0/1022
47	Y1	0.56	0/736	0.65	0/978
48	R2	0.40	0/583	0.52	0/771
48	Y2	0.40	0/583	0.52	0/771
49	R3	0.44	0/474	0.60	0/635
49	Y3	0.44	0/474	0.60	0/635
50	R4	0.37	0/578	0.64	0/776
50	Y4	0.37	0/578	0.64	0/776
51	R5	0.50	0/473	0.58	0/639
51	Y5	0.50	0/473	0.58	0/639
52	R6	0.34	0/460	0.51	0/613
52	Y6	0.34	0/460	0.51	0/613
53	R7	0.52	0/417	0.59	0/550
53	Y7	0.60	0/426	0.62	0/561
54	R8	0.55	0/525	0.76	0/691
54	Y8	0.55	0/525	0.76	0/691
55	R9	0.44	0/310	0.50	0/407
55	Y9	0.43	0/310	0.50	0/407
All	All	0.93	24/319989 (0.0%)	1.10	1680/478685 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	1
4	QD	0	1
4	XD	0	1
12	QL	0	2
12	XL	0	2
13	QM	0	1
27	RD	0	4
27	YD	0	4
28	RE	0	3
28	YE	0	3
30	RG	0	1
30	YG	0	1
31	RH	0	1
31	YH	0	1
32	RI	0	3
32	YI	0	3
35	RP	0	1
35	YP	0	1
37	RR	0	1
39	RT	0	1
39	YT	0	1
40	RU	0	2
40	YU	0	2
41	RV	0	2
41	YV	0	2
45	RZ	0	4
45	YZ	0	4
50	R4	0	1
50	Y4	0	1
54	R8	0	4
54	Y8	0	4
All	All	0	63

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	1	C	OP3-P	-10.70	1.48	1.61
22	QV	1	C	OP3-P	-10.69	1.48	1.61
25	YA	74	A	N9-C4	-6.89	1.33	1.37
25	RA	74	A	N9-C4	-6.79	1.33	1.37
23	XX	21	C	O3'-P	-6.62	1.53	1.61

The worst 5 of 1680 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1158	C	C2-N1-C1'	13.01	133.12	118.80
1	QA	1301	U	N1-C2-O2	12.90	131.83	122.80
1	XA	1158	C	N1-C2-O2	12.82	126.59	118.90
1	QA	328	C	N1-C2-O2	12.57	126.44	118.90
1	QA	1301	U	N3-C2-O2	-12.21	113.65	122.20

There are no chirality outliers.

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
4	QD	19	LEU	Peptide
12	QL	104	VAL	Peptide
12	QL	47	LYS	Peptide
13	QM	66	LEU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32244	0	16274	320	0
1	XA	32246	0	16277	343	2
2	QB	1907	0	1958	36	0
2	XB	1915	0	1969	25	0
3	QC	1605	0	1668	17	0
3	XC	1605	0	1668	15	0
4	QD	1703	0	1766	30	0
4	XD	1703	0	1767	29	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	12	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	18	0
7	XG	1257	0	1296	26	0
8	QH	1108	0	1165	14	0
8	XH	1108	0	1165	15	0
9	QI	1010	0	1037	24	0
9	XI	998	0	1024	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	QJ	801	0	849	17	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	23	0
11	XK	864	0	881	23	0
12	QL	975	0	1062	16	0
12	XL	956	0	1046	18	0
13	QM	955	0	1021	19	0
13	XM	946	0	1007	20	0
14	QN	492	0	529	8	0
14	XN	492	0	529	7	0
15	QO	734	0	771	4	0
15	XO	729	0	768	8	0
16	QP	705	0	725	11	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	14	0
17	XQ	834	0	904	17	0
18	QR	574	0	644	8	0
18	XR	574	0	644	6	0
19	QS	665	0	686	13	0
19	XS	674	0	699	9	0
20	QT	763	0	860	9	0
20	XT	763	0	861	11	0
21	QU	217	0	234	8	0
21	XU	217	0	234	8	0
22	QV	1644	0	836	10	0
22	QW	1640	0	837	57	0
22	XV	1644	0	836	9	0
22	XW	1640	0	837	71	0
23	QX	167	0	86	3	0
23	XX	230	0	120	17	0
24	QY	362	0	183	3	0
24	XY	362	0	184	3	0
25	RA	62071	0	31285	461	0
25	YA	62091	0	31290	472	1
26	RB	2573	0	1306	26	0
26	YB	2573	0	1306	28	1
27	RD	2115	0	2195	49	0
27	YD	2115	0	2195	48	0
28	RE	1568	0	1634	29	0
28	YE	1568	0	1634	33	0
29	RF	1585	0	1632	24	0
29	YF	1585	0	1632	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	RG	1474	0	1535	26	0
30	YG	1474	0	1535	32	0
31	RH	1336	0	1418	19	0
31	YH	1336	0	1418	20	0
32	RI	1136	0	1223	12	2
32	YI	1136	0	1223	14	0
33	RN	1104	0	1180	9	0
33	YN	1104	0	1180	8	0
34	RO	933	0	996	20	0
34	YO	933	0	996	19	0
35	RP	1145	0	1227	25	0
35	YP	1122	0	1204	25	0
36	RQ	1122	0	1179	31	0
36	YQ	1122	0	1179	24	0
37	RR	960	0	1021	14	0
37	YR	960	0	1021	9	0
38	RS	882	0	943	18	0
38	YS	882	0	943	20	0
39	RT	1141	0	1202	23	0
39	YT	1141	0	1202	25	0
40	RU	964	0	1022	33	0
40	YU	964	0	1022	24	0
41	RV	779	0	852	9	0
41	YV	779	0	852	7	4
42	RW	900	0	964	13	1
42	YW	900	0	964	12	0
43	RX	725	0	778	6	0
43	YX	725	0	778	7	0
44	RY	818	0	909	8	4
44	YY	818	0	909	15	1
45	RZ	1461	0	1493	28	0
45	YZ	1461	0	1493	26	0
46	R0	643	0	667	10	0
46	Y0	599	0	617	13	0
47	R1	763	0	848	14	0
47	Y1	729	0	802	10	0
48	R2	581	0	629	9	0
48	Y2	581	0	629	11	4
49	R3	469	0	518	6	0
49	Y3	469	0	518	3	0
50	R4	565	0	557	8	0
50	Y4	565	0	557	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	R5	459	0	476	6	0
51	Y5	459	0	479	4	4
52	R6	453	0	473	8	0
52	Y6	453	0	473	6	0
53	R7	409	0	454	4	0
53	Y7	418	0	467	5	0
54	R8	517	0	582	14	0
54	Y8	517	0	582	10	0
55	R9	307	0	335	4	0
55	Y9	307	0	335	6	0
56	QA	72	0	0	0	0
56	QC	1	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QV	6	0	0	0	0
56	QX	1	0	0	0	0
56	QY	1	0	0	0	0
56	R0	3	0	0	0	0
56	R8	1	0	0	0	0
56	RA	513	0	0	0	0
56	RB	11	0	0	0	0
56	RE	3	0	0	0	0
56	RN	1	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0
56	RR	2	0	0	0	0
56	RT	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	80	0	0	0	0
56	XC	1	0	0	0	0
56	XE	1	0	0	0	0
56	XL	1	0	0	0	0
56	XM	1	0	0	0	0
56	XQ	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	8	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	2	0	0	0	0
56	Y5	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YA	541	0	0	0	0
56	YB	12	0	0	0	0
56	YD	1	0	0	0	0
56	YE	3	0	0	0	0
56	YO	1	0	0	0	0
56	YP	4	0	0	0	0
56	YQ	3	0	0	0	0
56	YX	2	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	0	0
57	XD	8	0	0	0	0
58	QN	1	0	0	0	0
58	R4	1	0	0	0	0
58	R5	1	0	0	0	0
58	R6	1	0	0	0	0
58	R9	1	0	0	0	0
58	RY	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y4	1	0	0	0	0
58	Y5	1	0	0	0	0
58	Y6	1	0	0	0	0
58	Y9	1	0	0	0	0
58	YY	1	0	0	0	0
All	All	295646	0	199660	2768	12

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 2768 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)
7:XG:143:ARG:CD	22:XW:42:C:O3'	1.75	1.33
7:QG:143:ARG:HD3	22:QW:42:C:O3'	1.09	1.24
7:QG:143:ARG:CD	22:QW:42:C:O3'	1.88	1.20
23:XX:22:C:H6	23:XX:22:C:H5''	1.06	1.13
11:XK:54:ARG:HH22	22:XW:40:C:H4'	1.12	1.09

The worst 5 of 12 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:1411:C:O2'	26:YB:53:A:O2'[1_655]	1.11	1.09
32:RI:87:LYS:NZ	1:XA:359:U:OP1[4_555]	1.48	0.72
41:YV:49:THR:O	51:Y5:59:GLU:OE2[4_445]	1.56	0.64
44:RY:21:LYS:NZ	48:Y2:71:ASN:CB[3_555]	1.64	0.56
44:RY:19:LYS:O	48:Y2:71:ASN:ND2[3_555]	1.71	0.49

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	207 (89%)	25 (11%)	1 (0%)	30	62
2	XB	234/256 (91%)	208 (89%)	26 (11%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
4	QD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
4	XD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	QE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	19	51
5	XE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	19	51
6	QF	99/101 (98%)	99 (100%)	0	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	QK	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	XK	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
12	QL	123/132 (93%)	106 (86%)	17 (14%)	0	100	100
12	XL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	16	49
13	QM	118/126 (94%)	99 (84%)	18 (15%)	1 (1%)	16	49
13	XM	117/126 (93%)	98 (84%)	19 (16%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	36
14	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	36
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
16	XP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
17	QQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
19	XS	82/93 (88%)	67 (82%)	15 (18%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
27	RD	270/276 (98%)	247 (92%)	22 (8%)	1 (0%)	30	62
27	YD	270/276 (98%)	247 (92%)	22 (8%)	1 (0%)	30	62
28	RE	203/206 (98%)	165 (81%)	36 (18%)	2 (1%)	13	44
28	YE	203/206 (98%)	165 (81%)	36 (18%)	2 (1%)	13	44
29	RF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
29	YF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
30	RG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	22	54
30	YG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	22	54
31	RH	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	5	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	YH	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	5	32
32	RI	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	9	39
32	YI	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	9	39
33	RN	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	19	51
33	YN	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	19	51
34	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
34	YO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
35	RP	148/150 (99%)	117 (79%)	30 (20%)	1 (1%)	19	51
35	YP	145/150 (97%)	113 (78%)	31 (21%)	1 (1%)	19	51
36	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	19	51
36	YQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	19	51
37	RR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	46
37	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	46
38	RS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
38	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
39	RT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	8	38
39	YT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	8	38
40	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	46
40	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	46
41	RV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
41	YV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
42	RW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
42	YW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
43	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
43	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
44	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
44	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
45	RZ	181/206 (88%)	150 (83%)	29 (16%)	2 (1%)	12	43
45	YZ	181/206 (88%)	149 (82%)	30 (17%)	2 (1%)	12	43
46	R0	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
46	Y0	73/85 (86%)	67 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R1	95/98 (97%)	83 (87%)	12 (13%)	0	100	100
47	Y1	91/98 (93%)	77 (85%)	14 (15%)	0	100	100
48	R2	67/72 (93%)	64 (96%)	2 (3%)	1 (2%)	8	38
48	Y2	67/72 (93%)	64 (96%)	2 (3%)	1 (2%)	8	38
49	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
49	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	R4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	8	38
50	Y4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	8	38
51	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	R6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
52	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
53	R7	45/49 (92%)	45 (100%)	0	0	100	100
53	Y7	46/49 (94%)	46 (100%)	0	0	100	100
54	R8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	3	27
54	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	3	27
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11452/12128 (94%)	10311 (90%)	1088 (10%)	53 (0%)	25	57

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	RT	124	ASP
45	RZ	53	ILE
39	YT	124	ASP
45	YZ	53	ILE
14	QN	17	LYS

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	202 (100%)	1 (0%)	86	92
2	XB	204/220 (93%)	201 (98%)	3 (2%)	60	75
3	QC	159/188 (85%)	158 (99%)	1 (1%)	84	90
3	XC	159/188 (85%)	158 (99%)	1 (1%)	84	90
4	QD	180/181 (99%)	179 (99%)	1 (1%)	84	90
4	XD	180/181 (99%)	179 (99%)	1 (1%)	84	90
5	QE	116/123 (94%)	115 (99%)	1 (1%)	75	84
5	XE	116/123 (94%)	115 (99%)	1 (1%)	75	84
6	QF	90/90 (100%)	89 (99%)	1 (1%)	70	80
6	XF	90/90 (100%)	89 (99%)	1 (1%)	70	80
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	96 (98%)	2 (2%)	50	69
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	50	69
14	XN	49/50 (98%)	48 (98%)	1 (2%)	50	69
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	71 (99%)	1 (1%)	62	76
16	XP	72/74 (97%)	71 (99%)	1 (1%)	62	76
17	QQ	95/97 (98%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	62	76
19	XS	73/80 (91%)	72 (99%)	1 (1%)	62	76
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	212 (99%)	2 (1%)	75	84
27	YD	214/218 (98%)	212 (99%)	2 (1%)	75	84
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	165 (100%)	0	100	100
29	RF	161/166 (97%)	159 (99%)	2 (1%)	67	79
29	YF	161/166 (97%)	159 (99%)	2 (1%)	67	79
30	RG	155/156 (99%)	153 (99%)	2 (1%)	65	77
30	YG	155/156 (99%)	153 (99%)	2 (1%)	65	77
31	RH	145/148 (98%)	141 (97%)	4 (3%)	38	60
31	YH	145/148 (98%)	141 (97%)	4 (3%)	38	60
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	117/119 (98%)	116 (99%)	1 (1%)	75	84
33	YN	117/119 (98%)	116 (99%)	1 (1%)	75	84
34	RO	100/100 (100%)	98 (98%)	2 (2%)	50	69
34	YO	100/100 (100%)	98 (98%)	2 (2%)	50	69
35	RP	116/116 (100%)	114 (98%)	2 (2%)	56	73
35	YP	114/116 (98%)	113 (99%)	1 (1%)	75	84
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	111 (100%)	0	100	100
37	RR	100/101 (99%)	100 (100%)	0	100	100
37	YR	100/101 (99%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	RS	87/88 (99%)	86 (99%)	1 (1%)	70	80
38	YS	87/88 (99%)	86 (99%)	1 (1%)	70	80
39	RT	120/127 (94%)	119 (99%)	1 (1%)	79	85
39	YT	120/127 (94%)	119 (99%)	1 (1%)	79	85
40	RU	93/94 (99%)	93 (100%)	0	100	100
40	YU	93/94 (99%)	93 (100%)	0	100	100
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	82 (100%)	0	100	100
42	RW	92/92 (100%)	90 (98%)	2 (2%)	47	66
42	YW	92/92 (100%)	90 (98%)	2 (2%)	47	66
43	RX	74/78 (95%)	74 (100%)	0	100	100
43	YX	74/78 (95%)	74 (100%)	0	100	100
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	162/179 (90%)	161 (99%)	1 (1%)	84	90
45	YZ	162/179 (90%)	161 (99%)	1 (1%)	84	90
46	R0	65/67 (97%)	64 (98%)	1 (2%)	60	75
46	Y0	61/67 (91%)	60 (98%)	1 (2%)	58	74
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	78/83 (94%)	78 (100%)	0	100	100
48	R2	64/67 (96%)	64 (100%)	0	100	100
48	Y2	64/67 (96%)	64 (100%)	0	100	100
49	R3	51/52 (98%)	50 (98%)	1 (2%)	50	69
49	Y3	51/52 (98%)	50 (98%)	1 (2%)	50	69
50	R4	62/63 (98%)	61 (98%)	1 (2%)	58	74
50	Y4	62/63 (98%)	61 (98%)	1 (2%)	58	74
51	R5	51/52 (98%)	51 (100%)	0	100	100
51	Y5	51/52 (98%)	51 (100%)	0	100	100
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	51 (100%)	0	100	100
53	R7	40/42 (95%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	34 (100%)	0	100	100
55	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9687/10066 (96%)	9622 (99%)	65 (1%)	81	88

