



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 08:06 AM UTC

PDB ID : 4YPB / pdb_00004ypb
Title : Precleavage 70S structure of the P. vulgaris HigB DeltaH92 toxin bound to the AAA codon
Authors : Schureck, M.A.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2015-03-12
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

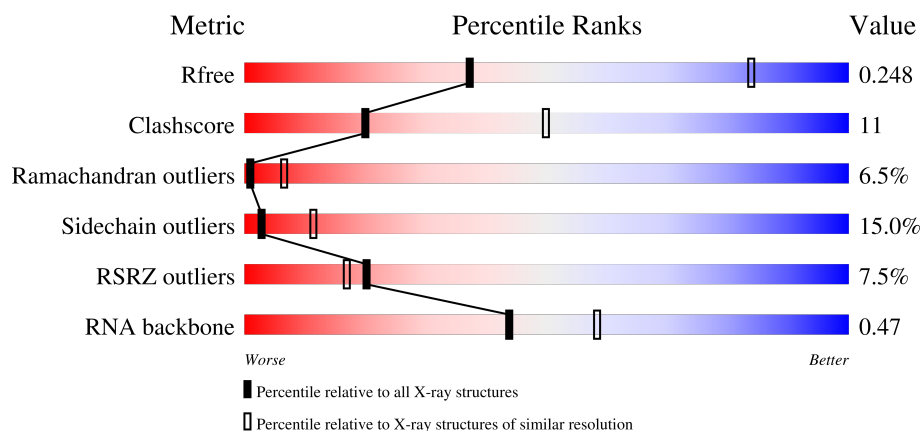
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	10% 55% 34% 10%
1	XA	1522	55% 35% 9%
2	QB	256	10% 52% 31% 9% 8%
2	XB	256	9% 49% 35% 8% 8%

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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	117	
24	XY	117	
25	RA	2916	
25	YA	2916	
26	RB	124	
26	YB	124	

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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	QA	1627	-	-	-	X
56	MG	QA	1663	-	-	-	X
56	MG	RA	3005	-	-	-	X
56	MG	YA	3280	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 297549 atoms, of which 18 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	1511	Total	C	N	O	P	0	0	0
			32472	14453	6011	10497	1511			
1	XA	1508	Total	C	N	O	P	0	0	0
			32409	14425	6001	10475	1508			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	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	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
3	XC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	154	Total	C	N	O	S	0	0	0
			1178	743	221	210	4			
5	XE	154	Total	C	N	O	S	0	0	0
			1178	743	221	210	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	128	Total	C	N	O	S	0	0	0
			1018	644	198	175	1			
9	XI	128	Total	C	N	O	S	0	0	0
			1018	644	198	175	1			

- 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			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	121	Total	C	N	O	S	0	0	0
			901	560	171	167	3			
11	XK	121	Total	C	N	O	S	0	0	0
			901	560	171	167	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			
13	XM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	71	Total	C	N	O	0	0	0
			585	373	116	96			
18	XR	71	Total	C	N	O	0	0	0
			585	373	116	96			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	82	Total	C	N	O	S	0	0	0
			656	419	121	114	2			
19	XS	82	Total	C	N	O	S	0	0	0
			656	419	121	114	2			

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

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

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

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

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
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
			1640	732	297	535	76			
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	20	Total	C	H	N	O	P	0	0	0
			449	199	9	89	132	20			
23	XX	20	Total	C	H	N	O	P	0	0	0
			449	199	9	89	132	20			

- Molecule 24 is a protein called Host inhibition of growth B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	QY	91	Total	C	N	O	0	0	0
			746	478	131	137			
24	XY	91	Total	C	N	O	0	0	0
			746	478	131	137			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QY	0	MET	-	initiating methionine	UNP Q7A225
QY	1	GLY	-	expression tag	UNP Q7A225
QY	92	LYS	-	expression tag	UNP Q7A225
QY	93	LEU	-	expression tag	UNP Q7A225
QY	94	GLY	-	expression tag	UNP Q7A225
QY	95	PRO	-	expression tag	UNP Q7A225
QY	96	GLU	-	expression tag	UNP Q7A225

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Chain	Residue	Modelled	Actual	Comment	Reference
QY	97	GLN	-	expression tag	UNP Q7A225
QY	98	LYS	-	expression tag	UNP Q7A225
QY	99	LEU	-	expression tag	UNP Q7A225
QY	100	ILE	-	expression tag	UNP Q7A225
QY	101	SER	-	expression tag	UNP Q7A225
QY	102	GLU	-	expression tag	UNP Q7A225
QY	103	GLU	-	expression tag	UNP Q7A225
QY	104	ASP	-	expression tag	UNP Q7A225
QY	105	LEU	-	expression tag	UNP Q7A225
QY	106	ASN	-	expression tag	UNP Q7A225
QY	107	SER	-	expression tag	UNP Q7A225
QY	108	ALA	-	expression tag	UNP Q7A225
QY	109	VAL	-	expression tag	UNP Q7A225
QY	110	ASP	-	expression tag	UNP Q7A225
QY	111	HIS	-	expression tag	UNP Q7A225
QY	112	HIS	-	expression tag	UNP Q7A225
QY	113	HIS	-	expression tag	UNP Q7A225
QY	114	HIS	-	expression tag	UNP Q7A225
QY	115	HIS	-	expression tag	UNP Q7A225
QY	116	HIS	-	expression tag	UNP Q7A225
XY	0	MET	-	initiating methionine	UNP Q7A225
XY	1	GLY	-	expression tag	UNP Q7A225
XY	92	LYS	-	expression tag	UNP Q7A225
XY	93	LEU	-	expression tag	UNP Q7A225
XY	94	GLY	-	expression tag	UNP Q7A225
XY	95	PRO	-	expression tag	UNP Q7A225
XY	96	GLU	-	expression tag	UNP Q7A225
XY	97	GLN	-	expression tag	UNP Q7A225
XY	98	LYS	-	expression tag	UNP Q7A225
XY	99	LEU	-	expression tag	UNP Q7A225
XY	100	ILE	-	expression tag	UNP Q7A225
XY	101	SER	-	expression tag	UNP Q7A225
XY	102	GLU	-	expression tag	UNP Q7A225
XY	103	GLU	-	expression tag	UNP Q7A225
XY	104	ASP	-	expression tag	UNP Q7A225
XY	105	LEU	-	expression tag	UNP Q7A225
XY	106	ASN	-	expression tag	UNP Q7A225
XY	107	SER	-	expression tag	UNP Q7A225
XY	108	ALA	-	expression tag	UNP Q7A225
XY	109	VAL	-	expression tag	UNP Q7A225
XY	110	ASP	-	expression tag	UNP Q7A225
XY	111	HIS	-	expression tag	UNP Q7A225

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Chain	Residue	Modelled	Actual	Comment	Reference
XY	112	HIS	-	expression tag	UNP Q7A225
XY	113	HIS	-	expression tag	UNP Q7A225
XY	114	HIS	-	expression tag	UNP Q7A225
XY	115	HIS	-	expression tag	UNP Q7A225
XY	116	HIS	-	expression tag	UNP Q7A225

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2891	Total	C	N	O	P	0	0	0
			62269	27713	11649	20016	2891			
25	YA	2875	Total	C	N	O	P	0	0	0
			61924	27560	11583	19906	2875			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	YB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	RF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			
29	YF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
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	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
31	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	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			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			
36	YQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	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	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	252	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	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			
46	Y0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	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	97	Total	C	N	O	S	0	0	0
			763	481	150	131	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	70	Total	C	N	O	S	0	0	0
			573	359	107	103	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	Y4	70	Total	C	N	O	S	0	0	0
			573	359	107	103	4			

- 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	57	Total	C	N	O	S	0	0	0
			442	278	88	71	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	48	Total	C	N	O	S	0	0	0
			417	259	86	68	4			
52	Y6	48	Total	C	N	O	S	0	0	0
			417	259	86	68	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	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	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	150	Total 150	Mg 150	0	0
56	QD	2	Total 2	Mg 2	0	0
56	QL	1	Total 1	Mg 1	0	0
56	QV	4	Total 4	Mg 4	0	0
56	QX	1	Total 1	Mg 1	0	0
56	RA	441	Total 441	Mg 441	0	0
56	RB	4	Total 4	Mg 4	0	0
56	RD	2	Total 2	Mg 2	0	0
56	RE	1	Total 1	Mg 1	0	0
56	RF	1	Total 1	Mg 1	0	0
56	RP	3	Total 3	Mg 3	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RT	1	Total 1	Mg 1	0	0
56	RV	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	R1	1	Total 1	Mg 1	0	0
56	R2	1	Total 1	Mg 1	0	0
56	R5	3	Total 3	Mg 3	0	0
56	XA	163	Total 163	Mg 163	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XD	1	Total 1	Mg 1	0	0
56	XF	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	XS	1	Total 1	Mg 1	0	0
56	XV	3	Total 3	Mg 3	0	0
56	YA	487	Total 487	Mg 487	0	0
56	YB	6	Total 6	Mg 6	0	0
56	YD	1	Total 1	Mg 1	0	0
56	YE	1	Total 1	Mg 1	0	0
56	YF	1	Total 1	Mg 1	0	0
56	YG	1	Total 1	Mg 1	0	0
56	YH	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	1	Total 1	Mg 1	0	0
56	YQ	2	Total 2	Mg 2	0	0
56	YV	1	Total 1	Mg 1	0	0
56	YW	1	Total 1	Mg 1	0	0
56	YY	1	Total 1	Mg 1	0	0
56	Y0	3	Total 3	Mg 3	0	0
56	Y1	1	Total 1	Mg 1	0	0

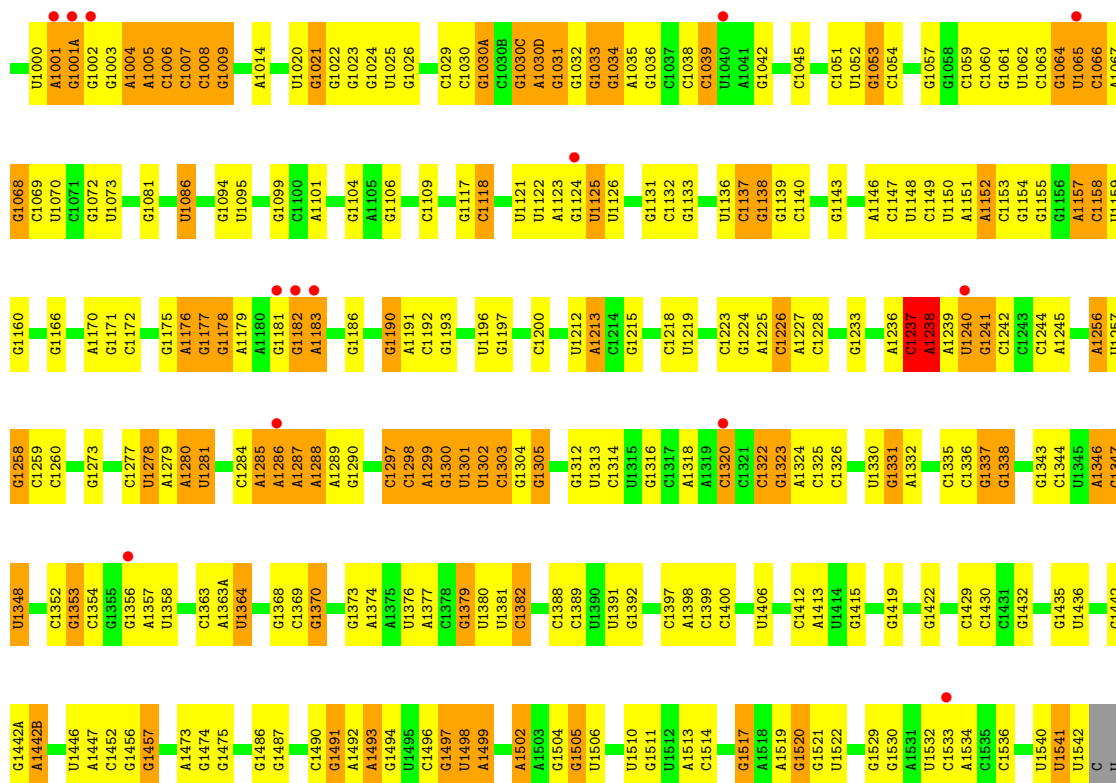
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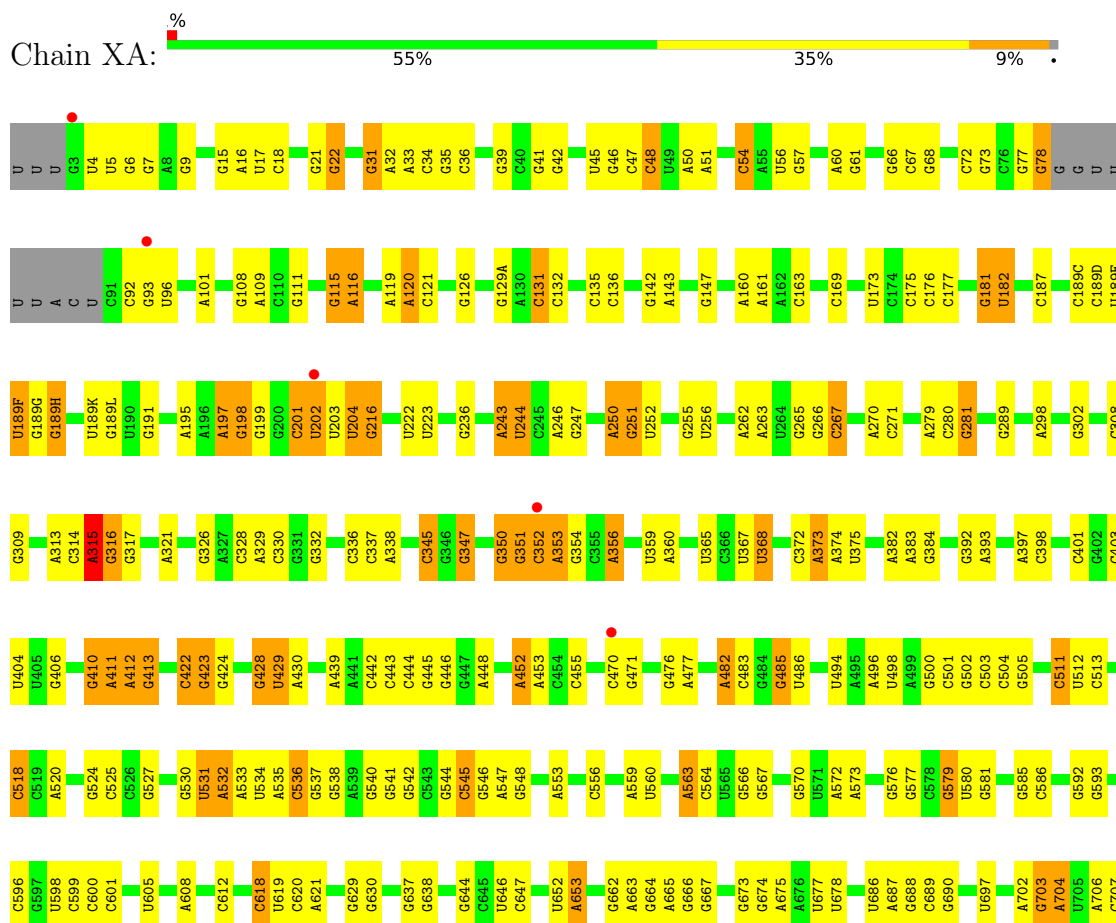
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	Y5	3	Total 3	Mg 3	0	0
56	Y7	1	Total 1	Mg 1	0	0

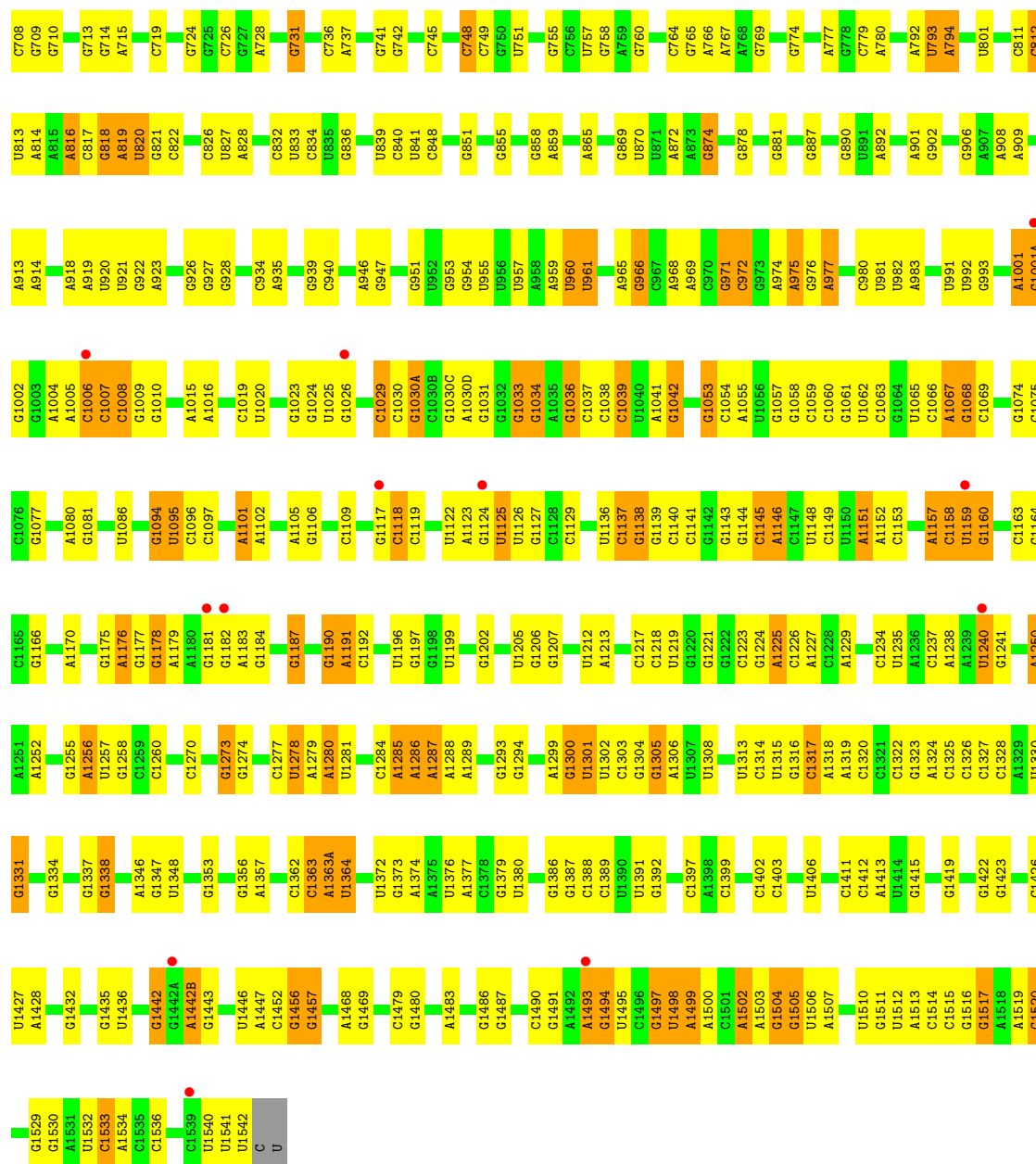
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QD	1	Total 1	Zn 1	0	0
57	QN	1	Total 1	Zn 1	0	0
57	XD	1	Total 1	Zn 1	0	0
57	XN	1	Total 1	Zn 1	0	0

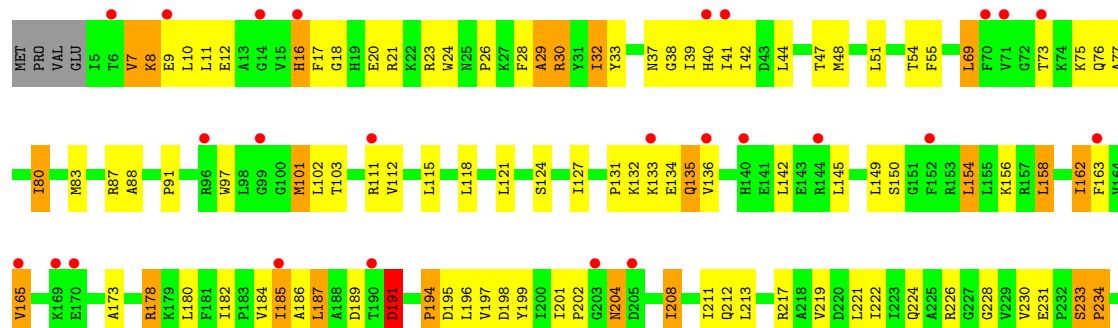


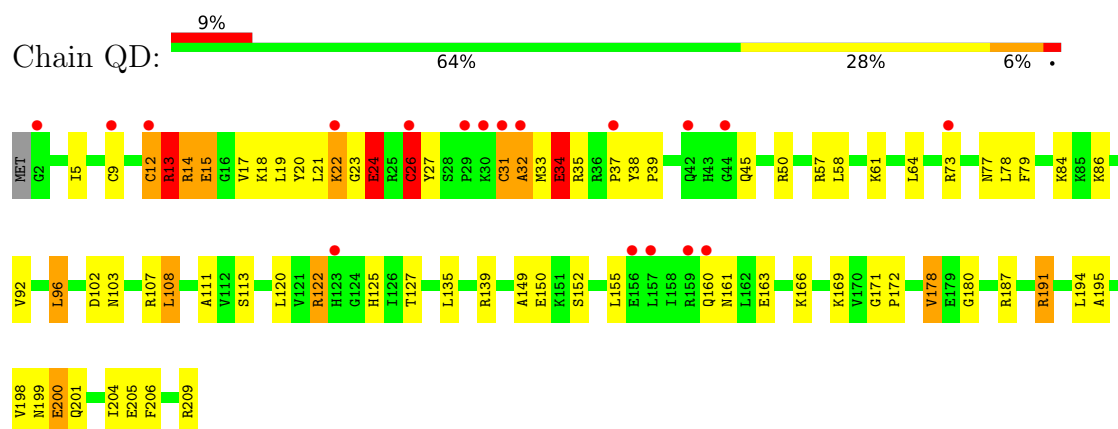
• Molecule 1: 16S rRNA



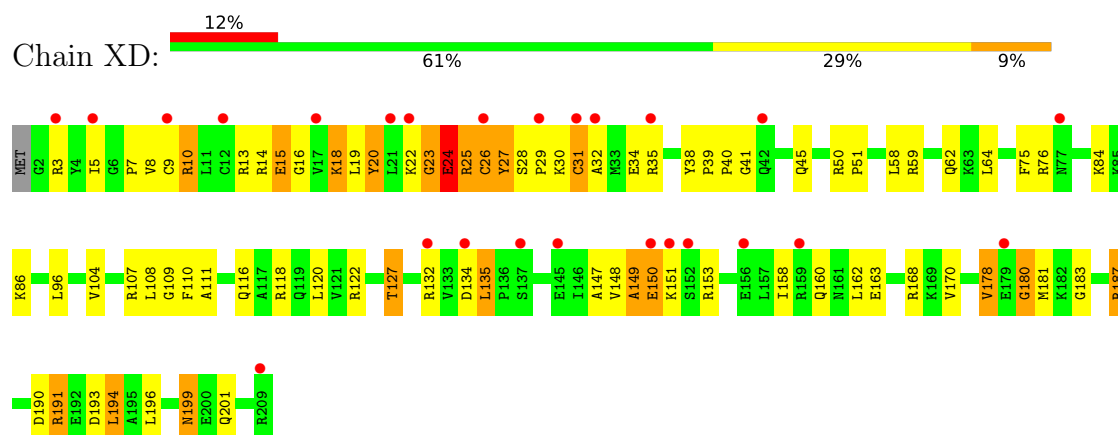


• Molecule 2: 30S ribosomal protein S2

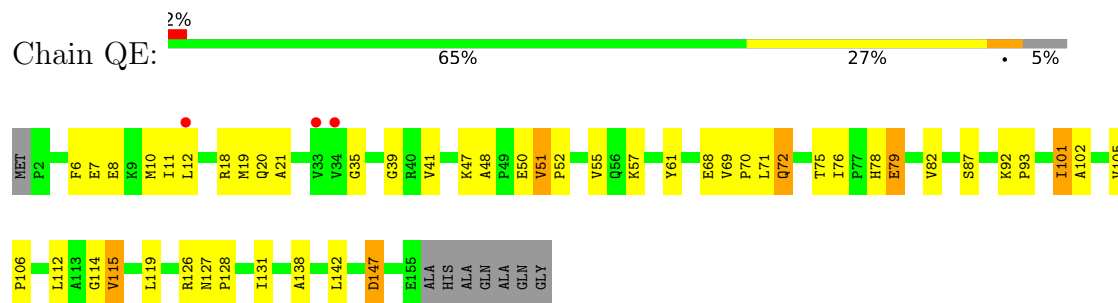




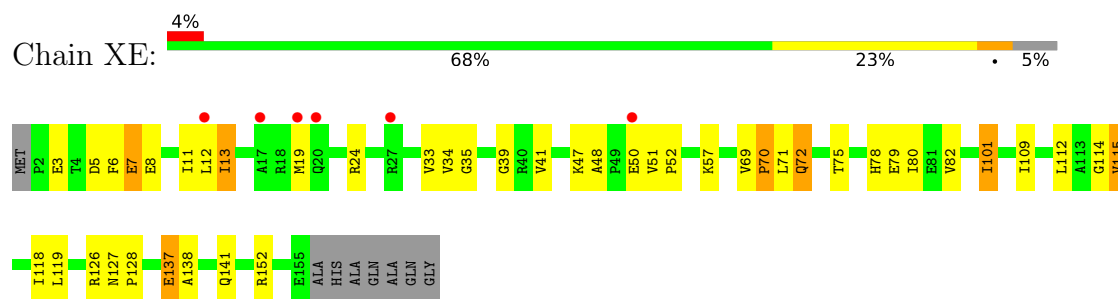
• Molecule 4: 30S ribosomal protein S4



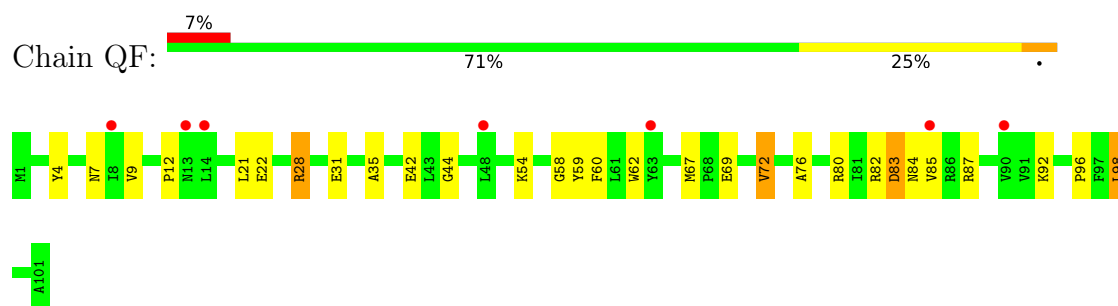
• Molecule 5: 30S ribosomal protein S5



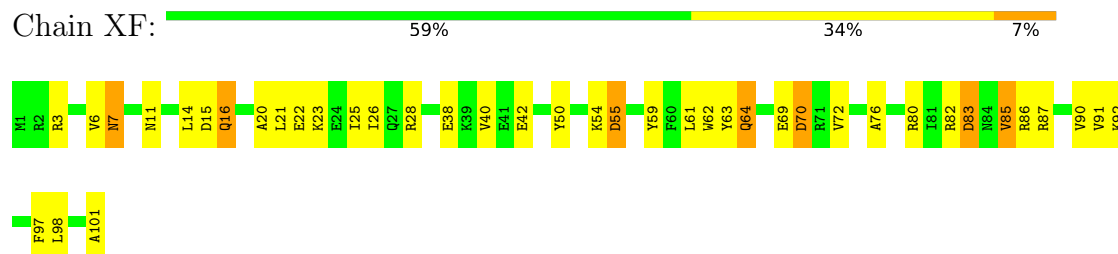
• Molecule 5: 30S ribosomal protein S5



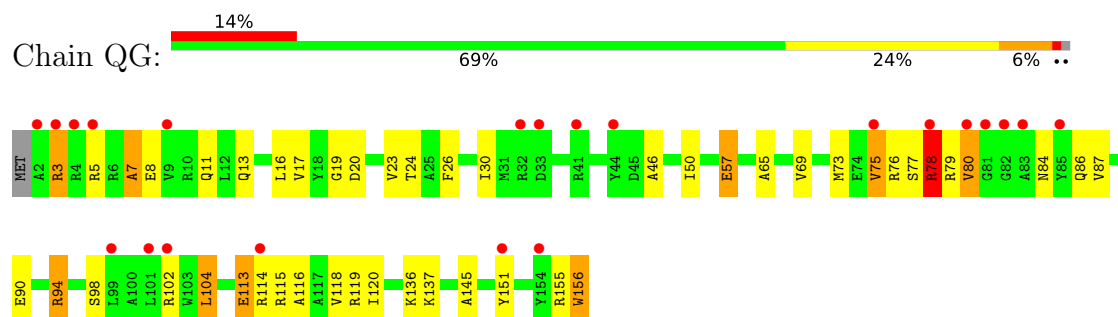
• Molecule 6: 30S ribosomal protein S6



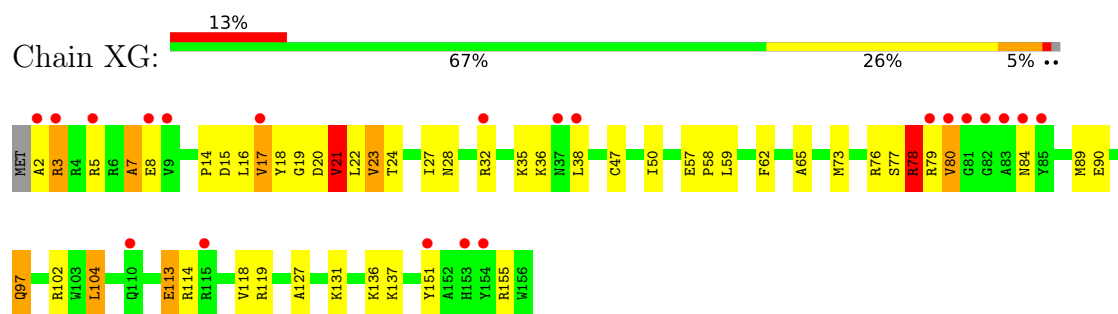
- Molecule 6: 30S ribosomal protein S6



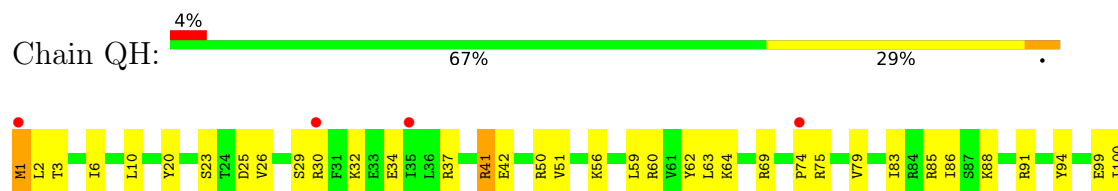
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7

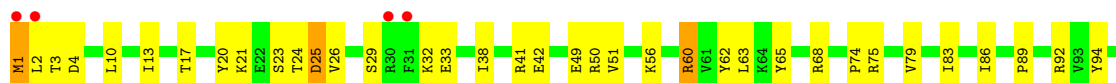


- Molecule 8: 30S ribosomal protein S8

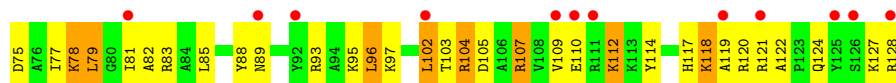
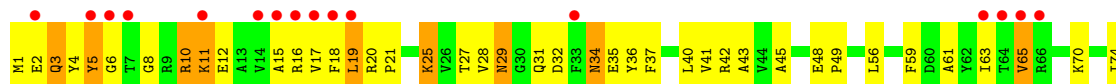
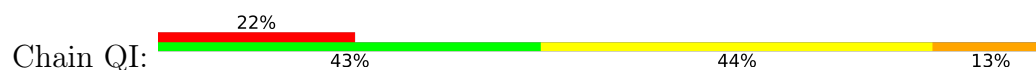