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	YS	3	ARG
42	YW	15	ARG
35	RP	125	VAL
35	RP	58	THR
42	YW	40	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
7	XG	28	ASN
35	YP	27	HIS
7	XG	68	ASN
14	XN	49	HIS
40	YU	94	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	297 (19%)	32 (2%)
1	XA	1498/1508 (99%)	282 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	2 (2%)
22	QW	76/77 (98%)	33 (43%)	2 (2%)
22	XV	76/77 (98%)	15 (19%)	2 (2%)
22	XW	76/77 (98%)	34 (44%)	2 (2%)
23	QX	7/25 (28%)	0	0
23	XX	10/25 (40%)	2 (20%)	0
24	QY	16/17 (94%)	4 (25%)	0
24	XY	16/17 (94%)	4 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	RA	2879/2915 (98%)	613 (21%)	41 (1%)
25	YA	2880/2915 (98%)	609 (21%)	41 (1%)
26	RB	119/122 (97%)	24 (20%)	0
26	YB	119/122 (97%)	24 (20%)	0
All	All	9346/9482 (98%)	1956 (20%)	149 (1%)

5 of 1956 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	32	A
1	QA	39	G
1	QA	41	G
1	QA	47	C

5 of 149 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	404	C
25	YA	2439	A
25	YA	856	C
25	YA	1379	A
25	RA	637	A

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1306 ligands modelled in this entry, 1304 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	QD	301	4	-	-	0/6/5/5
57	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	QA	1500/1508 (99%)	-0.13	16 (1%) 77 60	65, 113, 205, 388	0
1	XA	1500/1508 (99%)	-0.15	8 (0%) 87 72	59, 117, 222, 400	0
2	QB	235/256 (91%)	0.37	6 (2%) 57 41	103, 168, 244, 304	0
2	XB	236/256 (92%)	0.11	4 (1%) 69 50	93, 161, 229, 286	0
3	QC	205/239 (85%)	0.06	2 (0%) 79 62	111, 157, 211, 257	0
3	XC	205/239 (85%)	0.11	5 (2%) 59 44	91, 139, 206, 284	0
4	QD	208/209 (99%)	0.20	2 (0%) 79 62	63, 127, 183, 212	0
4	XD	208/209 (99%)	0.49	11 (5%) 33 26	73, 112, 164, 213	0
5	QE	151/162 (93%)	0.20	2 (1%) 74 56	83, 122, 165, 211	0
5	XE	151/162 (93%)	0.22	10 (6%) 26 21	69, 114, 158, 241	0
6	QF	101/101 (100%)	0.18	0 100 100	74, 119, 160, 190	0
6	XF	101/101 (100%)	0.22	3 (2%) 52 38	82, 126, 163, 232	0
7	QG	155/156 (99%)	0.10	3 (1%) 66 48	94, 134, 191, 284	0
7	XG	155/156 (99%)	0.25	4 (2%) 57 41	108, 158, 205, 249	0
8	QH	137/138 (99%)	0.04	2 (1%) 71 53	84, 127, 162, 189	0
8	XH	137/138 (99%)	0.19	3 (2%) 62 45	90, 123, 161, 180	0
9	QI	127/128 (99%)	0.40	13 (10%) 13 14	97, 156, 212, 304	0
9	XI	126/128 (98%)	0.30	11 (8%) 17 15	113, 173, 215, 258	0
10	QJ	99/105 (94%)	0.77	14 (14%) 7 10	130, 171, 227, 269	0
10	XJ	96/105 (91%)	0.39	4 (4%) 41 31	109, 175, 232, 260	0
11	QK	119/129 (92%)	0.23	4 (3%) 48 35	79, 120, 201, 273	0
11	XK	116/129 (89%)	0.24	1 (0%) 81 64	88, 126, 195, 263	0
12	QL	125/132 (94%)	0.94	15 (12%) 10 12	80, 116, 169, 249	0
12	XL	122/132 (92%)	0.55	14 (11%) 11 13	61, 99, 141, 240	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	120/126 (95%)	0.52	9 (7%) 22 18	97, 145, 199, 267	0
13	XM	119/126 (94%)	0.31	6 (5%) 35 27	101, 153, 216, 284	0
14	QN	60/61 (98%)	0.34	1 (1%) 69 50	107, 144, 190, 207	0
14	XN	60/61 (98%)	0.46	2 (3%) 49 36	102, 134, 173, 189	0
15	QO	88/89 (98%)	-0.07	0 100 100	67, 111, 147, 159	0
15	XO	87/89 (97%)	0.17	3 (3%) 48 35	80, 108, 156, 178	0
16	QP	84/88 (95%)	0.16	2 (2%) 59 44	94, 114, 160, 233	0
16	XP	84/88 (95%)	0.24	1 (1%) 76 57	87, 123, 161, 256	0
17	QQ	100/105 (95%)	0.11	1 (1%) 79 62	79, 113, 152, 230	0
17	XQ	100/105 (95%)	0.47	10 (10%) 14 14	85, 119, 164, 246	0
18	QR	70/88 (79%)	0.01	2 (2%) 54 39	72, 117, 168, 230	0
18	XR	70/88 (79%)	0.25	2 (2%) 54 39	83, 123, 187, 211	0
19	QS	83/93 (89%)	0.63	12 (14%) 7 10	107, 168, 223, 268	0
19	XS	84/93 (90%)	0.51	4 (4%) 36 28	102, 150, 205, 256	0
20	QT	99/106 (93%)	0.69	11 (11%) 12 13	72, 122, 187, 203	0
20	XT	99/106 (93%)	0.58	11 (11%) 12 13	92, 140, 202, 263	0
21	QU	25/27 (92%)	0.35	1 (4%) 43 32	107, 134, 199, 206	0
21	XU	25/27 (92%)	0.03	0 100 100	123, 145, 194, 197	0
22	QV	77/77 (100%)	0.17	2 (2%) 57 41	84, 123, 169, 246	0
22	QW	77/77 (100%)	1.20	10 (12%) 9 11	139, 313, 405, 436	0
22	XV	77/77 (100%)	0.05	2 (2%) 57 41	86, 119, 171, 232	0
22	XW	77/77 (100%)	0.82	5 (6%) 26 21	135, 350, 419, 437	0
23	QX	8/25 (32%)	0.79	1 (12%) 9 12	87, 89, 104, 143	0
23	XX	11/25 (44%)	0.89	1 (9%) 16 15	80, 88, 175, 184	0
24	QY	17/17 (100%)	-0.07	0 100 100	111, 139, 243, 275	0
24	XY	17/17 (100%)	0.01	0 100 100	105, 141, 239, 250	0
25	RA	2882/2915 (98%)	-0.14	25 (0%) 81 64	50, 90, 246, 448	0
25	YA	2883/2915 (98%)	-0.08	26 (0%) 81 64	45, 86, 245, 477	0
26	RB	120/122 (98%)	-0.20	1 (0%) 82 66	93, 129, 176, 215	0
26	YB	120/122 (98%)	-0.01	1 (0%) 82 66	107, 175, 227, 258	0
27	RD	272/276 (98%)	0.76	27 (9%) 14 14	50, 83, 132, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	YD	272/276 (98%)	0.55	16 (5%) 29 23	46, 82, 130, 294	0
28	RE	205/206 (99%)	0.33	7 (3%) 48 35	62, 102, 184, 262	0
28	YE	205/206 (99%)	0.59	18 (8%) 17 15	49, 103, 190, 326	0
29	RF	202/210 (96%)	0.54	11 (5%) 32 25	62, 103, 184, 233	0
29	YF	202/210 (96%)	0.20	7 (3%) 47 35	52, 92, 151, 220	0
30	RG	181/182 (99%)	0.17	4 (2%) 62 45	82, 137, 185, 287	0
30	YG	181/182 (99%)	0.34	2 (1%) 77 60	105, 165, 210, 256	0
31	RH	174/180 (96%)	0.23	1 (0%) 85 70	106, 176, 240, 355	0
31	YH	174/180 (96%)	0.65	8 (4%) 38 29	73, 130, 181, 270	0
32	RI	146/148 (98%)	0.57	11 (7%) 22 18	77, 144, 201, 258	0
32	YI	146/148 (98%)	0.46	8 (5%) 32 24	81, 142, 198, 251	0
33	RN	138/140 (98%)	0.54	8 (5%) 30 24	66, 108, 161, 194	0
33	YN	138/140 (98%)	0.52	9 (6%) 26 21	73, 109, 169, 195	0
34	RO	122/122 (100%)	0.24	4 (3%) 49 36	57, 99, 135, 164	0
34	YO	122/122 (100%)	0.13	3 (2%) 58 43	61, 91, 122, 142	0
35	RP	150/150 (100%)	0.61	9 (6%) 29 23	62, 112, 181, 243	0
35	YP	147/150 (98%)	0.36	7 (4%) 36 28	57, 103, 159, 195	0
36	RQ	141/141 (100%)	0.57	14 (9%) 14 14	70, 115, 185, 274	0
36	YQ	141/141 (100%)	0.61	13 (9%) 16 15	67, 113, 187, 294	0
37	RR	117/118 (99%)	0.09	5 (4%) 40 31	51, 93, 127, 246	0
37	YR	117/118 (99%)	0.40	5 (4%) 40 31	64, 94, 134, 214	0
38	RS	111/112 (99%)	0.23	2 (1%) 67 49	81, 133, 200, 253	0
38	YS	111/112 (99%)	0.87	10 (9%) 17 15	124, 175, 247, 333	0
39	RT	137/146 (93%)	0.32	2 (1%) 71 53	70, 111, 197, 271	0
39	YT	137/146 (93%)	0.43	9 (6%) 26 21	64, 109, 192, 233	0
40	RU	117/118 (99%)	0.60	6 (5%) 34 27	60, 103, 181, 251	0
40	YU	117/118 (99%)	0.64	7 (5%) 29 23	53, 93, 159, 213	0
41	RV	101/101 (100%)	0.55	6 (5%) 29 23	69, 122, 185, 288	0
41	YV	101/101 (100%)	0.45	3 (2%) 52 38	59, 113, 178, 321	0
42	RW	113/113 (100%)	0.21	5 (4%) 39 30	53, 81, 146, 249	0
42	YW	113/113 (100%)	0.24	4 (3%) 47 35	54, 81, 135, 258	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	RX	92/96 (95%)	0.35	4 (4%) 40 31	62, 96, 137, 202	0
43	YX	92/96 (95%)	0.09	0 100 100	50, 84, 128, 162	0
44	RY	107/110 (97%)	0.63	8 (7%) 22 18	77, 119, 185, 233	0
44	YY	107/110 (97%)	0.30	2 (1%) 66 48	62, 105, 157, 191	0
45	RZ	183/206 (88%)	0.13	0 100 100	107, 155, 233, 281	0
45	YZ	183/206 (88%)	0.11	2 (1%) 77 60	103, 168, 229, 303	0
46	R0	81/85 (95%)	0.39	5 (6%) 28 22	71, 104, 139, 233	0
46	Y0	75/85 (88%)	0.20	2 (2%) 56 41	80, 119, 149, 184	0
47	R1	97/98 (98%)	0.53	6 (6%) 28 22	61, 93, 187, 254	0
47	Y1	93/98 (94%)	0.67	8 (8%) 18 15	55, 94, 158, 196	0
48	R2	69/72 (95%)	0.54	4 (5%) 30 24	67, 120, 196, 265	0
48	Y2	69/72 (95%)	0.11	3 (4%) 40 31	60, 94, 173, 360	0
49	R3	59/60 (98%)	-0.03	0 100 100	64, 106, 171, 193	0
49	Y3	59/60 (98%)	0.15	1 (1%) 69 50	79, 106, 171, 207	0
50	R4	69/71 (97%)	0.29	0 100 100	118, 170, 258, 325	0
50	Y4	69/71 (97%)	0.27	1 (1%) 73 55	149, 197, 246, 317	0
51	R5	59/60 (98%)	0.14	1 (1%) 69 50	63, 96, 179, 245	0
51	Y5	59/60 (98%)	0.16	1 (1%) 69 50	63, 98, 192, 287	0
52	R6	53/54 (98%)	0.53	1 (1%) 66 48	136, 156, 204, 236	0
52	Y6	53/54 (98%)	0.45	0 100 100	129, 168, 237, 253	0
53	R7	47/49 (95%)	0.46	2 (4%) 40 31	48, 77, 119, 190	0
53	Y7	48/49 (97%)	0.30	3 (6%) 27 22	47, 68, 135, 168	0
54	R8	64/65 (98%)	0.89	5 (7%) 20 17	59, 98, 156, 238	0
54	Y8	64/65 (98%)	0.84	8 (12%) 9 12	67, 96, 145, 265	0
55	R9	37/37 (100%)	0.10	0 100 100	118, 151, 203, 237	0
55	Y9	37/37 (100%)	0.22	1 (2%) 56 41	118, 137, 202, 214	0
All	All	21014/21610 (97%)	0.16	628 (2%) 52 38	45, 114, 216, 477	0

The worst 5 of 628 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	RD	2	ALA	8.3
12	XL	28	LYS	7.4

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Mol	Chain	Res	Type	RSRZ
20	QT	9	ASN	7.4
35	RP	13	ASN	7.1
20	XT	9	ASN	6.7

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	MG	YA	3392	1/1	0.09	0.19	124,124,124,124	0
56	MG	XS	101	1/1	0.19	0.11	125,125,125,125	0
56	MG	YA	3357	1/1	0.20	0.14	204,204,204,204	0
56	MG	YA	3294	1/1	0.24	0.27	99,99,99,99	0
56	MG	YA	3173	1/1	0.29	0.23	78,78,78,78	0
56	MG	XV	108	1/1	0.36	0.13	130,130,130,130	0
56	MG	RA	3212	1/1	0.37	0.24	81,81,81,81	0
56	MG	RB	207	1/1	0.40	0.14	94,94,94,94	0
56	MG	RA	3337	1/1	0.41	0.24	85,85,85,85	0
56	MG	RA	3467	1/1	0.42	0.12	99,99,99,99	0
56	MG	YX	102	1/1	0.42	0.33	63,63,63,63	0
56	MG	RA	3430	1/1	0.43	0.12	171,171,171,171	0
56	MG	RA	3002	1/1	0.44	0.26	70,70,70,70	0
56	MG	QA	1668	1/1	0.46	0.23	84,84,84,84	0
56	MG	RA	3213	1/1	0.47	0.45	39,39,39,39	0
56	MG	YA	3184	1/1	0.47	0.17	66,66,66,66	0
56	MG	YA	3451	1/1	0.48	0.15	100,100,100,100	0
56	MG	YA	3361	1/1	0.49	0.12	83,83,83,83	0
56	MG	YB	207	1/1	0.49	0.13	113,113,113,113	0
56	MG	YA	3358	1/1	0.49	0.12	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3266	1/1	0.50	0.18	96,96,96,96	0
56	MG	XA	1662	1/1	0.50	0.14	107,107,107,107	0
56	MG	XA	1665	1/1	0.50	0.07	118,118,118,118	0
56	MG	YA	3449	1/1	0.51	0.09	89,89,89,89	0
56	MG	RA	3202	1/1	0.51	0.21	52,52,52,52	0
56	MG	RA	3318	1/1	0.52	0.13	53,53,53,53	0
56	MG	RA	3453	1/1	0.52	0.10	268,268,268,268	0
56	MG	QA	1624	1/1	0.53	0.17	72,72,72,72	0
56	MG	RA	3472	1/1	0.53	0.10	84,84,84,84	0
56	MG	RA	3485	1/1	0.53	0.22	73,73,73,73	0
56	MG	RA	3308	1/1	0.53	0.15	70,70,70,70	0
56	MG	YA	3319	1/1	0.54	0.20	108,108,108,108	0
56	MG	YA	3425	1/1	0.54	0.23	64,64,64,64	0
56	MG	YA	3471	1/1	0.55	0.14	78,78,78,78	0
56	MG	RA	3209	1/1	0.55	0.25	80,80,80,80	0
56	MG	RA	3357	1/1	0.55	0.17	80,80,80,80	0
56	MG	RA	3442	1/1	0.56	0.15	70,70,70,70	0
56	MG	YA	3485	1/1	0.56	0.07	94,94,94,94	0
56	MG	YA	3345	1/1	0.56	0.13	104,104,104,104	0
56	MG	XM	201	1/1	0.56	0.12	110,110,110,110	0
56	MG	YA	3456	1/1	0.57	0.29	84,84,84,84	0
56	MG	YA	3331	1/1	0.58	0.23	62,62,62,62	0
56	MG	YD	301	1/1	0.58	0.29	52,52,52,52	0
56	MG	RA	3322	1/1	0.58	0.20	74,74,74,74	0
56	MG	XA	1661	1/1	0.59	0.14	78,78,78,78	0
56	MG	RA	3108	1/1	0.59	0.21	52,52,52,52	0
58	ZN	R5	501	1/1	0.59	0.25	247,247,247,247	0
56	MG	RA	3283	1/1	0.60	0.22	69,69,69,69	0
56	MG	RA	3363	1/1	0.60	0.19	70,70,70,70	0
56	MG	RA	3287	1/1	0.60	0.25	102,102,102,102	0
56	MG	RA	3272	1/1	0.60	0.21	50,50,50,50	0
56	MG	QA	1638	1/1	0.61	0.32	62,62,62,62	0
56	MG	QA	1650	1/1	0.61	0.33	76,76,76,76	0
56	MG	YA	3212	1/1	0.61	0.22	72,72,72,72	0
56	MG	RA	3478	1/1	0.61	0.10	94,94,94,94	0
56	MG	RA	3304	1/1	0.61	0.27	71,71,71,71	0
56	MG	YA	3397	1/1	0.61	0.10	75,75,75,75	0
56	MG	RB	206	1/1	0.61	0.17	87,87,87,87	0
56	MG	RA	3098	1/1	0.61	0.20	44,44,44,44	0
56	MG	RA	3366	1/1	0.62	0.15	95,95,95,95	0
56	MG	YA	3512	1/1	0.62	0.24	82,82,82,82	0
56	MG	RA	3355	1/1	0.62	0.09	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3254	1/1	0.62	0.25	51,51,51,51	0
56	MG	YQ	203	1/1	0.62	0.13	82,82,82,82	0
56	MG	RB	205	1/1	0.62	0.23	85,85,85,85	0
56	MG	YA	3353	1/1	0.62	0.23	78,78,78,78	0
56	MG	RA	3460	1/1	0.63	0.11	65,65,65,65	0
56	MG	YA	3085	1/1	0.63	0.24	28,28,28,28	0
56	MG	YA	3309	1/1	0.63	0.11	99,99,99,99	0
56	MG	YA	3534	1/1	0.63	0.14	89,89,89,89	0
56	MG	QA	1664	1/1	0.63	0.29	84,84,84,84	0
56	MG	YB	209	1/1	0.63	0.10	75,75,75,75	0
56	MG	RA	3125	1/1	0.63	0.15	80,80,80,80	0
56	MG	YA	3195	1/1	0.63	0.31	71,71,71,71	0
56	MG	RA	3215	1/1	0.63	0.24	65,65,65,65	0
56	MG	Y8	101	1/1	0.63	0.23	74,74,74,74	0
56	MG	XA	1637	1/1	0.63	0.24	145,145,145,145	0
56	MG	YA	3320	1/1	0.64	0.18	85,85,85,85	0
56	MG	RA	3512	1/1	0.64	0.25	64,64,64,64	0
56	MG	RA	3374	1/1	0.64	0.13	73,73,73,73	0
56	MG	YA	3350	1/1	0.64	0.18	76,76,76,76	0
56	MG	RA	3505	1/1	0.64	0.32	67,67,67,67	0
56	MG	RA	3465	1/1	0.65	0.17	89,89,89,89	0
56	MG	YA	3077	1/1	0.65	0.14	52,52,52,52	0
56	MG	XA	1633	1/1	0.65	0.15	70,70,70,70	0
56	MG	RA	3409	1/1	0.65	0.57	81,81,81,81	0
56	MG	YA	3292	1/1	0.65	0.15	57,57,57,57	0
56	MG	YA	3346	1/1	0.65	0.09	82,82,82,82	0
56	MG	RA	3452	1/1	0.65	0.14	67,67,67,67	0
58	ZN	YY	202	1/1	0.65	0.28	234,234,234,234	0
56	MG	YA	3409	1/1	0.66	0.29	43,43,43,43	0
56	MG	YA	3414	1/1	0.66	0.16	67,67,67,67	0
56	MG	XA	1628	1/1	0.66	0.17	61,61,61,61	0
56	MG	RA	3282	1/1	0.66	0.14	100,100,100,100	0
56	MG	RA	3342	1/1	0.66	0.08	100,100,100,100	0
56	MG	RA	3353	1/1	0.66	0.11	74,74,74,74	0
56	MG	YA	3002	1/1	0.67	0.22	85,85,85,85	0
56	MG	QC	301	1/1	0.67	0.15	159,159,159,159	0
56	MG	RA	3470	1/1	0.67	0.25	92,92,92,92	0
56	MG	YA	3508	1/1	0.67	0.14	69,69,69,69	0
56	MG	QA	1670	1/1	0.67	0.12	86,86,86,86	0
56	MG	YA	3375	1/1	0.67	0.22	81,81,81,81	0
56	MG	YB	201	1/1	0.67	0.11	69,69,69,69	0
56	MG	RA	3418	1/1	0.67	0.19	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1678	1/1	0.67	0.23	71,71,71,71	0
56	MG	YA	3334	1/1	0.67	0.07	67,67,67,67	0
56	MG	YA	3336	1/1	0.67	0.20	45,45,45,45	0
56	MG	YA	3419	1/1	0.67	0.16	79,79,79,79	0
56	MG	XA	1627	1/1	0.67	0.14	43,43,43,43	0
56	MG	RA	3421	1/1	0.67	0.07	98,98,98,98	0
56	MG	RA	3316	1/1	0.67	0.23	59,59,59,59	0
56	MG	QA	1661	1/1	0.68	0.14	50,50,50,50	0
56	MG	YA	3228	1/1	0.68	0.26	77,77,77,77	0
56	MG	YA	3520	1/1	0.68	0.42	48,48,48,48	0
56	MG	YA	3344	1/1	0.68	0.25	73,73,73,73	0
56	MG	QX	101	1/1	0.68	0.11	53,53,53,53	0
56	MG	RA	3406	1/1	0.68	0.17	56,56,56,56	0
56	MG	YA	3155	1/1	0.68	0.16	60,60,60,60	0
56	MG	YA	3444	1/1	0.68	0.19	86,86,86,86	0
56	MG	RT	201	1/1	0.68	0.14	64,64,64,64	0
56	MG	YA	3179	1/1	0.68	0.13	96,96,96,96	0
56	MG	RA	3473	1/1	0.68	0.11	82,82,82,82	0
56	MG	YA	3194	1/1	0.68	0.22	28,28,28,28	0
56	MG	XX	101	1/1	0.68	0.16	81,81,81,81	0
56	MG	RA	3275	1/1	0.69	0.25	49,49,49,49	0
56	MG	YA	3394	1/1	0.69	0.22	80,80,80,80	0
56	MG	YA	3165	1/1	0.69	0.11	68,68,68,68	0
56	MG	RA	3006	1/1	0.69	0.14	54,54,54,54	0
56	MG	YA	3035	1/1	0.69	0.20	35,35,35,35	0
56	MG	YA	3182	1/1	0.69	0.11	85,85,85,85	0
56	MG	YA	3074	1/1	0.69	0.26	75,75,75,75	0
56	MG	XV	101	1/1	0.69	0.17	50,50,50,50	0
56	MG	RA	3321	1/1	0.69	0.17	73,73,73,73	0
56	MG	YA	3116	1/1	0.69	0.28	41,41,41,41	0
56	MG	YA	3362	1/1	0.69	0.14	70,70,70,70	0
56	MG	YA	3219	1/1	0.69	0.16	30,30,30,30	0
56	MG	YA	3390	1/1	0.69	0.20	63,63,63,63	0
56	MG	RA	3499	1/1	0.70	0.19	70,70,70,70	0
56	MG	RA	3179	1/1	0.70	0.23	84,84,84,84	0
56	MG	RA	3345	1/1	0.70	0.20	90,90,90,90	0
56	MG	YA	3203	1/1	0.70	0.12	100,100,100,100	0
56	MG	RB	202	1/1	0.70	0.11	76,76,76,76	0
56	MG	RA	3320	1/1	0.70	0.15	74,74,74,74	0
56	MG	RA	3134	1/1	0.70	0.17	30,30,30,30	0
56	MG	RA	3159	1/1	0.70	0.12	46,46,46,46	0
56	MG	YA	3470	1/1	0.70	0.14	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3262	1/1	0.70	0.20	77,77,77,77	0
58	ZN	R4	500	1/1	0.70	0.21	241,241,241,241	0
56	MG	RA	3216	1/1	0.70	0.27	88,88,88,88	0
56	MG	YA	3288	1/1	0.70	0.25	81,81,81,81	0
56	MG	YA	3284	1/1	0.71	0.18	51,51,51,51	0
56	MG	RA	3147	1/1	0.71	0.13	85,85,85,85	0
56	MG	YA	3291	1/1	0.71	0.26	37,37,37,37	0
56	MG	YA	3118	1/1	0.71	0.14	46,46,46,46	0
56	MG	RA	3007	1/1	0.71	0.15	84,84,84,84	0
56	MG	RA	3348	1/1	0.71	0.16	87,87,87,87	0
56	MG	YA	3169	1/1	0.71	0.25	74,74,74,74	0
56	MG	YB	210	1/1	0.71	0.10	83,83,83,83	0
56	MG	RA	3222	1/1	0.71	0.14	73,73,73,73	0
56	MG	YA	3450	1/1	0.71	0.14	90,90,90,90	0
56	MG	YA	3330	1/1	0.71	0.12	68,68,68,68	0
56	MG	YA	3364	1/1	0.71	0.21	68,68,68,68	0
56	MG	RB	201	1/1	0.71	0.14	68,68,68,68	0
56	MG	RA	3208	1/1	0.71	0.16	43,43,43,43	0
56	MG	RA	3341	1/1	0.71	0.15	85,85,85,85	0
56	MG	YA	3403	1/1	0.72	0.12	64,64,64,64	0
56	MG	YA	3312	1/1	0.72	0.33	76,76,76,76	0
56	MG	RA	3156	1/1	0.72	0.11	44,44,44,44	0
56	MG	YA	3006	1/1	0.72	0.24	49,49,49,49	0
56	MG	YA	3322	1/1	0.72	0.10	94,94,94,94	0
56	MG	RA	3117	1/1	0.72	0.13	39,39,39,39	0
56	MG	YA	3172	1/1	0.72	0.16	54,54,54,54	0
56	MG	RA	3085	1/1	0.72	0.21	26,26,26,26	0
56	MG	YA	3174	1/1	0.72	0.09	76,76,76,76	0
56	MG	YA	3130	1/1	0.72	0.26	68,68,68,68	0
56	MG	YA	3463	1/1	0.72	0.13	110,110,110,110	0
56	MG	YA	3299	1/1	0.72	0.23	104,104,104,104	0
56	MG	YA	3131	1/1	0.72	0.13	86,86,86,86	0
56	MG	YA	3348	1/1	0.72	0.12	61,61,61,61	0
56	MG	YA	3489	1/1	0.72	0.23	102,102,102,102	0
56	MG	RA	3356	1/1	0.73	0.09	45,45,45,45	0
56	MG	YA	3491	1/1	0.73	0.15	76,76,76,76	0
56	MG	YA	3501	1/1	0.73	0.07	85,85,85,85	0
56	MG	YP	204	1/1	0.73	0.22	55,55,55,55	0
56	MG	YA	3149	1/1	0.73	0.27	88,88,88,88	0
56	MG	YA	3183	1/1	0.73	0.19	44,44,44,44	0
56	MG	RA	3324	1/1	0.73	0.16	91,91,91,91	0
56	MG	YA	3373	1/1	0.73	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3481	1/1	0.73	0.23	87,87,87,87	0
56	MG	RA	3438	1/1	0.73	0.19	74,74,74,74	0
56	MG	YA	3301	1/1	0.74	0.17	60,60,60,60	0
56	MG	QV	106	1/1	0.74	0.32	95,95,95,95	0
56	MG	RA	3186	1/1	0.74	0.15	84,84,84,84	0
56	MG	YA	3264	1/1	0.74	0.35	82,82,82,82	0
56	MG	RA	3279	1/1	0.74	0.27	69,69,69,69	0
56	MG	RA	3488	1/1	0.74	0.17	66,66,66,66	0
56	MG	RA	3246	1/1	0.74	0.26	57,57,57,57	0
56	MG	RA	3450	1/1	0.74	0.12	79,79,79,79	0
56	MG	YA	3213	1/1	0.74	0.11	70,70,70,70	0
56	MG	YA	3422	1/1	0.74	0.23	61,61,61,61	0
56	MG	YA	3495	1/1	0.74	0.16	74,74,74,74	0
56	MG	XA	1666	1/1	0.74	0.11	45,45,45,45	0
56	MG	YA	3370	1/1	0.74	0.18	55,55,55,55	0
56	MG	RA	3365	1/1	0.74	0.19	70,70,70,70	0
56	MG	RA	3251	1/1	0.75	0.21	43,43,43,43	0
56	MG	YA	3170	1/1	0.75	0.21	43,43,43,43	0
56	MG	RA	3458	1/1	0.75	0.10	64,64,64,64	0
56	MG	RA	3325	1/1	0.75	0.13	66,66,66,66	0
56	MG	YA	3311	1/1	0.75	0.17	48,48,48,48	0
56	MG	YA	3229	1/1	0.75	0.14	75,75,75,75	0
56	MG	YA	3098	1/1	0.75	0.31	34,34,34,34	0
56	MG	YA	3360	1/1	0.75	0.17	81,81,81,81	0
56	MG	RA	3175	1/1	0.75	0.10	56,56,56,56	0
56	MG	QA	1616	1/1	0.75	0.15	72,72,72,72	0
56	MG	YA	3326	1/1	0.75	0.13	52,52,52,52	0
56	MG	YA	3369	1/1	0.75	0.15	45,45,45,45	0