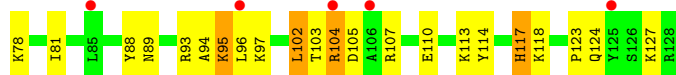
• Molecule 8: 30S ribosomal protein S8



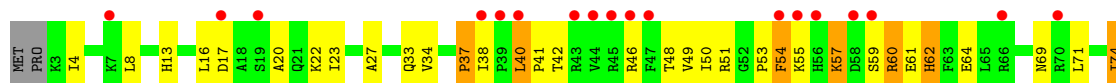
• Molecule 9: 30S ribosomal protein S9



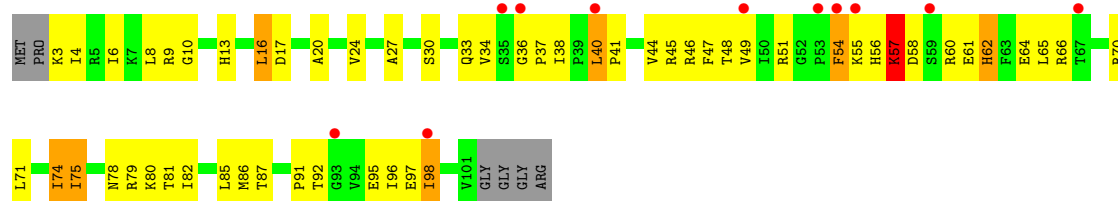
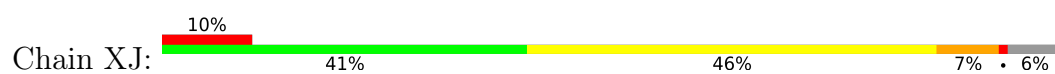
• Molecule 9: 30S ribosomal protein S9



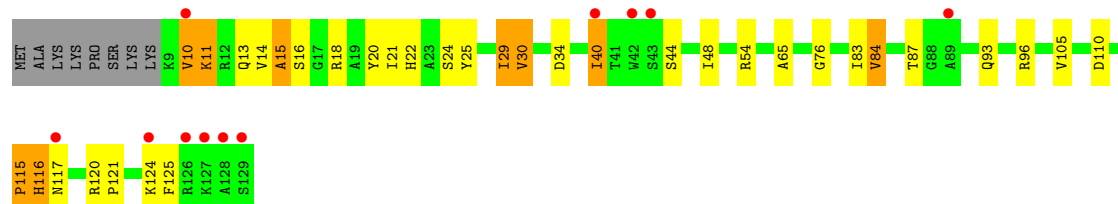
• Molecule 10: 30S ribosomal protein S10



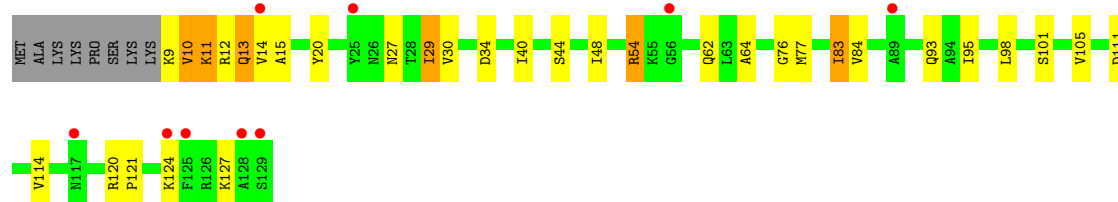
• Molecule 10: 30S ribosomal protein S10



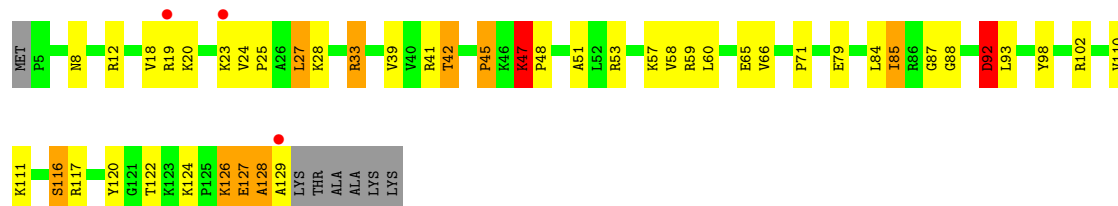
- Molecule 11: 30S ribosomal protein S11



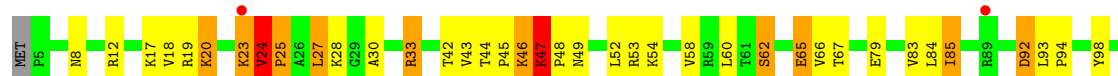
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

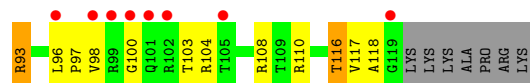
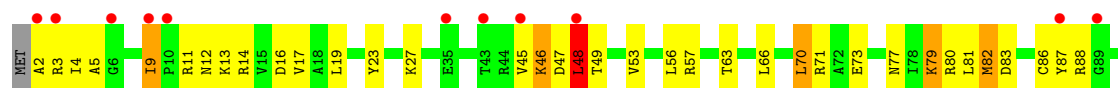


- Molecule 12: 30S ribosomal protein S12

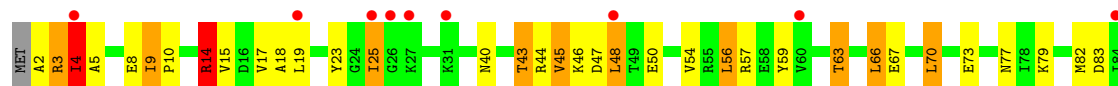




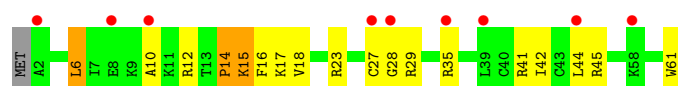
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



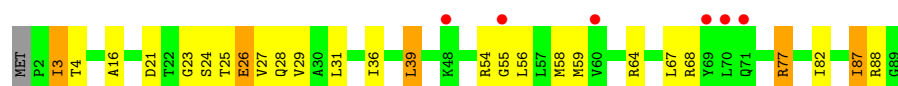
- Molecule 14: 30S ribosomal protein S14



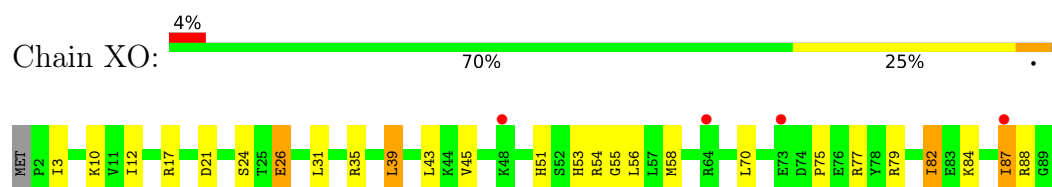
- Molecule 14: 30S ribosomal protein S14



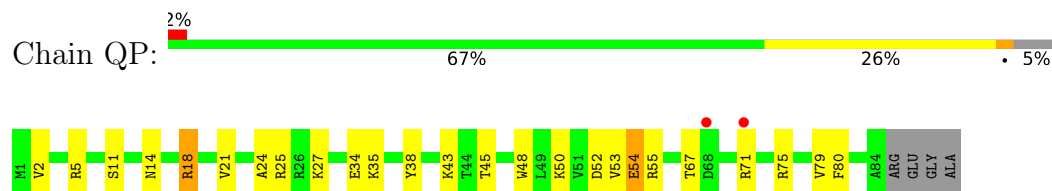
- Molecule 15: 30S ribosomal protein S15



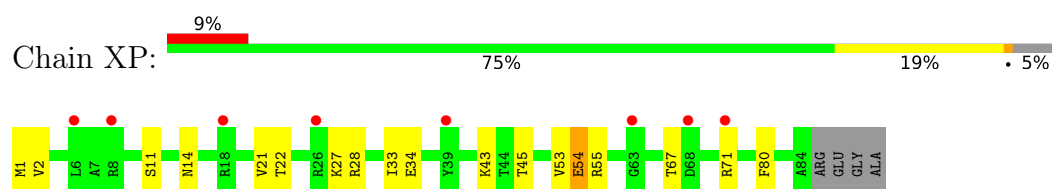
- Molecule 15: 30S ribosomal protein S15



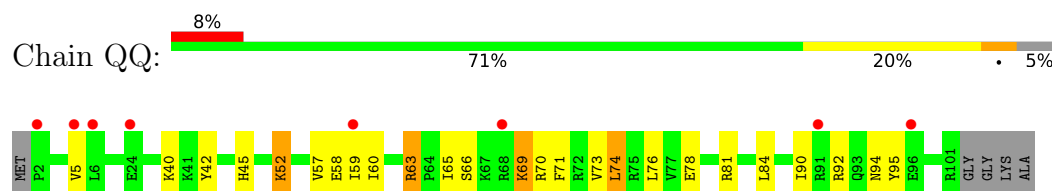
- Molecule 16: 30S ribosomal protein S16



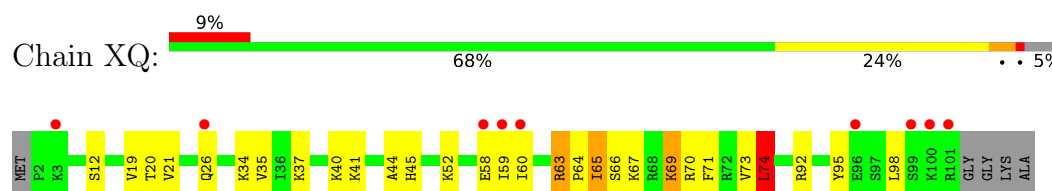
- Molecule 16: 30S ribosomal protein S16



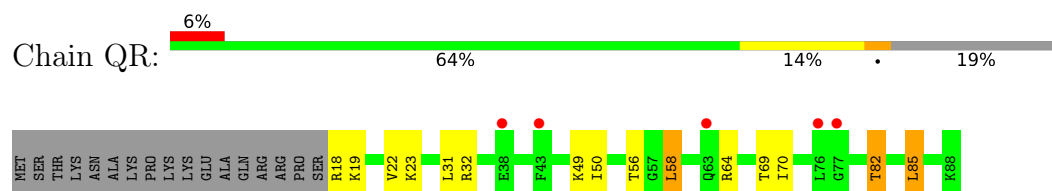
- Molecule 17: 30S ribosomal protein S17



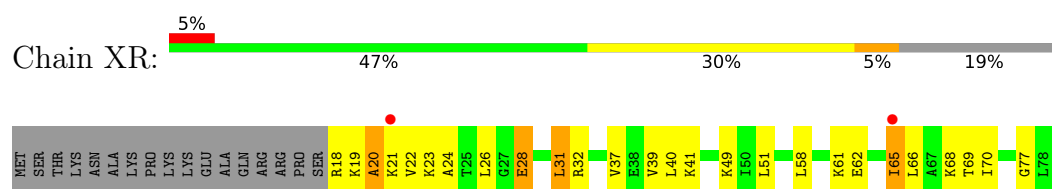
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

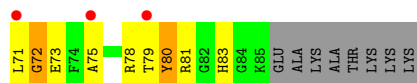
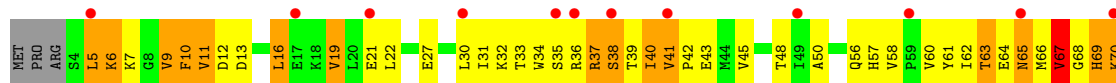


- Molecule 18: 30S ribosomal protein S18

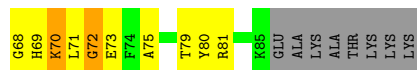
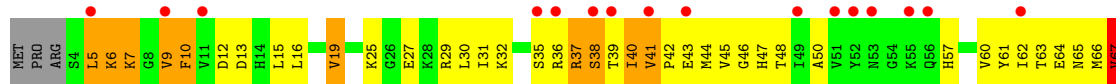




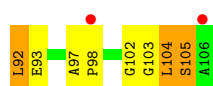
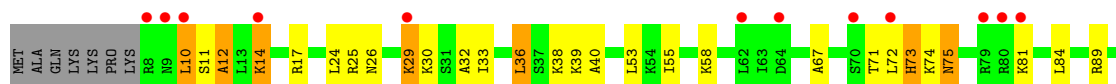
• Molecule 19: 30S ribosomal protein S19



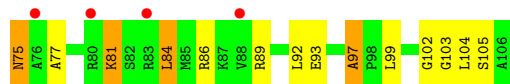
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20

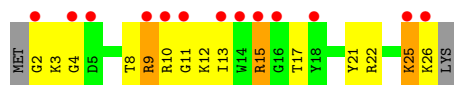


• Molecule 21: 30S ribosomal protein Thx





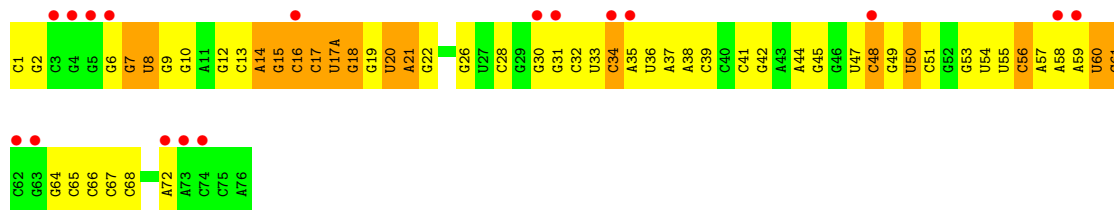
- Molecule 21: 30S ribosomal protein Thx



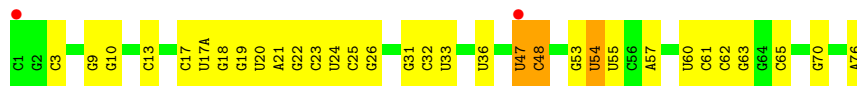
- Molecule 22: tRNA fMet



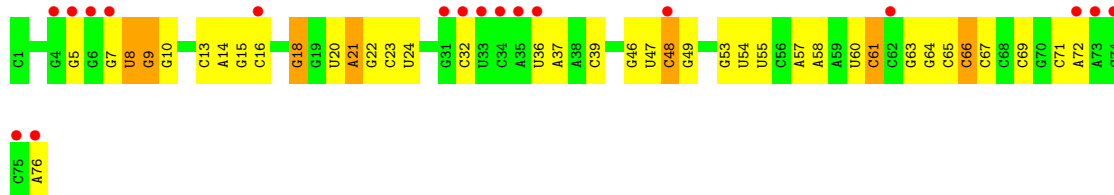
- Molecule 22: tRNA fMet



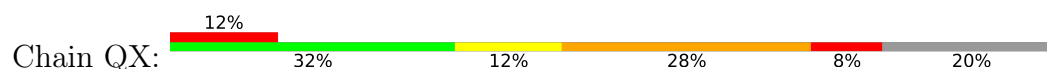
- Molecule 22: tRNA fMet

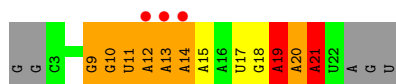


- Molecule 22: tRNA fMet

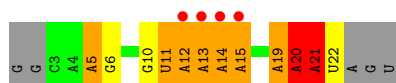
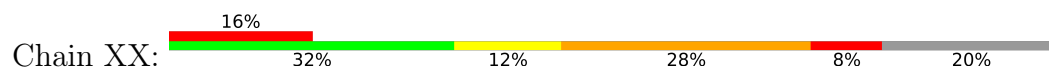


- Molecule 23: messenger RNA

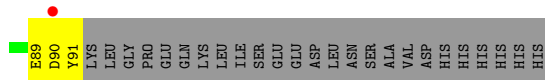




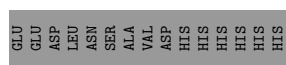
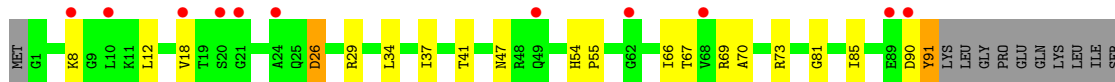
• Molecule 23: messenger RNA



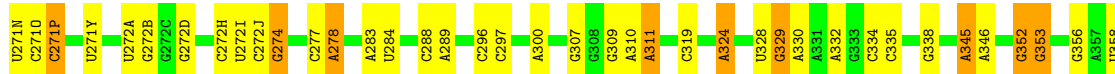
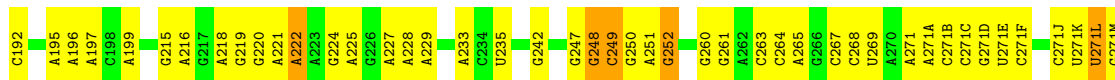
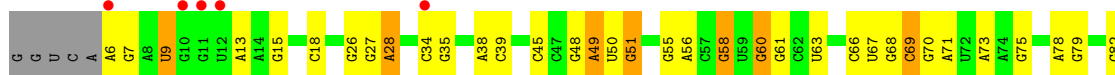
• Molecule 24: Host inhibition of growth B



• Molecule 24: Host inhibition of growth B



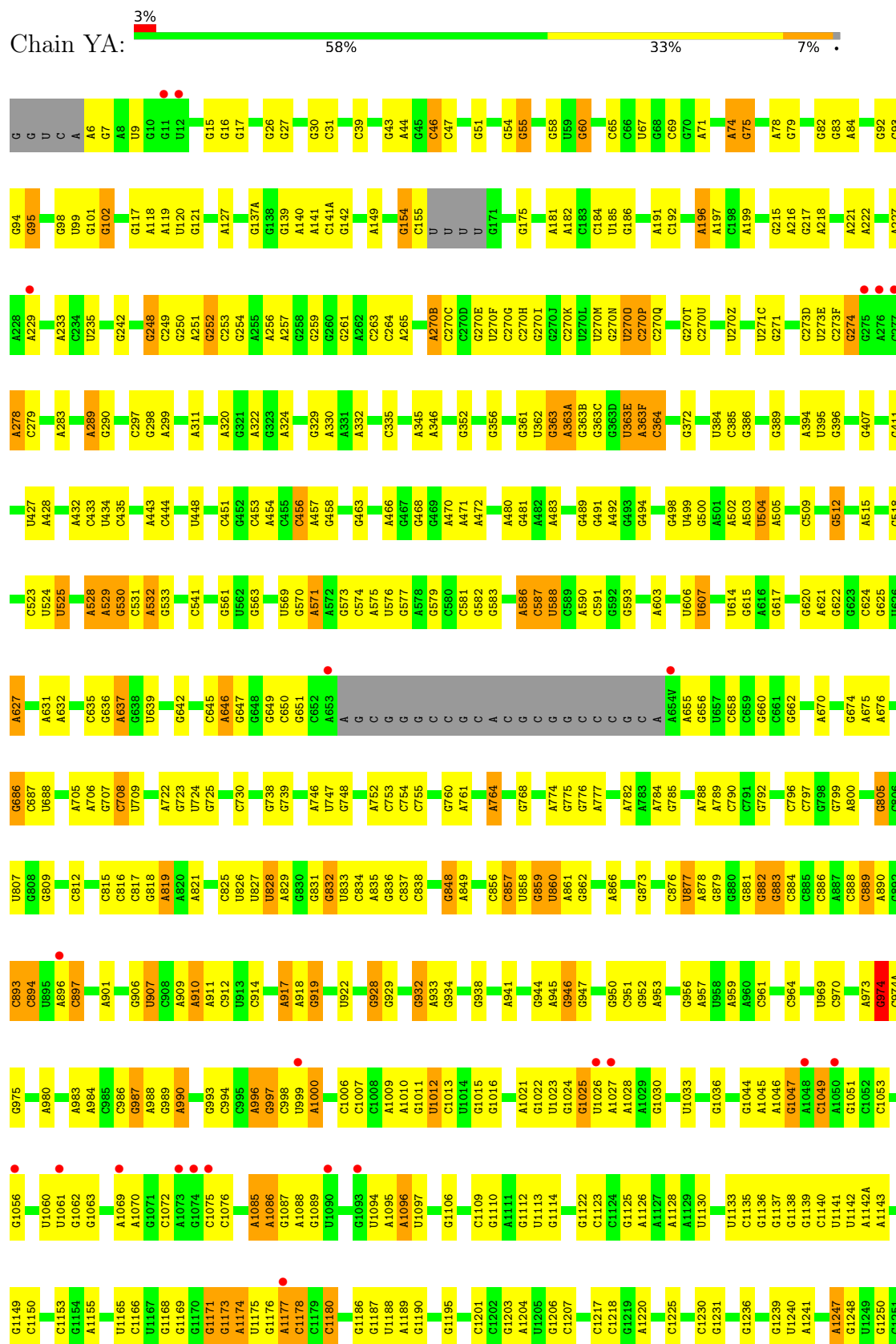
• Molecule 25: 23S rRNA



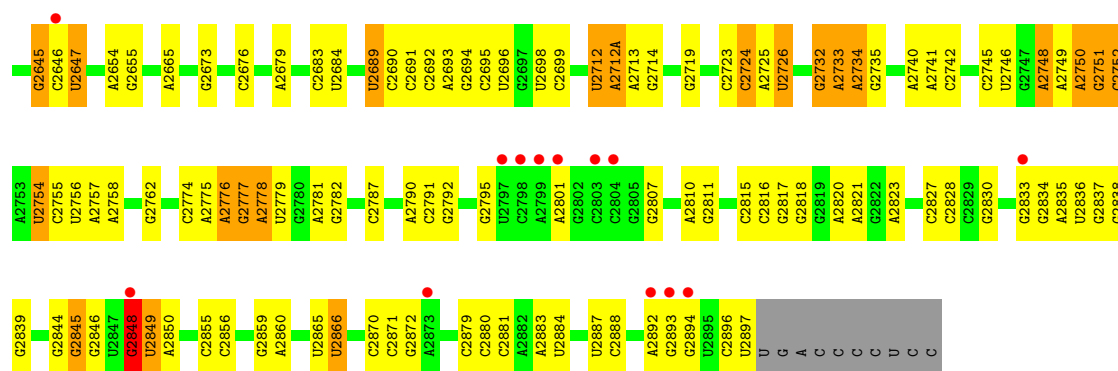
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A1566	A1567	G1466	C1376	G1285	U1188	G1093	C1013	G927	G849	G744	G651	C574	A470	U362
A1568	A1569	C1467	A1379	A1286	G1190	A1095	G1017	U930	G854	G748	A654	U576	G473	A363A
A1570	C1386	A1379	G1195	C1289	G1195	A1096	C1018	G931	C855	C749	G654A	C580	G481	U363E
A1571	A1301	U1199	U1198	U1300	U1198	A1098	U1019	G932	C856	A750	G654B	C581	C484	A363F
A1572	A1302	A1204	A1204	A1302	U1199	G1099	A1021	G934	C857	A752	G654D	C582	C486	C364
U1576	U1396	U1396	A1220	C1306	A1220	G1110	U1023	A941	C859	C753	C654F	C583	G370	G370
C1577	U1397	C1221	C1221	A1307	C1221	G1111	G1025	U943	C860	C755	G	A586	G372	A371
U1578	G1482	C1221A	G1222	A1308	C1221A	A1111	A1026	G944	C862	C756	A	C587	U373	G372
G1484	C1403	C1222	G1222	G1309	G1222	U1112	A1027	A945	C863	A764	C	U588	G493	A374
G1485	C1404	G1310	G1223	U1113	G1223	U1113	A1028	G946	C864	A764	G	C589	G494	A374
U1581	U1405	G1311	C1224	G1114	U1229	G1114	U1033	G947	C865	A774	C	A590	U505	U380
C1582	U1406	U1312	C1224	G1122	U1229	G1122	U1034	A953	C866	G775	G654N	C593	C509	U383
C1584	C1407	U1313	G1227	G1122	U1229	G1122	U1035	G956	U871	G775	C	C601	C509	U383
A1586	C1408	C1314	G1227	G1125	U1229	G1125	G1036	A957	A872	G775	G654P	G602	A512	U384
A1587	G1414	U1316	G1229	U1130	U1234	U1130	G1037	U958	C873	U779	C	G603	A513	C385
C1588	U1415	U1317	U1234	C1135	U1234	C1135	G1044	C961	C876	A782	G654R	A604	C517	U387
G1595	G1416	G1319	G1236	C1136	U1236	C1136	A1045	C961	U877	A783	G654T	C605	G518	G388
C1598	G1417	C1320	G1236	C1137	U1236	C1137	A1046	U969	A878	A784	A654U	C606	U519	G389
C1599	G1418	A1321	G1239	G1138	U1239	G1138	A1048	U970	C880	G785	A655	C612	G520	A394
C1600	U1420	A1322	U1240	G1139	U1240	G1139	C1049	C971	C881	C786	A656	G521	U395	U395
C1601	U1421	A1241	A1241	C1140	A1241	C1140	G1050	G972	C882	A788	U657	G522	G396	G396
U1602	G1422	U1329	A1246	U1141	U1246	U1141	G1051	A973	C883	A789	C588	U614	U523	A401
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G1674	U1453	G1364	A1274	C1179	A1274	C1179	G1003	G1003	A918	U833	G726	C640	C560	C461
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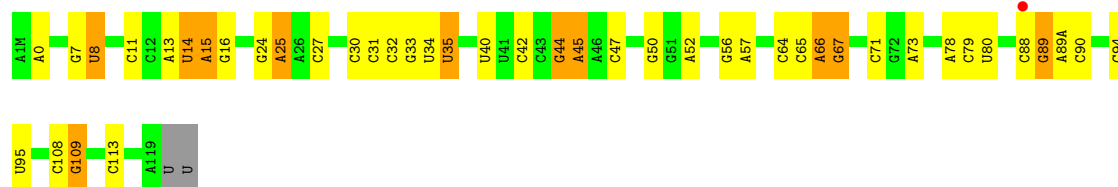
- Molecule 25: 23S rRNA



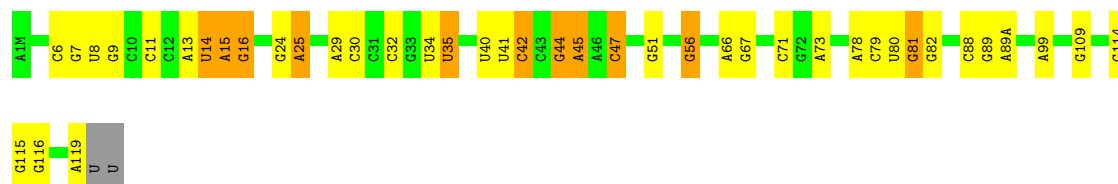
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G1256	A1365	G1460	A1545	G1767	C1882	U2074	C2350	G2445	
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A1262	G1368			A1773	A1885	G2080	C2356	A2448	G2543
U1263		G1465	A1554	A1779	C1886		C2357	U2449	
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G1266				A1785	A1889		G2368	G2458	G2557
	A1384	A1471	A1566	A1786	C1895	G2093	G2370		G2558
C1270	G1385		A1567	A1788	G1896		G2371	C2465	
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U1272	G1388	A1477	A1569	A1790	C1898	G2103	C2375	C2467	U2563
A1274	U1391		A1570	A1791	A1901	C2104	C2376	A2468	A2564
A1275				C1797	G1903	G2105	C2377	G2469	A2565
A1276	U1396		G1573	C1798	G1904	C2106	C2378		A2566
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U1278	G1400	G1484	U1575	C1799	G1906	C2108	C2380	U2473	C2568
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G1280	C1402	G1488	U1577	C1800	G1908	G2110	C2382	C2475	
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G1309	G1424	A1508	C1604	A1823	G1924	G2125	C2397	G2495	
U1313	G1425	C1509		G1835	G1925	G2126	C2398	C2496	
C1314	G1426	A1510		U1836	U1926	G2127	G2210		
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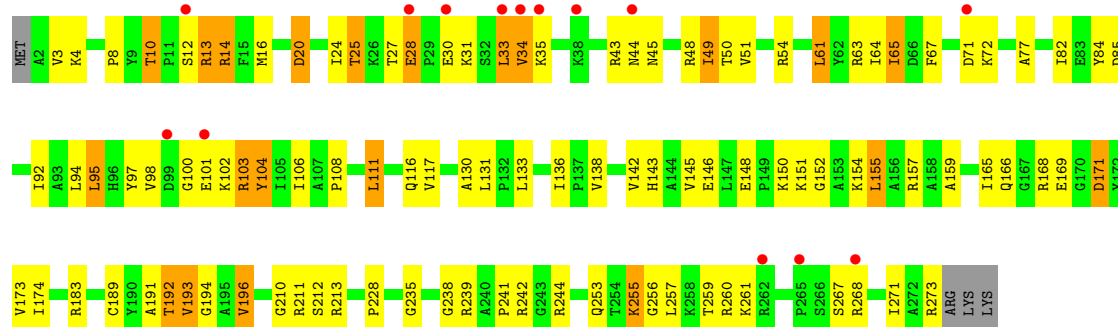
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA

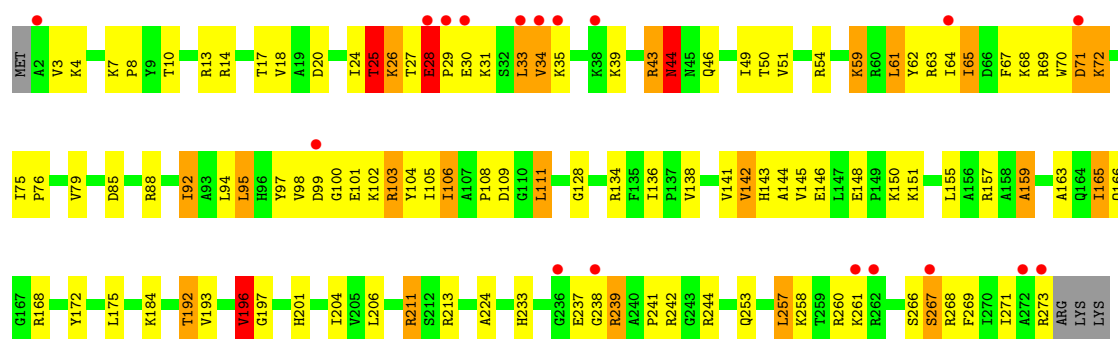


• Molecule 27: 50S ribosomal protein L2

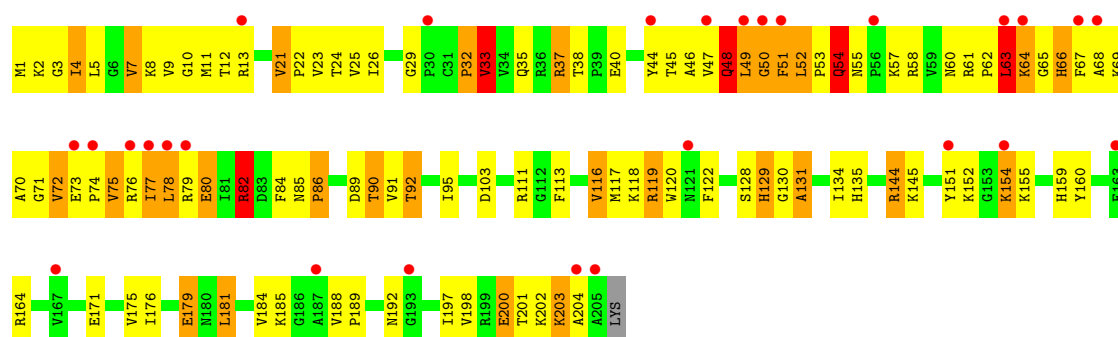


• Molecule 27: 50S ribosomal protein L2

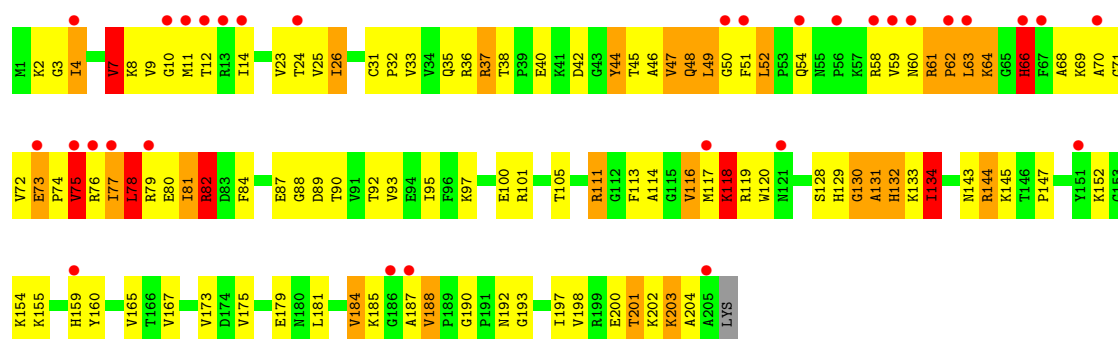




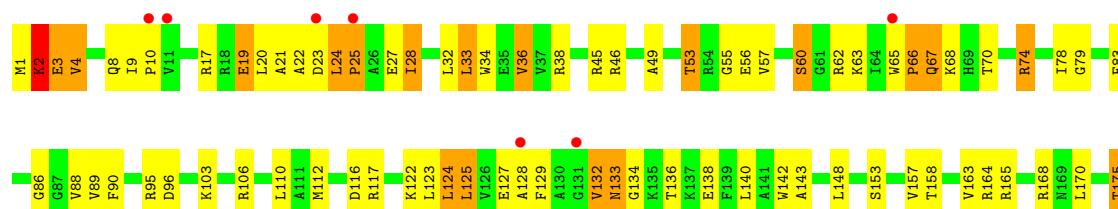
• Molecule 28: 50S ribosomal protein L3

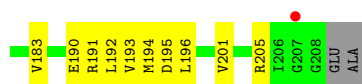


• Molecule 28: 50S ribosomal protein L3

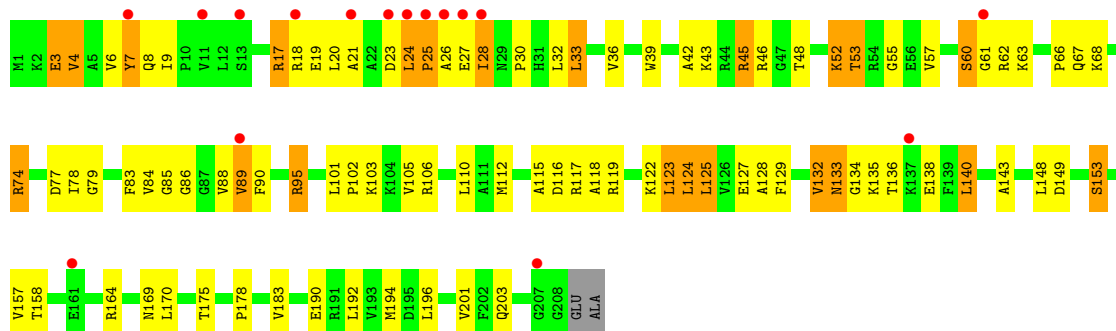


• Molecule 29: 50S ribosomal protein L4

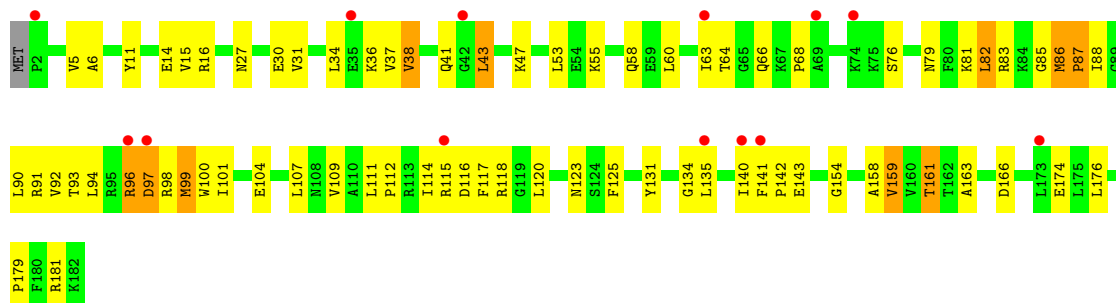




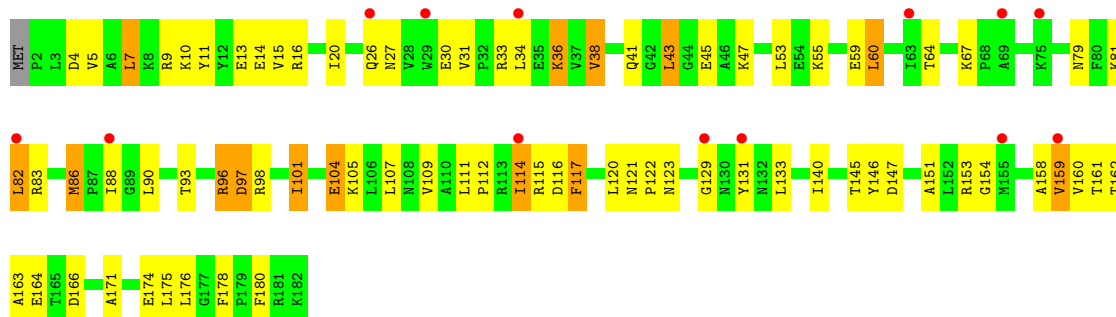
• Molecule 29: 50S ribosomal protein L4



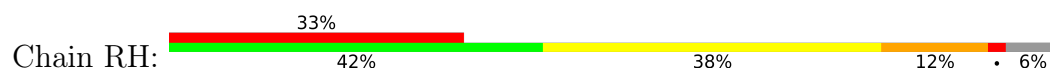
• Molecule 30: 50S ribosomal protein L5

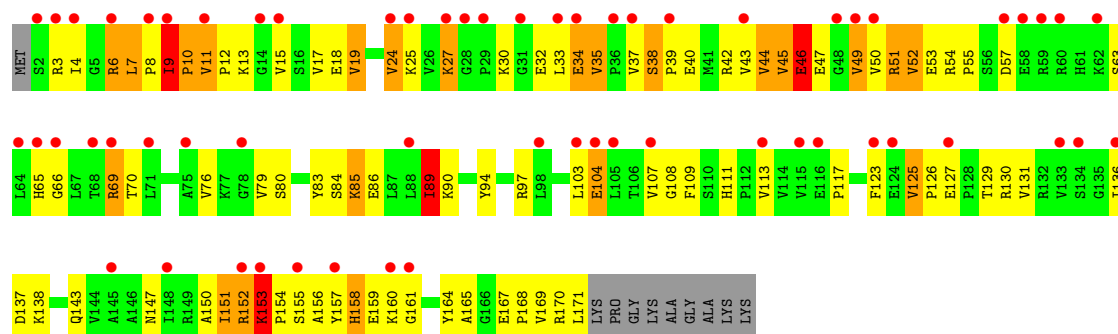


• Molecule 30: 50S ribosomal protein L5

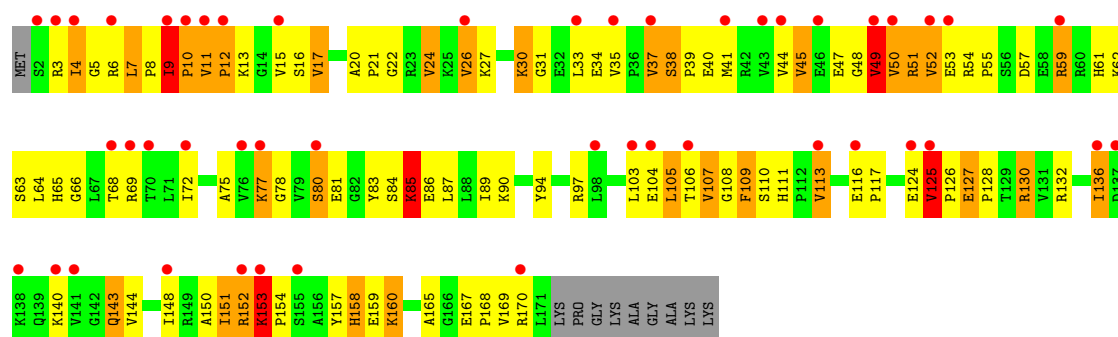


• Molecule 31: 50S ribosomal protein L6

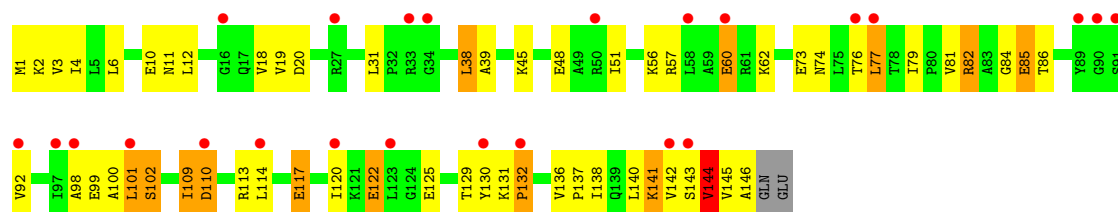




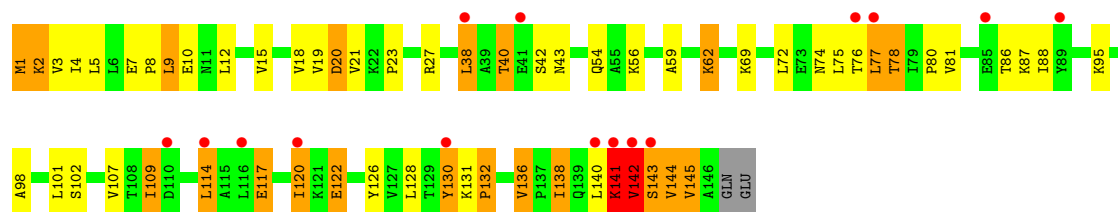
- Molecule 31: 50S ribosomal protein L6



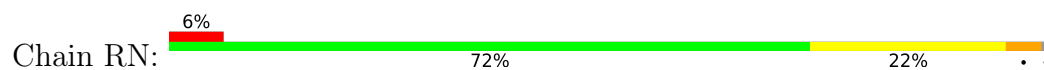
- Molecule 32: 50S ribosomal protein L9

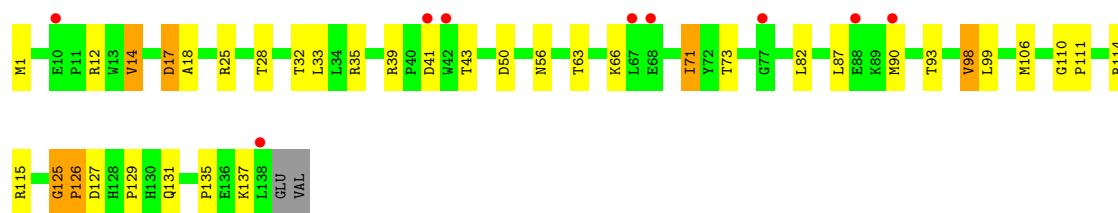


- Molecule 32: 50S ribosomal protein L9

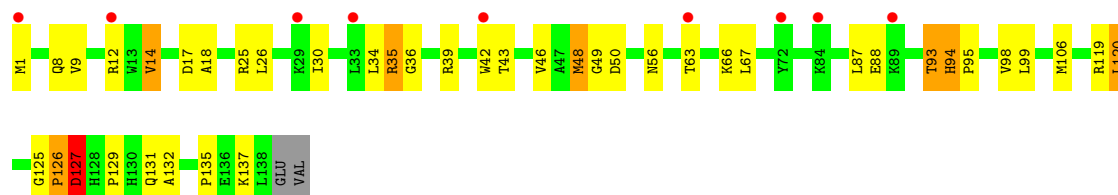


- Molecule 33: 50S ribosomal protein L13

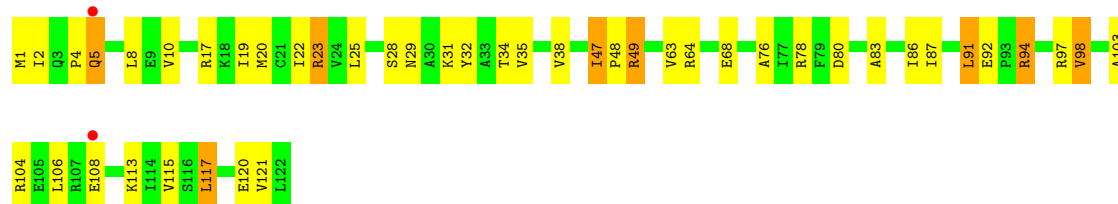




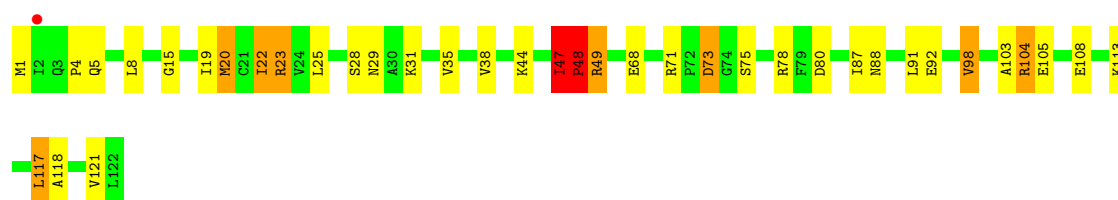
• Molecule 33: 50S ribosomal protein L13



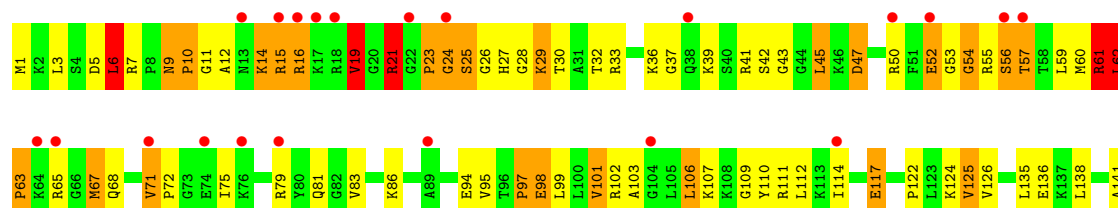
• Molecule 34: 50S ribosomal protein L14



• Molecule 34: 50S ribosomal protein L14

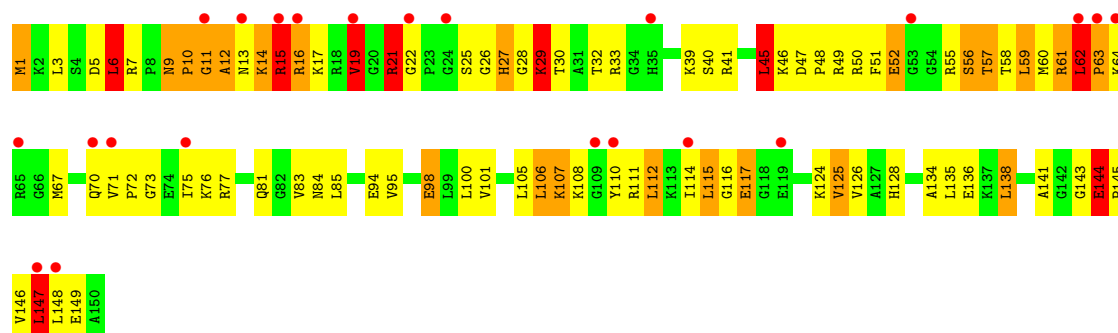


• Molecule 35: 50S ribosomal protein L15

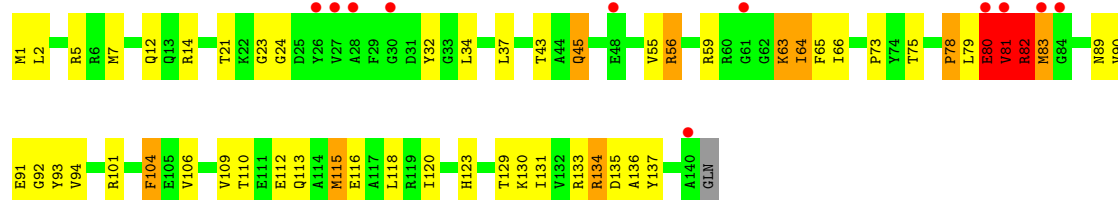




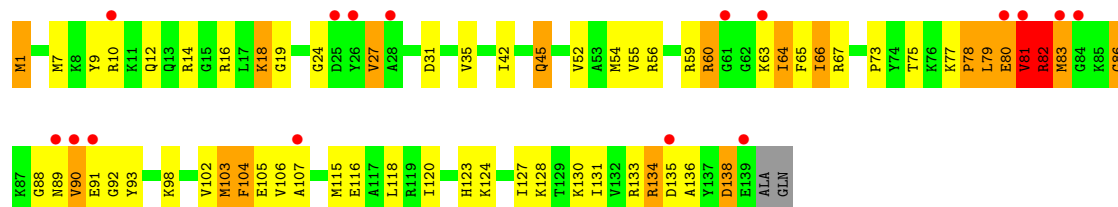
• Molecule 35: 50S ribosomal protein L15



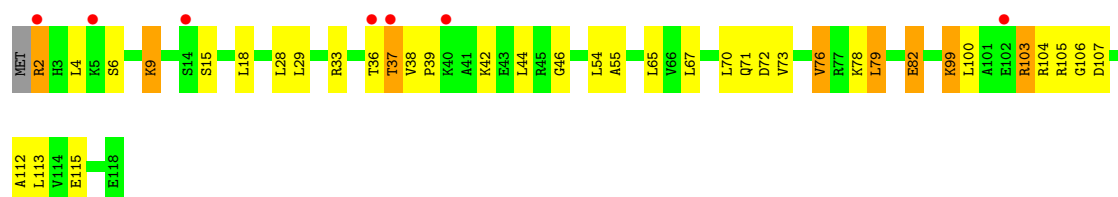
• Molecule 36: 50S ribosomal protein L16



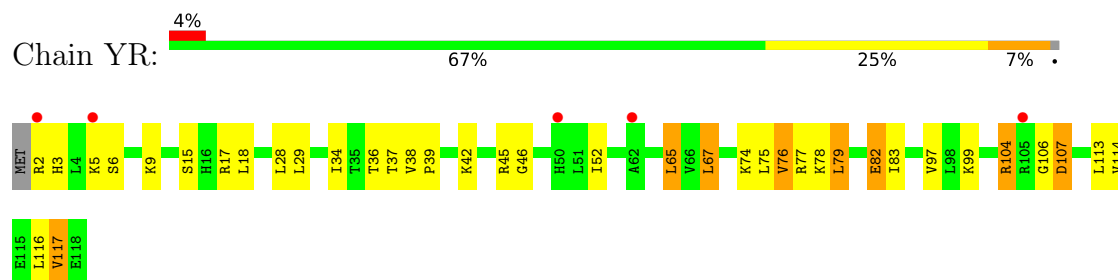
• Molecule 36: 50S ribosomal protein L16



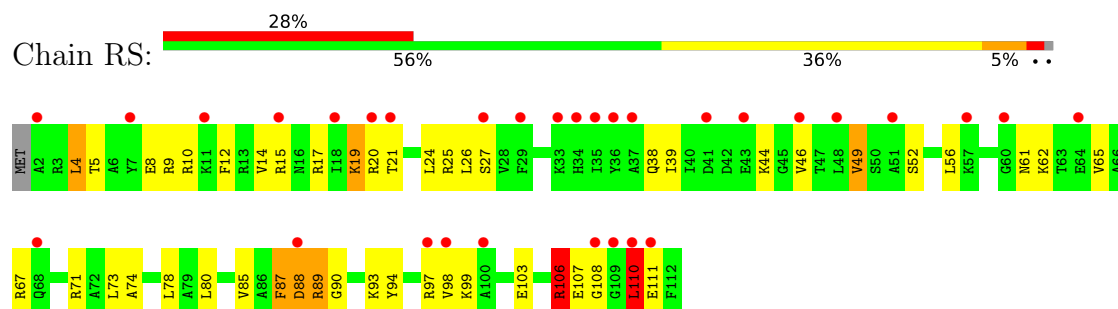
• Molecule 37: 50S ribosomal protein L17



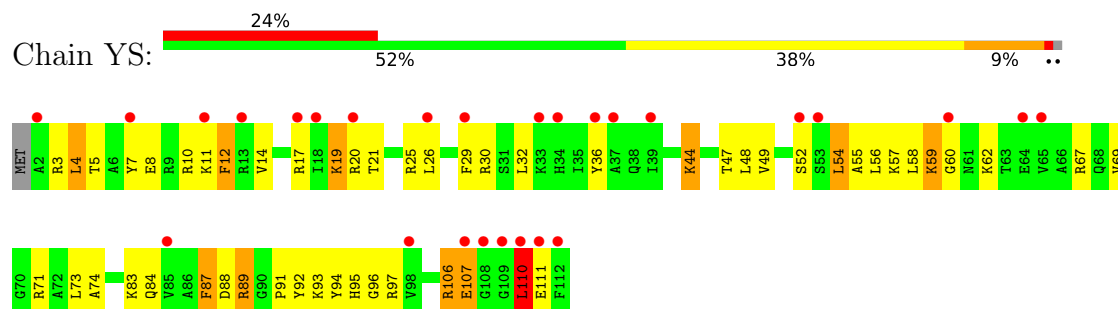
- Molecule 37: 50S ribosomal protein L17



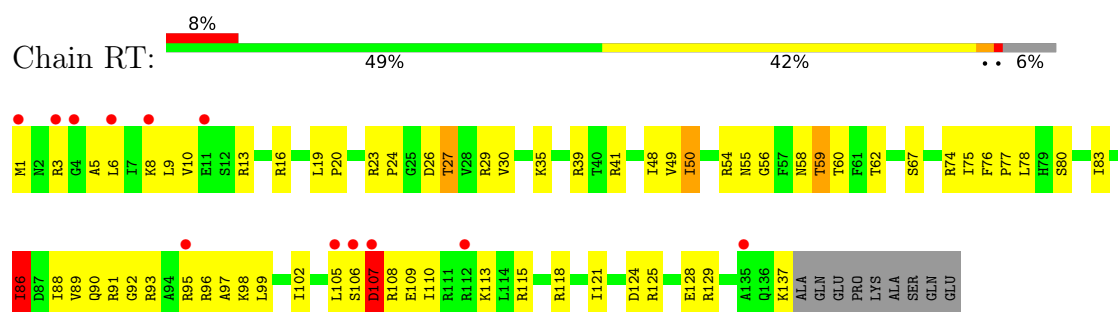
- Molecule 38: 50S ribosomal protein L18



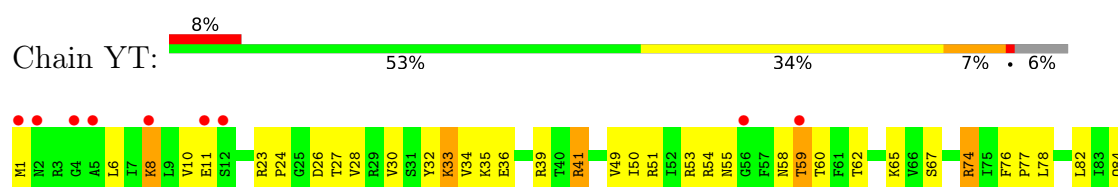
- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L19

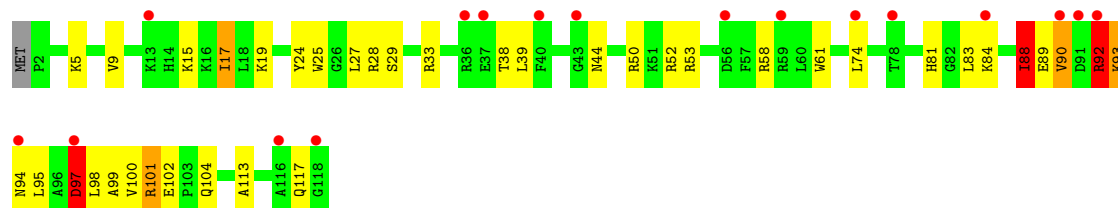




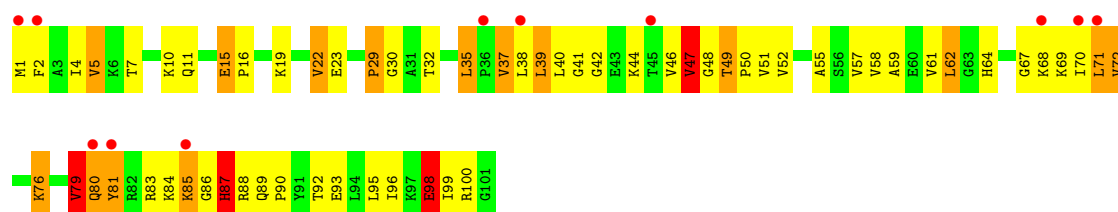
- Molecule 40: 50S ribosomal protein L20



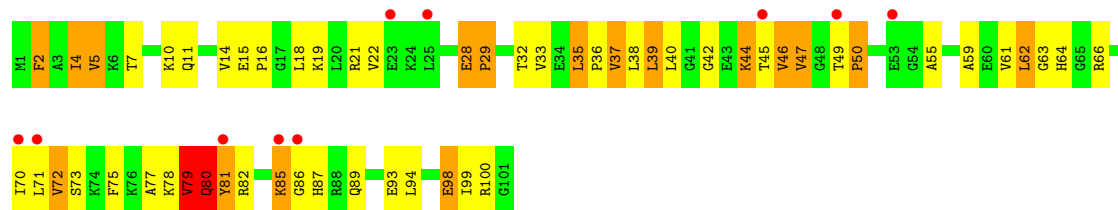
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21

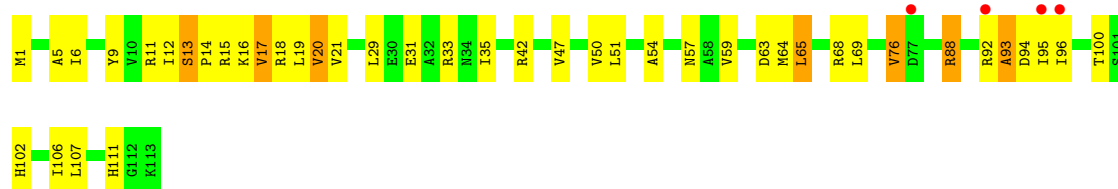


- Molecule 41: 50S ribosomal protein L21

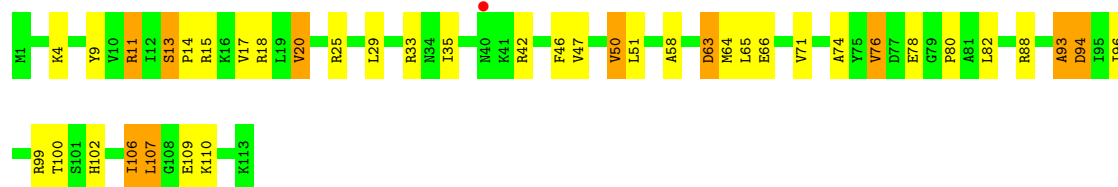


- Molecule 42: 50S ribosomal protein L22

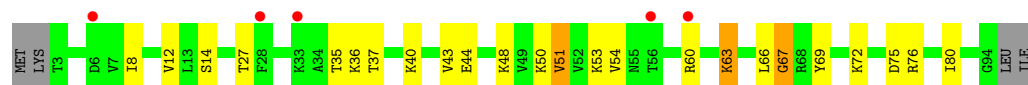
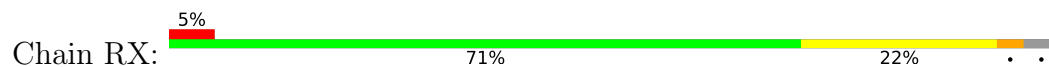




- Molecule 42: 50S ribosomal protein L22



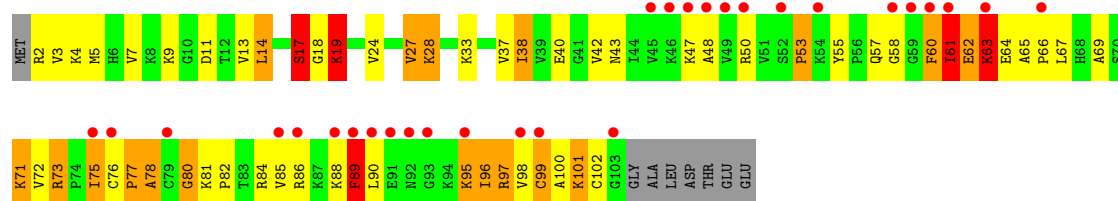
- Molecule 43: 50S ribosomal protein L23



- Molecule 43: 50S ribosomal protein L23

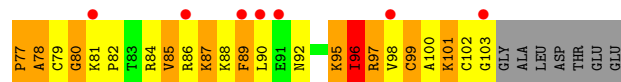


- Molecule 44: 50S ribosomal protein L24

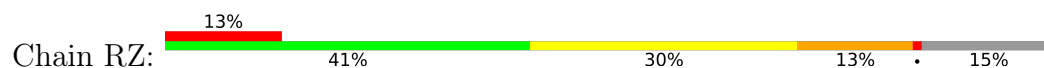


- Molecule 44: 50S ribosomal protein L24





• Molecule 45: 50S ribosomal protein L25



• Molecule 45: 50S ribosomal protein L25



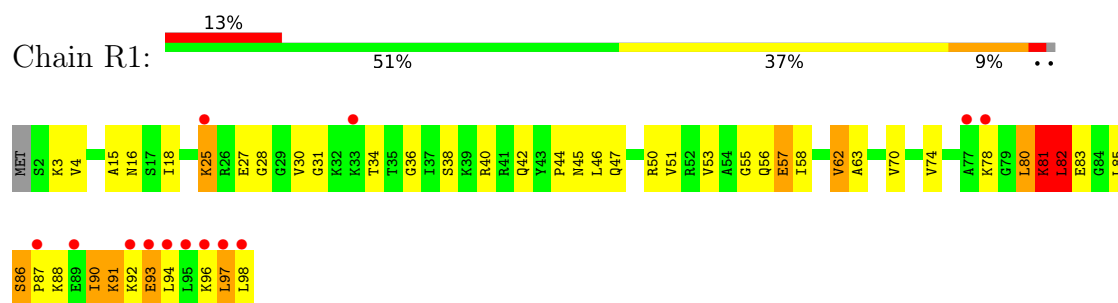
• Molecule 46: 50S ribosomal protein L27



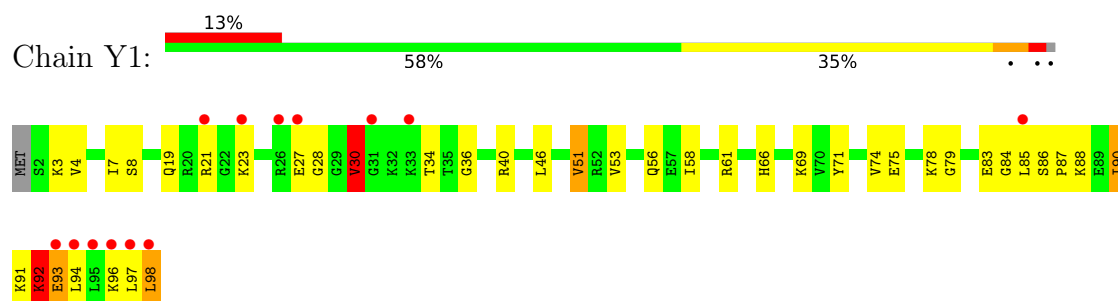
• Molecule 46: 50S ribosomal protein L27