56	MG	YE	303	1/1	0.75	0.10	61,61,61,61	0
56	MG	RA	3138	1/1	0.75	0.19	40,40,40,40	0
56	MG	XA	1648	1/1	0.75	0.09	68,68,68,68	0
56	MG	RA	3089	1/1	0.75	0.27	28,28,28,28	0
56	MG	YA	3383	1/1	0.75	0.13	59,59,59,59	0
58	ZN	RY	202	1/1	0.75	0.25	226,226,226,226	0
56	MG	YA	3386	1/1	0.75	0.14	68,68,68,68	0
56	MG	RA	3121	1/1	0.75	0.18	37,37,37,37	0
56	MG	RA	3082	1/1	0.75	0.21	28,28,28,28	0
58	ZN	Y5	501	1/1	0.75	0.28	124,124,124,124	0
56	MG	YA	3376	1/1	0.76	0.10	141,141,141,141	0
56	MG	YA	3201	1/1	0.76	0.11	62,62,62,62	0
56	MG	YA	3537	1/1	0.76	0.19	63,63,63,63	0
56	MG	YA	3384	1/1	0.76	0.28	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3453	1/1	0.76	0.18	80,80,80,80	0
56	MG	YA	3352	1/1	0.76	0.08	106,106,106,106	0
56	MG	YA	3283	1/1	0.76	0.18	80,80,80,80	0
56	MG	RA	3255	1/1	0.76	0.18	72,72,72,72	0
56	MG	RA	3314	1/1	0.76	0.17	56,56,56,56	0
56	MG	YA	3477	1/1	0.76	0.17	58,58,58,58	0
56	MG	YA	3137	1/1	0.76	0.12	73,73,73,73	0
56	MG	YA	3217	1/1	0.76	0.12	61,61,61,61	0
56	MG	Y7	101	1/1	0.76	0.17	82,82,82,82	0
56	MG	RA	3233	1/1	0.76	0.27	44,44,44,44	0
56	MG	RA	3377	1/1	0.76	0.15	81,81,81,81	0
56	MG	YA	3158	1/1	0.76	0.19	60,60,60,60	0
56	MG	RB	204	1/1	0.76	0.09	73,73,73,73	0
56	MG	RA	3317	1/1	0.76	0.24	65,65,65,65	0
56	MG	XA	1635	1/1	0.76	0.21	66,66,66,66	0
56	MG	RA	3471	1/1	0.77	0.19	65,65,65,65	0
56	MG	YA	3399	1/1	0.77	0.09	88,88,88,88	0
56	MG	YA	3461	1/1	0.77	0.16	76,76,76,76	0
56	MG	RA	3378	1/1	0.77	0.10	58,58,58,58	0
56	MG	YA	3407	1/1	0.77	0.18	72,72,72,72	0
56	MG	YA	3140	1/1	0.77	0.22	83,83,83,83	0
56	MG	RA	3201	1/1	0.77	0.16	89,89,89,89	0
56	MG	YA	3418	1/1	0.77	0.20	73,73,73,73	0
56	MG	RA	3227	1/1	0.77	0.12	50,50,50,50	0
56	MG	RA	3443	1/1	0.77	0.12	87,87,87,87	0
56	MG	YA	3306	1/1	0.77	0.23	102,102,102,102	0
56	MG	YA	3443	1/1	0.77	0.13	69,69,69,69	0
56	MG	YA	3269	1/1	0.77	0.13	46,46,46,46	0
56	MG	YA	3446	1/1	0.77	0.18	70,70,70,70	0
56	MG	YA	3342	1/1	0.77	0.16	49,49,49,49	0
56	MG	QA	1653	1/1	0.77	0.11	130,130,130,130	0
56	MG	RA	3280	1/1	0.77	0.30	73,73,73,73	0
56	MG	YA	3324	1/1	0.78	0.21	59,59,59,59	0
56	MG	QA	1649	1/1	0.78	0.07	62,62,62,62	0
56	MG	RA	3008	1/1	0.78	0.26	86,86,86,86	0
56	MG	RA	3047	1/1	0.78	0.12	71,71,71,71	0
56	MG	RA	3241	1/1	0.78	0.40	64,64,64,64	0
56	MG	RA	3153	1/1	0.78	0.10	38,38,38,38	0
56	MG	RA	3154	1/1	0.78	0.22	38,38,38,38	0
56	MG	RA	3292	1/1	0.78	0.17	56,56,56,56	0
56	MG	YA	3293	1/1	0.78	0.22	65,65,65,65	0
56	MG	RA	3294	1/1	0.78	0.27	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3047	1/1	0.78	0.24	31,31,31,31	0
56	MG	YA	3166	1/1	0.78	0.38	64,64,64,64	0
56	MG	YQ	201	1/1	0.78	0.12	72,72,72,72	0
56	MG	YA	3303	1/1	0.78	0.23	50,50,50,50	0
56	MG	XA	1663	1/1	0.78	0.14	64,64,64,64	0
56	MG	Y0	102	1/1	0.78	0.09	51,51,51,51	0
56	MG	YA	3227	1/1	0.78	0.20	49,49,49,49	0
56	MG	RA	3065	1/1	0.78	0.12	36,36,36,36	0
56	MG	RA	3260	1/1	0.78	0.21	45,45,45,45	0
56	MG	RA	3218	1/1	0.78	0.14	67,67,67,67	0
56	MG	YA	3111	1/1	0.78	0.13	39,39,39,39	0
56	MG	YA	3497	1/1	0.78	0.21	93,93,93,93	0
56	MG	XA	1679	1/1	0.78	0.14	86,86,86,86	0
56	MG	RA	3211	1/1	0.79	0.16	69,69,69,69	0
56	MG	XE	201	1/1	0.79	0.14	80,80,80,80	0
56	MG	RA	3457	1/1	0.79	0.10	97,97,97,97	0
56	MG	YA	3523	1/1	0.79	0.19	21,21,21,21	0
56	MG	RA	3495	1/1	0.79	0.24	15,15,15,15	0
56	MG	RA	3326	1/1	0.79	0.14	75,75,75,75	0
56	MG	RA	3334	1/1	0.79	0.09	58,58,58,58	0
56	MG	YB	205	1/1	0.79	0.15	76,76,76,76	0
56	MG	YA	3132	1/1	0.79	0.13	55,55,55,55	0
56	MG	RA	3300	1/1	0.79	0.17	68,68,68,68	0
56	MG	YA	3382	1/1	0.79	0.26	98,98,98,98	0
56	MG	YB	212	1/1	0.79	0.07	99,99,99,99	0
56	MG	RA	3266	1/1	0.79	0.16	52,52,52,52	0
56	MG	YA	3338	1/1	0.79	0.24	84,84,84,84	0
56	MG	RA	3009	1/1	0.79	0.19	38,38,38,38	0
56	MG	YA	3020	1/1	0.79	0.11	30,30,30,30	0
56	MG	YA	3026	1/1	0.79	0.27	55,55,55,55	0
56	MG	RA	3344	1/1	0.79	0.16	58,58,58,58	0
56	MG	Y0	101	1/1	0.79	0.19	54,54,54,54	0
56	MG	RA	3231	1/1	0.79	0.16	31,31,31,31	0
56	MG	RA	3087	1/1	0.79	0.23	64,64,64,64	0
56	MG	YA	3402	1/1	0.79	0.11	69,69,69,69	0
56	MG	RA	3352	1/1	0.79	0.17	75,75,75,75	0
56	MG	RO	201	1/1	0.79	0.29	79,79,79,79	0
56	MG	YA	3232	1/1	0.79	0.20	56,56,56,56	0
56	MG	YA	3249	1/1	0.79	0.26	64,64,64,64	0
56	MG	YA	3315	1/1	0.79	0.16	77,77,77,77	0
56	MG	RA	3029	1/1	0.80	0.22	26,26,26,26	0
56	MG	YA	3286	1/1	0.80	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3143	1/1	0.80	0.12	77,77,77,77	0
56	MG	YA	3028	1/1	0.80	0.29	23,23,23,23	0
56	MG	XA	1675	1/1	0.80	0.13	82,82,82,82	0
56	MG	YA	3156	1/1	0.80	0.15	60,60,60,60	0
56	MG	RA	3237	1/1	0.80	0.28	62,62,62,62	0
56	MG	YA	3161	1/1	0.80	0.16	56,56,56,56	0
56	MG	QV	101	1/1	0.80	0.22	45,45,45,45	0
56	MG	YA	3224	1/1	0.80	0.13	52,52,52,52	0
56	MG	YA	3398	1/1	0.80	0.25	78,78,78,78	0
56	MG	XA	1680	1/1	0.80	0.17	44,44,44,44	0
56	MG	RA	3177	1/1	0.80	0.12	74,74,74,74	0
56	MG	RA	3391	1/1	0.80	0.31	84,84,84,84	0
56	MG	RA	3393	1/1	0.80	0.14	69,69,69,69	0
56	MG	RA	3463	1/1	0.80	0.07	72,72,72,72	0
56	MG	XA	1650	1/1	0.80	0.17	114,114,114,114	0
56	MG	YA	3178	1/1	0.80	0.18	39,39,39,39	0
56	MG	RA	3394	1/1	0.80	0.09	53,53,53,53	0
56	MG	YA	3421	1/1	0.80	0.12	56,56,56,56	0
56	MG	RE	303	1/1	0.80	0.09	87,87,87,87	0
56	MG	RA	3400	1/1	0.80	0.10	85,85,85,85	0
56	MG	RP	202	1/1	0.80	0.29	56,56,56,56	0
56	MG	YA	3396	1/1	0.81	0.30	74,74,74,74	0
56	MG	RA	3313	1/1	0.81	0.16	63,63,63,63	0
56	MG	YA	3494	1/1	0.81	0.11	102,102,102,102	0
56	MG	YA	3171	1/1	0.81	0.26	44,44,44,44	0
56	MG	RA	3024	1/1	0.81	0.30	15,15,15,15	0
56	MG	RA	3351	1/1	0.81	0.20	63,63,63,63	0
56	MG	QA	1657	1/1	0.81	0.12	67,67,67,67	0
56	MG	YA	3404	1/1	0.81	0.15	73,73,73,73	0
56	MG	YA	3514	1/1	0.81	0.12	47,47,47,47	0
56	MG	XA	1668	1/1	0.81	0.24	95,95,95,95	0
56	MG	RA	3448	1/1	0.81	0.17	71,71,71,71	0
56	MG	RA	3329	1/1	0.81	0.09	76,76,76,76	0
56	MG	RA	3451	1/1	0.81	0.18	56,56,56,56	0
56	MG	RA	3293	1/1	0.81	0.16	70,70,70,70	0
56	MG	YB	204	1/1	0.81	0.07	118,118,118,118	0
56	MG	RY	201	1/1	0.81	0.22	67,67,67,67	0
56	MG	R0	102	1/1	0.81	0.10	54,54,54,54	0
56	MG	YA	3199	1/1	0.81	0.11	39,39,39,39	0
56	MG	R8	101	1/1	0.81	0.24	61,61,61,61	0
56	MG	YA	3305	1/1	0.81	0.15	41,41,41,41	0
56	MG	YA	3135	1/1	0.81	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1648	1/1	0.81	0.11	55,55,55,55	0
56	MG	RA	3405	1/1	0.81	0.20	55,55,55,55	0
56	MG	RA	3500	1/1	0.81	0.12	35,35,35,35	0
56	MG	YA	3146	1/1	0.81	0.12	67,67,67,67	0
56	MG	RA	3338	1/1	0.81	0.22	57,57,57,57	0
56	MG	YA	3004	1/1	0.81	0.12	56,56,56,56	0
56	MG	YA	3005	1/1	0.81	0.12	55,55,55,55	0
56	MG	YA	3464	1/1	0.81	0.18	56,56,56,56	0
56	MG	RA	3507	1/1	0.81	0.15	63,63,63,63	0
56	MG	RA	3133	1/1	0.81	0.14	92,92,92,92	0
56	MG	QA	1671	1/1	0.81	0.20	55,55,55,55	0
56	MG	YA	3480	1/1	0.81	0.10	81,81,81,81	0
56	MG	QA	1647	1/1	0.81	0.15	45,45,45,45	0
56	MG	YA	3033	1/1	0.81	0.20	41,41,41,41	0
56	MG	RA	3439	1/1	0.82	0.18	84,84,84,84	0
56	MG	RA	3261	1/1	0.82	0.13	63,63,63,63	0
56	MG	YA	3238	1/1	0.82	0.15	77,77,77,77	0
56	MG	YA	3439	1/1	0.82	0.09	70,70,70,70	0
56	MG	RA	3361	1/1	0.82	0.09	72,72,72,72	0
56	MG	YA	3177	1/1	0.82	0.23	63,63,63,63	0
56	MG	RA	3398	1/1	0.82	0.11	50,50,50,50	0
56	MG	RA	3242	1/1	0.82	0.23	71,71,71,71	0
56	MG	RA	3332	1/1	0.82	0.13	58,58,58,58	0
56	MG	YA	3328	1/1	0.82	0.09	72,72,72,72	0
56	MG	RA	3305	1/1	0.82	0.20	66,66,66,66	0
56	MG	YB	208	1/1	0.82	0.10	122,122,122,122	0
56	MG	YA	3455	1/1	0.82	0.14	66,66,66,66	0
56	MG	YA	3276	1/1	0.82	0.17	75,75,75,75	0
56	MG	QA	1603	1/1	0.82	0.21	34,34,34,34	0
56	MG	RA	3412	1/1	0.82	0.12	69,69,69,69	0
56	MG	XA	1676	1/1	0.82	0.12	99,99,99,99	0
56	MG	RA	3161	1/1	0.82	0.15	88,88,88,88	0
56	MG	XA	1611	1/1	0.82	0.15	34,34,34,34	0
56	MG	YA	3054	1/1	0.82	0.12	49,49,49,49	0
56	MG	YA	3059	1/1	0.82	0.23	40,40,40,40	0
56	MG	RA	3420	1/1	0.82	0.10	52,52,52,52	0
56	MG	RA	3039	1/1	0.82	0.14	27,27,27,27	0
56	MG	RA	3425	1/1	0.82	0.08	61,61,61,61	0
56	MG	YA	3302	1/1	0.82	0.18	109,109,109,109	0
56	MG	YA	3222	1/1	0.82	0.08	42,42,42,42	0
56	MG	RA	3379	1/1	0.82	0.14	84,84,84,84	0
56	MG	RA	3187	1/1	0.82	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3499	1/1	0.82	0.10	64,64,64,64	0
56	MG	YA	3113	1/1	0.82	0.13	33,33,33,33	0
56	MG	RA	3370	1/1	0.83	0.11	56,56,56,56	0
56	MG	RA	3158	1/1	0.83	0.29	51,51,51,51	0
56	MG	RA	3375	1/1	0.83	0.14	52,52,52,52	0
56	MG	RN	201	1/1	0.83	0.38	80,80,80,80	0
56	MG	YA	3259	1/1	0.83	0.16	56,56,56,56	0
56	MG	RA	3127	1/1	0.83	0.17	56,56,56,56	0
56	MG	RA	3433	1/1	0.83	0.14	66,66,66,66	0
56	MG	RA	3092	1/1	0.83	0.14	22,22,22,22	0
56	MG	YA	3105	1/1	0.83	0.08	60,60,60,60	0
56	MG	YA	3271	1/1	0.83	0.40	83,83,83,83	0
56	MG	RA	3172	1/1	0.83	0.20	59,59,59,59	0
56	MG	RA	3093	1/1	0.83	0.21	19,19,19,19	0
56	MG	YA	3180	1/1	0.83	0.10	45,45,45,45	0
56	MG	RA	3486	1/1	0.83	0.14	74,74,74,74	0
56	MG	RA	3214	1/1	0.83	0.26	72,72,72,72	0
56	MG	YA	3426	1/1	0.83	0.28	78,78,78,78	0
56	MG	RA	3445	1/1	0.83	0.09	47,47,47,47	0
56	MG	YA	3186	1/1	0.83	0.11	53,53,53,53	0
56	MG	RA	3296	1/1	0.83	0.19	66,66,66,66	0
56	MG	RA	3080	1/1	0.83	0.14	43,43,43,43	0
56	MG	RA	3145	1/1	0.83	0.11	40,40,40,40	0
56	MG	QA	1602	1/1	0.83	0.20	36,36,36,36	0
56	MG	RA	3058	1/1	0.83	0.26	72,72,72,72	0
56	MG	YA	3205	1/1	0.83	0.15	48,48,48,48	0
56	MG	YA	3018	1/1	0.83	0.26	14,14,14,14	0
56	MG	RA	3513	1/1	0.83	0.22	58,58,58,58	0
56	MG	YA	3148	1/1	0.83	0.19	51,51,51,51	0
56	MG	YA	3377	1/1	0.83	0.11	57,57,57,57	0
56	MG	RA	3061	1/1	0.83	0.42	26,26,26,26	0
56	MG	YA	3467	1/1	0.83	0.10	92,92,92,92	0
56	MG	QA	1611	1/1	0.83	0.19	35,35,35,35	0
56	MG	RA	3413	1/1	0.83	0.13	41,41,41,41	0
56	MG	YA	3475	1/1	0.83	0.23	66,66,66,66	0
56	MG	RA	3203	1/1	0.83	0.14	63,63,63,63	0
56	MG	YA	3040	1/1	0.83	0.12	61,61,61,61	0
56	MG	YA	3045	1/1	0.83	0.11	59,59,59,59	0
56	MG	YA	3230	1/1	0.83	0.15	70,70,70,70	0
56	MG	RA	3422	1/1	0.84	0.09	55,55,55,55	0
56	MG	YA	3168	1/1	0.84	0.11	68,68,68,68	0
56	MG	YA	3270	1/1	0.84	0.23	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1634	1/1	0.84	0.22	59,59,59,59	0
56	MG	YA	3029	1/1	0.84	0.16	27,27,27,27	0
56	MG	RA	3041	1/1	0.84	0.13	37,37,37,37	0
56	MG	RA	3328	1/1	0.84	0.19	65,65,65,65	0
56	MG	XA	1639	1/1	0.84	0.20	38,38,38,38	0
56	MG	XA	1640	1/1	0.84	0.11	48,48,48,48	0
56	MG	RA	3367	1/1	0.84	0.33	119,119,119,119	0
56	MG	YA	3486	1/1	0.84	0.12	58,58,58,58	0
56	MG	YA	3051	1/1	0.84	0.19	31,31,31,31	0
56	MG	RA	3249	1/1	0.84	0.12	76,76,76,76	0
56	MG	XA	1654	1/1	0.84	0.12	54,54,54,54	0
56	MG	YA	3296	1/1	0.84	0.18	49,49,49,49	0
56	MG	RA	3180	1/1	0.84	0.09	68,68,68,68	0
56	MG	RA	3441	1/1	0.84	0.20	87,87,87,87	0
56	MG	RA	3298	1/1	0.84	0.22	53,53,53,53	0
56	MG	YA	3093	1/1	0.84	0.17	47,47,47,47	0
56	MG	RA	3336	1/1	0.84	0.21	71,71,71,71	0
56	MG	YA	3100	1/1	0.84	0.17	44,44,44,44	0
56	MG	RA	3131	1/1	0.84	0.14	25,25,25,25	0
56	MG	RA	3132	1/1	0.84	0.17	50,50,50,50	0
56	MG	YA	3527	1/1	0.84	0.16	24,24,24,24	0
56	MG	RA	3381	1/1	0.84	0.24	77,77,77,77	0
56	MG	RA	3191	1/1	0.84	0.11	54,54,54,54	0
56	MG	YA	3538	1/1	0.84	0.24	45,45,45,45	0
56	MG	YA	3318	1/1	0.84	0.14	43,43,43,43	0
56	MG	RA	3306	1/1	0.84	0.17	31,31,31,31	0
56	MG	YA	3121	1/1	0.84	0.16	30,30,30,30	0
56	MG	YA	3216	1/1	0.84	0.11	49,49,49,49	0
56	MG	RA	3265	1/1	0.84	0.16	47,47,47,47	0
56	MG	QA	1631	1/1	0.84	0.09	123,123,123,123	0
56	MG	RA	3270	1/1	0.84	0.13	86,86,86,86	0
56	MG	RA	3223	1/1	0.84	0.17	52,52,52,52	0
56	MG	YA	3226	1/1	0.84	0.09	44,44,44,44	0
56	MG	YA	3332	1/1	0.84	0.14	47,47,47,47	0
56	MG	QA	1654	1/1	0.84	0.08	62,62,62,62	0
56	MG	RA	3407	1/1	0.84	0.11	54,54,54,54	0
56	MG	RA	3229	1/1	0.84	0.27	52,52,52,52	0
56	MG	RA	3469	1/1	0.84	0.24	85,85,85,85	0
56	MG	RA	3059	1/1	0.84	0.15	95,95,95,95	0
56	MG	RA	3164	1/1	0.84	0.12	60,60,60,60	0
56	MG	XA	1606	1/1	0.84	0.29	41,41,41,41	0
56	MG	YA	3347	1/1	0.84	0.19	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1626	1/1	0.84	0.13	51,51,51,51	0
56	MG	YA	3013	1/1	0.84	0.22	29,29,29,29	0
56	MG	QY	101	1/1	0.84	0.15	60,60,60,60	0
56	MG	YA	3460	1/1	0.84	0.05	84,84,84,84	0
56	MG	RA	3149	1/1	0.84	0.23	62,62,62,62	0
56	MG	YA	3335	1/1	0.85	0.20	46,46,46,46	0
56	MG	RA	3088	1/1	0.85	0.19	22,22,22,22	0
56	MG	RA	3170	1/1	0.85	0.07	43,43,43,43	0
56	MG	YA	3340	1/1	0.85	0.15	78,78,78,78	0
56	MG	RA	3432	1/1	0.85	0.08	57,57,57,57	0
56	MG	YA	3001	1/1	0.85	0.21	52,52,52,52	0
56	MG	R0	103	1/1	0.85	0.15	58,58,58,58	0
56	MG	YA	3506	1/1	0.85	0.15	70,70,70,70	0
56	MG	YA	3413	1/1	0.85	0.11	53,53,53,53	0
56	MG	YA	3003	1/1	0.85	0.29	17,17,17,17	0
56	MG	YA	3214	1/1	0.85	0.26	60,60,60,60	0
56	MG	RA	3049	1/1	0.85	0.17	20,20,20,20	0
56	MG	RA	3455	1/1	0.85	0.09	55,55,55,55	0
56	MG	RA	3484	1/1	0.85	0.09	84,84,84,84	0
56	MG	YA	3298	1/1	0.85	0.26	57,57,57,57	0
56	MG	YA	3008	1/1	0.85	0.27	18,18,18,18	0
56	MG	RA	3312	1/1	0.85	0.14	60,60,60,60	0
56	MG	YA	3225	1/1	0.85	0.12	35,35,35,35	0
56	MG	YA	3016	1/1	0.85	0.22	24,24,24,24	0
56	MG	YA	3017	1/1	0.85	0.25	16,16,16,16	0
56	MG	YA	3363	1/1	0.85	0.10	85,85,85,85	0
56	MG	YA	3115	1/1	0.85	0.14	43,43,43,43	0
56	MG	YA	3368	1/1	0.85	0.14	53,53,53,53	0
56	MG	RA	3173	1/1	0.85	0.11	51,51,51,51	0
56	MG	YA	3117	1/1	0.85	0.15	37,37,37,37	0
56	MG	XA	1630	1/1	0.85	0.08	41,41,41,41	0
56	MG	YA	3374	1/1	0.85	0.08	48,48,48,48	0
56	MG	YP	203	1/1	0.85	0.23	70,70,70,70	0
56	MG	QV	105	1/1	0.85	0.22	65,65,65,65	0
56	MG	YA	3243	1/1	0.85	0.21	51,51,51,51	0
56	MG	YA	3247	1/1	0.85	0.14	24,24,24,24	0
56	MG	RB	211	1/1	0.85	0.09	83,83,83,83	0
56	MG	QA	1615	1/1	0.85	0.09	43,43,43,43	0
56	MG	YA	3030	1/1	0.85	0.36	28,28,28,28	0
56	MG	XA	1636	1/1	0.85	0.09	93,93,93,93	0
56	MG	RA	3372	1/1	0.85	0.17	68,68,68,68	0
56	MG	RA	3373	1/1	0.85	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3187	1/1	0.85	0.09	39,39,39,39	0
56	MG	YA	3141	1/1	0.85	0.21	60,60,60,60	0
56	MG	RA	3291	1/1	0.85	0.13	75,75,75,75	0
56	MG	YA	3487	1/1	0.85	0.11	58,58,58,58	0
58	ZN	Y6	101	1/1	0.85	0.16	233,233,233,233	0
56	MG	XA	1608	1/1	0.86	0.07	78,78,78,78	0
56	MG	RA	3396	1/1	0.86	0.12	50,50,50,50	0
56	MG	XA	1612	1/1	0.86	0.15	41,41,41,41	0
56	MG	YA	3351	1/1	0.86	0.27	62,62,62,62	0
56	MG	YA	3114	1/1	0.86	0.19	66,66,66,66	0
56	MG	XA	1620	1/1	0.86	0.17	29,29,29,29	0
56	MG	XA	1671	1/1	0.86	0.17	39,39,39,39	0
56	MG	XA	1623	1/1	0.86	0.12	77,77,77,77	0
56	MG	RA	3474	1/1	0.86	0.12	46,46,46,46	0
56	MG	YA	3308	1/1	0.86	0.20	77,77,77,77	0
56	MG	RA	3128	1/1	0.86	0.08	58,58,58,58	0
56	MG	YA	3435	1/1	0.86	0.13	37,37,37,37	0
56	MG	YA	3436	1/1	0.86	0.13	60,60,60,60	0
56	MG	YA	3128	1/1	0.86	0.14	64,64,64,64	0
56	MG	RA	3482	1/1	0.86	0.21	65,65,65,65	0
56	MG	RA	3050	1/1	0.86	0.25	20,20,20,20	0
56	MG	RA	3116	1/1	0.86	0.09	71,71,71,71	0
56	MG	RA	3051	1/1	0.86	0.11	38,38,38,38	0
56	MG	YA	3372	1/1	0.86	0.14	74,74,74,74	0
56	MG	YA	3257	1/1	0.86	0.21	38,38,38,38	0
56	MG	RA	3339	1/1	0.86	0.21	34,34,34,34	0
56	MG	RA	3461	1/1	0.86	0.11	67,67,67,67	0
56	MG	RA	3020	1/1	0.86	0.34	29,29,29,29	0
56	MG	QA	1644	1/1	0.86	0.09	58,58,58,58	0
56	MG	YA	3380	1/1	0.86	0.15	65,65,65,65	0
56	MG	XA	1644	1/1	0.86	0.13	64,64,64,64	0
56	MG	XA	1645	1/1	0.86	0.09	57,57,57,57	0
56	MG	RA	3141	1/1	0.86	0.17	55,55,55,55	0
56	MG	YA	3468	1/1	0.86	0.21	50,50,50,50	0
56	MG	RA	3382	1/1	0.86	0.20	61,61,61,61	0
56	MG	RA	3126	1/1	0.86	0.17	32,32,32,32	0
56	MG	YA	3157	1/1	0.86	0.10	71,71,71,71	0
56	MG	YA	3393	1/1	0.86	0.10	46,46,46,46	0
56	MG	RA	3331	1/1	0.86	0.14	65,65,65,65	0
56	MG	RA	3040	1/1	0.86	0.15	25,25,25,25	0
56	MG	YA	3341	1/1	0.86	0.16	92,92,92,92	0
56	MG	YA	3101	1/1	0.86	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3218	1/1	0.86	0.10	62,62,62,62	0
56	MG	YA	3104	1/1	0.86	0.24	42,42,42,42	0
56	MG	YA	3221	1/1	0.86	0.12	51,51,51,51	0
56	MG	RA	3183	1/1	0.87	0.10	43,43,43,43	0
56	MG	YA	3185	1/1	0.87	0.10	49,49,49,49	0
56	MG	YA	3261	1/1	0.87	0.24	56,56,56,56	0
56	MG	YA	3483	1/1	0.87	0.15	66,66,66,66	0
56	MG	RA	3490	1/1	0.87	0.13	33,33,33,33	0
56	MG	YA	3263	1/1	0.87	0.17	43,43,43,43	0
56	MG	RA	3267	1/1	0.87	0.25	55,55,55,55	0
56	MG	YA	3488	1/1	0.87	0.18	87,87,87,87	0
56	MG	RA	3167	1/1	0.87	0.12	81,81,81,81	0
56	MG	RA	3414	1/1	0.87	0.14	67,67,67,67	0
56	MG	YA	3196	1/1	0.87	0.09	48,48,48,48	0
56	MG	YA	3038	1/1	0.87	0.16	25,25,25,25	0
56	MG	RA	3271	1/1	0.87	0.15	77,77,77,77	0
56	MG	YA	3343	1/1	0.87	0.09	44,44,44,44	0
56	MG	YA	3278	1/1	0.87	0.11	105,105,105,105	0
56	MG	YA	3504	1/1	0.87	0.18	53,53,53,53	0
56	MG	RA	3376	1/1	0.87	0.10	79,79,79,79	0
56	MG	RA	3168	1/1	0.87	0.13	63,63,63,63	0
56	MG	YA	3510	1/1	0.87	0.13	71,71,71,71	0
56	MG	YA	3211	1/1	0.87	0.08	45,45,45,45	0
56	MG	QA	1663	1/1	0.87	0.19	58,58,58,58	0
56	MG	RA	3197	1/1	0.87	0.20	44,44,44,44	0
56	MG	RA	3466	1/1	0.87	0.10	57,57,57,57	0
56	MG	YA	3525	1/1	0.87	0.26	15,15,15,15	0
56	MG	QV	104	1/1	0.87	0.17	116,116,116,116	0
56	MG	YA	3532	1/1	0.87	0.17	50,50,50,50	0
56	MG	QA	1635	1/1	0.87	0.10	64,64,64,64	0
56	MG	RA	3385	1/1	0.87	0.06	61,61,61,61	0
56	MG	YA	3427	1/1	0.87	0.17	53,53,53,53	0
56	MG	YA	3541	1/1	0.87	0.14	35,35,35,35	0
56	MG	YA	3429	1/1	0.87	0.25	58,58,58,58	0
56	MG	RA	3053	1/1	0.87	0.15	32,32,32,32	0
56	MG	YA	3359	1/1	0.87	0.18	56,56,56,56	0
56	MG	YB	206	1/1	0.87	0.10	49,49,49,49	0
56	MG	YA	3220	1/1	0.87	0.11	41,41,41,41	0
56	MG	RB	208	1/1	0.87	0.12	65,65,65,65	0
56	MG	RA	3259	1/1	0.87	0.17	69,69,69,69	0
56	MG	RA	3290	1/1	0.87	0.15	60,60,60,60	0
56	MG	YB	211	1/1	0.87	0.09	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3447	1/1	0.87	0.16	64,64,64,64	0
56	MG	YA	3103	1/1	0.87	0.17	40,40,40,40	0
56	MG	YE	302	1/1	0.87	0.25	83,83,83,83	0
56	MG	RA	3364	1/1	0.87	0.09	93,93,93,93	0
56	MG	XA	1647	1/1	0.87	0.09	66,66,66,66	0
56	MG	YA	3452	1/1	0.87	0.12	78,78,78,78	0
56	MG	RA	3113	1/1	0.87	0.14	87,87,87,87	0
56	MG	YA	3007	1/1	0.87	0.16	39,39,39,39	0
56	MG	RA	3479	1/1	0.87	0.09	56,56,56,56	0
56	MG	XA	1653	1/1	0.87	0.23	51,51,51,51	0
56	MG	YA	3317	1/1	0.87	0.11	49,49,49,49	0
56	MG	RA	3068	1/1	0.87	0.15	33,33,33,33	0
56	MG	XA	1659	1/1	0.87	0.22	71,71,71,71	0
56	MG	YA	3378	1/1	0.87	0.14	67,67,67,67	0
56	MG	RA	3340	1/1	0.87	0.08	53,53,53,53	0
56	MG	YA	3469	1/1	0.87	0.17	90,90,90,90	0
56	MG	RA	3368	1/1	0.87	0.10	27,27,27,27	0
56	MG	RA	3076	1/1	0.87	0.28	35,35,35,35	0
56	MG	YA	3256	1/1	0.87	0.22	34,34,34,34	0
56	MG	RA	3392	1/1	0.88	0.17	32,32,32,32	0
56	MG	YA	3204	1/1	0.88	0.24	61,61,61,61	0
56	MG	YA	3274	1/1	0.88	0.31	65,65,65,65	0
56	MG	RA	3178	1/1	0.88	0.11	63,63,63,63	0
56	MG	YA	3210	1/1	0.88	0.40	60,60,60,60	0
56	MG	XV	106	1/1	0.88	0.29	70,70,70,70	0
56	MG	YA	3070	1/1	0.88	0.13	47,47,47,47	0
56	MG	YA	3152	1/1	0.88	0.18	60,60,60,60	0
56	MG	RA	3307	1/1	0.88	0.07	83,83,83,83	0
56	MG	YA	3075	1/1	0.88	0.15	12,12,12,12	0
56	MG	RA	3026	1/1	0.88	0.20	24,24,24,24	0
56	MG	RA	3289	1/1	0.88	0.13	70,70,70,70	0
56	MG	YA	3086	1/1	0.88	0.20	28,28,28,28	0
56	MG	YA	3516	1/1	0.88	0.09	30,30,30,30	0
56	MG	YA	3356	1/1	0.88	0.25	53,53,53,53	0
56	MG	YA	3295	1/1	0.88	0.09	67,67,67,67	0
56	MG	RA	3447	1/1	0.88	0.13	49,49,49,49	0
56	MG	RA	3165	1/1	0.88	0.18	42,42,42,42	0
56	MG	YA	3528	1/1	0.88	0.10	54,54,54,54	0
56	MG	RR	202	1/1	0.88	0.15	80,80,80,80	0
56	MG	YA	3440	1/1	0.88	0.12	56,56,56,56	0
56	MG	XA	1649	1/1	0.88	0.11	67,67,67,67	0
56	MG	QA	1646	1/1	0.88	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3445	1/1	0.88	0.12	71,71,71,71	0
56	MG	QA	1601	1/1	0.88	0.21	47,47,47,47	0