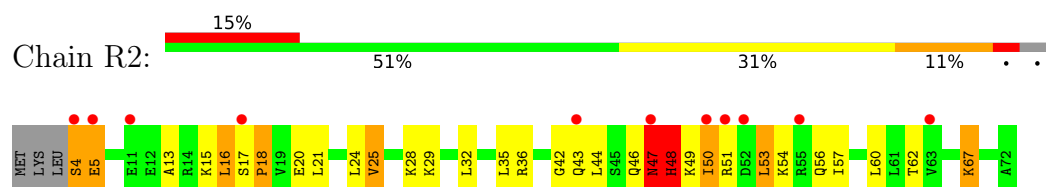
- Molecule 47: 50S ribosomal protein L28



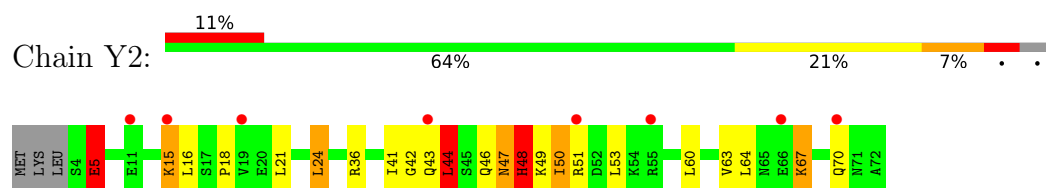
- Molecule 47: 50S ribosomal protein L28



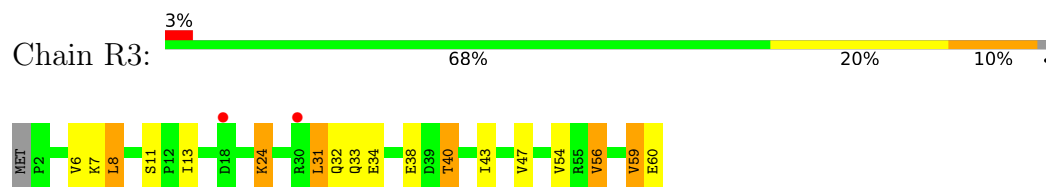
- Molecule 48: 50S ribosomal protein L29



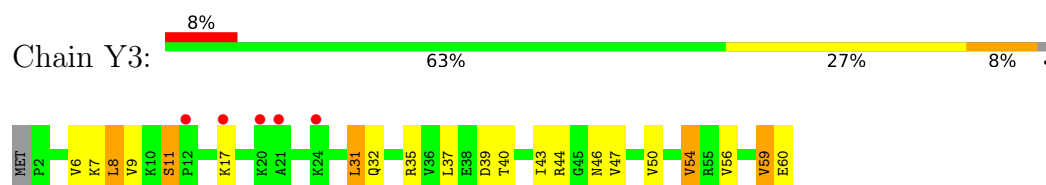
- Molecule 48: 50S ribosomal protein L29



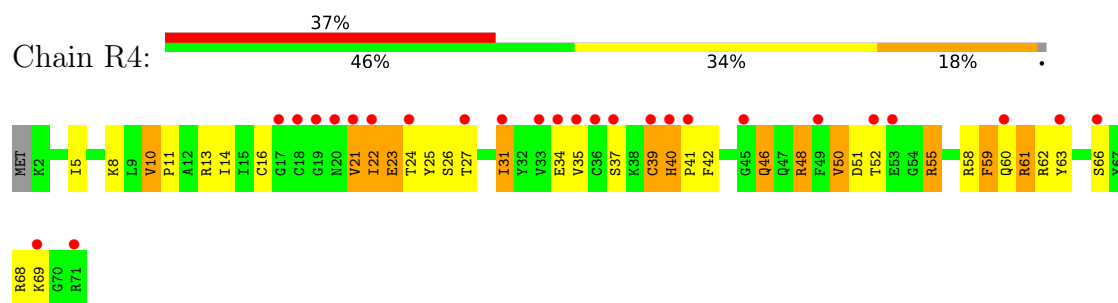
- Molecule 49: 50S ribosomal protein L30



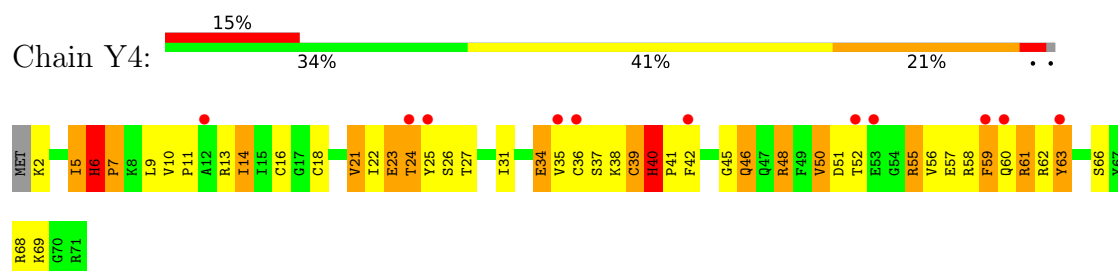
- Molecule 49: 50S ribosomal protein L30



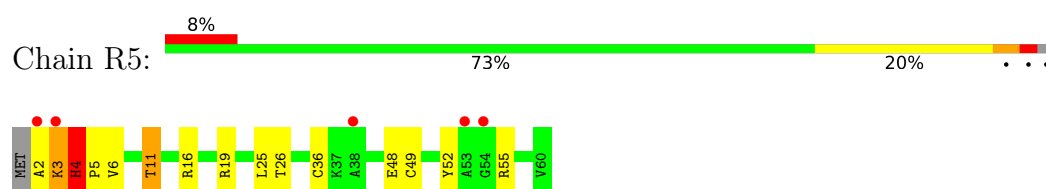
- Molecule 50: 50S ribosomal protein L31



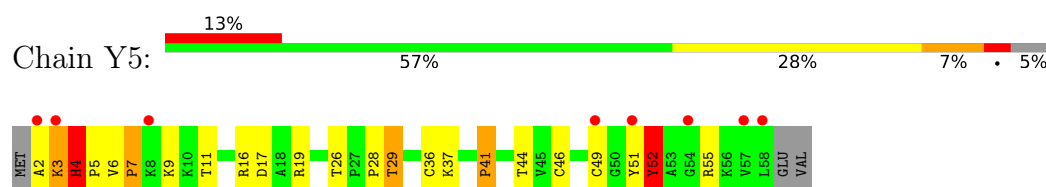
- Molecule 50: 50S ribosomal protein L31



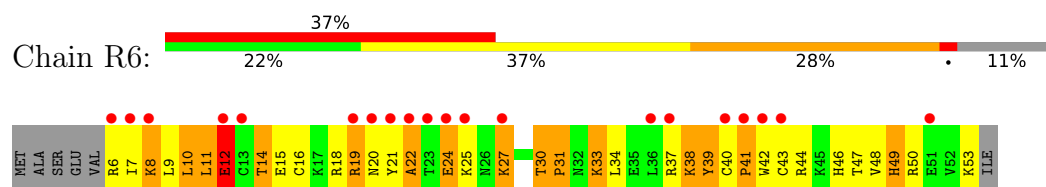
- Molecule 51: 50S ribosomal protein L32



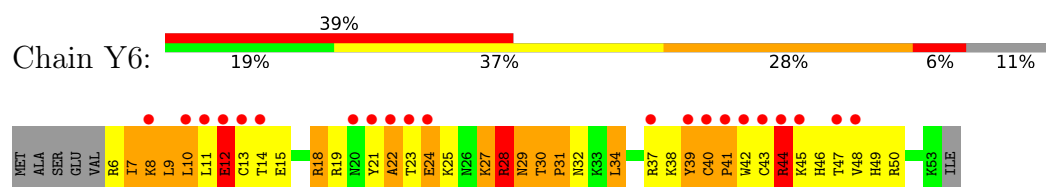
- Molecule 51: 50S ribosomal protein L32



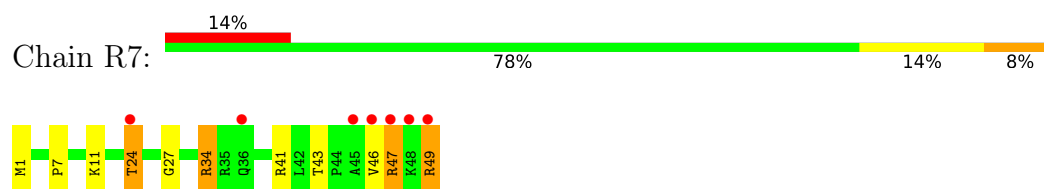
- Molecule 52: 50S ribosomal protein L33



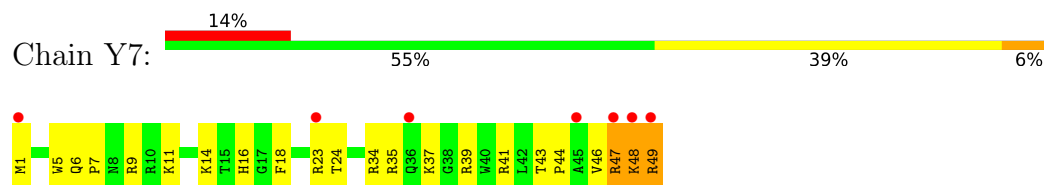
- Molecule 52: 50S ribosomal protein L33



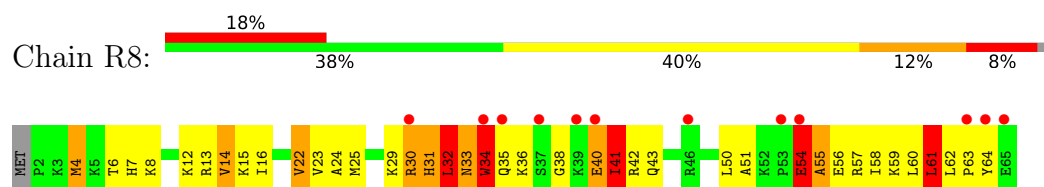
• Molecule 53: 50S ribosomal protein L34



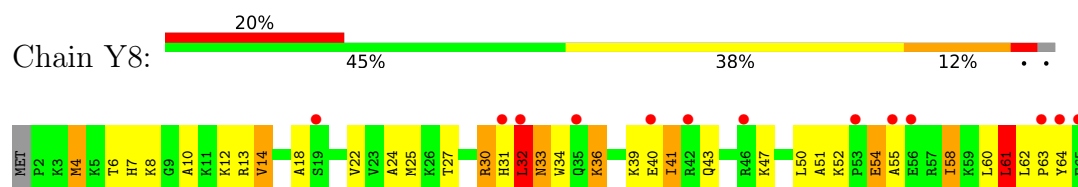
• Molecule 53: 50S ribosomal protein L34



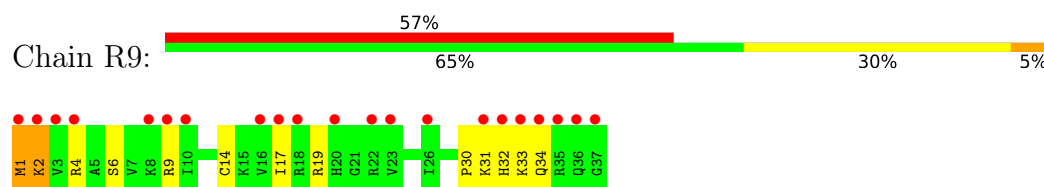
• Molecule 54: 50S ribosomal protein L35



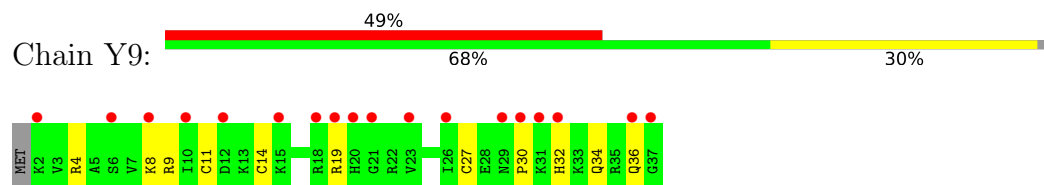
• Molecule 54: 50S ribosomal protein L35



• 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, α , β , γ	214.11Å 453.88Å 607.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.40 34.93 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.93-3.40) 98.8 (34.93-3.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.234 0.214 , 0.248	Depositor DCC
R_{free} test set	44426 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	72.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	297549	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	QA	0.18	0/36346	0.37	6/56724 (0.0%)
1	XA	0.18	0/36276	0.36	1/56615 (0.0%)
2	QB	0.33	0/1950	0.81	2/2630 (0.1%)
2	XB	0.33	0/1950	0.82	2/2630 (0.1%)
3	QC	0.33	0/1636	0.77	0/2205
3	XC	0.36	0/1636	0.79	0/2205
4	QD	0.36	0/1733	0.84	2/2318 (0.1%)
4	XD	0.36	0/1733	0.83	3/2318 (0.1%)
5	QE	0.37	0/1195	0.87	0/1609
5	XE	0.41	0/1195	0.80	0/1609
6	QF	0.31	0/856	0.74	0/1154
6	XF	0.33	0/856	0.75	0/1154
7	QG	0.33	0/1276	0.80	2/1709 (0.1%)
7	XG	0.36	0/1276	0.85	2/1709 (0.1%)
8	QH	0.33	0/1136	0.82	0/1527
8	XH	0.36	0/1136	0.81	2/1527 (0.1%)
9	QI	0.34	0/1037	0.84	1/1389 (0.1%)
9	XI	0.35	0/1037	0.83	2/1389 (0.1%)
10	QJ	0.31	0/814	0.77	0/1095
10	XJ	0.32	0/814	0.78	0/1095
11	QK	0.39	0/916	0.82	1/1234 (0.1%)
11	XK	0.38	0/916	0.86	1/1234 (0.1%)
12	QL	0.39	0/991	0.89	2/1327 (0.2%)
12	XL	0.43	1/991 (0.1%)	0.92	8/1327 (0.6%)
13	QM	0.37	0/947	0.85	0/1270
13	XM	0.35	0/947	0.85	0/1270
14	QN	0.32	0/501	0.80	0/664
14	XN	0.35	0/501	0.80	0/664
15	QO	0.31	0/745	0.70	0/992
15	XO	0.35	0/745	0.75	0/992
16	QP	0.33	0/721	0.75	0/970
16	XP	0.34	0/721	0.75	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.32	0/847	0.79	0/1131
17	XQ	0.34	0/847	0.74	0/1131
18	QR	0.33	0/590	0.78	0/782
18	XR	0.33	0/590	0.77	0/782
19	QS	0.37	0/670	0.86	1/901 (0.1%)
19	XS	0.41	0/670	0.88	0/901
20	QT	0.35	0/765	0.79	1/1007 (0.1%)
20	XT	0.34	0/765	0.80	1/1007 (0.1%)
21	QU	0.29	0/221	0.78	0/288
21	XU	0.28	0/221	0.74	0/288
22	QV	0.19	0/1832	0.36	0/2855
22	QW	0.13	0/1832	0.29	0/2855
22	XV	0.20	0/1832	0.36	0/2855
22	XW	0.12	0/1832	0.28	0/2855
23	QX	0.37	0/417	0.51	0/649
23	XX	0.34	0/417	0.50	0/649
24	QY	0.43	0/762	0.73	1/1028 (0.1%)
24	XY	0.34	0/762	0.73	0/1028
25	RA	0.23	0/69742	0.41	10/108874 (0.0%)
25	YA	0.22	1/69356 (0.0%)	0.40	6/108271 (0.0%)
26	RB	0.18	0/2928	0.36	0/4568
26	YB	0.18	0/2928	0.36	0/4568
27	RD	0.43	0/2165	0.88	4/2919 (0.1%)
27	YD	0.47	0/2165	0.93	5/2919 (0.2%)
28	RE	0.44	0/1601	0.95	7/2160 (0.3%)
28	YE	0.44	0/1601	0.94	6/2160 (0.3%)
29	RF	0.45	0/1662	0.92	4/2249 (0.2%)
29	YF	0.41	0/1662	0.91	2/2249 (0.1%)
30	RG	0.34	0/1499	0.78	2/2016 (0.1%)
30	YG	0.35	0/1499	0.78	0/2016
31	RH	0.38	0/1332	1.03	10/1802 (0.6%)
31	YH	0.43	0/1332	1.01	8/1802 (0.4%)
32	RI	0.35	0/1151	0.85	1/1558 (0.1%)
32	YI	0.40	0/1151	0.93	4/1558 (0.3%)
33	RN	0.36	0/1131	0.85	3/1525 (0.2%)
33	YN	0.38	0/1131	0.87	2/1525 (0.1%)
34	RO	0.39	0/943	0.87	2/1269 (0.2%)
34	YO	0.43	0/943	0.87	2/1269 (0.2%)
35	RP	0.45	0/1162	0.98	6/1544 (0.4%)
35	YP	0.47	0/1162	0.97	3/1544 (0.2%)
36	RQ	0.45	0/1133	0.88	1/1515 (0.1%)
36	YQ	0.46	0/1128	0.91	2/1508 (0.1%)
37	RR	0.39	0/974	0.80	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.42	0/974	0.80	1/1302 (0.1%)
38	RS	0.32	0/892	0.77	1/1187 (0.1%)
38	YS	0.36	0/892	0.83	1/1187 (0.1%)
39	RT	0.35	0/1155	0.79	2/1542 (0.1%)
39	YT	0.39	0/1155	0.81	0/1542
40	RU	0.42	0/982	0.86	3/1306 (0.2%)
40	YU	0.41	0/982	0.91	4/1306 (0.3%)
41	RV	0.52	0/790	1.01	4/1057 (0.4%)
41	YV	0.48	0/790	1.02	5/1057 (0.5%)
42	RW	0.43	0/911	0.84	3/1220 (0.2%)
42	YW	0.42	0/911	0.82	2/1220 (0.2%)
43	RX	0.40	0/739	0.85	0/993
43	YX	0.45	0/739	0.89	1/993 (0.1%)
44	RY	0.45	0/798	0.97	0/1064
44	YY	0.45	0/798	0.94	0/1064
45	RZ	0.46	2/1435 (0.1%)	0.95	4/1947 (0.2%)
45	YZ	0.43	0/1493	0.96	6/2026 (0.3%)
46	R0	0.40	0/666	0.86	0/885
46	Y0	0.40	0/666	0.87	1/885 (0.1%)
47	R1	0.42	0/770	0.85	0/1022
47	Y1	0.49	0/770	0.84	0/1022
48	R2	0.33	0/583	0.92	1/771 (0.1%)
48	Y2	0.41	0/583	0.90	1/771 (0.1%)
49	R3	0.37	0/474	0.77	0/635
49	Y3	0.37	0/474	0.81	0/635
50	R4	0.34	0/586	0.77	0/785
50	Y4	0.43	0/586	0.82	1/785 (0.1%)
51	R5	0.44	0/473	1.06	2/639 (0.3%)
51	Y5	0.42	0/456	0.99	5/617 (0.8%)
52	R6	0.41	0/424	0.98	2/565 (0.4%)
52	Y6	0.56	0/424	1.09	2/565 (0.4%)
53	R7	0.42	0/438	0.80	0/575
53	Y7	0.44	0/438	0.83	2/575 (0.3%)
54	R8	0.56	0/525	1.13	5/691 (0.7%)
54	Y8	0.54	0/525	1.13	3/691 (0.4%)
55	R9	0.34	0/310	0.72	0/407
55	Y9	0.31	0/302	0.71	0/397
All	All	0.28	4/321792 (0.0%)	0.56	193/481138 (0.0%)

All (4) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	RZ	157	LEU	C-N	6.51	1.41	1.33
25	YA	1545	A	O3'-P	5.37	1.67	1.61
12	XL	25	PRO	N-CD	5.10	1.54	1.47
45	RZ	158	PRO	N-CD	5.06	1.54	1.47

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Y8	41	ILE	N-CA-C	-12.63	101.71	113.71
54	R8	41	ILE	N-CA-C	-11.89	102.42	113.71
31	YH	9	ILE	C-N-CD	-11.87	94.49	120.60
36	YQ	82	ARG	N-CA-C	11.20	124.88	109.54
25	RA	859	G	C1'-C2'-O2'	-10.35	96.28	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32472	0	16393	493	0
1	XA	32409	0	16361	457	0
2	QB	1915	0	1969	58	0
2	XB	1915	0	1969	63	0
3	QC	1612	0	1677	50	0
3	XC	1612	0	1677	50	0
4	QD	1703	0	1765	47	0
4	XD	1703	0	1765	44	0
5	QE	1178	0	1234	28	0
5	XE	1178	0	1234	23	0
6	QF	843	0	857	18	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	31	0
7	XG	1257	0	1296	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	QH	1116	0	1177	30	0
8	XH	1116	0	1177	27	0
9	QI	1018	0	1049	52	0
9	XI	1018	0	1049	45	0
10	QJ	801	0	849	35	0
10	XJ	801	0	849	46	0
11	QK	901	0	926	28	0
11	XK	901	0	926	24	0
12	QL	975	0	1062	27	0
12	XL	975	0	1062	24	0
13	QM	937	0	995	29	0
13	XM	937	0	995	56	0
14	QN	492	0	528	15	0
14	XN	492	0	528	21	0
15	QO	734	0	771	16	0
15	XO	734	0	771	16	0
16	QP	705	0	725	15	0
16	XP	705	0	725	11	0
17	QQ	834	0	904	16	0
17	XQ	834	0	904	19	0
18	QR	585	0	657	11	0
18	XR	585	0	657	20	0
19	QS	656	0	678	48	0
19	XS	656	0	678	46	0
20	QT	763	0	861	23	0
20	XT	763	0	861	28	0
21	QU	217	0	234	12	0
21	XU	217	0	234	16	0
22	QV	1640	0	837	26	0
22	QW	1640	0	837	45	0
22	XV	1640	0	837	18	0
22	XW	1640	0	837	23	0
23	QX	440	9	224	18	0
23	XX	440	9	224	16	0
24	QY	746	0	742	16	0
24	XY	746	0	742	17	0
25	RA	62269	0	31392	834	0
25	YA	61924	0	31213	697	0
26	RB	2617	0	1328	29	0
26	YB	2617	0	1328	34	0
27	RD	2115	0	2195	66	0
27	YD	2115	0	2195	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	RE	1568	0	1634	123	0
28	YE	1568	0	1634	83	0
29	RF	1627	0	1680	56	0
29	YF	1627	0	1680	59	0
30	RG	1474	0	1535	52	0
30	YG	1474	0	1535	52	0
31	RH	1307	0	1382	89	0
31	YH	1307	0	1382	69	0
32	RI	1136	0	1223	32	0
32	YI	1136	0	1223	62	0
33	RN	1104	0	1180	15	0
33	YN	1104	0	1180	24	0
34	RO	933	0	996	31	0
34	YO	933	0	996	28	0
35	RP	1145	0	1228	98	0
35	YP	1145	0	1228	101	0
36	RQ	1112	0	1170	41	0
36	YQ	1107	0	1166	44	0
37	RR	960	0	1021	18	0
37	YR	960	0	1021	23	0
38	RS	882	0	943	31	0
38	YS	882	0	943	36	0
39	RT	1141	0	1202	46	0
39	YT	1141	0	1202	39	0
40	RU	964	0	1022	42	0
40	YU	964	0	1022	32	0
41	RV	779	0	852	64	0
41	YV	779	0	852	54	0
42	RW	900	0	964	25	0
42	YW	900	0	964	21	0
43	RX	725	0	778	15	0
43	YX	725	0	778	16	0
44	RY	785	0	878	52	0
44	YY	785	0	878	57	0
45	RZ	1404	0	1437	81	0
45	YZ	1461	0	1493	51	0
46	R0	657	0	683	17	0
46	Y0	657	0	683	26	0
47	R1	763	0	848	31	0
47	Y1	763	0	848	24	0
48	R2	581	0	629	19	0
48	Y2	581	0	629	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	R3	469	0	518	11	0
49	Y3	469	0	518	9	0
50	R4	573	0	565	26	0
50	Y4	573	0	565	44	0
51	R5	459	0	480	10	0
51	Y5	442	0	465	25	0
52	R6	417	0	441	29	0
52	Y6	417	0	441	49	0
53	R7	430	0	480	6	0
53	Y7	430	0	480	13	0
54	R8	517	0	582	42	0
54	Y8	517	0	582	38	0
55	R9	307	0	338	11	0
55	Y9	299	0	326	7	0
56	QA	150	0	0	0	0
56	QD	2	0	0	0	0
56	QL	1	0	0	0	0
56	QV	4	0	0	0	0
56	QX	1	0	0	0	0
56	R0	3	0	0	0	0
56	R1	1	0	0	0	0
56	R2	1	0	0	0	0
56	R5	3	0	0	0	0
56	RA	441	0	0	0	0
56	RB	4	0	0	0	0
56	RD	2	0	0	0	0
56	RE	1	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RQ	2	0	0	0	0
56	RR	1	0	0	0	0
56	RT	1	0	0	0	0
56	RV	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	163	0	0	0	0
56	XD	1	0	0	0	0
56	XF	1	0	0	0	0
56	XL	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	3	0	0	0	0
56	Y0	3	0	0	0	0
56	Y1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Y5	3	0	0	0	0
56	Y7	1	0	0	0	0
56	YA	487	0	0	0	0
56	YB	6	0	0	0	0
56	YD	1	0	0	0	0
56	YE	1	0	0	0	0
56	YF	1	0	0	0	0
56	YG	1	0	0	0	0
56	YH	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	1	0	0	0	0
56	YQ	2	0	0	0	0
56	YV	1	0	0	0	0
56	YW	1	0	0	0	0
56	YY	1	0	0	0	0
57	QD	1	0	0	0	0
57	QN	1	0	0	0	0
57	XD	1	0	0	0	0
57	XN	1	0	0	0	0
All	All	297531	18	201516	5466	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5466 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)
41:YV:49:THR:CG2	41:YV:50:PRO:HD3	1.35	1.56
44:RY:76:CYS:SG	44:RY:77:PRO:HD2	1.44	1.55
31:RH:9:ILE:CG2	31:RH:10:PRO:HA	1.36	1.51
41:RV:49:THR:CG2	41:RV:50:PRO:HD3	1.50	1.41
32:YI:77:LEU:HB2	32:YI:142:VAL:CG2	1.54	1.37

There are no symmetry-related clashes.

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	234/256 (91%)	186 (80%)	29 (12%)	19 (8%)	1	4
2	XB	234/256 (91%)	189 (81%)	27 (12%)	18 (8%)	1	5
3	QC	204/239 (85%)	162 (79%)	26 (13%)	16 (8%)	1	4
3	XC	204/239 (85%)	159 (78%)	33 (16%)	12 (6%)	1	8
4	QD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	1	10
4	XD	206/209 (99%)	168 (82%)	24 (12%)	14 (7%)	1	6
5	QE	152/162 (94%)	136 (90%)	12 (8%)	4 (3%)	4	21
5	XE	152/162 (94%)	137 (90%)	10 (7%)	5 (3%)	3	17
6	QF	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
6	XF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	QG	153/156 (98%)	136 (89%)	13 (8%)	4 (3%)	4	21
7	XG	153/156 (98%)	134 (88%)	15 (10%)	4 (3%)	4	21
8	QH	136/138 (99%)	126 (93%)	7 (5%)	3 (2%)	5	24
8	XH	136/138 (99%)	123 (90%)	10 (7%)	3 (2%)	5	24
9	QI	126/128 (98%)	94 (75%)	24 (19%)	8 (6%)	1	7
9	XI	126/128 (98%)	96 (76%)	23 (18%)	7 (6%)	1	9
10	QJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	2	15
10	XJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	1	10
11	QK	119/129 (92%)	100 (84%)	14 (12%)	5 (4%)	2	14
11	XK	119/129 (92%)	105 (88%)	10 (8%)	4 (3%)	3	17
12	QL	123/132 (93%)	99 (80%)	16 (13%)	8 (6%)	1	6
12	XL	123/132 (93%)	97 (79%)	18 (15%)	8 (6%)	1	6
13	QM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	3
13	XM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	3
14	QN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	50 (86%)	5 (9%)	3 (5%)	1	10
15	QO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	XO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	QP	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
16	XP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
17	QQ	98/105 (93%)	90 (92%)	7 (7%)	1 (1%)	12	40
17	XQ	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	6	25
18	QR	69/88 (78%)	61 (88%)	8 (12%)	0	100	100
18	XR	69/88 (78%)	62 (90%)	6 (9%)	1 (1%)	9	31
19	QS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	1
19	XS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	1
20	QT	97/106 (92%)	79 (81%)	15 (16%)	3 (3%)	3	18
20	XT	97/106 (92%)	80 (82%)	14 (14%)	3 (3%)	3	18
21	QU	23/27 (85%)	17 (74%)	5 (22%)	1 (4%)	2	13
21	XU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	0	4
24	QY	89/117 (76%)	80 (90%)	9 (10%)	0	100	100
24	XY	89/117 (76%)	84 (94%)	5 (6%)	0	100	100
27	RD	270/276 (98%)	224 (83%)	38 (14%)	8 (3%)	3	18
27	YD	270/276 (98%)	229 (85%)	31 (12%)	10 (4%)	2	16
28	RE	203/206 (98%)	141 (70%)	36 (18%)	26 (13%)	0	1
28	YE	203/206 (98%)	133 (66%)	37 (18%)	33 (16%)	0	0
29	RF	206/210 (98%)	167 (81%)	26 (13%)	13 (6%)	1	7
29	YF	206/210 (98%)	168 (82%)	22 (11%)	16 (8%)	1	4
30	RG	179/182 (98%)	141 (79%)	26 (14%)	12 (7%)	1	6
30	YG	179/182 (98%)	147 (82%)	21 (12%)	11 (6%)	1	7
31	RH	168/180 (93%)	104 (62%)	37 (22%)	27 (16%)	0	0
31	YH	168/180 (93%)	98 (58%)	42 (25%)	28 (17%)	0	0
32	RI	144/148 (97%)	110 (76%)	28 (19%)	6 (4%)	2	14
32	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	2	14
33	RN	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	1	10
33	YN	136/140 (97%)	110 (81%)	19 (14%)	7 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	RO	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	44
34	YO	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	44
35	RP	148/150 (99%)	99 (67%)	23 (16%)	26 (18%)	0	0
35	YP	148/150 (99%)	103 (70%)	22 (15%)	23 (16%)	0	0
36	RQ	138/141 (98%)	110 (80%)	17 (12%)	11 (8%)	1	4
36	YQ	137/141 (97%)	111 (81%)	15 (11%)	11 (8%)	1	4
37	RR	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	16
37	YR	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	4	21
38	RS	109/112 (97%)	84 (77%)	17 (16%)	8 (7%)	1	5
38	YS	109/112 (97%)	85 (78%)	13 (12%)	11 (10%)	0	3
39	RT	135/146 (92%)	108 (80%)	25 (18%)	2 (2%)	8	30
39	YT	135/146 (92%)	113 (84%)	17 (13%)	5 (4%)	2	16
40	RU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	7	28
40	YU	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	4	21
41	RV	99/101 (98%)	71 (72%)	13 (13%)	15 (15%)	0	0
41	YV	99/101 (98%)	70 (71%)	15 (15%)	14 (14%)	0	0
42	RW	111/113 (98%)	107 (96%)	1 (1%)	3 (3%)	4	20
42	YW	111/113 (98%)	104 (94%)	3 (3%)	4 (4%)	2	16
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	24
43	YX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	24
44	RY	100/110 (91%)	57 (57%)	28 (28%)	15 (15%)	0	0
44	YY	100/110 (91%)	58 (58%)	26 (26%)	16 (16%)	0	0
45	RZ	174/206 (84%)	119 (68%)	33 (19%)	22 (13%)	0	1
45	YZ	181/206 (88%)	122 (67%)	42 (23%)	17 (9%)	0	3
46	R0	81/85 (95%)	73 (90%)	5 (6%)	3 (4%)	2	16
46	Y0	81/85 (95%)	67 (83%)	11 (14%)	3 (4%)	2	16
47	R1	95/98 (97%)	71 (75%)	12 (13%)	12 (13%)	0	1
47	Y1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	7
48	R2	67/72 (93%)	54 (81%)	8 (12%)	5 (8%)	1	5
48	Y2	67/72 (93%)	56 (84%)	5 (8%)	6 (9%)	0	3
49	R3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Y3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
50	R4	68/71 (96%)	43 (63%)	12 (18%)	13 (19%)	0	0
50	Y4	68/71 (96%)	37 (54%)	15 (22%)	16 (24%)	0	0
51	R5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	16
51	Y5	55/60 (92%)	48 (87%)	3 (6%)	4 (7%)	1	5
52	R6	46/54 (85%)	22 (48%)	15 (33%)	9 (20%)	0	0
52	Y6	46/54 (85%)	16 (35%)	17 (37%)	13 (28%)	0	0
53	R7	47/49 (96%)	47 (100%)	0	0	100	100
53	Y7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
54	R8	62/65 (95%)	48 (77%)	7 (11%)	7 (11%)	0	2
54	Y8	62/65 (95%)	48 (77%)	7 (11%)	7 (11%)	0	2
55	R9	35/37 (95%)	34 (97%)	0	1 (3%)	3	19
55	Y9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11647/12362 (94%)	9400 (81%)	1486 (13%)	761 (6%)	1	6

5 of 761 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	29	ALA
2	QB	165	VAL
2	QB	195	ASP
2	QB	238	LEU
3	QC	64	VAL

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	204/220 (93%)	176 (86%)	28 (14%)	3	14
2	XB	204/220 (93%)	175 (86%)	29 (14%)	3	13
3	QC	160/188 (85%)	143 (89%)	17 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	XC	160/188 (85%)	140 (88%)	20 (12%)	4	18
4	QD	180/181 (99%)	156 (87%)	24 (13%)	4	15
4	XD	180/181 (99%)	153 (85%)	27 (15%)	3	11
5	QE	119/123 (97%)	107 (90%)	12 (10%)	7	25
5	XE	119/123 (97%)	106 (89%)	13 (11%)	6	22
6	QF	90/90 (100%)	84 (93%)	6 (7%)	15	41
6	XF	90/90 (100%)	74 (82%)	16 (18%)	2	7
7	QG	126/127 (99%)	112 (89%)	14 (11%)	6	21
7	XG	126/127 (99%)	107 (85%)	19 (15%)	3	11
8	QH	119/119 (100%)	108 (91%)	11 (9%)	8	29
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	22
9	QI	99/99 (100%)	78 (79%)	21 (21%)	1	3
9	XI	99/99 (100%)	83 (84%)	16 (16%)	2	10
10	QJ	89/92 (97%)	78 (88%)	11 (12%)	4	18
10	XJ	89/92 (97%)	76 (85%)	13 (15%)	3	12
11	QK	92/99 (93%)	83 (90%)	9 (10%)	7	27
11	XK	92/99 (93%)	83 (90%)	9 (10%)	7	27
12	QL	104/109 (95%)	89 (86%)	15 (14%)	3	13
12	XL	104/109 (95%)	82 (79%)	22 (21%)	1	3
13	QM	94/101 (93%)	80 (85%)	14 (15%)	3	12
13	XM	94/101 (93%)	83 (88%)	11 (12%)	5	20
14	QN	49/50 (98%)	46 (94%)	3 (6%)	17	43
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	25
15	QO	79/80 (99%)	71 (90%)	8 (10%)	7	25
15	XO	79/80 (99%)	72 (91%)	7 (9%)	9	31
16	QP	72/74 (97%)	65 (90%)	7 (10%)	8	28
16	XP	72/74 (97%)	65 (90%)	7 (10%)	8	28
17	QQ	95/97 (98%)	90 (95%)	5 (5%)	20	47
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	38
18	QR	62/77 (80%)	57 (92%)	5 (8%)	11	36
18	XR	62/77 (80%)	55 (89%)	7 (11%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	QS	71/80 (89%)	52 (73%)	19 (27%)	0	1
19	XS	71/80 (89%)	56 (79%)	15 (21%)	1	3
20	QT	76/82 (93%)	61 (80%)	15 (20%)	1	5
20	XT	76/82 (93%)	63 (83%)	13 (17%)	2	9
21	QU	20/22 (91%)	19 (95%)	1 (5%)	22	49
21	XU	20/22 (91%)	18 (90%)	2 (10%)	7	26
24	QY	78/102 (76%)	76 (97%)	2 (3%)	40	61
24	XY	78/102 (76%)	74 (95%)	4 (5%)	21	48
27	RD	214/218 (98%)	175 (82%)	39 (18%)	2	7
27	YD	214/218 (98%)	173 (81%)	41 (19%)	1	6
28	RE	165/166 (99%)	133 (81%)	32 (19%)	1	5
28	YE	165/166 (99%)	131 (79%)	34 (21%)	1	4
29	RF	165/166 (99%)	139 (84%)	26 (16%)	2	10
29	YF	165/166 (99%)	141 (86%)	24 (14%)	3	13
30	RG	155/156 (99%)	144 (93%)	11 (7%)	13	39
30	YG	155/156 (99%)	138 (89%)	17 (11%)	6	22
31	RH	142/148 (96%)	120 (84%)	22 (16%)	2	10
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	5
32	RI	122/124 (98%)	100 (82%)	22 (18%)	2	7
32	YI	122/124 (98%)	98 (80%)	24 (20%)	1	5
33	RN	117/119 (98%)	105 (90%)	12 (10%)	7	24
33	YN	117/119 (98%)	105 (90%)	12 (10%)	7	24
34	RO	100/100 (100%)	88 (88%)	12 (12%)	5	19
34	YO	100/100 (100%)	86 (86%)	14 (14%)	3	13
35	RP	116/116 (100%)	85 (73%)	31 (27%)	0	1
35	YP	116/116 (100%)	82 (71%)	34 (29%)	0	1
36	RQ	110/111 (99%)	94 (86%)	16 (14%)	3	13
36	YQ	110/111 (99%)	90 (82%)	20 (18%)	2	7
37	RR	100/101 (99%)	81 (81%)	19 (19%)	1	6
37	YR	100/101 (99%)	84 (84%)	16 (16%)	2	10
38	RS	87/88 (99%)	78 (90%)	9 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	12
39	RT	120/127 (94%)	99 (82%)	21 (18%)	2	8
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	8
40	RU	93/94 (99%)	85 (91%)	8 (9%)	10	33
40	YU	93/94 (99%)	84 (90%)	9 (10%)	8	28
41	RV	82/82 (100%)	67 (82%)	15 (18%)	2	7
41	YV	82/82 (100%)	64 (78%)	18 (22%)	1	3
42	RW	92/92 (100%)	78 (85%)	14 (15%)	3	10
42	YW	92/92 (100%)	79 (86%)	13 (14%)	3	13
43	RX	74/78 (95%)	64 (86%)	10 (14%)	4	15
43	YX	74/78 (95%)	66 (89%)	8 (11%)	6	22
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	1
44	YY	85/91 (93%)	62 (73%)	23 (27%)	0	1
45	RZ	155/179 (87%)	123 (79%)	32 (21%)	1	4
45	YZ	162/179 (90%)	132 (82%)	30 (18%)	1	7
46	R0	66/67 (98%)	60 (91%)	6 (9%)	9	30
46	Y0	66/67 (98%)	59 (89%)	7 (11%)	6	23
47	R1	82/83 (99%)	68 (83%)	14 (17%)	2	9
47	Y1	82/83 (99%)	71 (87%)	11 (13%)	4	15
48	R2	64/67 (96%)	52 (81%)	12 (19%)	1	6
48	Y2	64/67 (96%)	55 (86%)	9 (14%)	3	13
49	R3	51/52 (98%)	43 (84%)	8 (16%)	2	10
49	Y3	51/52 (98%)	42 (82%)	9 (18%)	2	8
50	R4	62/63 (98%)	49 (79%)	13 (21%)	1	4
50	Y4	62/63 (98%)	45 (73%)	17 (27%)	0	1
51	R5	51/52 (98%)	43 (84%)	8 (16%)	2	10
51	Y5	49/52 (94%)	43 (88%)	6 (12%)	5	19
52	R6	47/52 (90%)	34 (72%)	13 (28%)	0	1
52	Y6	47/52 (90%)	29 (62%)	18 (38%)	0	0
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2	9
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	R8	54/55 (98%)	43 (80%)	11 (20%)	1	4
54	Y8	54/55 (98%)	44 (82%)	10 (18%)	1	7
55	R9	34/34 (100%)	32 (94%)	2 (6%)	18	44
55	Y9	33/34 (97%)	33 (100%)	0	100	100
All	All	9854/10270 (96%)	8372 (85%)	1482 (15%)	3	11

5 of 1482 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	XN	58	LYS
32	YI	88	ILE
18	XR	82	THR
14	XN	41	ARG
28	YE	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
37	YR	3	HIS
45	YZ	118	GLN
51	Y5	23	HIS
37	RR	50	HIS
36	RQ	113	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1522 (99%)	296 (19%)	46 (3%)
1	XA	1506/1522 (98%)	290 (19%)	38 (2%)
22	QV	76/77 (98%)	13 (17%)	0
22	QW	76/77 (98%)	20 (26%)	2 (2%)
22	XV	76/77 (98%)	12 (15%)	1 (1%)
22	XW	76/77 (98%)	18 (23%)	0
23	QX	19/25 (76%)	8 (42%)	2 (10%)
23	XX	19/25 (76%)	9 (47%)	1 (5%)
25	RA	2888/2916 (99%)	591 (20%)	42 (1%)
25	YA	2872/2916 (98%)	567 (19%)	41 (1%)
26	RB	121/124 (97%)	20 (16%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	YB	121/124 (97%)	21 (17%)	1 (0%)
All	All	9359/9482 (98%)	1865 (19%)	175 (1%)

5 of 1865 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G

5 of 175 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	792	A
25	YA	883	G
1	XA	960	U
1	XA	1532	U
25	YA	1427	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	A2M	XX	19	56,23	22,25,26	1.55	4 (18%)	30,36,39	2.20	12 (40%)
23	A2M	QX	21	1,23	22,25,26	1.50	4 (18%)	30,36,39	2.21	11 (36%)
23	A2M	QX	20	23	22,25,26	1.57	3 (13%)	30,36,39	2.25	9 (30%)
23	A2M	QX	19	23	22,25,26	1.51	5 (22%)	30,36,39	2.11	11 (36%)
23	A2M	XX	21	1,23	22,25,26	1.48	5 (22%)	30,36,39	2.18	12 (40%)
23	A2M	XX	20	23	22,25,26	1.49	4 (18%)	30,36,39	2.33	11 (36%)

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
23	A2M	XX	19	56,23	-	2/9/27/28	0/3/3/3
23	A2M	QX	21	1,23	-	5/9/27/28	0/3/3/3
23	A2M	QX	20	23	-	2/9/27/28	0/3/3/3
23	A2M	QX	19	23	-	2/9/27/28	0/3/3/3
23	A2M	XX	21	1,23	-	4/9/27/28	0/3/3/3
23	A2M	XX	20	23	-	0/9/27/28	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A2M	C5-C4	5.06	1.48	1.39
23	XX	19	A2M	C5-C4	4.67	1.47	1.39
23	QX	21	A2M	C5-C4	4.58	1.47	1.39
23	XX	21	A2M	C5-C4	4.49	1.47	1.39
23	XX	20	A2M	C5-C4	4.48	1.47	1.39

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	20	A2M	C5-C4-N3	-6.57	117.67	126.72
23	XX	20	A2M	C5-C4-N3	-6.29	118.05	126.72
23	QX	21	A2M	C5-C4-N3	-5.67	118.91	126.72
23	XX	21	A2M	C5-C4-N3	-5.09	119.71	126.72
23	QX	20	A2M	N3-C4-N9	4.84	135.40	127.17

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	QX	20	A2M	O4'-C4'-C5'-O5'
23	QX	20	A2M	C3'-C4'-C5'-O5'
23	QX	21	A2M	C1'-C2'-O2'-CM'
23	XX	21	A2M	C1'-C2'-O2'-CM'
23	QX	21	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	QX	21	A2M	2	0
23	QX	19	A2M	1	0
23	XX	21	A2M	2	0
23	XX	20	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1312 ligands modelled in this entry, 1312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1511/1522 (99%)	-0.03	21 (1%) 73 59	39, 80, 190, 435	0
1	XA	1508/1522 (99%)	-0.08	17 (1%) 78 65	27, 78, 175, 487	0
2	QB	236/256 (92%)	0.83	25 (10%) 11 11	58, 138, 241, 336	0
2	XB	236/256 (92%)	0.86	23 (9%) 13 13	52, 119, 215, 332	0
3	QC	206/239 (86%)	0.56	8 (3%) 43 31	61, 111, 200, 469	0
3	XC	206/239 (86%)	0.47	7 (3%) 48 35	44, 103, 197, 564	0
4	QD	208/209 (99%)	0.51	18 (8%) 16 14	35, 66, 119, 173	0
4	XD	208/209 (99%)	0.70	25 (12%) 9 9	41, 82, 132, 198	0
5	QE	154/162 (95%)	0.39	3 (1%) 66 51	34, 74, 138, 244	0
5	XE	154/162 (95%)	0.30	6 (3%) 43 31	31, 68, 144, 340	0
6	QF	101/101 (100%)	0.68	7 (6%) 23 18	58, 117, 161, 183	0
6	XF	101/101 (100%)	0.24	0 100 100	29, 68, 110, 175	0
7	QG	155/156 (99%)	0.91	22 (14%) 6 8	80, 130, 214, 347	0
7	XG	155/156 (99%)	0.82	21 (13%) 7 8	54, 101, 179, 252	0
8	QH	138/138 (100%)	0.34	5 (3%) 46 33	41, 81, 119, 179	0
8	XH	138/138 (100%)	0.31	5 (3%) 46 33	48, 79, 128, 182	0
9	QI	128/128 (100%)	1.19	28 (21%) 2 4	78, 156, 267, 359	0
9	XI	128/128 (100%)	1.11	21 (16%) 4 6	61, 115, 202, 350	0
10	QJ	99/105 (94%)	1.37	22 (22%) 2 4	74, 149, 278, 339	0
10	XJ	99/105 (94%)	1.10	11 (11%) 10 11	63, 133, 253, 371	0
11	QK	121/129 (93%)	0.65	11 (9%) 15 14	43, 102, 182, 301	0
11	XK	121/129 (93%)	0.56	9 (7%) 20 17	32, 71, 159, 258	0
12	QL	125/132 (94%)	0.28	3 (2%) 59 45	27, 62, 103, 271	0
12	XL	125/132 (94%)	0.35	4 (3%) 50 37	30, 64, 103, 263	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	118/126 (93%)	1.06	19 (16%) 4 6	75, 133, 248, 348	0
13	XM	118/126 (93%)	1.02	14 (11%) 9 10	64, 114, 183, 467	0
14	QN	60/61 (98%)	1.22	9 (15%) 5 7	79, 110, 169, 205	0
14	XN	60/61 (98%)	1.05	6 (10%) 12 12	60, 93, 133, 240	0
15	QO	88/89 (98%)	0.68	6 (6%) 23 19	37, 86, 136, 170	0
15	XO	88/89 (98%)	0.47	4 (4%) 38 28	34, 74, 110, 161	0
16	QP	84/88 (95%)	0.37	2 (2%) 59 45	38, 68, 111, 260	0
16	XP	84/88 (95%)	0.83	8 (9%) 14 13	63, 90, 138, 347	0
17	QQ	100/105 (95%)	0.51	8 (8%) 18 16	33, 79, 110, 133	0
17	XQ	100/105 (95%)	0.65	9 (9%) 15 14	35, 82, 118, 188	0
18	QR	71/88 (80%)	0.83	5 (7%) 22 18	64, 114, 191, 248	0
18	XR	71/88 (80%)	0.48	4 (5%) 30 23	33, 66, 181, 270	0
19	QS	82/93 (88%)	1.21	15 (18%) 3 5	78, 148, 306, 418	0
19	XS	82/93 (88%)	1.36	16 (19%) 3 4	57, 126, 215, 401	0
20	QT	99/106 (93%)	0.86	14 (14%) 6 8	54, 85, 160, 222	0
20	XT	99/106 (93%)	0.98	13 (13%) 7 8	61, 107, 176, 212	0
21	QU	25/27 (92%)	2.21	14 (56%) 0 0	94, 130, 197, 278	0
21	XU	25/27 (92%)	2.79	13 (52%) 0 0	74, 113, 170, 194	0
22	QV	77/77 (100%)	0.20	2 (2%) 57 42	46, 83, 132, 187	0
22	QW	77/77 (100%)	1.45	17 (22%) 2 4	86, 279, 383, 409	0
22	XV	77/77 (100%)	-0.08	2 (2%) 57 42	42, 79, 123, 172	0
22	XW	77/77 (100%)	1.43	18 (23%) 2 3	115, 271, 335, 411	0
23	QX	17/25 (68%)	1.09	3 (17%) 4 5	53, 218, 306, 334	0
23	XX	17/25 (68%)	1.05	4 (23%) 2 3	45, 237, 354, 390	0
24	QY	91/117 (77%)	0.84	13 (14%) 6 8	83, 126, 163, 188	0
24	XY	91/117 (77%)	0.72	11 (12%) 8 9	82, 127, 165, 185	0
25	RA	2891/2916 (99%)	0.00	72 (2%) 58 43	20, 56, 239, 588	0
25	YA	2875/2916 (98%)	-0.10	76 (2%) 57 42	20, 54, 248, 583	0
26	RB	122/124 (98%)	0.03	1 (0%) 82 71	46, 96, 148, 214	0
26	YB	122/124 (98%)	0.08	0 100 100	55, 86, 136, 215	0
27	RD	272/276 (98%)	0.51	14 (5%) 33 25	17, 54, 102, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	YD	272/276 (98%)	0.28	18 (6%) 24 19	12, 35, 83, 212	0
28	RE	205/206 (99%)	0.88	27 (13%) 7 8	25, 73, 159, 362	0
28	YE	205/206 (99%)	0.87	31 (15%) 5 7	26, 73, 168, 563	0
29	RF	208/210 (99%)	0.26	8 (3%) 44 31	13, 44, 168, 316	0
29	YF	208/210 (99%)	0.60	16 (7%) 19 16	22, 67, 240, 535	0
30	RG	181/182 (99%)	0.73	13 (7%) 21 18	62, 110, 161, 194	0
30	YG	181/182 (99%)	0.64	13 (7%) 21 18	42, 97, 165, 199	0
31	RH	170/180 (94%)	1.76	60 (35%) 1 1	59, 182, 468, 582	0
31	YH	170/180 (94%)	1.61	47 (27%) 1 2	58, 146, 370, 574	0
32	RI	146/148 (98%)	1.03	24 (16%) 4 6	51, 113, 183, 290	0
32	YI	146/148 (98%)	0.86	15 (10%) 12 12	36, 92, 188, 341	0
33	RN	138/140 (98%)	0.56	9 (6%) 25 20	25, 75, 121, 188	0
33	YN	138/140 (98%)	0.55	9 (6%) 25 20	26, 81, 141, 196	0
34	RO	122/122 (100%)	0.21	2 (1%) 70 56	26, 58, 90, 120	0
34	YO	122/122 (100%)	0.12	1 (0%) 82 71	27, 58, 91, 116	0
35	RP	150/150 (100%)	0.94	22 (14%) 6 7	19, 68, 152, 324	0
35	YP	150/150 (100%)	0.98	22 (14%) 6 7	27, 66, 149, 278	0
36	RQ	140/141 (99%)	0.77	11 (7%) 18 16	30, 70, 115, 294	0
36	YQ	139/141 (98%)	0.73	16 (11%) 9 10	35, 70, 127, 273	0
37	RR	117/118 (99%)	0.43	7 (5%) 27 21	26, 65, 100, 156	0
37	YR	117/118 (99%)	0.56	5 (4%) 40 29	33, 65, 115, 161	0
38	RS	111/112 (99%)	1.30	31 (27%) 1 2	59, 112, 201, 486	0
38	YS	111/112 (99%)	1.23	27 (24%) 2 3	54, 93, 171, 315	0
39	RT	137/146 (93%)	0.62	12 (8%) 15 14	36, 78, 172, 561	0
39	YT	137/146 (93%)	0.61	12 (8%) 15 14	29, 80, 263, 460	0
40	RU	117/118 (99%)	0.50	5 (4%) 40 29	20, 56, 126, 223	0
40	YU	117/118 (99%)	0.90	17 (14%) 6 7	32, 74, 147, 342	0
41	RV	101/101 (100%)	0.59	11 (10%) 10 11	23, 79, 142, 406	0
41	YV	101/101 (100%)	0.86	10 (9%) 13 12	27, 102, 149, 576	0
42	RW	113/113 (100%)	0.25	4 (3%) 47 34	23, 53, 113, 248	0
42	YW	113/113 (100%)	0.30	1 (0%) 81 68	26, 61, 118, 368	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RX	92/96 (95%)	0.61	5 (5%) 31 24	37, 69, 114, 140	0
43	YX	92/96 (95%)	0.28	2 (2%) 62 47	26, 55, 107, 126	0
44	RY	102/110 (92%)	1.53	29 (28%) 1 2	33, 78, 230, 539	0
44	YY	102/110 (92%)	1.43	23 (22%) 2 4	40, 95, 248, 579	0
45	RZ	176/206 (85%)	0.99	27 (15%) 5 7	54, 109, 230, 333	0
45	YZ	183/206 (88%)	0.98	29 (15%) 5 6	55, 111, 190, 333	0
46	R0	83/85 (97%)	0.79	12 (14%) 6 7	30, 69, 179, 363	0
46	Y0	83/85 (97%)	0.82	7 (8%) 17 15	29, 70, 166, 209	0
47	R1	97/98 (98%)	1.01	13 (13%) 7 8	27, 64, 206, 399	0
47	Y1	97/98 (98%)	0.88	13 (13%) 7 8	17, 46, 207, 422	0
48	R2	69/72 (95%)	0.87	11 (15%) 5 6	35, 87, 189, 288	0
48	Y2	69/72 (95%)	0.67	8 (11%) 9 10	28, 69, 119, 233	0
49	R3	59/60 (98%)	0.18	2 (3%) 48 35	36, 63, 116, 167	0
49	Y3	59/60 (98%)	0.50	5 (8%) 16 15	39, 80, 135, 184	0
50	R4	70/71 (98%)	1.80	26 (37%) 1 1	105, 280, 598, 608	0
50	Y4	70/71 (98%)	1.12	11 (15%) 5 6	92, 189, 571, 588	0
51	R5	59/60 (98%)	0.52	5 (8%) 16 15	21, 60, 201, 299	0
51	Y5	57/60 (95%)	1.06	8 (14%) 6 8	15, 71, 193, 303	0
52	R6	48/54 (88%)	2.19	20 (41%) 0 1	71, 128, 199, 285	0
52	Y6	48/54 (88%)	2.24	21 (43%) 0 1	60, 111, 181, 219	0
53	R7	49/49 (100%)	0.86	7 (14%) 6 8	15, 36, 127, 208	0
53	Y7	49/49 (100%)	0.75	7 (14%) 6 8	10, 29, 97, 215	0
54	R8	64/65 (98%)	1.26	12 (18%) 3 4	22, 50, 116, 225	0
54	Y8	64/65 (98%)	1.22	13 (20%) 3 4	22, 52, 96, 236	0
55	R9	37/37 (100%)	2.42	21 (56%) 0 0	99, 140, 190, 246	0
55	Y9	36/37 (97%)	2.19	18 (50%) 0 0	88, 155, 219, 248	0
All	All	21218/21844 (97%)	0.43	1595 (7%) 20 17	10, 78, 219, 608	0

The worst 5 of 1595 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	YY	91	GLU	11.3
52	Y6	41	PRO	10.4