56	MG	QA	1667	1/1	0.88	0.20	52,52,52,52	0
56	MG	QA	1623	1/1	0.88	0.12	37,37,37,37	0
56	MG	RA	3295	1/1	0.88	0.17	53,53,53,53	0
56	MG	RA	3192	1/1	0.88	0.14	49,49,49,49	0
56	MG	XA	1607	1/1	0.88	0.16	64,64,64,64	0
56	MG	RA	3297	1/1	0.88	0.15	50,50,50,50	0
56	MG	YA	3313	1/1	0.88	0.24	60,60,60,60	0
56	MG	YA	3242	1/1	0.88	0.08	50,50,50,50	0
56	MG	YA	3025	1/1	0.88	0.09	38,38,38,38	0
56	MG	RA	3504	1/1	0.88	0.14	123,123,123,123	0
56	MG	RA	3349	1/1	0.88	0.14	70,70,70,70	0
56	MG	YA	3251	1/1	0.88	0.38	56,56,56,56	0
56	MG	YO	201	1/1	0.88	0.28	52,52,52,52	0
56	MG	RA	3140	1/1	0.88	0.15	50,50,50,50	0
56	MG	YA	3255	1/1	0.88	0.15	46,46,46,46	0
56	MG	YA	3129	1/1	0.88	0.09	51,51,51,51	0
56	MG	RA	3299	1/1	0.88	0.20	76,76,76,76	0
56	MG	YA	3387	1/1	0.88	0.14	58,58,58,58	0
56	MG	RA	3198	1/1	0.88	0.14	66,66,66,66	0
56	MG	RA	3303	1/1	0.88	0.16	62,62,62,62	0
56	MG	RA	3111	1/1	0.88	0.24	26,26,26,26	0
56	MG	YA	3333	1/1	0.88	0.26	36,36,36,36	0
56	MG	YA	3482	1/1	0.88	0.13	67,67,67,67	0
56	MG	RA	3070	1/1	0.88	0.10	27,27,27,27	0
56	MG	YA	3198	1/1	0.88	0.11	70,70,70,70	0
56	MG	RA	3389	1/1	0.88	0.19	104,104,104,104	0
56	MG	RA	3359	1/1	0.88	0.27	37,37,37,37	0
56	MG	YA	3401	1/1	0.88	0.15	62,62,62,62	0
56	MG	RA	3309	1/1	0.89	0.29	63,63,63,63	0
56	MG	YA	3511	1/1	0.89	0.17	67,67,67,67	0
56	MG	RA	3195	1/1	0.89	0.09	36,36,36,36	0
56	MG	RA	3501	1/1	0.89	0.09	58,58,58,58	0
56	MG	RA	3054	1/1	0.89	0.09	42,42,42,42	0
56	MG	QA	1655	1/1	0.89	0.13	51,51,51,51	0
56	MG	YA	3202	1/1	0.89	0.11	73,73,73,73	0
56	MG	RA	3181	1/1	0.89	0.10	47,47,47,47	0
56	MG	YA	3087	1/1	0.89	0.11	24,24,24,24	0
56	MG	YA	3089	1/1	0.89	0.16	42,42,42,42	0
56	MG	RA	3101	1/1	0.89	0.10	37,37,37,37	0
56	MG	RA	3274	1/1	0.89	0.07	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3099	1/1	0.89	0.19	16,16,16,16	0
56	MG	RA	3319	1/1	0.89	0.11	44,44,44,44	0
56	MG	RA	3016	1/1	0.89	0.14	24,24,24,24	0
56	MG	YA	3215	1/1	0.89	0.12	69,69,69,69	0
56	MG	YA	3391	1/1	0.89	0.10	46,46,46,46	0
56	MG	YA	3102	1/1	0.89	0.14	18,18,18,18	0
56	MG	YA	3167	1/1	0.89	0.08	66,66,66,66	0
56	MG	RA	3205	1/1	0.89	0.12	49,49,49,49	0
56	MG	YA	3022	1/1	0.89	0.16	20,20,20,20	0
56	MG	RA	3256	1/1	0.89	0.23	61,61,61,61	0
56	MG	RA	3323	1/1	0.89	0.15	57,57,57,57	0
56	MG	YA	3472	1/1	0.89	0.11	74,74,74,74	0
56	MG	RA	3281	1/1	0.89	0.28	57,57,57,57	0
56	MG	RA	3480	1/1	0.89	0.09	44,44,44,44	0
56	MG	RA	3258	1/1	0.89	0.19	106,106,106,106	0
56	MG	YA	3176	1/1	0.89	0.11	65,65,65,65	0
56	MG	RA	3135	1/1	0.89	0.23	52,52,52,52	0
56	MG	YA	3034	1/1	0.89	0.23	35,35,35,35	0
56	MG	RA	3189	1/1	0.89	0.38	75,75,75,75	0
56	MG	RA	3419	1/1	0.89	0.07	65,65,65,65	0
56	MG	YA	3355	1/1	0.89	0.17	51,51,51,51	0
56	MG	RP	201	1/1	0.89	0.08	46,46,46,46	0
56	MG	RA	3288	1/1	0.89	0.11	59,59,59,59	0
56	MG	YA	3304	1/1	0.89	0.09	57,57,57,57	0
56	MG	YA	3239	1/1	0.89	0.30	48,48,48,48	0
56	MG	YA	3240	1/1	0.89	0.12	36,36,36,36	0
56	MG	RA	3137	1/1	0.89	0.14	84,84,84,84	0
56	MG	RA	3494	1/1	0.89	0.14	45,45,45,45	0
56	MG	RA	3119	1/1	0.89	0.12	41,41,41,41	0
56	MG	YA	3058	1/1	0.89	0.12	49,49,49,49	0
56	MG	R0	101	1/1	0.89	0.43	70,70,70,70	0
56	MG	YA	3253	1/1	0.89	0.22	67,67,67,67	0
56	MG	RA	3395	1/1	0.90	0.10	55,55,55,55	0
56	MG	RA	3169	1/1	0.90	0.11	21,21,21,21	0
56	MG	RB	210	1/1	0.90	0.10	78,78,78,78	0
56	MG	RA	3273	1/1	0.90	0.24	51,51,51,51	0
56	MG	RE	302	1/1	0.90	0.09	84,84,84,84	0
56	MG	RA	3244	1/1	0.90	0.10	33,33,33,33	0
56	MG	RA	3444	1/1	0.90	0.17	73,73,73,73	0
56	MG	RA	3199	1/1	0.90	0.11	44,44,44,44	0
56	MG	RA	3347	1/1	0.90	0.21	33,33,33,33	0
56	MG	RA	3247	1/1	0.90	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1605	1/1	0.90	0.30	35,35,35,35	0
56	MG	YA	3522	1/1	0.90	0.20	27,27,27,27	0
56	MG	RA	3184	1/1	0.90	0.14	51,51,51,51	0
56	MG	RA	3221	1/1	0.90	0.06	58,58,58,58	0
56	MG	QA	1636	1/1	0.90	0.10	39,39,39,39	0
56	MG	RA	3204	1/1	0.90	0.14	50,50,50,50	0
56	MG	RA	3456	1/1	0.90	0.10	51,51,51,51	0
56	MG	RA	3144	1/1	0.90	0.08	53,53,53,53	0
56	MG	XA	1605	1/1	0.90	0.17	34,34,34,34	0
56	MG	QA	1620	1/1	0.90	0.08	85,85,85,85	0
56	MG	XA	1667	1/1	0.90	0.20	48,48,48,48	0
56	MG	YA	3188	1/1	0.90	0.15	42,42,42,42	0
56	MG	YA	3323	1/1	0.90	0.13	48,48,48,48	0
56	MG	YA	3381	1/1	0.90	0.13	55,55,55,55	0
56	MG	RA	3384	1/1	0.90	0.12	43,43,43,43	0
56	MG	RA	3230	1/1	0.90	0.14	44,44,44,44	0
56	MG	RA	3001	1/1	0.90	0.18	28,28,28,28	0
56	MG	YA	3465	1/1	0.90	0.14	88,88,88,88	0
56	MG	YA	3329	1/1	0.90	0.17	54,54,54,54	0
56	MG	RA	3508	1/1	0.90	0.16	33,33,33,33	0
56	MG	XA	1677	1/1	0.90	0.09	62,62,62,62	0
56	MG	YA	3139	1/1	0.90	0.12	36,36,36,36	0
56	MG	XA	1617	1/1	0.90	0.16	22,22,22,22	0
56	MG	XA	1618	1/1	0.90	0.10	45,45,45,45	0
56	MG	RA	3426	1/1	0.90	0.13	49,49,49,49	0
56	MG	YP	201	1/1	0.90	0.42	68,68,68,68	0
56	MG	YP	202	1/1	0.90	0.13	76,76,76,76	0
56	MG	RA	3427	1/1	0.90	0.22	58,58,58,58	0
56	MG	YA	3479	1/1	0.90	0.20	84,84,84,84	0
56	MG	YA	3206	1/1	0.90	0.06	41,41,41,41	0
56	MG	XL	201	1/1	0.90	0.17	74,74,74,74	0
56	MG	YA	3062	1/1	0.90	0.13	23,23,23,23	0
56	MG	YY	201	1/1	0.90	0.27	66,66,66,66	0
56	MG	XA	1624	1/1	0.90	0.19	58,58,58,58	0
56	MG	YA	3153	1/1	0.90	0.26	59,59,59,59	0
56	MG	XQ	201	1/1	0.90	0.08	108,108,108,108	0
56	MG	RA	3031	1/1	0.90	0.22	30,30,30,30	0
56	MG	RA	3235	1/1	0.90	0.15	44,44,44,44	0
56	MG	YA	3290	1/1	0.90	0.17	57,57,57,57	0
56	MG	RA	3012	1/1	0.90	0.17	24,24,24,24	0
56	MG	YA	3159	1/1	0.90	0.14	39,39,39,39	0
58	ZN	Y4	500	1/1	0.90	0.15	242,242,242,242	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3436	1/1	0.90	0.13	41,41,41,41	0
56	MG	QA	1632	1/1	0.90	0.25	27,27,27,27	0
56	MG	RA	3033	1/1	0.91	0.15	20,20,20,20	0
56	MG	RA	3038	1/1	0.91	0.15	22,22,22,22	0
56	MG	YA	3389	1/1	0.91	0.10	57,57,57,57	0
56	MG	RA	3207	1/1	0.91	0.08	47,47,47,47	0
56	MG	RB	203	1/1	0.91	0.07	64,64,64,64	0
56	MG	XV	102	1/1	0.91	0.08	53,53,53,53	0
56	MG	YA	3236	1/1	0.91	0.16	60,60,60,60	0
56	MG	YA	3492	1/1	0.91	0.12	76,76,76,76	0
56	MG	YA	3237	1/1	0.91	0.21	47,47,47,47	0
56	MG	YA	3395	1/1	0.91	0.29	54,54,54,54	0
56	MG	XA	1629	1/1	0.91	0.06	51,51,51,51	0
56	MG	RA	3060	1/1	0.91	0.27	16,16,16,16	0
56	MG	YA	3500	1/1	0.91	0.12	103,103,103,103	0
56	MG	YA	3094	1/1	0.91	0.11	43,43,43,43	0
56	MG	YA	3503	1/1	0.91	0.29	52,52,52,52	0
56	MG	RA	3182	1/1	0.91	0.14	69,69,69,69	0
56	MG	YA	3400	1/1	0.91	0.11	67,67,67,67	0
56	MG	YA	3507	1/1	0.91	0.09	61,61,61,61	0
56	MG	RA	3096	1/1	0.91	0.14	60,60,60,60	0
56	MG	YA	3244	1/1	0.91	0.18	45,45,45,45	0
56	MG	RA	3434	1/1	0.91	0.14	38,38,38,38	0
56	MG	RA	3435	1/1	0.91	0.06	61,61,61,61	0
56	MG	QA	1627	1/1	0.91	0.14	35,35,35,35	0
56	MG	RA	3437	1/1	0.91	0.21	64,64,64,64	0
56	MG	RA	3018	1/1	0.91	0.19	14,14,14,14	0
56	MG	XA	1642	1/1	0.91	0.13	71,71,71,71	0
56	MG	XA	1643	1/1	0.91	0.07	73,73,73,73	0
56	MG	RA	3107	1/1	0.91	0.12	26,26,26,26	0
56	MG	QA	1610	1/1	0.91	0.16	19,19,19,19	0
56	MG	YA	3260	1/1	0.91	0.22	51,51,51,51	0
56	MG	RA	3284	1/1	0.91	0.11	53,53,53,53	0
56	MG	RA	3402	1/1	0.91	0.20	64,64,64,64	0
56	MG	YA	3535	1/1	0.91	0.22	52,52,52,52	0
56	MG	RA	3045	1/1	0.91	0.18	24,24,24,24	0
56	MG	RQ	202	1/1	0.91	0.08	74,74,74,74	0
56	MG	YA	3193	1/1	0.91	0.26	42,42,42,42	0
56	MG	RA	3022	1/1	0.91	0.10	27,27,27,27	0
56	MG	YA	3123	1/1	0.91	0.15	75,75,75,75	0
56	MG	YA	3124	1/1	0.91	0.13	48,48,48,48	0
56	MG	YA	3126	1/1	0.91	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3220	1/1	0.91	0.08	63,63,63,63	0
56	MG	QA	1652	1/1	0.91	0.06	45,45,45,45	0
56	MG	YA	3280	1/1	0.91	0.14	72,72,72,72	0
56	MG	QA	1662	1/1	0.91	0.20	41,41,41,41	0
56	MG	RA	3491	1/1	0.91	0.09	39,39,39,39	0
56	MG	QA	1618	1/1	0.91	0.25	67,67,67,67	0
56	MG	YA	3134	1/1	0.91	0.08	60,60,60,60	0
56	MG	RA	3263	1/1	0.91	0.16	43,43,43,43	0
56	MG	YA	3208	1/1	0.91	0.10	67,67,67,67	0
56	MG	XA	1604	1/1	0.91	0.15	64,64,64,64	0
56	MG	RA	3030	1/1	0.91	0.27	8,8,8,8	0
56	MG	RA	3454	1/1	0.91	0.08	47,47,47,47	0
56	MG	YA	3367	1/1	0.91	0.11	51,51,51,51	0
56	MG	RA	3122	1/1	0.91	0.14	34,34,34,34	0
56	MG	YA	3142	1/1	0.91	0.14	32,32,32,32	0
56	MG	YA	3297	1/1	0.91	0.15	51,51,51,51	0
56	MG	YA	3046	1/1	0.91	0.19	20,20,20,20	0
56	MG	RA	3502	1/1	0.91	0.08	43,43,43,43	0
56	MG	YA	3300	1/1	0.91	0.17	91,91,91,91	0
56	MG	RA	3380	1/1	0.91	0.18	57,57,57,57	0
56	MG	RA	3148	1/1	0.91	0.20	36,36,36,36	0
56	MG	XA	1615	1/1	0.91	0.12	25,25,25,25	0
56	MG	QA	1641	1/1	0.91	0.10	37,37,37,37	0
56	MG	YA	3061	1/1	0.91	0.15	22,22,22,22	0
56	MG	YA	3478	1/1	0.91	0.19	74,74,74,74	0
58	ZN	R6	101	1/1	0.91	0.13	213,213,213,213	0
56	MG	RA	3459	1/1	0.91	0.11	53,53,53,53	0
56	MG	RA	3423	1/1	0.91	0.12	57,57,57,57	0
56	MG	YA	3072	1/1	0.91	0.15	3,3,3,3	0
56	MG	XA	1622	1/1	0.91	0.07	53,53,53,53	0
56	MG	RA	3066	1/1	0.92	0.20	29,29,29,29	0
56	MG	RA	3174	1/1	0.92	0.06	40,40,40,40	0
56	MG	YA	3272	1/1	0.92	0.14	33,33,33,33	0
56	MG	RA	3401	1/1	0.92	0.08	41,41,41,41	0
56	MG	YA	3056	1/1	0.92	0.23	28,28,28,28	0
56	MG	YA	3277	1/1	0.92	0.12	38,38,38,38	0
56	MG	XA	1631	1/1	0.92	0.13	38,38,38,38	0
56	MG	RA	3067	1/1	0.92	0.13	28,28,28,28	0
56	MG	RA	3124	1/1	0.92	0.09	36,36,36,36	0
56	MG	YA	3509	1/1	0.92	0.09	54,54,54,54	0
56	MG	RA	3302	1/1	0.92	0.10	46,46,46,46	0
56	MG	YA	3069	1/1	0.92	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3287	1/1	0.92	0.18	59,59,59,59	0
56	MG	RA	3052	1/1	0.92	0.09	41,41,41,41	0
56	MG	RA	3240	1/1	0.92	0.10	47,47,47,47	0
56	MG	YA	3519	1/1	0.92	0.11	34,34,34,34	0
56	MG	YA	3073	1/1	0.92	0.09	39,39,39,39	0
56	MG	YA	3437	1/1	0.92	0.04	60,60,60,60	0
56	MG	YA	3438	1/1	0.92	0.14	56,56,56,56	0
56	MG	RQ	201	1/1	0.92	0.23	74,74,74,74	0
56	MG	RA	3371	1/1	0.92	0.14	82,82,82,82	0
56	MG	YA	3076	1/1	0.92	0.09	20,20,20,20	0