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Mol	Chain	Res	Type	RSRZ
28	YE	59	VAL	10.4
11	QK	129	SER	10.0
21	XU	2	GLY	9.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	A2M	XX	21	23/24	0.77	0.14	108,164,164,164	0
23	A2M	QX	21	23/24	0.80	0.14	108,155,155,155	0
23	A2M	XX	19	23/24	0.87	0.14	99,99,108,108	0
23	A2M	QX	19	23/24	0.88	0.14	108,108,108,108	0
23	A2M	QX	20	23/24	0.89	0.11	108,114,114,114	0
23	A2M	XX	20	23/24	0.90	0.13	107,107,108,108	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	YA	3163	1/1	0.28	0.20	40,40,40,40	0
56	MG	YA	3215	1/1	0.30	0.34	79,79,79,79	0
56	MG	RA	3075	1/1	0.35	0.24	35,35,35,35	0
56	MG	QA	1630	1/1	0.40	0.25	64,64,64,64	0
56	MG	RA	3020	1/1	0.41	0.21	11,11,11,11	0
56	MG	XA	1625	1/1	0.42	0.19	80,80,80,80	0
56	MG	XD	302	1/1	0.43	0.23	85,85,85,85	0
56	MG	YH	201	1/1	0.45	0.24	118,118,118,118	0
56	MG	YA	3357	1/1	0.47	0.25	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3417	1/1	0.50	0.36	66,66,66,66	0
56	MG	QA	1733	1/1	0.52	0.36	86,86,86,86	0
56	MG	RA	3413	1/1	0.53	0.18	63,63,63,63	0
56	MG	RA	3380	1/1	0.53	0.19	61,61,61,61	0
56	MG	YA	3127	1/1	0.55	0.19	51,51,51,51	0
56	MG	YA	3396	1/1	0.57	0.10	54,54,54,54	0
56	MG	QA	1719	1/1	0.57	0.25	70,70,70,70	0
56	MG	RA	3220	1/1	0.59	0.23	43,43,43,43	0
56	MG	YA	3155	1/1	0.60	0.11	41,41,41,41	0
56	MG	YA	3304	1/1	0.60	0.28	71,71,71,71	0
56	MG	YA	3311	1/1	0.60	0.27	74,74,74,74	0
56	MG	YA	3182	1/1	0.61	0.16	58,58,58,58	0
56	MG	YA	3196	1/1	0.61	0.28	35,35,35,35	0
56	MG	YA	3083	1/1	0.61	0.28	58,58,58,58	0
56	MG	YA	3416	1/1	0.61	0.17	9,9,9,9	0
56	MG	QA	1669	1/1	0.61	0.17	71,71,71,71	0
56	MG	XA	1630	1/1	0.62	0.20	40,40,40,40	0
56	MG	QD	303	1/1	0.62	0.17	69,69,69,69	0
56	MG	RA	3343	1/1	0.62	0.23	61,61,61,61	0
56	MG	YA	3427	1/1	0.63	0.11	30,30,30,30	0
56	MG	QA	1702	1/1	0.63	0.23	81,81,81,81	0
56	MG	YA	3412	1/1	0.64	0.20	61,61,61,61	0
56	MG	RA	3357	1/1	0.64	0.23	51,51,51,51	0
56	MG	RA	3131	1/1	0.64	0.23	78,78,78,78	0
56	MG	RA	3355	1/1	0.64	0.14	58,58,58,58	0
56	MG	QA	1648	1/1	0.65	0.13	58,58,58,58	0
56	MG	XA	1658	1/1	0.65	0.18	35,35,35,35	0
56	MG	QA	1747	1/1	0.65	0.13	61,61,61,61	0
56	MG	YA	3328	1/1	0.66	0.26	38,38,38,38	0
56	MG	RA	3396	1/1	0.66	0.26	37,37,37,37	0
56	MG	RA	3211	1/1	0.66	0.17	11,11,11,11	0
56	MG	RA	3114	1/1	0.66	0.17	19,19,19,19	0
56	MG	YA	3294	1/1	0.66	0.09	56,56,56,56	0
56	MG	XA	1691	1/1	0.66	0.15	50,50,50,50	0
56	MG	YG	201	1/1	0.66	0.13	56,56,56,56	0
56	MG	XA	1696	1/1	0.66	0.19	71,71,71,71	0
56	MG	QA	1677	1/1	0.67	0.18	60,60,60,60	0
56	MG	RA	3101	1/1	0.67	0.28	37,37,37,37	0
56	MG	YA	3379	1/1	0.67	0.13	53,53,53,53	0
56	MG	YA	3392	1/1	0.67	0.21	60,60,60,60	0
56	MG	YA	3233	1/1	0.67	0.25	49,49,49,49	0
56	MG	YA	3223	1/1	0.68	0.16	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	RA	3277	1/1	0.68	0.21	67,67,67,67	0
56	MG	YA	3086	1/1	0.68	0.17	23,23,23,23	0
56	MG	QA	1724	1/1	0.68	0.10	63,63,63,63	0
56	MG	YA	3031	1/1	0.68	0.27	26,26,26,26	0
56	MG	RA	3299	1/1	0.69	0.23	48,48,48,48	0
56	MG	YA	3326	1/1	0.69	0.20	51,51,51,51	0
56	MG	XA	1755	1/1	0.69	0.14	68,68,68,68	0
56	MG	YA	3242	1/1	0.69	0.23	42,42,42,42	0
56	MG	YA	3484	1/1	0.69	0.22	24,24,24,24	0
56	MG	QA	1683	1/1	0.69	0.32	46,46,46,46	0
56	MG	QA	1693	1/1	0.69	0.24	66,66,66,66	0
56	MG	YA	3472	1/1	0.70	0.25	69,69,69,69	0
56	MG	YA	3128	1/1	0.70	0.13	37,37,37,37	0
56	MG	RY	201	1/1	0.70	0.17	43,43,43,43	0
56	MG	RA	3225	1/1	0.70	0.14	40,40,40,40	0
56	MG	RA	3182	1/1	0.71	0.23	58,58,58,58	0
56	MG	QA	1603	1/1	0.71	0.10	52,52,52,52	0
56	MG	QA	1708	1/1	0.72	0.30	42,42,42,42	0
56	MG	XA	1730	1/1	0.72	0.18	47,47,47,47	0
56	MG	RA	3399	1/1	0.72	0.37	47,47,47,47	0
56	MG	YA	3415	1/1	0.72	0.26	68,68,68,68	0
56	MG	XA	1629	1/1	0.72	0.13	53,53,53,53	0
56	MG	RA	3166	1/1	0.72	0.18	31,31,31,31	0
56	MG	XA	1656	1/1	0.72	0.23	45,45,45,45	0
56	MG	RA	3084	1/1	0.72	0.22	27,27,27,27	0
56	MG	YB	202	1/1	0.72	0.27	38,38,38,38	0
56	MG	YA	3378	1/1	0.72	0.11	52,52,52,52	0
56	MG	RA	3421	1/1	0.72	0.09	59,59,59,59	0
56	MG	RA	3215	1/1	0.73	0.14	41,41,41,41	0
56	MG	QA	1721	1/1	0.73	0.13	41,41,41,41	0
56	MG	RA	3360	1/1	0.73	0.18	51,51,51,51	0
56	MG	RA	3134	1/1	0.73	0.23	38,38,38,38	0
56	MG	YA	3040	1/1	0.73	0.28	25,25,25,25	0
56	MG	YA	3082	1/1	0.73	0.14	20,20,20,20	0
56	MG	QA	1729	1/1	0.73	0.16	31,31,31,31	0
56	MG	RA	3111	1/1	0.73	0.09	40,40,40,40	0
56	MG	RA	3406	1/1	0.73	0.30	59,59,59,59	0
56	MG	RA	3335	1/1	0.73	0.22	52,52,52,52	0
56	MG	YA	3485	1/1	0.73	0.24	22,22,22,22	0
56	MG	QA	1750	1/1	0.73	0.16	68,68,68,68	0
56	MG	XA	1700	1/1	0.73	0.24	79,79,79,79	0
56	MG	YA	3366	1/1	0.73	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1699	1/1	0.74	0.22	78,78,78,78	0
56	MG	RA	3326	1/1	0.74	0.22	56,56,56,56	0
56	MG	YA	3276	1/1	0.74	0.23	31,31,31,31	0
56	MG	RA	3168	1/1	0.74	0.27	54,54,54,54	0
56	MG	RA	3171	1/1	0.74	0.19	51,51,51,51	0
56	MG	YA	3132	1/1	0.74	0.36	60,60,60,60	0
56	MG	XA	1759	1/1	0.74	0.21	63,63,63,63	0
56	MG	QA	1699	1/1	0.74	0.12	55,55,55,55	0
56	MG	RA	3232	1/1	0.74	0.26	45,45,45,45	0
56	MG	RA	3204	1/1	0.74	0.19	52,52,52,52	0
56	MG	YA	3068	1/1	0.74	0.18	32,32,32,32	0
56	MG	QA	1695	1/1	0.74	0.23	47,47,47,47	0
56	MG	RA	3017	1/1	0.75	0.10	17,17,17,17	0
56	MG	RA	3261	1/1	0.75	0.33	45,45,45,45	0
56	MG	YA	3481	1/1	0.75	0.33	44,44,44,44	0
56	MG	RA	3005	1/1	0.75	0.42	32,32,32,32	0
56	MG	YA	3422	1/1	0.76	0.11	58,58,58,58	0
56	MG	RA	3214	1/1	0.76	0.11	33,33,33,33	0
56	MG	QA	1722	1/1	0.76	0.21	52,52,52,52	0
56	MG	RA	3405	1/1	0.76	0.12	43,43,43,43	0
56	MG	YA	3099	1/1	0.76	0.33	68,68,68,68	0
56	MG	QA	1732	1/1	0.76	0.15	54,54,54,54	0
56	MG	RA	3330	1/1	0.76	0.14	43,43,43,43	0
56	MG	YA	3231	1/1	0.76	0.24	30,30,30,30	0
56	MG	RA	3264	1/1	0.76	0.26	42,42,42,42	0
56	MG	XA	1701	1/1	0.77	0.20	42,42,42,42	0
56	MG	RA	3316	1/1	0.77	0.22	57,57,57,57	0
56	MG	YA	3315	1/1	0.77	0.22	53,53,53,53	0
56	MG	XA	1742	1/1	0.77	0.28	73,73,73,73	0
56	MG	XA	1754	1/1	0.77	0.19	55,55,55,55	0
56	MG	QA	1663	1/1	0.77	0.41	68,68,68,68	0
56	MG	QA	1636	1/1	0.77	0.31	56,56,56,56	0
56	MG	RA	3300	1/1	0.77	0.15	40,40,40,40	0
56	MG	RA	3307	1/1	0.77	0.10	49,49,49,49	0
56	MG	YA	3152	1/1	0.77	0.24	54,54,54,54	0
56	MG	XA	1641	1/1	0.77	0.17	51,51,51,51	0
56	MG	YA	3406	1/1	0.77	0.24	60,60,60,60	0
56	MG	YA	3195	1/1	0.78	0.16	51,51,51,51	0
56	MG	RA	3083	1/1	0.78	0.17	5,5,5,5	0
56	MG	YA	3321	1/1	0.78	0.11	60,60,60,60	0
56	MG	YA	3420	1/1	0.78	0.16	23,23,23,23	0
56	MG	YA	3214	1/1	0.78	0.34	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3393	1/1	0.78	0.13	38,38,38,38	0
56	MG	XA	1693	1/1	0.78	0.11	36,36,36,36	0
56	MG	RA	3262	1/1	0.78	0.13	48,48,48,48	0
56	MG	RA	3347	1/1	0.78	0.30	83,83,83,83	0
56	MG	RA	3129	1/1	0.78	0.08	14,14,14,14	0
56	MG	RA	3229	1/1	0.78	0.08	44,44,44,44	0
56	MG	RA	3410	1/1	0.78	0.38	70,70,70,70	0
56	MG	QA	1742	1/1	0.78	0.07	22,22,22,22	0
56	MG	YA	3278	1/1	0.79	0.24	52,52,52,52	0
56	MG	YA	3280	1/1	0.79	0.46	40,40,40,40	0
56	MG	YA	3287	1/1	0.79	0.19	47,47,47,47	0
56	MG	YA	3153	1/1	0.79	0.23	37,37,37,37	0
56	MG	YA	3480	1/1	0.79	0.10	65,65,65,65	0
56	MG	RA	3293	1/1	0.79	0.22	58,58,58,58	0
56	MG	YA	3159	1/1	0.79	0.23	28,28,28,28	0
56	MG	R2	101	1/1	0.79	0.26	62,62,62,62	0
56	MG	XA	1705	1/1	0.79	0.20	38,38,38,38	0
56	MG	QA	1627	1/1	0.79	0.65	72,72,72,72	0
56	MG	RA	3339	1/1	0.79	0.22	44,44,44,44	0
56	MG	Y5	102	1/1	0.79	0.22	47,47,47,47	0
56	MG	RA	3254	1/1	0.80	0.14	46,46,46,46	0
56	MG	RA	3102	1/1	0.80	0.17	10,10,10,10	0
56	MG	RA	3423	1/1	0.80	0.18	42,42,42,42	0
56	MG	RA	3435	1/1	0.80	0.26	64,64,64,64	0
56	MG	YA	3408	1/1	0.80	0.18	73,73,73,73	0
56	MG	YA	3275	1/1	0.80	0.28	41,41,41,41	0
56	MG	RD	301	1/1	0.80	0.09	24,24,24,24	0
56	MG	RQ	202	1/1	0.80	0.21	48,48,48,48	0
56	MG	QA	1703	1/1	0.80	0.24	47,47,47,47	0
56	MG	YA	3149	1/1	0.80	0.19	54,54,54,54	0
56	MG	RA	3014	1/1	0.80	0.36	3,3,3,3	0
56	MG	YA	3437	1/1	0.80	0.23	89,89,89,89	0
56	MG	YA	3448	1/1	0.80	0.25	51,51,51,51	0
56	MG	XA	1607	1/1	0.80	0.40	43,43,43,43	0
56	MG	QA	1734	1/1	0.80	0.25	52,52,52,52	0
56	MG	XA	1627	1/1	0.80	0.12	57,57,57,57	0
56	MG	QA	1728	1/1	0.80	0.18	48,48,48,48	0
56	MG	RA	3227	1/1	0.80	0.14	53,53,53,53	0
56	MG	XF	201	1/1	0.80	0.12	39,39,39,39	0
56	MG	RA	3408	1/1	0.80	0.46	53,53,53,53	0
56	MG	RA	3133	1/1	0.80	0.29	52,52,52,52	0
56	MG	RA	3206	1/1	0.80	0.12	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1637	1/1	0.81	0.14	49,49,49,49	0
56	MG	RA	3249	1/1	0.81	0.09	47,47,47,47	0
56	MG	YA	3426	1/1	0.81	0.14	34,34,34,34	0
56	MG	XA	1719	1/1	0.81	0.11	50,50,50,50	0
56	MG	RA	3128	1/1	0.81	0.17	43,43,43,43	0
56	MG	RA	3184	1/1	0.81	0.19	24,24,24,24	0
56	MG	XA	1750	1/1	0.81	0.11	44,44,44,44	0
56	MG	XA	1611	1/1	0.81	0.25	46,46,46,46	0
56	MG	RA	3148	1/1	0.81	0.12	19,19,19,19	0
56	MG	YA	3397	1/1	0.81	0.14	58,58,58,58	0
56	MG	QA	1735	1/1	0.81	0.39	66,66,66,66	0
56	MG	YA	3129	1/1	0.81	0.24	41,41,41,41	0
56	MG	RA	3037	1/1	0.81	0.26	24,24,24,24	0
56	MG	YA	3318	1/1	0.81	0.27	43,43,43,43	0
56	MG	QA	1637	1/1	0.81	0.37	53,53,53,53	0
56	MG	YA	3395	1/1	0.82	0.09	46,46,46,46	0
56	MG	QA	1745	1/1	0.82	0.09	44,44,44,44	0
56	MG	RA	3391	1/1	0.82	0.20	19,19,19,19	0
56	MG	XA	1632	1/1	0.82	0.28	46,46,46,46	0
56	MG	XA	1635	1/1	0.82	0.23	36,36,36,36	0
56	MG	RA	3051	1/1	0.82	0.26	62,62,62,62	0
56	MG	RB	203	1/1	0.82	0.27	37,37,37,37	0
56	MG	XA	1648	1/1	0.82	0.21	53,53,53,53	0
56	MG	XA	1652	1/1	0.82	0.35	48,48,48,48	0
56	MG	RA	3105	1/1	0.82	0.19	33,33,33,33	0
56	MG	RA	3276	1/1	0.82	0.26	50,50,50,50	0
56	MG	YA	3007	1/1	0.82	0.42	38,38,38,38	0
56	MG	RA	3069	1/1	0.82	0.27	23,23,23,23	0
56	MG	YA	3188	1/1	0.82	0.28	38,38,38,38	0
56	MG	RA	3279	1/1	0.82	0.14	26,26,26,26	0
56	MG	QA	1646	1/1	0.82	0.22	36,36,36,36	0
56	MG	YA	3204	1/1	0.82	0.14	10,10,10,10	0
56	MG	QA	1720	1/1	0.82	0.21	53,53,53,53	0
56	MG	YA	3371	1/1	0.82	0.27	57,57,57,57	0
56	MG	QA	1608	1/1	0.82	0.36	25,25,25,25	0
56	MG	RA	3256	1/1	0.82	0.43	93,93,93,93	0
56	MG	YA	3390	1/1	0.82	0.13	54,54,54,54	0
56	MG	YA	3095	1/1	0.82	0.20	52,52,52,52	0
56	MG	YA	3268	1/1	0.83	0.29	49,49,49,49	0
56	MG	QA	1725	1/1	0.83	0.13	64,64,64,64	0
56	MG	YA	3048	1/1	0.83	0.13	22,22,22,22	0
56	MG	XA	1620	1/1	0.83	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3279	1/1	0.83	0.09	54,54,54,54	0
56	MG	XA	1624	1/1	0.83	0.18	59,59,59,59	0
56	MG	YA	3179	1/1	0.83	0.18	41,41,41,41	0
56	MG	RA	3297	1/1	0.83	0.20	47,47,47,47	0
56	MG	YA	3187	1/1	0.83	0.18	19,19,19,19	0
56	MG	RA	3233	1/1	0.83	0.19	25,25,25,25	0
56	MG	RA	3331	1/1	0.83	0.17	69,69,69,69	0
56	MG	YA	3317	1/1	0.83	0.26	48,48,48,48	0
56	MG	RQ	201	1/1	0.83	0.09	23,23,23,23	0
56	MG	YA	3436	1/1	0.83	0.34	51,51,51,51	0
56	MG	XA	1763	1/1	0.83	0.10	52,52,52,52	0
56	MG	RA	3108	1/1	0.83	0.30	33,33,33,33	0
56	MG	RA	3253	1/1	0.83	0.33	59,59,59,59	0
56	MG	YA	3331	1/1	0.83	0.13	24,24,24,24	0
56	MG	RA	3311	1/1	0.83	0.29	55,55,55,55	0
56	MG	YA	3482	1/1	0.83	0.22	69,69,69,69	0
56	MG	YA	3227	1/1	0.83	0.18	53,53,53,53	0
56	MG	YA	3140	1/1	0.83	0.10	58,58,58,58	0
56	MG	YA	3013	1/1	0.83	0.30	0,0,0,0	0
56	MG	RA	3345	1/1	0.83	0.18	42,42,42,42	0
56	MG	YA	3244	1/1	0.83	0.18	54,54,54,54	0
56	MG	YA	3391	1/1	0.83	0.16	44,44,44,44	0
56	MG	YA	3211	1/1	0.84	0.13	22,22,22,22	0
56	MG	XA	1683	1/1	0.84	0.19	31,31,31,31	0
56	MG	XA	1686	1/1	0.84	0.41	64,64,64,64	0
56	MG	YA	3220	1/1	0.84	0.14	33,33,33,33	0
56	MG	RA	3057	1/1	0.84	0.34	2,2,2,2	0
56	MG	RA	3273	1/1	0.84	0.10	44,44,44,44	0
56	MG	RA	3404	1/1	0.84	0.19	48,48,48,48	0
56	MG	QA	1618	1/1	0.84	0.16	29,29,29,29	0
56	MG	RA	3198	1/1	0.84	0.20	26,26,26,26	0
56	MG	YA	3401	1/1	0.84	0.14	43,43,43,43	0
56	MG	XA	1621	1/1	0.84	0.25	38,38,38,38	0
56	MG	YA	3265	1/1	0.84	0.21	40,40,40,40	0
56	MG	RA	3340	1/1	0.84	0.24	72,72,72,72	0
56	MG	XA	1715	1/1	0.84	0.34	52,52,52,52	0
56	MG	QA	1673	1/1	0.84	0.16	70,70,70,70	0
56	MG	XA	1727	1/1	0.84	0.36	78,78,78,78	0
56	MG	XA	1729	1/1	0.84	0.18	47,47,47,47	0
56	MG	YA	3145	1/1	0.84	0.14	68,68,68,68	0
56	MG	QA	1674	1/1	0.84	0.18	27,27,27,27	0
56	MG	RA	3236	1/1	0.84	0.30	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3303	1/1	0.84	0.35	69,69,69,69	0
56	MG	XA	1743	1/1	0.84	0.11	53,53,53,53	0
56	MG	RA	3420	1/1	0.84	0.14	35,35,35,35	0
56	MG	RA	3352	1/1	0.84	0.23	62,62,62,62	0
56	MG	QA	1738	1/1	0.84	0.07	32,32,32,32	0
56	MG	RA	3213	1/1	0.84	0.34	21,21,21,21	0
56	MG	RA	3438	1/1	0.84	0.16	23,23,23,23	0
56	MG	RA	3095	1/1	0.84	0.31	45,45,45,45	0
56	MG	QA	1665	1/1	0.84	0.16	51,51,51,51	0
56	MG	RA	3218	1/1	0.84	0.13	13,13,13,13	0
56	MG	RA	3178	1/1	0.84	0.13	32,32,32,32	0
56	MG	XA	1672	1/1	0.84	0.08	44,44,44,44	0
56	MG	RA	3049	1/1	0.85	0.18	19,19,19,19	0
56	MG	YA	3389	1/1	0.85	0.18	49,49,49,49	0
56	MG	QA	1656	1/1	0.85	0.29	26,26,26,26	0
56	MG	YA	3249	1/1	0.85	0.19	34,34,34,34	0
56	MG	RA	3147	1/1	0.85	0.11	41,41,41,41	0
56	MG	QA	1692	1/1	0.85	0.32	65,65,65,65	0
56	MG	YA	3270	1/1	0.85	0.23	49,49,49,49	0
56	MG	RA	3281	1/1	0.85	0.09	57,57,57,57	0
56	MG	XA	1612	1/1	0.85	0.11	39,39,39,39	0
56	MG	RA	3157	1/1	0.85	0.10	43,43,43,43	0
56	MG	YA	3164	1/1	0.85	0.14	38,38,38,38	0
56	MG	QA	1743	1/1	0.85	0.13	57,57,57,57	0
56	MG	QA	1662	1/1	0.85	0.15	40,40,40,40	0
56	MG	YA	3184	1/1	0.85	0.27	28,28,28,28	0
56	MG	RA	3350	1/1	0.85	0.20	45,45,45,45	0
56	MG	RA	3351	1/1	0.85	0.11	75,75,75,75	0
56	MG	YA	3423	1/1	0.85	0.16	23,23,23,23	0
56	MG	QA	1628	1/1	0.85	0.07	68,68,68,68	0
56	MG	RA	3259	1/1	0.85	0.28	46,46,46,46	0
56	MG	RA	3309	1/1	0.85	0.29	45,45,45,45	0
56	MG	QA	1622	1/1	0.85	0.22	29,29,29,29	0
56	MG	YA	3438	1/1	0.85	0.21	68,68,68,68	0
56	MG	YA	3319	1/1	0.85	0.16	47,47,47,47	0
56	MG	YA	3451	1/1	0.85	0.14	38,38,38,38	0
56	MG	RA	3439	1/1	0.85	0.25	50,50,50,50	0
56	MG	YA	3121	1/1	0.85	0.15	52,52,52,52	0
56	MG	XA	1738	1/1	0.85	0.14	45,45,45,45	0
56	MG	RA	3440	1/1	0.85	0.16	12,12,12,12	0
56	MG	YA	3333	1/1	0.85	0.12	47,47,47,47	0
56	MG	YA	3346	1/1	0.85	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3041	1/1	0.85	0.18	7,7,7,7	0
56	MG	RA	3100	1/1	0.85	0.25	52,52,52,52	0
56	MG	RA	3329	1/1	0.85	0.12	46,46,46,46	0
56	MG	YA	3234	1/1	0.85	0.12	30,30,30,30	0
56	MG	RA	3358	1/1	0.86	0.07	45,45,45,45	0
56	MG	RA	3169	1/1	0.86	0.19	47,47,47,47	0
56	MG	RA	3070	1/1	0.86	0.27	25,25,25,25	0
56	MG	RA	3431	1/1	0.86	0.37	40,40,40,40	0
56	MG	QA	1680	1/1	0.86	0.12	48,48,48,48	0
56	MG	RA	3180	1/1	0.86	0.18	53,53,53,53	0
56	MG	QA	1672	1/1	0.86	0.30	54,54,54,54	0
56	MG	YA	3001	1/1	0.86	0.40	73,73,73,73	0
56	MG	QA	1675	1/1	0.86	0.21	42,42,42,42	0
56	MG	QA	1647	1/1	0.86	0.19	55,55,55,55	0
56	MG	RA	3202	1/1	0.86	0.15	22,22,22,22	0
56	MG	YA	3425	1/1	0.86	0.57	62,62,62,62	0
56	MG	RA	3270	1/1	0.86	0.19	51,51,51,51	0
56	MG	YA	3045	1/1	0.86	0.19	3,3,3,3	0
56	MG	YA	3433	1/1	0.86	0.13	34,34,34,34	0
56	MG	RA	3127	1/1	0.86	0.32	52,52,52,52	0
56	MG	YA	3342	1/1	0.86	0.38	66,66,66,66	0
56	MG	YA	3252	1/1	0.86	0.30	47,47,47,47	0
56	MG	YA	3447	1/1	0.86	0.09	38,38,38,38	0
56	MG	YA	3355	1/1	0.86	0.25	63,63,63,63	0
56	MG	YA	3260	1/1	0.86	0.22	32,32,32,32	0
56	MG	YA	3059	1/1	0.86	0.09	15,15,15,15	0
56	MG	YA	3473	1/1	0.86	0.11	30,30,30,30	0
56	MG	YA	3178	1/1	0.86	0.12	36,36,36,36	0
56	MG	RR	201	1/1	0.86	0.24	31,31,31,31	0
56	MG	YA	3074	1/1	0.86	0.30	21,21,21,21	0
56	MG	YA	3483	1/1	0.86	0.31	58,58,58,58	0
56	MG	YA	3384	1/1	0.86	0.37	64,64,64,64	0
56	MG	RA	3318	1/1	0.86	0.10	32,32,32,32	0
56	MG	RA	3060	1/1	0.86	0.16	14,14,14,14	0
56	MG	RA	3416	1/1	0.86	0.34	58,58,58,58	0
56	MG	QV	101	1/1	0.86	0.10	31,31,31,31	0
56	MG	YA	3283	1/1	0.86	0.09	37,37,37,37	0
56	MG	Y5	103	1/1	0.86	0.19	41,41,41,41	0
56	MG	RA	3412	1/1	0.87	0.16	34,34,34,34	0
56	MG	YA	3383	1/1	0.87	0.13	34,34,34,34	0
56	MG	YA	3090	1/1	0.87	0.07	43,43,43,43	0
56	MG	YA	3091	1/1	0.87	0.15	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3342	1/1	0.87	0.35	61,61,61,61	0
56	MG	YA	3097	1/1	0.87	0.17	21,21,21,21	0
56	MG	RA	3290	1/1	0.87	0.10	40,40,40,40	0
56	MG	QA	1626	1/1	0.87	0.18	46,46,46,46	0
56	MG	RA	3141	1/1	0.87	0.09	31,31,31,31	0
56	MG	RA	3298	1/1	0.87	0.06	52,52,52,52	0
56	MG	RA	3121	1/1	0.87	0.10	45,45,45,45	0
56	MG	RA	3258	1/1	0.87	0.19	51,51,51,51	0
56	MG	XA	1745	1/1	0.87	0.15	45,45,45,45	0
56	MG	XA	1748	1/1	0.87	0.18	66,66,66,66	0
56	MG	XA	1636	1/1	0.87	0.28	57,57,57,57	0
56	MG	RA	3124	1/1	0.87	0.20	32,32,32,32	0
56	MG	RA	3191	1/1	0.87	0.12	15,15,15,15	0
56	MG	YA	3421	1/1	0.87	0.14	68,68,68,68	0
56	MG	XA	1757	1/1	0.87	0.30	60,60,60,60	0
56	MG	YA	3291	1/1	0.87	0.21	33,33,33,33	0
56	MG	RA	3043	1/1	0.87	0.22	17,17,17,17	0
56	MG	RA	3359	1/1	0.87	0.08	16,16,16,16	0
56	MG	QA	1625	1/1	0.87	0.21	66,66,66,66	0
56	MG	YA	3307	1/1	0.87	0.22	46,46,46,46	0
56	MG	RA	3231	1/1	0.87	0.22	50,50,50,50	0
56	MG	YA	3313	1/1	0.87	0.17	25,25,25,25	0
56	MG	RA	3324	1/1	0.87	0.21	45,45,45,45	0
56	MG	YA	3441	1/1	0.87	0.14	49,49,49,49	0
56	MG	YA	3004	1/1	0.87	0.22	12,12,12,12	0
56	MG	YA	3006	1/1	0.87	0.29	32,32,32,32	0
56	MG	XA	1677	1/1	0.87	0.15	36,36,36,36	0
56	MG	YA	3458	1/1	0.87	0.16	51,51,51,51	0
56	MG	YA	3462	1/1	0.87	0.14	48,48,48,48	0
56	MG	QA	1632	1/1	0.87	0.24	57,57,57,57	0
56	MG	YA	3322	1/1	0.87	0.20	55,55,55,55	0
56	MG	RA	3274	1/1	0.87	0.23	44,44,44,44	0
56	MG	XA	1689	1/1	0.87	0.21	31,31,31,31	0
56	MG	QA	1712	1/1	0.87	0.14	46,46,46,46	0
56	MG	YA	3208	1/1	0.87	0.20	27,27,27,27	0
56	MG	QA	1716	1/1	0.87	0.21	36,36,36,36	0
56	MG	YA	3053	1/1	0.87	0.24	27,27,27,27	0
56	MG	RA	3247	1/1	0.87	0.30	26,26,26,26	0
56	MG	YF	301	1/1	0.87	0.20	37,37,37,37	0
56	MG	XA	1609	1/1	0.87	0.08	79,79,79,79	0
56	MG	RA	3176	1/1	0.87	0.17	34,34,34,34	0
56	MG	RA	3288	1/1	0.87	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3341	1/1	0.87	0.14	31,31,31,31	0
56	MG	YA	3372	1/1	0.88	0.11	37,37,37,37	0
56	MG	RA	3125	1/1	0.88	0.15	26,26,26,26	0
56	MG	RA	3239	1/1	0.88	0.21	45,45,45,45	0
56	MG	RA	3061	1/1	0.88	0.24	17,17,17,17	0
56	MG	RA	3422	1/1	0.88	0.09	43,43,43,43	0
56	MG	YA	3386	1/1	0.88	0.30	54,54,54,54	0
56	MG	XA	1731	1/1	0.88	0.26	47,47,47,47	0
56	MG	XA	1737	1/1	0.88	0.29	14,14,14,14	0
56	MG	YA	3250	1/1	0.88	0.27	27,27,27,27	0
56	MG	RA	3319	1/1	0.88	0.05	50,50,50,50	0
56	MG	YA	3098	1/1	0.88	0.12	47,47,47,47	0
56	MG	YA	3263	1/1	0.88	0.13	41,41,41,41	0
56	MG	XA	1634	1/1	0.88	0.10	46,46,46,46	0
56	MG	RA	3068	1/1	0.88	0.28	13,13,13,13	0
56	MG	RA	3278	1/1	0.88	0.19	46,46,46,46	0
56	MG	XA	1747	1/1	0.88	0.10	45,45,45,45	0
56	MG	YA	3410	1/1	0.88	0.10	28,28,28,28	0
56	MG	RA	3379	1/1	0.88	0.23	26,26,26,26	0
56	MG	YA	3277	1/1	0.88	0.16	38,38,38,38	0
56	MG	RA	3251	1/1	0.88	0.07	63,63,63,63	0
56	MG	RA	3382	1/1	0.88	0.20	28,28,28,28	0
56	MG	RA	3389	1/1	0.88	0.14	22,22,22,22	0
56	MG	RA	3216	1/1	0.88	0.25	36,36,36,36	0
56	MG	XA	1758	1/1	0.88	0.35	51,51,51,51	0
56	MG	RA	3092	1/1	0.88	0.12	41,41,41,41	0
56	MG	QA	1614	1/1	0.88	0.10	38,38,38,38	0
56	MG	YA	3300	1/1	0.88	0.16	48,48,48,48	0
56	MG	YA	3430	1/1	0.88	0.14	55,55,55,55	0
56	MG	YA	3431	1/1	0.88	0.19	52,52,52,52	0
56	MG	RA	3291	1/1	0.88	0.23	31,31,31,31	0
56	MG	XA	1681	1/1	0.88	0.14	22,22,22,22	0
56	MG	RA	3400	1/1	0.88	0.14	30,30,30,30	0
56	MG	YA	3309	1/1	0.88	0.12	30,30,30,30	0
56	MG	R1	101	1/1	0.88	0.23	46,46,46,46	0
56	MG	YA	3446	1/1	0.88	0.14	20,20,20,20	0
56	MG	RA	3292	1/1	0.88	0.39	31,31,31,31	0
56	MG	RA	3192	1/1	0.88	0.28	15,15,15,15	0
56	MG	RA	3099	1/1	0.88	0.20	25,25,25,25	0
56	MG	YA	3017	1/1	0.88	0.40	30,30,30,30	0