56	MG	YA	3531	1/1	0.92	0.05	23,23,23,23	0
56	MG	RR	201	1/1	0.92	0.08	58,58,58,58	0
56	MG	YA	3081	1/1	0.92	0.08	42,42,42,42	0
56	MG	RA	3097	1/1	0.92	0.16	36,36,36,36	0
56	MG	QA	1608	1/1	0.92	0.10	35,35,35,35	0
56	MG	YA	3448	1/1	0.92	0.30	67,67,67,67	0
56	MG	YA	3164	1/1	0.92	0.14	46,46,46,46	0
56	MG	RA	3100	1/1	0.92	0.10	23,23,23,23	0
56	MG	XA	1646	1/1	0.92	0.12	29,29,29,29	0
56	MG	RA	3496	1/1	0.92	0.14	26,26,26,26	0
56	MG	YA	3371	1/1	0.92	0.24	59,59,59,59	0
56	MG	RA	3130	1/1	0.92	0.18	47,47,47,47	0
56	MG	YA	3097	1/1	0.92	0.23	21,21,21,21	0
56	MG	RA	3071	1/1	0.92	0.07	37,37,37,37	0
56	MG	RA	3013	1/1	0.92	0.15	25,25,25,25	0
56	MG	XA	1652	1/1	0.92	0.07	68,68,68,68	0
56	MG	RA	3056	1/1	0.92	0.13	62,62,62,62	0
56	MG	RA	3285	1/1	0.92	0.13	60,60,60,60	0
56	MG	RA	3315	1/1	0.92	0.19	40,40,40,40	0
56	MG	YA	3241	1/1	0.92	0.23	31,31,31,31	0
56	MG	YA	3019	1/1	0.92	0.29	34,34,34,34	0
56	MG	XA	1660	1/1	0.92	0.14	55,55,55,55	0
56	MG	RA	3163	1/1	0.92	0.07	38,38,38,38	0
56	MG	YA	3023	1/1	0.92	0.20	24,24,24,24	0
56	MG	RA	3003	1/1	0.92	0.18	39,39,39,39	0
56	MG	YA	3388	1/1	0.92	0.10	46,46,46,46	0
56	MG	YQ	202	1/1	0.92	0.17	108,108,108,108	0
56	MG	RA	3350	1/1	0.92	0.15	61,61,61,61	0
56	MG	QA	1621	1/1	0.92	0.08	47,47,47,47	0
56	MG	QA	1617	1/1	0.92	0.08	42,42,42,42	0
56	MG	QA	1659	1/1	0.92	0.11	67,67,67,67	0
56	MG	RA	3139	1/1	0.92	0.16	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3122	1/1	0.92	0.11	26,26,26,26	0
56	MG	XA	1670	1/1	0.92	0.07	36,36,36,36	0
56	MG	RA	3262	1/1	0.92	0.09	61,61,61,61	0
56	MG	YA	3036	1/1	0.92	0.20	16,16,16,16	0
56	MG	QA	1606	1/1	0.92	0.10	49,49,49,49	0
56	MG	RA	3120	1/1	0.92	0.09	55,55,55,55	0
56	MG	YA	3043	1/1	0.92	0.17	42,42,42,42	0
56	MG	RA	3200	1/1	0.92	0.12	43,43,43,43	0
56	MG	YA	3268	1/1	0.92	0.05	44,44,44,44	0
56	MG	RA	3476	1/1	0.92	0.16	73,73,73,73	0
56	MG	QA	1633	1/1	0.93	0.06	63,63,63,63	0
56	MG	XA	1614	1/1	0.93	0.12	26,26,26,26	0
56	MG	RA	3410	1/1	0.93	0.12	49,49,49,49	0
56	MG	YA	3385	1/1	0.93	0.11	46,46,46,46	0
56	MG	RA	3245	1/1	0.93	0.17	35,35,35,35	0
56	MG	YA	3063	1/1	0.93	0.09	34,34,34,34	0
56	MG	YA	3067	1/1	0.93	0.19	31,31,31,31	0
56	MG	YA	3068	1/1	0.93	0.12	29,29,29,29	0
56	MG	XC	301	1/1	0.93	0.10	112,112,112,112	0
56	MG	YA	3314	1/1	0.93	0.10	53,53,53,53	0
56	MG	YA	3231	1/1	0.93	0.14	40,40,40,40	0
56	MG	YA	3316	1/1	0.93	0.14	52,52,52,52	0
56	MG	RA	3276	1/1	0.93	0.07	60,60,60,60	0
56	MG	YA	3498	1/1	0.93	0.17	52,52,52,52	0
56	MG	RA	3277	1/1	0.93	0.19	39,39,39,39	0
56	MG	RA	3415	1/1	0.93	0.14	50,50,50,50	0
56	MG	YA	3163	1/1	0.93	0.05	60,60,60,60	0
56	MG	YA	3502	1/1	0.93	0.12	54,54,54,54	0
56	MG	RA	3416	1/1	0.93	0.08	38,38,38,38	0
56	MG	RA	3511	1/1	0.93	0.08	80,80,80,80	0
56	MG	RA	3023	1/1	0.93	0.09	30,30,30,30	0
56	MG	RA	3196	1/1	0.93	0.07	44,44,44,44	0
56	MG	YA	3079	1/1	0.93	0.28	23,23,23,23	0
56	MG	RA	3248	1/1	0.93	0.10	87,87,87,87	0
56	MG	YA	3082	1/1	0.93	0.13	31,31,31,31	0
56	MG	RA	3217	1/1	0.93	0.09	87,87,87,87	0
56	MG	RA	3105	1/1	0.93	0.10	48,48,48,48	0
56	MG	YA	3513	1/1	0.93	0.08	95,95,95,95	0
56	MG	XA	1632	1/1	0.93	0.11	51,51,51,51	0
56	MG	RA	3042	1/1	0.93	0.10	54,54,54,54	0
56	MG	YA	3175	1/1	0.93	0.08	33,33,33,33	0
56	MG	RA	3424	1/1	0.93	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3420	1/1	0.93	0.15	55,55,55,55	0
56	MG	RA	3150	1/1	0.93	0.07	31,31,31,31	0
56	MG	RA	3468	1/1	0.93	0.24	54,54,54,54	0
56	MG	YA	3526	1/1	0.93	0.19	13,13,13,13	0
56	MG	RA	3286	1/1	0.93	0.28	54,54,54,54	0
56	MG	RB	209	1/1	0.93	0.08	87,87,87,87	0
56	MG	QA	1604	1/1	0.93	0.11	20,20,20,20	0
56	MG	YA	3428	1/1	0.93	0.11	32,32,32,32	0
56	MG	RA	3428	1/1	0.93	0.19	46,46,46,46	0
56	MG	YA	3431	1/1	0.93	0.11	55,55,55,55	0
56	MG	YA	3432	1/1	0.93	0.08	44,44,44,44	0
56	MG	RE	301	1/1	0.93	0.08	28,28,28,28	0
56	MG	YA	3539	1/1	0.93	0.17	53,53,53,53	0
56	MG	RA	3429	1/1	0.93	0.14	80,80,80,80	0
56	MG	RA	3109	1/1	0.93	0.11	50,50,50,50	0
56	MG	RA	3225	1/1	0.93	0.11	17,17,17,17	0
56	MG	YA	3106	1/1	0.93	0.18	31,31,31,31	0
56	MG	YA	3190	1/1	0.93	0.21	54,54,54,54	0
56	MG	QA	1642	1/1	0.93	0.17	40,40,40,40	0
56	MG	QA	1672	1/1	0.93	0.06	75,75,75,75	0
56	MG	QA	1609	1/1	0.93	0.10	24,24,24,24	0
56	MG	RA	3354	1/1	0.93	0.09	54,54,54,54	0
56	MG	RA	3481	1/1	0.93	0.11	58,58,58,58	0
56	MG	RA	3264	1/1	0.93	0.19	41,41,41,41	0
56	MG	YA	3281	1/1	0.93	0.14	35,35,35,35	0
56	MG	RA	3483	1/1	0.93	0.09	70,70,70,70	0
56	MG	XA	1657	1/1	0.93	0.11	55,55,55,55	0
56	MG	RA	3091	1/1	0.93	0.20	18,18,18,18	0
56	MG	RA	3118	1/1	0.93	0.17	33,33,33,33	0
56	MG	RA	3014	1/1	0.93	0.12	17,17,17,17	0
56	MG	YA	3365	1/1	0.93	0.08	53,53,53,53	0
56	MG	YA	3458	1/1	0.93	0.09	54,54,54,54	0
56	MG	YA	3459	1/1	0.93	0.13	48,48,48,48	0
56	MG	YA	3366	1/1	0.93	0.18	49,49,49,49	0
56	MG	RA	3487	1/1	0.93	0.15	48,48,48,48	0
56	MG	YA	3037	1/1	0.93	0.19	20,20,20,20	0
56	MG	QA	1665	1/1	0.93	0.05	42,42,42,42	0
56	MG	YA	3039	1/1	0.93	0.17	16,16,16,16	0
56	MG	RA	3362	1/1	0.93	0.10	37,37,37,37	0
56	MG	Y5	502	1/1	0.93	0.07	40,40,40,40	0
56	MG	XA	1603	1/1	0.93	0.14	16,16,16,16	0
56	MG	RA	3327	1/1	0.93	0.15	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QV	103	1/1	0.93	0.09	49,49,49,49	0
56	MG	QA	1637	1/1	0.93	0.17	55,55,55,55	0
56	MG	YA	3050	1/1	0.93	0.18	23,23,23,23	0
56	MG	RA	3330	1/1	0.93	0.12	54,54,54,54	0
58	ZN	R9	101	1/1	0.93	0.27	122,122,122,122	0
56	MG	RA	3498	1/1	0.93	0.08	29,29,29,29	0
56	MG	YA	3379	1/1	0.93	0.20	45,45,45,45	0
56	MG	YA	3055	1/1	0.93	0.10	26,26,26,26	0
56	MG	RA	3074	1/1	0.93	0.07	56,56,56,56	0
58	ZN	Y9	101	1/1	0.93	0.19	197,197,197,197	0
56	MG	RA	3160	1/1	0.94	0.10	45,45,45,45	0
56	MG	QA	1613	1/1	0.94	0.06	45,45,45,45	0
56	MG	RA	3028	1/1	0.94	0.06	20,20,20,20	0
56	MG	YA	3307	1/1	0.94	0.24	55,55,55,55	0
56	MG	QA	1622	1/1	0.94	0.13	51,51,51,51	0
56	MG	YA	3442	1/1	0.94	0.06	68,68,68,68	0
56	MG	YA	3192	1/1	0.94	0.08	56,56,56,56	0
56	MG	YA	3310	1/1	0.94	0.13	31,31,31,31	0
56	MG	YA	3517	1/1	0.94	0.11	53,53,53,53	0
56	MG	XA	1619	1/1	0.94	0.11	48,48,48,48	0
56	MG	RA	3239	1/1	0.94	0.24	50,50,50,50	0
56	MG	RA	3073	1/1	0.94	0.13	30,30,30,30	0
56	MG	RA	3449	1/1	0.94	0.07	59,59,59,59	0
56	MG	YA	3524	1/1	0.94	0.23	7,7,7,7	0
56	MG	YA	3197	1/1	0.94	0.05	119,119,119,119	0
56	MG	RA	3417	1/1	0.94	0.13	63,63,63,63	0
56	MG	YA	3258	1/1	0.94	0.13	30,30,30,30	0
56	MG	YA	3084	1/1	0.94	0.09	22,22,22,22	0
56	MG	YA	3529	1/1	0.94	0.10	46,46,46,46	0
56	MG	QA	1628	1/1	0.94	0.10	44,44,44,44	0
56	MG	RA	3044	1/1	0.94	0.22	18,18,18,18	0
56	MG	YA	3321	1/1	0.94	0.10	51,51,51,51	0
56	MG	RA	3243	1/1	0.94	0.21	54,54,54,54	0
56	MG	YA	3150	1/1	0.94	0.07	51,51,51,51	0
56	MG	QA	1629	1/1	0.94	0.05	60,60,60,60	0
56	MG	YA	3325	1/1	0.94	0.06	56,56,56,56	0
56	MG	YA	3540	1/1	0.94	0.11	29,29,29,29	0
56	MG	YA	3462	1/1	0.94	0.08	78,78,78,78	0
56	MG	YA	3092	1/1	0.94	0.21	21,21,21,21	0
56	MG	YB	202	1/1	0.94	0.07	50,50,50,50	0
56	MG	YB	203	1/1	0.94	0.07	75,75,75,75	0
56	MG	YA	3154	1/1	0.94	0.17	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3032	1/1	0.94	0.18	30,30,30,30	0
56	MG	YA	3466	1/1	0.94	0.08	36,36,36,36	0
56	MG	RA	3386	1/1	0.94	0.06	43,43,43,43	0
56	MG	RA	3492	1/1	0.94	0.10	21,21,21,21	0
56	MG	RA	3084	1/1	0.94	0.08	51,51,51,51	0
56	MG	RA	3106	1/1	0.94	0.19	31,31,31,31	0
56	MG	RA	3219	1/1	0.94	0.07	49,49,49,49	0
56	MG	RA	3048	1/1	0.94	0.07	24,24,24,24	0
56	MG	RA	3086	1/1	0.94	0.13	28,28,28,28	0
56	MG	YA	3337	1/1	0.94	0.07	45,45,45,45	0
56	MG	YA	3279	1/1	0.94	0.25	56,56,56,56	0
56	MG	RA	3462	1/1	0.94	0.07	40,40,40,40	0
56	MG	RA	3253	1/1	0.94	0.16	58,58,58,58	0
56	MG	YA	3282	1/1	0.94	0.24	33,33,33,33	0
56	MG	RA	3335	1/1	0.94	0.06	51,51,51,51	0
56	MG	YA	3049	1/1	0.94	0.18	21,21,21,21	0
56	MG	YA	3484	1/1	0.94	0.07	40,40,40,40	0
56	MG	YA	3285	1/1	0.94	0.14	30,30,30,30	0
56	MG	YA	3109	1/1	0.94	0.15	45,45,45,45	0
56	MG	RA	3503	1/1	0.94	0.06	56,56,56,56	0
56	MG	XV	104	1/1	0.94	0.05	65,65,65,65	0
56	MG	RA	3176	1/1	0.94	0.15	51,51,51,51	0
56	MG	RA	3399	1/1	0.94	0.07	60,60,60,60	0
56	MG	RA	3004	1/1	0.94	0.15	28,28,28,28	0
56	MG	RA	3110	1/1	0.94	0.10	42,42,42,42	0
56	MG	RA	3509	1/1	0.94	0.21	7,7,7,7	0
56	MG	RA	3034	1/1	0.94	0.20	23,23,23,23	0
56	MG	YA	3424	1/1	0.94	0.13	49,49,49,49	0
56	MG	XA	1651	1/1	0.94	0.07	52,52,52,52	0
56	MG	YA	3235	1/1	0.94	0.12	57,57,57,57	0
56	MG	RA	3228	1/1	0.94	0.17	32,32,32,32	0
56	MG	YA	3064	1/1	0.94	0.08	41,41,41,41	0
56	MG	RA	3112	1/1	0.94	0.08	28,28,28,28	0
56	MG	QA	1669	1/1	0.94	0.06	56,56,56,56	0
56	MG	XA	1656	1/1	0.94	0.07	45,45,45,45	0
56	MG	RA	3343	1/1	0.94	0.14	36,36,36,36	0
56	MG	QF	201	1/1	0.95	0.07	55,55,55,55	0
56	MG	RA	3075	1/1	0.95	0.09	39,39,39,39	0
56	MG	RA	3232	1/1	0.95	0.13	30,30,30,30	0
56	MG	RA	3185	1/1	0.95	0.09	60,60,60,60	0
56	MG	RA	3210	1/1	0.95	0.15	55,55,55,55	0
56	MG	RA	3236	1/1	0.95	0.22	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3248	1/1	0.95	0.13	20,20,20,20	0
56	MG	YA	3066	1/1	0.95	0.10	22,22,22,22	0
56	MG	YA	3521	1/1	0.95	0.15	13,13,13,13	0
56	MG	RA	3035	1/1	0.95	0.12	27,27,27,27	0
56	MG	RA	3238	1/1	0.95	0.10	57,57,57,57	0
56	MG	YA	3189	1/1	0.95	0.05	42,42,42,42	0
56	MG	RA	3094	1/1	0.95	0.21	21,21,21,21	0
56	MG	XA	1658	1/1	0.95	0.06	58,58,58,58	0
56	MG	YA	3071	1/1	0.95	0.11	92,92,92,92	0
56	MG	YA	3009	1/1	0.95	0.07	37,37,37,37	0
56	MG	RA	3268	1/1	0.95	0.16	48,48,48,48	0
56	MG	YA	3138	1/1	0.95	0.08	56,56,56,56	0
56	MG	RA	3037	1/1	0.95	0.07	9,9,9,9	0
56	MG	YA	3533	1/1	0.95	0.26	73,73,73,73	0
56	MG	QA	1639	1/1	0.95	0.05	46,46,46,46	0
56	MG	RA	3489	1/1	0.95	0.18	70,70,70,70	0
56	MG	RA	3171	1/1	0.95	0.12	39,39,39,39	0
56	MG	XA	1664	1/1	0.95	0.14	31,31,31,31	0
56	MG	YA	3145	1/1	0.95	0.07	32,32,32,32	0