56	MG	QA	1606	1/1	0.88	0.20	18,18,18,18	0
56	MG	YA	3464	1/1	0.88	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3467	1/1	0.88	0.21	68,68,68,68	0
56	MG	YA	3194	1/1	0.88	0.10	17,17,17,17	0
56	MG	RA	3174	1/1	0.88	0.08	26,26,26,26	0
56	MG	YA	3479	1/1	0.88	0.15	52,52,52,52	0
56	MG	XA	1615	1/1	0.88	0.19	37,37,37,37	0
56	MG	RA	3175	1/1	0.88	0.27	46,46,46,46	0
56	MG	YA	3050	1/1	0.88	0.35	24,24,24,24	0
56	MG	YA	3210	1/1	0.88	0.19	25,25,25,25	0
56	MG	RA	3268	1/1	0.88	0.25	48,48,48,48	0
56	MG	YA	3344	1/1	0.88	0.20	35,35,35,35	0
56	MG	YA	3056	1/1	0.88	0.29	1,1,1,1	0
56	MG	XA	1706	1/1	0.88	0.12	37,37,37,37	0
56	MG	YA	3067	1/1	0.88	0.29	19,19,19,19	0
56	MG	XA	1710	1/1	0.88	0.25	48,48,48,48	0
56	MG	YQ	201	1/1	0.88	0.14	44,44,44,44	0
56	MG	YY	201	1/1	0.88	0.13	31,31,31,31	0
56	MG	YA	3369	1/1	0.88	0.08	35,35,35,35	0
56	MG	QA	1668	1/1	0.88	0.18	45,45,45,45	0
56	MG	YA	3026	1/1	0.89	0.28	30,30,30,30	0
56	MG	YA	3398	1/1	0.89	0.15	55,55,55,55	0
56	MG	YA	3285	1/1	0.89	0.16	26,26,26,26	0
56	MG	RA	3237	1/1	0.89	0.09	23,23,23,23	0
56	MG	QA	1731	1/1	0.89	0.06	34,34,34,34	0
56	MG	YA	3180	1/1	0.89	0.37	58,58,58,58	0
56	MG	RA	3320	1/1	0.89	0.42	63,63,63,63	0
56	MG	RA	3245	1/1	0.89	0.13	34,34,34,34	0
56	MG	RA	3366	1/1	0.89	0.07	67,67,67,67	0
56	MG	XA	1725	1/1	0.89	0.30	44,44,44,44	0
56	MG	RA	3367	1/1	0.89	0.09	46,46,46,46	0
56	MG	QA	1657	1/1	0.89	0.13	20,20,20,20	0
56	MG	RA	3434	1/1	0.89	0.16	37,37,37,37	0
56	MG	QA	1687	1/1	0.89	0.21	52,52,52,52	0
56	MG	RA	3436	1/1	0.89	0.17	8,8,8,8	0
56	MG	RA	3063	1/1	0.89	0.30	29,29,29,29	0
56	MG	RA	3002	1/1	0.89	0.26	42,42,42,42	0
56	MG	RA	3390	1/1	0.89	0.28	49,49,49,49	0
56	MG	RB	202	1/1	0.89	0.23	29,29,29,29	0
56	MG	RA	3150	1/1	0.89	0.16	40,40,40,40	0
56	MG	RA	3151	1/1	0.89	0.21	52,52,52,52	0
56	MG	YA	3329	1/1	0.89	0.20	45,45,45,45	0
56	MG	YA	3096	1/1	0.89	0.22	40,40,40,40	0
56	MG	RA	3394	1/1	0.89	0.21	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3334	1/1	0.89	0.38	52,52,52,52	0
56	MG	YA	3335	1/1	0.89	0.26	16,16,16,16	0
56	MG	XA	1753	1/1	0.89	0.20	70,70,70,70	0
56	MG	XA	1665	1/1	0.89	0.23	26,26,26,26	0
56	MG	YA	3109	1/1	0.89	0.30	14,14,14,14	0
56	MG	YA	3347	1/1	0.89	0.21	29,29,29,29	0
56	MG	YA	3116	1/1	0.89	0.22	16,16,16,16	0
56	MG	YA	3469	1/1	0.89	0.13	68,68,68,68	0
56	MG	RA	3156	1/1	0.89	0.11	30,30,30,30	0
56	MG	XA	1675	1/1	0.89	0.26	46,46,46,46	0
56	MG	YA	3476	1/1	0.89	0.09	45,45,45,45	0
56	MG	YA	3368	1/1	0.89	0.20	59,59,59,59	0
56	MG	QA	1715	1/1	0.89	0.21	72,72,72,72	0
56	MG	YA	3256	1/1	0.89	0.06	29,29,29,29	0
56	MG	YA	3258	1/1	0.89	0.13	46,46,46,46	0
56	MG	RA	3165	1/1	0.89	0.22	25,25,25,25	0
56	MG	RA	3194	1/1	0.89	0.17	21,21,21,21	0
56	MG	RA	3230	1/1	0.89	0.18	20,20,20,20	0
56	MG	XA	1603	1/1	0.89	0.18	24,24,24,24	0
56	MG	YB	203	1/1	0.89	0.26	27,27,27,27	0
56	MG	RA	3306	1/1	0.89	0.41	63,63,63,63	0
56	MG	XA	1608	1/1	0.89	0.24	30,30,30,30	0
56	MG	RA	3012	1/1	0.89	0.43	29,29,29,29	0
56	MG	RA	3201	1/1	0.89	0.12	57,57,57,57	0
56	MG	YA	3157	1/1	0.89	0.16	32,32,32,32	0
56	MG	RA	3050	1/1	0.89	0.29	6,6,6,6	0
56	MG	QA	1705	1/1	0.89	0.14	37,37,37,37	0
56	MG	YA	3114	1/1	0.90	0.17	20,20,20,20	0
56	MG	RA	3312	1/1	0.90	0.15	26,26,26,26	0
56	MG	YA	3261	1/1	0.90	0.17	40,40,40,40	0
56	MG	QA	1723	1/1	0.90	0.22	46,46,46,46	0
56	MG	YA	3123	1/1	0.90	0.16	30,30,30,30	0
56	MG	RA	3022	1/1	0.90	0.30	17,17,17,17	0
56	MG	RA	3073	1/1	0.90	0.41	35,35,35,35	0
56	MG	YA	3271	1/1	0.90	0.16	32,32,32,32	0
56	MG	QA	1609	1/1	0.90	0.19	27,27,27,27	0
56	MG	YA	3130	1/1	0.90	0.21	37,37,37,37	0
56	MG	YA	3402	1/1	0.90	0.20	70,70,70,70	0
56	MG	YA	3403	1/1	0.90	0.20	42,42,42,42	0
56	MG	RA	3374	1/1	0.90	0.13	51,51,51,51	0
56	MG	RA	3427	1/1	0.90	0.13	35,35,35,35	0
56	MG	QA	1717	1/1	0.90	0.33	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3146	1/1	0.90	0.15	24,24,24,24	0
56	MG	YA	3282	1/1	0.90	0.21	49,49,49,49	0
56	MG	QA	1737	1/1	0.90	0.23	43,43,43,43	0
56	MG	YA	3151	1/1	0.90	0.11	26,26,26,26	0
56	MG	RA	3089	1/1	0.90	0.23	18,18,18,18	0
56	MG	YA	3289	1/1	0.90	0.08	44,44,44,44	0
56	MG	YA	3012	1/1	0.90	0.19	14,14,14,14	0
56	MG	XA	1702	1/1	0.90	0.33	46,46,46,46	0
56	MG	RA	3046	1/1	0.90	0.20	7,7,7,7	0
56	MG	YA	3022	1/1	0.90	0.22	49,49,49,49	0
56	MG	YA	3428	1/1	0.90	0.18	55,55,55,55	0
56	MG	YA	3429	1/1	0.90	0.18	38,38,38,38	0
56	MG	RA	3093	1/1	0.90	0.07	27,27,27,27	0
56	MG	XA	1631	1/1	0.90	0.16	14,14,14,14	0
56	MG	XA	1713	1/1	0.90	0.14	48,48,48,48	0
56	MG	QV	103	1/1	0.90	0.13	45,45,45,45	0
56	MG	YA	3312	1/1	0.90	0.26	63,63,63,63	0
56	MG	YA	3047	1/1	0.90	0.15	10,10,10,10	0
56	MG	RA	3096	1/1	0.90	0.08	44,44,44,44	0
56	MG	YA	3443	1/1	0.90	0.16	17,17,17,17	0
56	MG	YA	3445	1/1	0.90	0.13	19,19,19,19	0
56	MG	QA	1638	1/1	0.90	0.26	64,64,64,64	0
56	MG	YA	3051	1/1	0.90	0.26	38,38,38,38	0
56	MG	RA	3004	1/1	0.90	0.26	16,16,16,16	0
56	MG	QA	1696	1/1	0.90	0.37	67,67,67,67	0
56	MG	RA	3010	1/1	0.90	0.15	14,14,14,14	0
56	MG	XA	1643	1/1	0.90	0.19	23,23,23,23	0
56	MG	YA	3463	1/1	0.90	0.13	53,53,53,53	0
56	MG	XA	1733	1/1	0.90	0.12	47,47,47,47	0
56	MG	XA	1645	1/1	0.90	0.14	35,35,35,35	0
56	MG	YA	3079	1/1	0.90	0.20	34,34,34,34	0
56	MG	RA	3104	1/1	0.90	0.28	28,28,28,28	0
56	MG	QA	1688	1/1	0.90	0.07	31,31,31,31	0
56	MG	YA	3084	1/1	0.90	0.12	11,11,11,11	0
56	MG	YA	3341	1/1	0.90	0.48	71,71,71,71	0
56	MG	XA	1654	1/1	0.90	0.33	42,42,42,42	0
56	MG	QA	1681	1/1	0.90	0.32	37,37,37,37	0
56	MG	YA	3224	1/1	0.90	0.22	22,22,22,22	0
56	MG	RA	3167	1/1	0.90	0.15	54,54,54,54	0
56	MG	RA	3066	1/1	0.90	0.18	31,31,31,31	0
56	MG	XA	1749	1/1	0.90	0.20	39,39,39,39	0
56	MG	R5	102	1/1	0.90	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3239	1/1	0.90	0.24	40,40,40,40	0
56	MG	QA	1746	1/1	0.90	0.22	56,56,56,56	0
56	MG	XA	1676	1/1	0.90	0.06	32,32,32,32	0
56	MG	YA	3101	1/1	0.90	0.29	25,25,25,25	0
56	MG	YO	201	1/1	0.90	0.14	49,49,49,49	0
56	MG	YA	3103	1/1	0.90	0.22	17,17,17,17	0
56	MG	RA	3116	1/1	0.90	0.24	18,18,18,18	0
56	MG	YA	3255	1/1	0.90	0.32	33,33,33,33	0
56	MG	YA	3111	1/1	0.90	0.30	53,53,53,53	0
56	MG	YA	3181	1/1	0.91	0.21	33,33,33,33	0
56	MG	YA	3405	1/1	0.91	0.32	47,47,47,47	0
56	MG	RA	3161	1/1	0.91	0.06	39,39,39,39	0
56	MG	YA	3407	1/1	0.91	0.15	4,4,4,4	0
56	MG	RA	3304	1/1	0.91	0.17	37,37,37,37	0
56	MG	YA	3409	1/1	0.91	0.24	10,10,10,10	0
56	MG	RA	3305	1/1	0.91	0.29	42,42,42,42	0
56	MG	RA	3110	1/1	0.91	0.32	8,8,8,8	0
56	MG	YA	3078	1/1	0.91	0.19	9,9,9,9	0
56	MG	YA	3308	1/1	0.91	0.24	26,26,26,26	0
56	MG	QA	1727	1/1	0.91	0.19	43,43,43,43	0
56	MG	RA	3308	1/1	0.91	0.18	47,47,47,47	0
56	MG	RA	3426	1/1	0.91	0.29	65,65,65,65	0
56	MG	RA	3072	1/1	0.91	0.24	32,32,32,32	0
56	MG	RA	3029	1/1	0.91	0.17	16,16,16,16	0
56	MG	RA	3036	1/1	0.91	0.20	26,26,26,26	0
56	MG	QA	1643	1/1	0.91	0.17	35,35,35,35	0
56	MG	RA	3373	1/1	0.91	0.25	31,31,31,31	0
56	MG	QA	1748	1/1	0.91	0.14	47,47,47,47	0
56	MG	YA	3222	1/1	0.91	0.30	25,25,25,25	0
56	MG	YA	3324	1/1	0.91	0.23	75,75,75,75	0
56	MG	QA	1605	1/1	0.91	0.18	31,31,31,31	0
56	MG	QA	1676	1/1	0.91	0.16	31,31,31,31	0
56	MG	YA	3225	1/1	0.91	0.17	17,17,17,17	0
56	MG	YA	3330	1/1	0.91	0.08	31,31,31,31	0
56	MG	YA	3440	1/1	0.91	0.25	62,62,62,62	0
56	MG	QA	1635	1/1	0.91	0.29	38,38,38,38	0
56	MG	RA	3386	1/1	0.91	0.12	17,17,17,17	0
56	MG	RB	204	1/1	0.91	0.10	47,47,47,47	0
56	MG	XA	1673	1/1	0.91	0.11	44,44,44,44	0
56	MG	RA	3325	1/1	0.91	0.21	46,46,46,46	0
56	MG	QA	1718	1/1	0.91	0.27	47,47,47,47	0
56	MG	RA	3132	1/1	0.91	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1617	1/1	0.91	0.09	33,33,33,33	0
56	MG	YA	3459	1/1	0.91	0.16	43,43,43,43	0
56	MG	QA	1610	1/1	0.91	0.10	60,60,60,60	0
56	MG	YA	3352	1/1	0.91	0.18	35,35,35,35	0
56	MG	XS	300	1/1	0.91	0.14	29,29,29,29	0
56	MG	YA	3465	1/1	0.91	0.06	41,41,41,41	0
56	MG	RA	3333	1/1	0.91	0.15	35,35,35,35	0
56	MG	YA	3468	1/1	0.91	0.17	47,47,47,47	0
56	MG	YA	3361	1/1	0.91	0.31	68,68,68,68	0
56	MG	XA	1687	1/1	0.91	0.10	30,30,30,30	0
56	MG	RA	3397	1/1	0.91	0.19	49,49,49,49	0
56	MG	QA	1671	1/1	0.91	0.15	43,43,43,43	0
56	MG	QA	1631	1/1	0.91	0.19	33,33,33,33	0
56	MG	RA	3401	1/1	0.91	0.07	41,41,41,41	0
56	MG	RA	3402	1/1	0.91	0.21	57,57,57,57	0
56	MG	RA	3403	1/1	0.91	0.19	43,43,43,43	0
56	MG	RA	3197	1/1	0.91	0.09	30,30,30,30	0
56	MG	QA	1741	1/1	0.91	0.19	37,37,37,37	0
56	MG	RA	3103	1/1	0.91	0.31	43,43,43,43	0
56	MG	QA	1706	1/1	0.91	0.30	52,52,52,52	0
56	MG	QA	1660	1/1	0.91	0.19	14,14,14,14	0
56	MG	YB	204	1/1	0.91	0.08	49,49,49,49	0
56	MG	XA	1712	1/1	0.91	0.23	34,34,34,34	0
56	MG	YA	3049	1/1	0.91	0.30	12,12,12,12	0
56	MG	QA	1710	1/1	0.91	0.16	46,46,46,46	0
56	MG	YA	3172	1/1	0.91	0.21	53,53,53,53	0
56	MG	YA	3173	1/1	0.91	0.25	52,52,52,52	0
56	MG	XA	1714	1/1	0.91	0.24	55,55,55,55	0
56	MG	RA	3349	1/1	0.91	0.18	55,55,55,55	0
56	MG	RA	3415	1/1	0.91	0.14	53,53,53,53	0
56	MG	RA	3407	1/1	0.92	0.20	4,4,4,4	0
56	MG	RA	3091	1/1	0.92	0.10	27,27,27,27	0
56	MG	YA	3259	1/1	0.92	0.18	46,46,46,46	0
56	MG	QA	1624	1/1	0.92	0.12	31,31,31,31	0
56	MG	XA	1680	1/1	0.92	0.12	24,24,24,24	0
56	MG	RA	3411	1/1	0.92	0.27	29,29,29,29	0
56	MG	YA	3400	1/1	0.92	0.13	36,36,36,36	0
56	MG	RA	3241	1/1	0.92	0.23	27,27,27,27	0
56	MG	XA	1685	1/1	0.92	0.24	38,38,38,38	0
56	MG	RA	3209	1/1	0.92	0.26	19,19,19,19	0
56	MG	YA	3404	1/1	0.92	0.16	20,20,20,20	0
56	MG	RA	3323	1/1	0.92	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XV	103	1/1	0.92	0.23	47,47,47,47	0
56	MG	YA	3134	1/1	0.92	0.33	32,32,32,32	0
56	MG	RA	3142	1/1	0.92	0.18	24,24,24,24	0
56	MG	RA	3371	1/1	0.92	0.26	51,51,51,51	0
56	MG	XA	1617	1/1	0.92	0.20	49,49,49,49	0
56	MG	YA	3411	1/1	0.92	0.30	63,63,63,63	0
56	MG	XA	1694	1/1	0.92	0.16	38,38,38,38	0
56	MG	RA	3282	1/1	0.92	0.11	42,42,42,42	0
56	MG	XA	1698	1/1	0.92	0.11	44,44,44,44	0
56	MG	RA	3065	1/1	0.92	0.26	10,10,10,10	0
56	MG	RA	3250	1/1	0.92	0.18	22,22,22,22	0
56	MG	YA	3156	1/1	0.92	0.26	15,15,15,15	0
56	MG	QA	1711	1/1	0.92	0.24	53,53,53,53	0
56	MG	YA	3424	1/1	0.92	0.24	46,46,46,46	0
56	MG	YA	3292	1/1	0.92	0.25	35,35,35,35	0
56	MG	YA	3158	1/1	0.92	0.21	40,40,40,40	0
56	MG	YA	3296	1/1	0.92	0.14	51,51,51,51	0
56	MG	RA	3118	1/1	0.92	0.22	31,31,31,31	0
56	MG	RA	3181	1/1	0.92	0.08	40,40,40,40	0
56	MG	YA	3041	1/1	0.92	0.19	30,30,30,30	0
56	MG	RA	3334	1/1	0.92	0.21	40,40,40,40	0
56	MG	YA	3432	1/1	0.92	0.28	78,78,78,78	0
56	MG	RA	3432	1/1	0.92	0.23	91,91,91,91	0
56	MG	YA	3175	1/1	0.92	0.11	30,30,30,30	0
56	MG	XA	1711	1/1	0.92	0.24	39,39,39,39	0
56	MG	RA	3294	1/1	0.92	0.07	10,10,10,10	0
56	MG	RA	3255	1/1	0.92	0.18	38,38,38,38	0
56	MG	RA	3047	1/1	0.92	0.15	25,25,25,25	0
56	MG	YA	3442	1/1	0.92	0.16	42,42,42,42	0
56	MG	QA	1649	1/1	0.92	0.18	31,31,31,31	0
56	MG	RA	3186	1/1	0.92	0.26	45,45,45,45	0
56	MG	QA	1645	1/1	0.92	0.13	41,41,41,41	0
56	MG	YA	3060	1/1	0.92	0.23	3,3,3,3	0
56	MG	YA	3193	1/1	0.92	0.19	18,18,18,18	0
56	MG	YA	3066	1/1	0.92	0.07	27,27,27,27	0
56	MG	XA	1726	1/1	0.92	0.40	59,59,59,59	0
56	MG	RA	3398	1/1	0.92	0.14	45,45,45,45	0
56	MG	YA	3070	1/1	0.92	0.24	3,3,3,3	0
56	MG	QA	1602	1/1	0.92	0.26	35,35,35,35	0
56	MG	XA	1646	1/1	0.92	0.31	64,64,64,64	0
56	MG	RA	3053	1/1	0.92	0.25	21,21,21,21	0
56	MG	YA	3212	1/1	0.92	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1732	1/1	0.92	0.11	32,32,32,32	0
56	MG	RA	3348	1/1	0.92	0.24	45,45,45,45	0
56	MG	YA	3470	1/1	0.92	0.11	35,35,35,35	0
56	MG	YA	3217	1/1	0.92	0.15	23,23,23,23	0
56	MG	YA	3343	1/1	0.92	0.20	64,64,64,64	0
56	MG	XA	1735	1/1	0.92	0.21	16,16,16,16	0
56	MG	RA	3054	1/1	0.92	0.16	11,11,11,11	0
56	MG	QA	1641	1/1	0.92	0.20	32,32,32,32	0
56	MG	XA	1657	1/1	0.92	0.16	31,31,31,31	0
56	MG	YA	3092	1/1	0.92	0.54	52,52,52,52	0
56	MG	YA	3094	1/1	0.92	0.07	43,43,43,43	0
56	MG	QA	1686	1/1	0.92	0.41	72,72,72,72	0
56	MG	XA	1744	1/1	0.92	0.23	36,36,36,36	0
56	MG	XA	1659	1/1	0.92	0.31	27,27,27,27	0
56	MG	XA	1662	1/1	0.92	0.21	44,44,44,44	0
56	MG	QA	1709	1/1	0.92	0.21	36,36,36,36	0
56	MG	YB	206	1/1	0.92	0.05	48,48,48,48	0
56	MG	XA	1669	1/1	0.92	0.19	29,29,29,29	0
56	MG	YA	3247	1/1	0.92	0.22	41,41,41,41	0
56	MG	R0	103	1/1	0.92	0.14	19,19,19,19	0
56	MG	YN	201	1/1	0.92	0.09	34,34,34,34	0
56	MG	YA	3105	1/1	0.92	0.19	50,50,50,50	0
56	MG	YA	3251	1/1	0.92	0.17	54,54,54,54	0
56	MG	YQ	202	1/1	0.92	0.04	27,27,27,27	0
56	MG	YV	201	1/1	0.92	0.17	22,22,22,22	0
56	MG	YA	3106	1/1	0.92	0.21	15,15,15,15	0
56	MG	YA	3253	1/1	0.92	0.20	19,19,19,19	0
56	MG	RA	3275	1/1	0.92	0.32	48,48,48,48	0
56	MG	Y7	101	1/1	0.92	0.18	45,45,45,45	0
56	MG	RA	3332	1/1	0.93	0.25	40,40,40,40	0
56	MG	YA	3362	1/1	0.93	0.27	66,66,66,66	0
56	MG	YA	3046	1/1	0.93	0.17	14,14,14,14	0
56	MG	YA	3199	1/1	0.93	0.29	45,45,45,45	0
56	MG	YA	3201	1/1	0.93	0.21	20,20,20,20	0
56	MG	XA	1601	1/1	0.93	0.18	8,8,8,8	0
56	MG	XA	1697	1/1	0.93	0.14	42,42,42,42	0
56	MG	YA	3377	1/1	0.93	0.14	47,47,47,47	0
56	MG	QA	1679	1/1	0.93	0.10	34,34,34,34	0
56	MG	RA	3146	1/1	0.93	0.07	26,26,26,26	0
56	MG	YA	3381	1/1	0.93	0.08	48,48,48,48	0
56	MG	YA	3382	1/1	0.93	0.20	37,37,37,37	0
56	MG	QA	1613	1/1	0.93	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3094	1/1	0.93	0.37	35,35,35,35	0
56	MG	RA	3188	1/1	0.93	0.18	51,51,51,51	0
56	MG	YA	3388	1/1	0.93	0.11	28,28,28,28	0
56	MG	XA	1703	1/1	0.93	0.20	46,46,46,46	0
56	MG	RA	3067	1/1	0.93	0.14	28,28,28,28	0
56	MG	RA	3018	1/1	0.93	0.27	10,10,10,10	0
56	MG	RA	3152	1/1	0.93	0.29	19,19,19,19	0
56	MG	YA	3393	1/1	0.93	0.16	21,21,21,21	0
56	MG	RA	3153	1/1	0.93	0.17	25,25,25,25	0
56	MG	RA	3123	1/1	0.93	0.25	31,31,31,31	0
56	MG	QA	1698	1/1	0.93	0.14	41,41,41,41	0
56	MG	YA	3077	1/1	0.93	0.19	16,16,16,16	0
56	MG	YA	3399	1/1	0.93	0.11	57,57,57,57	0
56	MG	RA	3158	1/1	0.93	0.27	61,61,61,61	0
56	MG	QA	1670	1/1	0.93	0.30	48,48,48,48	0
56	MG	YA	3081	1/1	0.93	0.21	7,7,7,7	0
56	MG	YA	3241	1/1	0.93	0.13	33,33,33,33	0
56	MG	RA	3302	1/1	0.93	0.10	46,46,46,46	0
56	MG	XA	1721	1/1	0.93	0.09	52,52,52,52	0
56	MG	RA	3162	1/1	0.93	0.20	49,49,49,49	0
56	MG	RA	3164	1/1	0.93	0.13	51,51,51,51	0
56	MG	RA	3028	1/1	0.93	0.20	10,10,10,10	0
56	MG	XA	1633	1/1	0.93	0.12	25,25,25,25	0
56	MG	RA	3003	1/1	0.93	0.15	8,8,8,8	0
56	MG	QA	1701	1/1	0.93	0.05	42,42,42,42	0
56	MG	RA	3059	1/1	0.93	0.17	24,24,24,24	0
56	MG	RA	3425	1/1	0.93	0.07	38,38,38,38	0
56	MG	XA	1640	1/1	0.93	0.14	29,29,29,29	0
56	MG	YA	3417	1/1	0.93	0.25	22,22,22,22	0
56	MG	YA	3418	1/1	0.93	0.13	16,16,16,16	0
56	MG	XA	1736	1/1	0.93	0.14	23,23,23,23	0
56	MG	RA	3363	1/1	0.93	0.32	34,34,34,34	0
56	MG	QA	1736	1/1	0.93	0.18	33,33,33,33	0
56	MG	XA	1741	1/1	0.93	0.06	55,55,55,55	0
56	MG	XA	1644	1/1	0.93	0.20	25,25,25,25	0
56	MG	RA	3429	1/1	0.93	0.17	50,50,50,50	0
56	MG	YA	3107	1/1	0.93	0.20	14,14,14,14	0
56	MG	QA	1634	1/1	0.93	0.21	41,41,41,41	0
56	MG	RA	3368	1/1	0.93	0.23	46,46,46,46	0
56	MG	RA	3433	1/1	0.93	0.17	39,39,39,39	0
56	MG	XA	1653	1/1	0.93	0.12	35,35,35,35	0
56	MG	YA	3118	1/1	0.93	0.10	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3313	1/1	0.93	0.20	20,20,20,20	0
56	MG	RA	3372	1/1	0.93	0.12	7,7,7,7	0
56	MG	YA	3435	1/1	0.93	0.06	22,22,22,22	0
56	MG	XA	1751	1/1	0.93	0.12	70,70,70,70	0
56	MG	RA	3265	1/1	0.93	0.18	29,29,29,29	0
56	MG	RA	3437	1/1	0.93	0.14	24,24,24,24	0
56	MG	YA	3439	1/1	0.93	0.12	43,43,43,43	0
56	MG	RA	3317	1/1	0.93	0.12	40,40,40,40	0
56	MG	XA	1756	1/1	0.93	0.23	61,61,61,61	0
56	MG	YA	3133	1/1	0.93	0.12	25,25,25,25	0
56	MG	RA	3378	1/1	0.93	0.25	2,2,2,2	0
56	MG	XA	1664	1/1	0.93	0.31	30,30,30,30	0
56	MG	YA	3295	1/1	0.93	0.23	52,52,52,52	0
56	MG	YA	3141	1/1	0.93	0.20	24,24,24,24	0
56	MG	RA	3219	1/1	0.93	0.14	9,9,9,9	0
56	MG	YA	3302	1/1	0.93	0.19	51,51,51,51	0
56	MG	YA	3457	1/1	0.93	0.22	49,49,49,49	0
56	MG	RB	201	1/1	0.93	0.24	28,28,28,28	0
56	MG	RA	3269	1/1	0.93	0.14	33,33,33,33	0
56	MG	RA	3109	1/1	0.93	0.26	18,18,18,18	0
56	MG	RA	3321	1/1	0.93	0.15	33,33,33,33	0
56	MG	RA	3272	1/1	0.93	0.14	46,46,46,46	0
56	MG	YA	3154	1/1	0.93	0.15	16,16,16,16	0
56	MG	YA	3466	1/1	0.93	0.24	49,49,49,49	0
56	MG	RP	202	1/1	0.93	0.08	18,18,18,18	0
56	MG	YA	3003	1/1	0.93	0.26	4,4,4,4	0
56	MG	YA	3314	1/1	0.93	0.04	47,47,47,47	0
56	MG	RP	203	1/1	0.93	0.09	4,4,4,4	0
56	MG	RA	3222	1/1	0.93	0.27	45,45,45,45	0
56	MG	RA	3135	1/1	0.93	0.12	32,32,32,32	0
56	MG	YA	3475	1/1	0.93	0.12	49,49,49,49	0
56	MG	YA	3161	1/1	0.93	0.14	39,39,39,39	0
56	MG	RA	3226	1/1	0.93	0.16	33,33,33,33	0
56	MG	RA	3328	1/1	0.93	0.27	42,42,42,42	0
56	MG	YA	3165	1/1	0.93	0.21	34,34,34,34	0
56	MG	YA	3166	1/1	0.93	0.21	24,24,24,24	0
56	MG	YA	3169	1/1	0.93	0.13	20,20,20,20	0
56	MG	R0	101	1/1	0.93	0.27	44,44,44,44	0
56	MG	YA	3020	1/1	0.93	0.16	18,18,18,18	0
56	MG	XA	1688	1/1	0.93	0.07	41,41,41,41	0
56	MG	YA	3025	1/1	0.93	0.26	16,16,16,16	0
56	MG	RA	3137	1/1	0.93	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3029	1/1	0.93	0.09	15,15,15,15	0
56	MG	YA	3339	1/1	0.93	0.27	62,62,62,62	0
56	MG	YA	3030	1/1	0.93	0.23	3,3,3,3	0
56	MG	XA	1690	1/1	0.93	0.13	65,65,65,65	0
56	MG	YA	3183	1/1	0.93	0.18	49,49,49,49	0
56	MG	YA	3035	1/1	0.93	0.12	29,29,29,29	0
56	MG	YA	3036	1/1	0.93	0.24	10,10,10,10	0
56	MG	YA	3038	1/1	0.93	0.30	45,45,45,45	0
56	MG	YA	3192	1/1	0.93	0.30	23,23,23,23	0
56	MG	YW	201	1/1	0.93	0.10	52,52,52,52	0
56	MG	YA	3354	1/1	0.93	0.15	50,50,50,50	0
56	MG	Y0	102	1/1	0.93	0.05	37,37,37,37	0
56	MG	RA	3140	1/1	0.93	0.14	34,34,34,34	0
56	MG	QA	1685	1/1	0.93	0.09	11,11,11,11	0
56	MG	YA	3359	1/1	0.93	0.03	42,42,42,42	0
56	MG	RA	3155	1/1	0.94	0.16	12,12,12,12	0
56	MG	YA	3136	1/1	0.94	0.17	22,22,22,22	0
56	MG	YA	3027	1/1	0.94	0.18	14,14,14,14	0
56	MG	YA	3269	1/1	0.94	0.17	30,30,30,30	0
56	MG	QA	1655	1/1	0.94	0.24	31,31,31,31	0
56	MG	XA	1718	1/1	0.94	0.10	31,31,31,31	0
56	MG	QA	1615	1/1	0.94	0.10	29,29,29,29	0
56	MG	YA	3032	1/1	0.94	0.17	16,16,16,16	0
56	MG	YA	3150	1/1	0.94	0.14	9,9,9,9	0
56	MG	YA	3034	1/1	0.94	0.14	21,21,21,21	0
56	MG	XA	1720	1/1	0.94	0.07	44,44,44,44	0
56	MG	RA	3015	1/1	0.94	0.15	9,9,9,9	0
56	MG	YA	3037	1/1	0.94	0.13	10,10,10,10	0
56	MG	XA	1723	1/1	0.94	0.19	58,58,58,58	0
56	MG	XA	1724	1/1	0.94	0.20	33,33,33,33	0
56	MG	RA	3160	1/1	0.94	0.21	31,31,31,31	0
56	MG	RA	3248	1/1	0.94	0.19	38,38,38,38	0
56	MG	QA	1707	1/1	0.94	0.26	57,57,57,57	0
56	MG	RT	201	1/1	0.94	0.13	44,44,44,44	0
56	MG	YA	3293	1/1	0.94	0.40	68,68,68,68	0
56	MG	QA	1666	1/1	0.94	0.10	23,23,23,23	0
56	MG	QA	1700	1/1	0.94	0.26	31,31,31,31	0
56	MG	RA	3130	1/1	0.94	0.19	12,12,12,12	0
56	MG	YA	3297	1/1	0.94	0.28	35,35,35,35	0
56	MG	YA	3298	1/1	0.94	0.20	21,21,21,21	0
56	MG	QV	104	1/1	0.94	0.16	58,58,58,58	0
56	MG	XA	1667	1/1	0.94	0.22	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3171	1/1	0.94	0.11	26,26,26,26	0
56	MG	YA	3055	1/1	0.94	0.18	12,12,12,12	0
56	MG	RA	3212	1/1	0.94	0.21	18,18,18,18	0
56	MG	RA	3023	1/1	0.94	0.11	47,47,47,47	0
56	MG	R5	103	1/1	0.94	0.07	25,25,25,25	0
56	MG	YA	3061	1/1	0.94	0.23	0,0,0,0	0
56	MG	XA	1739	1/1	0.94	0.20	51,51,51,51	0
56	MG	RA	3074	1/1	0.94	0.15	27,27,27,27	0
56	MG	RA	3356	1/1	0.94	0.09	39,39,39,39	0
56	MG	QA	1639	1/1	0.94	0.31	48,48,48,48	0
56	MG	YA	3316	1/1	0.94	0.09	30,30,30,30	0
56	MG	XA	1679	1/1	0.94	0.08	37,37,37,37	0
56	MG	RA	3260	1/1	0.94	0.17	22,22,22,22	0
56	MG	XA	1746	1/1	0.94	0.12	47,47,47,47	0
56	MG	RA	3107	1/1	0.94	0.17	20,20,20,20	0
56	MG	RA	3217	1/1	0.94	0.09	27,27,27,27	0
56	MG	XA	1684	1/1	0.94	0.08	33,33,33,33	0
56	MG	RA	3361	1/1	0.94	0.17	52,52,52,52	0
56	MG	XA	1613	1/1	0.94	0.08	22,22,22,22	0