56	MG	YA	3327	1/1	0.95	0.06	20,20,20,20	0
56	MG	XA	1625	1/1	0.95	0.06	55,55,55,55	0
56	MG	XA	1626	1/1	0.95	0.07	30,30,30,30	0
56	MG	YA	3024	1/1	0.95	0.16	14,14,14,14	0
56	MG	RA	3194	1/1	0.95	0.23	59,59,59,59	0
56	MG	YA	3273	1/1	0.95	0.14	28,28,28,28	0
56	MG	YA	3151	1/1	0.95	0.07	37,37,37,37	0
56	MG	RA	3358	1/1	0.95	0.06	38,38,38,38	0
56	MG	RA	3493	1/1	0.95	0.18	70,70,70,70	0
56	MG	QA	1651	1/1	0.95	0.08	45,45,45,45	0
56	MG	YA	3474	1/1	0.95	0.10	41,41,41,41	0
56	MG	XA	1673	1/1	0.95	0.05	36,36,36,36	0
56	MG	XA	1674	1/1	0.95	0.07	93,93,93,93	0
56	MG	RA	3099	1/1	0.95	0.10	30,30,30,30	0
56	MG	RA	3155	1/1	0.95	0.08	48,48,48,48	0
56	MG	RA	3019	1/1	0.95	0.09	29,29,29,29	0
56	MG	YA	3160	1/1	0.95	0.06	73,73,73,73	0
56	MG	RA	3333	1/1	0.95	0.17	37,37,37,37	0
56	MG	RA	3278	1/1	0.95	0.22	41,41,41,41	0
56	MG	RA	3157	1/1	0.95	0.08	26,26,26,26	0
56	MG	YA	3410	1/1	0.95	0.11	76,76,76,76	0
56	MG	YA	3411	1/1	0.95	0.07	57,57,57,57	0
56	MG	YA	3412	1/1	0.95	0.27	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1625	1/1	0.95	0.07	43,43,43,43	0
56	MG	YA	3289	1/1	0.95	0.08	50,50,50,50	0
56	MG	YA	3415	1/1	0.95	0.09	43,43,43,43	0
56	MG	YA	3349	1/1	0.95	0.16	54,54,54,54	0
56	MG	RA	3021	1/1	0.95	0.06	29,29,29,29	0
56	MG	QA	1630	1/1	0.95	0.07	42,42,42,42	0
56	MG	XA	1641	1/1	0.95	0.06	54,54,54,54	0
56	MG	RA	3311	1/1	0.95	0.14	63,63,63,63	0
56	MG	YA	3423	1/1	0.95	0.08	91,91,91,91	0
56	MG	YA	3107	1/1	0.95	0.10	55,55,55,55	0
56	MG	RA	3506	1/1	0.95	0.15	46,46,46,46	0
56	MG	QA	1614	1/1	0.95	0.06	63,63,63,63	0
56	MG	YA	3112	1/1	0.95	0.14	18,18,18,18	0
56	MG	YA	3233	1/1	0.95	0.14	64,64,64,64	0
56	MG	RA	3162	1/1	0.95	0.12	49,49,49,49	0
56	MG	YA	3052	1/1	0.95	0.11	30,30,30,30	0
56	MG	RA	3090	1/1	0.95	0.08	31,31,31,31	0
56	MG	RA	3475	1/1	0.95	0.14	44,44,44,44	0
56	MG	XV	107	1/1	0.95	0.07	23,23,23,23	0
56	MG	YA	3207	1/1	0.96	0.20	54,54,54,54	0
56	MG	RA	3146	1/1	0.96	0.19	40,40,40,40	0
56	MG	YA	3095	1/1	0.96	0.08	24,24,24,24	0
56	MG	YA	3518	1/1	0.96	0.15	32,32,32,32	0
56	MG	RA	3010	1/1	0.96	0.06	29,29,29,29	0
56	MG	RA	3129	1/1	0.96	0.10	46,46,46,46	0
56	MG	YA	3275	1/1	0.96	0.24	33,33,33,33	0
56	MG	RA	3011	1/1	0.96	0.08	42,42,42,42	0
56	MG	YA	3041	1/1	0.96	0.08	21,21,21,21	0
56	MG	XV	105	1/1	0.96	0.10	42,42,42,42	0
56	MG	RA	3115	1/1	0.96	0.07	45,45,45,45	0
56	MG	XA	1655	1/1	0.96	0.09	31,31,31,31	0
56	MG	XA	1621	1/1	0.96	0.09	48,48,48,48	0
56	MG	RA	3224	1/1	0.96	0.05	40,40,40,40	0
56	MG	RA	3269	1/1	0.96	0.17	65,65,65,65	0
56	MG	QA	1658	1/1	0.96	0.09	80,80,80,80	0
56	MG	RA	3369	1/1	0.96	0.13	40,40,40,40	0
56	MG	RA	3005	1/1	0.96	0.21	27,27,27,27	0
56	MG	RA	3497	1/1	0.96	0.26	21,21,21,21	0
56	MG	RA	3188	1/1	0.96	0.08	45,45,45,45	0
56	MG	QA	1645	1/1	0.96	0.09	51,51,51,51	0
56	MG	RA	3346	1/1	0.96	0.06	46,46,46,46	0
56	MG	RA	3250	1/1	0.96	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3011	1/1	0.96	0.06	25,25,25,25	0
56	MG	YA	3406	1/1	0.96	0.06	29,29,29,29	0
56	MG	YA	3473	1/1	0.96	0.09	65,65,65,65	0
56	MG	YA	3012	1/1	0.96	0.12	22,22,22,22	0
56	MG	YA	3119	1/1	0.96	0.19	44,44,44,44	0
56	MG	RA	3408	1/1	0.96	0.08	61,61,61,61	0
56	MG	YA	3065	1/1	0.96	0.22	21,21,21,21	0
56	MG	YA	3014	1/1	0.96	0.19	27,27,27,27	0
56	MG	YA	3354	1/1	0.96	0.23	43,43,43,43	0
56	MG	QA	1607	1/1	0.96	0.07	37,37,37,37	0
56	MG	YA	3125	1/1	0.96	0.18	23,23,23,23	0
56	MG	XA	1669	1/1	0.96	0.12	63,63,63,63	0
56	MG	RA	3017	1/1	0.96	0.13	20,20,20,20	0
56	MG	RA	3411	1/1	0.96	0.05	42,42,42,42	0
56	MG	RA	3254	1/1	0.96	0.18	27,27,27,27	0
56	MG	YE	301	1/1	0.96	0.10	37,37,37,37	0
56	MG	YA	3021	1/1	0.96	0.12	20,20,20,20	0
56	MG	RA	3193	1/1	0.96	0.07	54,54,54,54	0
56	MG	YA	3133	1/1	0.96	0.09	27,27,27,27	0
56	MG	YA	3490	1/1	0.96	0.10	52,52,52,52	0
56	MG	QA	1643	1/1	0.96	0.09	58,58,58,58	0
56	MG	RA	3446	1/1	0.96	0.38	55,55,55,55	0
56	MG	YA	3493	1/1	0.96	0.07	102,102,102,102	0
56	MG	YA	3191	1/1	0.96	0.09	93,93,93,93	0
56	MG	RA	3510	1/1	0.96	0.06	21,21,21,21	0
56	MG	YA	3496	1/1	0.96	0.12	59,59,59,59	0
56	MG	RA	3257	1/1	0.96	0.10	39,39,39,39	0
56	MG	YA	3430	1/1	0.96	0.07	65,65,65,65	0
56	MG	YA	3027	1/1	0.96	0.07	28,28,28,28	0
56	MG	YA	3080	1/1	0.96	0.18	21,21,21,21	0
56	MG	RA	3062	1/1	0.96	0.05	36,36,36,36	0
56	MG	RA	3078	1/1	0.96	0.12	42,42,42,42	0
56	MG	RA	3383	1/1	0.96	0.16	32,32,32,32	0
56	MG	YA	3144	1/1	0.96	0.18	41,41,41,41	0
56	MG	YA	3505	1/1	0.96	0.09	105,105,105,105	0
56	MG	YA	3200	1/1	0.96	0.08	55,55,55,55	0
56	MG	YA	3031	1/1	0.96	0.07	24,24,24,24	0
56	MG	YA	3441	1/1	0.96	0.05	77,77,77,77	0
56	MG	YA	3032	1/1	0.96	0.13	24,24,24,24	0
56	MG	QA	1612	1/1	0.96	0.04	34,34,34,34	0
56	MG	RA	3081	1/1	0.96	0.09	16,16,16,16	0
56	MG	RA	3095	1/1	0.96	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3310	1/1	0.96	0.07	38,38,38,38	0
56	MG	RA	3440	1/1	0.97	0.06	64,64,64,64	0
56	MG	YA	3267	1/1	0.97	0.12	23,23,23,23	0
56	MG	RA	3143	1/1	0.97	0.08	56,56,56,56	0
56	MG	YA	3078	1/1	0.97	0.06	41,41,41,41	0
56	MG	YA	3530	1/1	0.97	0.04	52,52,52,52	0
56	MG	RA	3055	1/1	0.97	0.05	46,46,46,46	0
56	MG	YA	3476	1/1	0.97	0.11	49,49,49,49	0
56	MG	YA	3127	1/1	0.97	0.15	38,38,38,38	0
56	MG	RA	3360	1/1	0.97	0.18	45,45,45,45	0
56	MG	RA	3036	1/1	0.97	0.06	24,24,24,24	0
56	MG	RA	3057	1/1	0.97	0.12	14,14,14,14	0
56	MG	RA	3226	1/1	0.97	0.12	10,10,10,10	0
56	MG	YA	3223	1/1	0.97	0.09	43,43,43,43	0
56	MG	RA	3166	1/1	0.97	0.04	39,39,39,39	0
56	MG	QA	1660	1/1	0.97	0.04	80,80,80,80	0
56	MG	QA	1619	1/1	0.97	0.07	53,53,53,53	0
56	MG	YA	3088	1/1	0.97	0.06	38,38,38,38	0
56	MG	YA	3433	1/1	0.97	0.15	50,50,50,50	0
56	MG	YA	3434	1/1	0.97	0.04	64,64,64,64	0
56	MG	YA	3136	1/1	0.97	0.07	53,53,53,53	0
56	MG	QA	1634	1/1	0.97	0.09	57,57,57,57	0
56	MG	YA	3048	1/1	0.97	0.05	19,19,19,19	0
56	MG	RA	3103	1/1	0.97	0.05	45,45,45,45	0
56	MG	XA	1638	1/1	0.97	0.03	69,69,69,69	0
56	MG	RA	3190	1/1	0.97	0.03	47,47,47,47	0
56	MG	RA	3397	1/1	0.97	0.07	57,57,57,57	0
56	MG	YA	3053	1/1	0.97	0.14	9,9,9,9	0
56	MG	YA	3015	1/1	0.97	0.08	18,18,18,18	0
56	MG	RA	3152	1/1	0.97	0.21	38,38,38,38	0
56	MG	RA	3301	1/1	0.97	0.18	49,49,49,49	0
56	MG	YA	3147	1/1	0.97	0.04	51,51,51,51	0
56	MG	YA	3057	1/1	0.97	0.13	20,20,20,20	0
56	MG	RA	3234	1/1	0.97	0.11	32,32,32,32	0
56	MG	XA	1609	1/1	0.97	0.09	82,82,82,82	0
56	MG	RA	3104	1/1	0.97	0.11	62,62,62,62	0
56	MG	RA	3025	1/1	0.97	0.08	22,22,22,22	0
56	MG	RA	3403	1/1	0.97	0.09	41,41,41,41	0
56	MG	YA	3108	1/1	0.97	0.05	27,27,27,27	0
56	MG	YA	3454	1/1	0.97	0.13	49,49,49,49	0
56	MG	YX	101	1/1	0.97	0.15	118,118,118,118	0
56	MG	YA	3250	1/1	0.97	0.17	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3431	1/1	0.97	0.04	38,38,38,38	0
56	MG	YA	3457	1/1	0.97	0.06	104,104,104,104	0
56	MG	YA	3252	1/1	0.97	0.24	22,22,22,22	0
56	MG	XA	1616	1/1	0.97	0.05	35,35,35,35	0
56	MG	RA	3404	1/1	0.97	0.06	50,50,50,50	0
56	MG	YA	3515	1/1	0.97	0.07	48,48,48,48	0
57	SF4	QD	301	8/8	0.97	0.08	78,114,135,135	0
56	MG	RA	3136	1/1	0.97	0.09	54,54,54,54	0
56	MG	RA	3077	1/1	0.97	0.09	23,23,23,23	0
56	MG	RA	3464	1/1	0.97	0.09	72,72,72,72	0
56	MG	RA	3015	1/1	0.97	0.06	20,20,20,20	0
56	MG	XV	103	1/1	0.97	0.08	51,51,51,51	0
56	MG	YA	3209	1/1	0.97	0.06	48,48,48,48	0
56	MG	RA	3027	1/1	0.97	0.12	20,20,20,20	0
56	MG	RA	3043	1/1	0.97	0.09	15,15,15,15	0
56	MG	QA	1656	1/1	0.97	0.05	46,46,46,46	0
56	MG	RA	3142	1/1	0.97	0.14	38,38,38,38	0
56	MG	RA	3206	1/1	0.98	0.04	39,39,39,39	0
56	MG	YA	3096	1/1	0.98	0.03	39,39,39,39	0
56	MG	YA	3416	1/1	0.98	0.05	70,70,70,70	0
56	MG	YA	3417	1/1	0.98	0.06	63,63,63,63	0
56	MG	RA	3102	1/1	0.98	0.09	18,18,18,18	0
56	MG	XA	1610	1/1	0.98	0.07	40,40,40,40	0
56	MG	RA	3063	1/1	0.98	0.07	25,25,25,25	0
56	MG	YA	3234	1/1	0.98	0.07	63,63,63,63	0
56	MG	YA	3265	1/1	0.98	0.09	26,26,26,26	0
56	MG	RA	3114	1/1	0.98	0.06	42,42,42,42	0
56	MG	YA	3181	1/1	0.98	0.07	24,24,24,24	0
56	MG	YA	3010	1/1	0.98	0.09	24,24,24,24	0
56	MG	XA	1613	1/1	0.98	0.06	40,40,40,40	0
56	MG	RA	3069	1/1	0.98	0.06	28,28,28,28	0
56	MG	RA	3064	1/1	0.98	0.09	24,24,24,24	0
56	MG	RA	3151	1/1	0.98	0.06	31,31,31,31	0
56	MG	QA	1666	1/1	0.98	0.05	48,48,48,48	0
56	MG	XA	1672	1/1	0.98	0.04	44,44,44,44	0
56	MG	RA	3079	1/1	0.98	0.07	24,24,24,24	0
56	MG	YA	3245	1/1	0.98	0.24	8,8,8,8	0
56	MG	YA	3083	1/1	0.98	0.07	29,29,29,29	0
56	MG	XA	1601	1/1	0.98	0.18	28,28,28,28	0
56	MG	YA	3339	1/1	0.98	0.12	20,20,20,20	0
56	MG	XA	1602	1/1	0.98	0.04	56,56,56,56	0
57	SF4	XD	301	8/8	0.98	0.09	64,81,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3072	1/1	0.98	0.09	23,23,23,23	0
56	MG	QV	102	1/1	0.98	0.07	63,63,63,63	0
56	MG	YA	3405	1/1	0.98	0.08	27,27,27,27	0
56	MG	YA	3042	1/1	0.98	0.09	38,38,38,38	0
56	MG	RA	3388	1/1	0.98	0.06	26,26,26,26	0
56	MG	YA	3091	1/1	0.98	0.06	34,34,34,34	0
56	MG	YA	3044	1/1	0.98	0.15	28,28,28,28	0
56	MG	QH	201	1/1	0.98	0.16	64,64,64,64	0
56	MG	YA	3120	1/1	0.98	0.06	35,35,35,35	0
56	MG	RA	3083	1/1	0.98	0.12	42,42,42,42	0
56	MG	RA	3123	1/1	0.99	0.04	25,25,25,25	0
56	MG	QA	1640	1/1	0.99	0.05	33,33,33,33	0
56	MG	YA	3246	1/1	0.99	0.07	24,24,24,24	0
56	MG	YA	3090	1/1	0.99	0.03	40,40,40,40	0
58	ZN	QN	101	1/1	0.99	0.05	104,104,104,104	0
56	MG	RA	3477	1/1	0.99	0.13	74,74,74,74	0
56	MG	YA	3110	1/1	0.99	0.04	30,30,30,30	0
56	MG	YA	3536	1/1	0.99	0.09	52,52,52,52	0
56	MG	RA	3387	1/1	0.99	0.04	38,38,38,38	0
56	MG	YA	3162	1/1	0.99	0.04	32,32,32,32	0
58	ZN	XN	101	1/1	0.99	0.04	111,111,111,111	0
56	MG	YA	3408	1/1	0.99	0.05	27,27,27,27	0
56	MG	YA	3060	1/1	0.99	0.04	22,22,22,22	0
56	MG	RA	3046	1/1	0.99	0.05	13,13,13,13	0
56	MG	RA	3252	1/1	0.99	0.19	19,19,19,19	0
56	MG	RA	3390	1/1	0.99	0.04	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.