56	MG	YA	3085	1/1	0.94	0.16	17,17,17,17	0
56	MG	YA	3200	1/1	0.94	0.08	1,1,1,1	0
56	MG	RA	3080	1/1	0.94	0.23	17,17,17,17	0
56	MG	YA	3089	1/1	0.94	0.21	7,7,7,7	0
56	MG	YA	3453	1/1	0.94	0.07	35,35,35,35	0
56	MG	YA	3456	1/1	0.94	0.09	28,28,28,28	0
56	MG	RA	3364	1/1	0.94	0.21	39,39,39,39	0
56	MG	QA	1744	1/1	0.94	0.05	56,56,56,56	0
56	MG	QA	1611	1/1	0.94	0.18	28,28,28,28	0
56	MG	YA	3460	1/1	0.94	0.28	35,35,35,35	0
56	MG	YA	3340	1/1	0.94	0.36	29,29,29,29	0
56	MG	RA	3221	1/1	0.94	0.21	22,22,22,22	0
56	MG	RA	3085	1/1	0.94	0.13	13,13,13,13	0
56	MG	RA	3223	1/1	0.94	0.16	26,26,26,26	0
56	MG	XA	1761	1/1	0.94	0.14	23,23,23,23	0
56	MG	XA	1695	1/1	0.94	0.24	52,52,52,52	0
56	MG	QA	1653	1/1	0.94	0.17	20,20,20,20	0
56	MG	YA	3351	1/1	0.94	0.17	42,42,42,42	0
56	MG	RA	3115	1/1	0.94	0.23	46,46,46,46	0
56	MG	YA	3353	1/1	0.94	0.20	8,8,8,8	0
56	MG	YA	3102	1/1	0.94	0.19	22,22,22,22	0
56	MG	RA	3062	1/1	0.94	0.25	5,5,5,5	0
56	MG	RA	3183	1/1	0.94	0.16	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3117	1/1	0.94	0.17	28,28,28,28	0
56	MG	RA	3327	1/1	0.94	0.21	46,46,46,46	0
56	MG	YA	3108	1/1	0.94	0.14	33,33,33,33	0
56	MG	YA	3364	1/1	0.94	0.38	50,50,50,50	0
56	MG	YA	3365	1/1	0.94	0.14	22,22,22,22	0
56	MG	YA	3235	1/1	0.94	0.24	27,27,27,27	0
56	MG	RA	3185	1/1	0.94	0.24	54,54,54,54	0
56	MG	YA	3240	1/1	0.94	0.20	17,17,17,17	0
56	MG	YA	3110	1/1	0.94	0.15	29,29,29,29	0
56	MG	QA	1704	1/1	0.94	0.19	31,31,31,31	0
56	MG	RA	3120	1/1	0.94	0.25	40,40,40,40	0
56	MG	YE	301	1/1	0.94	0.09	4,4,4,4	0
56	MG	YA	3010	1/1	0.94	0.20	4,4,4,4	0
56	MG	YA	3248	1/1	0.94	0.09	30,30,30,30	0
56	MG	YA	3011	1/1	0.94	0.19	0,0,0,0	0
56	MG	RA	3235	1/1	0.94	0.11	28,28,28,28	0
56	MG	XA	1707	1/1	0.94	0.28	35,35,35,35	0
56	MG	YA	3124	1/1	0.94	0.18	8,8,8,8	0
56	MG	YA	3385	1/1	0.94	0.22	46,46,46,46	0
56	MG	YA	3014	1/1	0.94	0.20	18,18,18,18	0
56	MG	RA	3441	1/1	0.94	0.17	14,14,14,14	0
56	MG	YA	3019	1/1	0.94	0.18	14,14,14,14	0
56	MG	RA	3283	1/1	0.94	0.13	18,18,18,18	0
56	MG	Y0	103	1/1	0.94	0.19	27,27,27,27	0
56	MG	YA	3131	1/1	0.94	0.16	11,11,11,11	0
56	MG	RA	3285	1/1	0.94	0.12	28,28,28,28	0
56	MG	RA	3064	1/1	0.94	0.16	18,18,18,18	0
56	MG	RA	3025	1/1	0.95	0.10	12,12,12,12	0
56	MG	RA	3026	1/1	0.95	0.21	24,24,24,24	0
56	MG	YA	3273	1/1	0.95	0.08	24,24,24,24	0
56	MG	XA	1647	1/1	0.95	0.05	47,47,47,47	0
56	MG	QA	1652	1/1	0.95	0.13	23,23,23,23	0
56	MG	XA	1651	1/1	0.95	0.16	25,25,25,25	0
56	MG	XA	1728	1/1	0.95	0.19	52,52,52,52	0
56	MG	RA	3370	1/1	0.95	0.37	43,43,43,43	0
56	MG	RA	3126	1/1	0.95	0.14	31,31,31,31	0
56	MG	QA	1658	1/1	0.95	0.34	46,46,46,46	0
56	MG	XA	1655	1/1	0.95	0.18	39,39,39,39	0
56	MG	RA	3033	1/1	0.95	0.21	8,8,8,8	0
56	MG	RA	3263	1/1	0.95	0.35	31,31,31,31	0
56	MG	QA	1690	1/1	0.95	0.09	27,27,27,27	0
56	MG	QA	1612	1/1	0.95	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1660	1/1	0.95	0.08	37,37,37,37	0
56	MG	YA	3065	1/1	0.95	0.10	29,29,29,29	0
56	MG	RA	3266	1/1	0.95	0.19	31,31,31,31	0
56	MG	XA	1740	1/1	0.95	0.23	44,44,44,44	0
56	MG	XA	1663	1/1	0.95	0.15	30,30,30,30	0
56	MG	YA	3069	1/1	0.95	0.09	14,14,14,14	0
56	MG	RE	301	1/1	0.95	0.17	1,1,1,1	0
56	MG	YA	3419	1/1	0.95	0.13	2,2,2,2	0
56	MG	YA	3299	1/1	0.95	0.15	23,23,23,23	0
56	MG	YA	3071	1/1	0.95	0.16	17,17,17,17	0
56	MG	YA	3301	1/1	0.95	0.17	34,34,34,34	0
56	MG	RA	3267	1/1	0.95	0.16	28,28,28,28	0
56	MG	RA	3322	1/1	0.95	0.07	15,15,15,15	0
56	MG	RA	3040	1/1	0.95	0.20	4,4,4,4	0
56	MG	YA	3185	1/1	0.95	0.12	35,35,35,35	0
56	MG	RA	3173	1/1	0.95	0.25	5,5,5,5	0
56	MG	QA	1714	1/1	0.95	0.08	25,25,25,25	0
56	MG	RA	3271	1/1	0.95	0.04	23,23,23,23	0
56	MG	RV	201	1/1	0.95	0.15	4,4,4,4	0
56	MG	QA	1749	1/1	0.95	0.09	41,41,41,41	0
56	MG	XA	1678	1/1	0.95	0.10	41,41,41,41	0
56	MG	XA	1752	1/1	0.95	0.12	44,44,44,44	0
56	MG	YA	3197	1/1	0.95	0.23	22,22,22,22	0
56	MG	RA	3395	1/1	0.95	0.18	27,27,27,27	0
56	MG	RA	3045	1/1	0.95	0.23	4,4,4,4	0
56	MG	QA	1682	1/1	0.95	0.29	51,51,51,51	0
56	MG	XA	1682	1/1	0.95	0.09	26,26,26,26	0
56	MG	YA	3205	1/1	0.95	0.27	43,43,43,43	0
56	MG	RA	3016	1/1	0.95	0.17	6,6,6,6	0
56	MG	QA	1601	1/1	0.95	0.17	17,17,17,17	0
56	MG	QA	1740	1/1	0.95	0.36	49,49,49,49	0
56	MG	RA	3019	1/1	0.95	0.16	17,17,17,17	0
56	MG	RA	3143	1/1	0.95	0.10	58,58,58,58	0
56	MG	XA	1604	1/1	0.95	0.19	9,9,9,9	0
56	MG	RA	3076	1/1	0.95	0.21	15,15,15,15	0
56	MG	YA	3449	1/1	0.95	0.17	36,36,36,36	0
56	MG	YA	3450	1/1	0.95	0.09	43,43,43,43	0
56	MG	YA	3218	1/1	0.95	0.12	36,36,36,36	0
56	MG	YA	3452	1/1	0.95	0.12	47,47,47,47	0
56	MG	RA	3336	1/1	0.95	0.14	48,48,48,48	0
56	MG	YA	3336	1/1	0.95	0.21	17,17,17,17	0
56	MG	YA	3221	1/1	0.95	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	3338	1/1	0.95	0.39	67,67,67,67	0
56	MG	RA	3078	1/1	0.95	0.18	14,14,14,14	0
56	MG	RA	3234	1/1	0.95	0.06	23,23,23,23	0
56	MG	RA	3079	1/1	0.95	0.20	10,10,10,10	0
56	MG	YA	3226	1/1	0.95	0.15	19,19,19,19	0
56	MG	RA	3286	1/1	0.95	0.15	20,20,20,20	0
56	MG	YA	3228	1/1	0.95	0.11	25,25,25,25	0
56	MG	YA	3350	1/1	0.95	0.06	22,22,22,22	0
56	MG	RA	3112	1/1	0.95	0.13	22,22,22,22	0
56	MG	QA	1684	1/1	0.95	0.17	32,32,32,32	0
56	MG	RA	3346	1/1	0.95	0.14	37,37,37,37	0
56	MG	RA	3238	1/1	0.95	0.06	11,11,11,11	0
56	MG	YA	3236	1/1	0.95	0.25	14,14,14,14	0
56	MG	YA	3356	1/1	0.95	0.17	30,30,30,30	0
56	MG	YA	3237	1/1	0.95	0.19	37,37,37,37	0
56	MG	RA	3081	1/1	0.95	0.19	4,4,4,4	0
56	MG	YA	3360	1/1	0.95	0.12	44,44,44,44	0
56	MG	RA	3240	1/1	0.95	0.21	26,26,26,26	0
56	MG	RA	3195	1/1	0.95	0.26	29,29,29,29	0
56	MG	RA	3295	1/1	0.95	0.27	46,46,46,46	0
56	MG	YA	3243	1/1	0.95	0.19	38,38,38,38	0
56	MG	RA	3082	1/1	0.95	0.24	0,0,0,0	0
56	MG	YA	3246	1/1	0.95	0.22	29,29,29,29	0
56	MG	YA	3486	1/1	0.95	0.05	19,19,19,19	0
56	MG	YA	3487	1/1	0.95	0.18	18,18,18,18	0
56	MG	YA	3021	1/1	0.95	0.19	17,17,17,17	0
56	MG	RA	3154	1/1	0.95	0.22	41,41,41,41	0
56	MG	QA	1616	1/1	0.95	0.10	29,29,29,29	0
56	MG	RA	3056	1/1	0.95	0.16	14,14,14,14	0
56	MG	RA	3301	1/1	0.95	0.07	41,41,41,41	0
56	MG	RA	3119	1/1	0.95	0.11	8,8,8,8	0
56	MG	YA	3380	1/1	0.95	0.09	31,31,31,31	0
56	MG	RA	3205	1/1	0.95	0.11	19,19,19,19	0
56	MG	YA	3254	1/1	0.95	0.16	26,26,26,26	0
56	MG	XA	1639	1/1	0.95	0.23	48,48,48,48	0
56	MG	XA	1716	1/1	0.95	0.24	25,25,25,25	0
56	MG	YA	3033	1/1	0.95	0.14	10,10,10,10	0
56	MG	XA	1717	1/1	0.95	0.22	46,46,46,46	0
56	MG	QA	1664	1/1	0.95	0.17	17,17,17,17	0
56	MG	RA	3362	1/1	0.95	0.16	52,52,52,52	0
56	MG	Y0	101	1/1	0.95	0.10	18,18,18,18	0
56	MG	YA	3147	1/1	0.95	0.25	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3087	1/1	0.95	0.16	20,20,20,20	0
56	MG	Y1	101	1/1	0.95	0.24	24,24,24,24	0
56	MG	RA	3210	1/1	0.95	0.20	50,50,50,50	0
56	MG	YA	3039	1/1	0.95	0.16	14,14,14,14	0
56	MG	YA	3394	1/1	0.95	0.16	64,64,64,64	0
57	ZN	XD	301	1/1	0.95	0.28	48,48,48,48	0
56	MG	RA	3136	1/1	0.96	0.33	28,28,28,28	0
56	MG	YA	3167	1/1	0.96	0.22	30,30,30,30	0
56	MG	YA	3168	1/1	0.96	0.20	19,19,19,19	0
56	MG	XA	1638	1/1	0.96	0.23	34,34,34,34	0
56	MG	QA	1642	1/1	0.96	0.13	39,39,39,39	0
56	MG	YA	3281	1/1	0.96	0.10	27,27,27,27	0
56	MG	RP	201	1/1	0.96	0.06	21,21,21,21	0
56	MG	XA	1760	1/1	0.96	0.21	47,47,47,47	0
56	MG	YA	3284	1/1	0.96	0.11	14,14,14,14	0
56	MG	RA	3224	1/1	0.96	0.14	19,19,19,19	0
56	MG	YA	3286	1/1	0.96	0.12	20,20,20,20	0
56	MG	YA	3176	1/1	0.96	0.18	17,17,17,17	0
56	MG	YA	3177	1/1	0.96	0.20	35,35,35,35	0
56	MG	XA	1642	1/1	0.96	0.09	39,39,39,39	0
56	MG	YA	3080	1/1	0.96	0.31	15,15,15,15	0
56	MG	RA	3138	1/1	0.96	0.11	10,10,10,10	0
56	MG	RA	3077	1/1	0.96	0.13	16,16,16,16	0
56	MG	YA	3414	1/1	0.96	0.23	29,29,29,29	0
56	MG	XA	1704	1/1	0.96	0.18	46,46,46,46	0
56	MG	XV	102	1/1	0.96	0.08	34,34,34,34	0
56	MG	RA	3097	1/1	0.96	0.36	48,48,48,48	0
56	MG	RA	3409	1/1	0.96	0.25	69,69,69,69	0
56	MG	YA	3002	1/1	0.96	0.15	0,0,0,0	0
56	MG	RA	3228	1/1	0.96	0.19	18,18,18,18	0
56	MG	YA	3189	1/1	0.96	0.10	12,12,12,12	0
56	MG	YA	3191	1/1	0.96	0.25	9,9,9,9	0
56	MG	XA	1708	1/1	0.96	0.20	32,32,32,32	0
56	MG	RA	3296	1/1	0.96	0.10	29,29,29,29	0
56	MG	YA	3093	1/1	0.96	0.19	17,17,17,17	0
56	MG	RA	3199	1/1	0.96	0.20	39,39,39,39	0
56	MG	YA	3009	1/1	0.96	0.17	7,7,7,7	0
56	MG	RA	3369	1/1	0.96	0.35	38,38,38,38	0
56	MG	R0	102	1/1	0.96	0.28	39,39,39,39	0
56	MG	RA	3414	1/1	0.96	0.30	54,54,54,54	0
56	MG	QA	1691	1/1	0.96	0.18	20,20,20,20	0
56	MG	RA	3008	1/1	0.96	0.31	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	R5	101	1/1	0.96	0.14	14,14,14,14	0
56	MG	RA	3203	1/1	0.96	0.21	26,26,26,26	0
56	MG	YA	3209	1/1	0.96	0.18	9,9,9,9	0
56	MG	YA	3104	1/1	0.96	0.20	47,47,47,47	0
56	MG	RA	3418	1/1	0.96	0.11	28,28,28,28	0
56	MG	QA	1620	1/1	0.96	0.11	13,13,13,13	0
56	MG	XA	1661	1/1	0.96	0.19	23,23,23,23	0
56	MG	YA	3325	1/1	0.96	0.18	14,14,14,14	0
56	MG	RA	3337	1/1	0.96	0.06	41,41,41,41	0
56	MG	YA	3327	1/1	0.96	0.27	54,54,54,54	0
56	MG	YA	3444	1/1	0.96	0.18	5,5,5,5	0
56	MG	YA	3216	1/1	0.96	0.13	13,13,13,13	0
56	MG	RA	3377	1/1	0.96	0.29	24,24,24,24	0
56	MG	QL	201	1/1	0.96	0.05	38,38,38,38	0
56	MG	YA	3028	1/1	0.96	0.13	18,18,18,18	0
56	MG	YA	3112	1/1	0.96	0.12	14,14,14,14	0
56	MG	YA	3113	1/1	0.96	0.18	25,25,25,25	0
56	MG	QA	1621	1/1	0.96	0.10	29,29,29,29	0
56	MG	YA	3115	1/1	0.96	0.20	40,40,40,40	0
56	MG	XA	1666	1/1	0.96	0.34	39,39,39,39	0
56	MG	RA	3208	1/1	0.96	0.23	35,35,35,35	0
56	MG	YA	3120	1/1	0.96	0.25	33,33,33,33	0
56	MG	QV	102	1/1	0.96	0.13	28,28,28,28	0
56	MG	YA	3230	1/1	0.96	0.19	38,38,38,38	0
56	MG	XA	1670	1/1	0.96	0.22	36,36,36,36	0
56	MG	YA	3345	1/1	0.96	0.22	38,38,38,38	0
56	MG	YA	3232	1/1	0.96	0.15	38,38,38,38	0
56	MG	RA	3428	1/1	0.96	0.10	33,33,33,33	0
56	MG	RA	3383	1/1	0.96	0.25	44,44,44,44	0
56	MG	XA	1674	1/1	0.96	0.18	32,32,32,32	0
56	MG	XA	1734	1/1	0.96	0.10	27,27,27,27	0
56	MG	XA	1614	1/1	0.96	0.13	19,19,19,19	0
56	MG	RA	3031	1/1	0.96	0.24	6,6,6,6	0
56	MG	XA	1616	1/1	0.96	0.15	25,25,25,25	0
56	MG	RA	3387	1/1	0.96	0.23	16,16,16,16	0
56	MG	YA	3042	1/1	0.96	0.20	7,7,7,7	0
56	MG	YA	3358	1/1	0.96	0.22	27,27,27,27	0
56	MG	YA	3043	1/1	0.96	0.12	9,9,9,9	0
56	MG	YA	3138	1/1	0.96	0.05	18,18,18,18	0
56	MG	YA	3245	1/1	0.96	0.12	33,33,33,33	0
56	MG	YA	3044	1/1	0.96	0.20	12,12,12,12	0
56	MG	XA	1619	1/1	0.96	0.15	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3142	1/1	0.96	0.26	14,14,14,14	0
56	MG	YA	3144	1/1	0.96	0.04	24,24,24,24	0
56	MG	YA	3367	1/1	0.96	0.12	30,30,30,30	0
56	MG	RA	3106	1/1	0.96	0.16	57,57,57,57	0
56	MG	QA	1640	1/1	0.96	0.25	53,53,53,53	0
56	MG	YA	3370	1/1	0.96	0.14	24,24,24,24	0
56	MG	XA	1623	1/1	0.96	0.12	20,20,20,20	0
56	MG	YA	3148	1/1	0.96	0.14	32,32,32,32	0
56	MG	YA	3373	1/1	0.96	0.08	35,35,35,35	0
56	MG	RA	3035	1/1	0.96	0.07	17,17,17,17	0
56	MG	RA	3071	1/1	0.96	0.22	9,9,9,9	0
56	MG	RA	3246	1/1	0.96	0.11	25,25,25,25	0
56	MG	XA	1628	1/1	0.96	0.33	44,44,44,44	0
56	MG	RA	3090	1/1	0.96	0.15	4,4,4,4	0
56	MG	QA	1661	1/1	0.96	0.06	23,23,23,23	0
56	MG	QA	1604	1/1	0.96	0.15	17,17,17,17	0
56	MG	YA	3262	1/1	0.96	0.14	36,36,36,36	0
56	MG	RA	3159	1/1	0.96	0.21	5,5,5,5	0
56	MG	RA	3187	1/1	0.96	0.24	48,48,48,48	0
56	MG	YA	3387	1/1	0.96	0.05	27,27,27,27	0
56	MG	YA	3266	1/1	0.96	0.17	42,42,42,42	0
56	MG	YA	3063	1/1	0.96	0.11	20,20,20,20	0
56	MG	YA	3064	1/1	0.96	0.18	5,5,5,5	0
56	MG	XA	1692	1/1	0.96	0.09	36,36,36,36	0
56	MG	RA	3039	1/1	0.96	0.16	21,21,21,21	0
56	MG	YA	3272	1/1	0.96	0.17	26,26,26,26	0
56	MG	QA	1713	1/1	0.96	0.21	38,38,38,38	0
57	ZN	QN	101	1/1	0.96	0.05	76,76,76,76	0
56	MG	RA	3287	1/1	0.96	0.06	17,17,17,17	0
56	MG	RD	302	1/1	0.97	0.14	9,9,9,9	0
56	MG	RA	3315	1/1	0.97	0.14	30,30,30,30	0
56	MG	RA	3122	1/1	0.97	0.23	8,8,8,8	0
56	MG	QA	1644	1/1	0.97	0.16	23,23,23,23	0
56	MG	YA	3332	1/1	0.97	0.17	25,25,25,25	0
56	MG	QX	101	1/1	0.97	0.14	17,17,17,17	0
56	MG	YA	3100	1/1	0.97	0.18	3,3,3,3	0
56	MG	RA	3244	1/1	0.97	0.12	16,16,16,16	0
56	MG	RA	3177	1/1	0.97	0.18	16,16,16,16	0
56	MG	YA	3337	1/1	0.97	0.05	23,23,23,23	0
56	MG	YA	3338	1/1	0.97	0.27	15,15,15,15	0
56	MG	RA	3149	1/1	0.97	0.27	2,2,2,2	0
56	MG	RA	3179	1/1	0.97	0.22	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1619	1/1	0.97	0.18	12,12,12,12	0
56	MG	YA	3257	1/1	0.97	0.27	36,36,36,36	0
56	MG	QA	1650	1/1	0.97	0.20	19,19,19,19	0
56	MG	YA	3434	1/1	0.97	0.08	42,42,42,42	0
56	MG	RA	3365	1/1	0.97	0.23	21,21,21,21	0
56	MG	RA	3021	1/1	0.97	0.16	4,4,4,4	0
56	MG	QA	1651	1/1	0.97	0.14	29,29,29,29	0
56	MG	XA	1650	1/1	0.97	0.28	16,16,16,16	0
56	MG	YA	3349	1/1	0.97	0.18	24,24,24,24	0
56	MG	RA	3252	1/1	0.97	0.10	21,21,21,21	0
56	MG	YA	3264	1/1	0.97	0.20	16,16,16,16	0
56	MG	QA	1694	1/1	0.97	0.04	27,27,27,27	0
56	MG	RA	3044	1/1	0.97	0.16	1,1,1,1	0
56	MG	RA	3088	1/1	0.97	0.12	27,27,27,27	0
56	MG	RA	3024	1/1	0.97	0.23	7,7,7,7	0
56	MG	RA	3257	1/1	0.97	0.03	25,25,25,25	0
56	MG	YA	3117	1/1	0.97	0.17	14,14,14,14	0
56	MG	QA	1667	1/1	0.97	0.14	27,27,27,27	0
56	MG	YA	3052	1/1	0.97	0.19	1,1,1,1	0
56	MG	RA	3375	1/1	0.97	0.10	25,25,25,25	0
56	MG	YA	3122	1/1	0.97	0.36	14,14,14,14	0
56	MG	XA	1606	1/1	0.97	0.20	14,14,14,14	0
56	MG	YA	3198	1/1	0.97	0.19	17,17,17,17	0
56	MG	YA	3454	1/1	0.97	0.06	44,44,44,44	0
56	MG	RA	3190	1/1	0.97	0.18	19,19,19,19	0
56	MG	YA	3126	1/1	0.97	0.12	10,10,10,10	0
56	MG	YA	3058	1/1	0.97	0.07	34,34,34,34	0
56	MG	YA	3202	1/1	0.97	0.12	15,15,15,15	0
56	MG	RA	3424	1/1	0.97	0.06	26,26,26,26	0
56	MG	YA	3461	1/1	0.97	0.06	37,37,37,37	0
56	MG	XL	201	1/1	0.97	0.04	45,45,45,45	0
56	MG	QA	1633	1/1	0.97	0.15	23,23,23,23	0
56	MG	YA	3062	1/1	0.97	0.12	0,0,0,0	0
56	MG	XV	101	1/1	0.97	0.12	39,39,39,39	0
56	MG	YA	3374	1/1	0.97	0.12	28,28,28,28	0
56	MG	YA	3288	1/1	0.97	0.17	25,25,25,25	0
56	MG	XA	1610	1/1	0.97	0.14	15,15,15,15	0
56	MG	YA	3290	1/1	0.97	0.15	82,82,82,82	0
56	MG	RA	3027	1/1	0.97	0.16	2,2,2,2	0
56	MG	YA	3135	1/1	0.97	0.14	14,14,14,14	0
56	MG	QA	1629	1/1	0.97	0.20	26,26,26,26	0
56	MG	YA	3474	1/1	0.97	0.08	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	RA	3381	1/1	0.97	0.23	0,0,0,0	0
56	MG	YA	3139	1/1	0.97	0.20	36,36,36,36	0
56	MG	YA	3477	1/1	0.97	0.20	38,38,38,38	0
56	MG	YA	3478	1/1	0.97	0.17	46,46,46,46	0
56	MG	QA	1730	1/1	0.97	0.10	58,58,58,58	0
56	MG	YA	3219	1/1	0.97	0.23	39,39,39,39	0
56	MG	XA	1668	1/1	0.97	0.16	20,20,20,20	0
56	MG	RA	3430	1/1	0.97	0.41	50,50,50,50	0
56	MG	YA	3143	1/1	0.97	0.07	23,23,23,23	0
56	MG	XA	1722	1/1	0.97	0.11	38,38,38,38	0
56	MG	YA	3073	1/1	0.97	0.13	15,15,15,15	0
56	MG	RA	3030	1/1	0.97	0.13	13,13,13,13	0
56	MG	RA	3385	1/1	0.97	0.19	2,2,2,2	0
56	MG	YB	201	1/1	0.97	0.21	31,31,31,31	0
56	MG	YA	3305	1/1	0.97	0.17	21,21,21,21	0
56	MG	YA	3306	1/1	0.97	0.17	22,22,22,22	0
56	MG	RA	3139	1/1	0.97	0.12	41,41,41,41	0
56	MG	YB	205	1/1	0.97	0.07	48,48,48,48	0
56	MG	RA	3303	1/1	0.97	0.14	34,34,34,34	0
56	MG	YA	3229	1/1	0.97	0.28	43,43,43,43	0
56	MG	YA	3310	1/1	0.97	0.22	28,28,28,28	0
56	MG	QA	1678	1/1	0.97	0.05	29,29,29,29	0
56	MG	RA	3200	1/1	0.97	0.28	31,31,31,31	0
56	MG	YA	3015	1/1	0.97	0.13	9,9,9,9	0
56	MG	RA	3032	1/1	0.97	0.11	5,5,5,5	0
56	MG	RA	3392	1/1	0.97	0.19	36,36,36,36	0
56	MG	QA	1654	1/1	0.97	0.12	20,20,20,20	0
56	MG	RA	3034	1/1	0.97	0.14	9,9,9,9	0
56	MG	YA	3088	1/1	0.97	0.14	5,5,5,5	0
56	MG	RA	3170	1/1	0.97	0.25	26,26,26,26	0
56	MG	YA	3320	1/1	0.97	0.21	38,38,38,38	0
56	MG	RA	3144	1/1	0.97	0.20	10,10,10,10	0
56	MG	RA	3145	1/1	0.97	0.11	9,9,9,9	0
56	MG	YA	3323	1/1	0.97	0.28	37,37,37,37	0
56	MG	Y5	101	1/1	0.97	0.07	22,22,22,22	0
56	MG	YA	3413	1/1	0.97	0.18	7,7,7,7	0
56	MG	YA	3162	1/1	0.97	0.22	44,44,44,44	0
56	MG	RA	3207	1/1	0.97	0.08	18,18,18,18	0
56	MG	RA	3314	1/1	0.97	0.12	19,19,19,19	0
56	MG	RA	3354	1/1	0.97	0.20	34,34,34,34	0
56	MG	YA	3016	1/1	0.98	0.07	2,2,2,2	0
56	MG	RA	3419	1/1	0.98	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3455	1/1	0.98	0.36	42,42,42,42	0
56	MG	YA	3018	1/1	0.98	0.13	18,18,18,18	0
56	MG	XA	1626	1/1	0.98	0.22	22,22,22,22	0
56	MG	RA	3013	1/1	0.98	0.15	0,0,0,0	0
56	MG	RA	3388	1/1	0.98	0.29	15,15,15,15	0
56	MG	QA	1659	1/1	0.98	0.17	25,25,25,25	0
56	MG	YA	3119	1/1	0.98	0.10	10,10,10,10	0
56	MG	YA	3024	1/1	0.98	0.13	13,13,13,13	0
56	MG	QA	1697	1/1	0.98	0.15	30,30,30,30	0
56	MG	YA	3174	1/1	0.98	0.08	15,15,15,15	0
56	MG	YA	3072	1/1	0.98	0.21	19,19,19,19	0
56	MG	RA	3163	1/1	0.98	0.12	34,34,34,34	0
56	MG	RA	3048	1/1	0.98	0.21	5,5,5,5	0
56	MG	YA	3125	1/1	0.98	0.05	13,13,13,13	0
56	MG	YA	3348	1/1	0.98	0.16	30,30,30,30	0
56	MG	YA	3076	1/1	0.98	0.10	26,26,26,26	0
56	MG	YA	3471	1/1	0.98	0.09	28,28,28,28	0
56	MG	QA	1739	1/1	0.98	0.23	42,42,42,42	0
56	MG	YA	3238	1/1	0.98	0.09	14,14,14,14	0
56	MG	QA	1623	1/1	0.98	0.31	35,35,35,35	0
56	MG	RA	3038	1/1	0.98	0.09	2,2,2,2	0
56	MG	RA	3098	1/1	0.98	0.22	44,44,44,44	0
56	MG	RA	3280	1/1	0.98	0.07	17,17,17,17	0
56	MG	RA	3052	1/1	0.98	0.18	4,4,4,4	0
56	MG	RA	3189	1/1	0.98	0.28	6,6,6,6	0
56	MG	RA	3310	1/1	0.98	0.18	17,17,17,17	0
56	MG	XA	1602	1/1	0.98	0.26	8,8,8,8	0
56	MG	RA	3007	1/1	0.98	0.16	5,5,5,5	0
56	MG	YA	3137	1/1	0.98	0.12	5,5,5,5	0
56	MG	XA	1762	1/1	0.98	0.05	53,53,53,53	0
56	MG	YA	3363	1/1	0.98	0.34	56,56,56,56	0
56	MG	RA	3284	1/1	0.98	0.21	48,48,48,48	0
56	MG	XA	1605	1/1	0.98	0.12	6,6,6,6	0
56	MG	QD	302	1/1	0.98	0.07	23,23,23,23	0
56	MG	RA	3172	1/1	0.98	0.04	28,28,28,28	0
56	MG	RA	3193	1/1	0.98	0.21	0,0,0,0	0
56	MG	RA	3055	1/1	0.98	0.30	10,10,10,10	0
56	MG	XA	1649	1/1	0.98	0.09	12,12,12,12	0
56	MG	RA	3289	1/1	0.98	0.17	23,23,23,23	0
56	MG	YD	301	1/1	0.98	0.20	2,2,2,2	0
56	MG	RA	3376	1/1	0.98	0.14	5,5,5,5	0
56	MG	RA	3086	1/1	0.98	0.07	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3196	1/1	0.98	0.21	18,18,18,18	0
56	MG	YA	3375	1/1	0.98	0.31	51,51,51,51	0
56	MG	YA	3376	1/1	0.98	0.09	38,38,38,38	0
56	MG	YA	3206	1/1	0.98	0.09	12,12,12,12	0
56	MG	YP	201	1/1	0.98	0.04	7,7,7,7	0
56	MG	RA	3009	1/1	0.98	0.09	6,6,6,6	0
56	MG	YA	3005	1/1	0.98	0.14	1,1,1,1	0
56	MG	RA	3242	1/1	0.98	0.07	30,30,30,30	0
56	MG	RA	3243	1/1	0.98	0.06	37,37,37,37	0
56	MG	QA	1689	1/1	0.98	0.26	42,42,42,42	0
56	MG	YA	3267	1/1	0.98	0.20	32,32,32,32	0
56	MG	YA	3213	1/1	0.98	0.18	33,33,33,33	0
56	MG	XA	1618	1/1	0.98	0.14	15,15,15,15	0
56	MG	YA	3057	1/1	0.98	0.13	3,3,3,3	0
56	MG	RA	3353	1/1	0.98	0.33	30,30,30,30	0
56	MG	RF	301	1/1	0.98	0.04	24,24,24,24	0
56	MG	RA	3384	1/1	0.98	0.07	8,8,8,8	0
56	MG	YA	3274	1/1	0.98	0.23	35,35,35,35	0
57	ZN	QD	301	1/1	0.98	0.23	29,29,29,29	0
56	MG	RA	3058	1/1	0.98	0.13	1,1,1,1	0
56	MG	RA	3001	1/1	0.98	0.05	41,41,41,41	0
57	ZN	XN	101	1/1	0.98	0.03	67,67,67,67	0
56	MG	RA	3113	1/1	0.99	0.10	17,17,17,17	0
56	MG	YA	3023	1/1	0.99	0.21	2,2,2,2	0
56	MG	XA	1671	1/1	0.99	0.05	0,0,0,0	0
56	MG	YA	3008	1/1	0.99	0.06	2,2,2,2	0
56	MG	QA	1607	1/1	0.99	0.21	12,12,12,12	0
56	MG	YA	3170	1/1	0.99	0.23	7,7,7,7	0
56	MG	YA	3054	1/1	0.99	0.24	1,1,1,1	0
56	MG	YA	3186	1/1	0.99	0.22	1,1,1,1	0
56	MG	YA	3203	1/1	0.99	0.23	30,30,30,30	0
56	MG	YA	3075	1/1	0.99	0.15	8,8,8,8	0
56	MG	YA	3087	1/1	0.99	0.10	14,14,14,14	0
56	MG	YA	3160	1/1	0.99	0.16	25,25,25,25	0
56	MG	YA	3207	1/1	0.99	0.06	13,13,13,13	0
56	MG	YA	3190	1/1	0.99	0.26	22,22,22,22	0
56	MG	XA	1709	1/1	0.99	0.17	23,23,23,23	0
56	MG	XA	1622	1/1	0.99	0.25	37,37,37,37	0
56	MG	RA	3011	1/1	0.99	0.11	1,1,1,1	0
56	MG	QA	1726	1/1	0.99	0.03	23,23,23,23	0
56	MG	RA	3042	1/1	1.00	0.09	7,7,7,7	0
56	MG	RA	3006	1/1	1.00	0.02	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3344	1/1	1.00	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.