



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:50 AM UTC

PDB ID : 4V7J / pdb_00004v7j
Title : Structure of RelE nuclease bound to the 70S ribosome (precleavage state)
Authors : Neubauer, C.; Gao, Y.-G.; Andersen, K.R.; Dunham, C.M.; Kelley, A.C.;
Hentschel, J.; Gerdes, K.; Ramakrishnan, V.; Brodersen, D.E.
Deposited on : 2009-11-02
Resolution : 3.30 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:

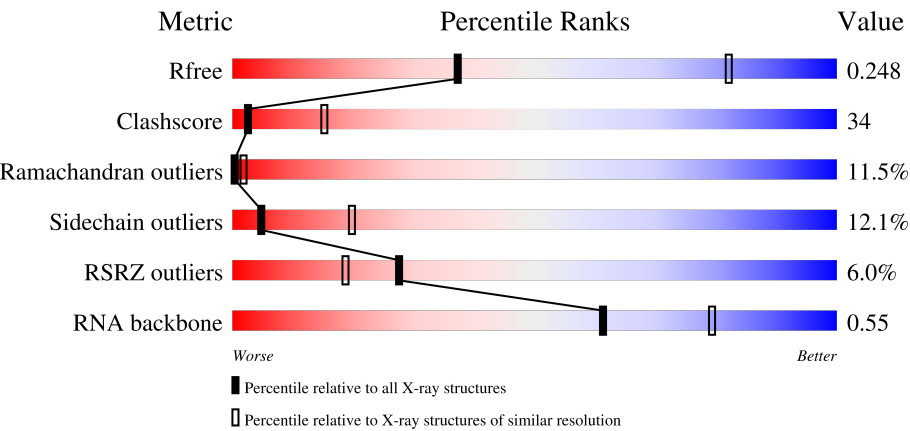
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	Ab	256	4% 23% 54% 13% 9%
1	Bb	256	4% 24% 54% 13% 9%
2	Ac	239	5% 28% 44% 14% 14%
2	Bc	239	3% 28% 44% 14% 14%

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Mol	Chain	Length	Quality of chain
3	Ad	209	
3	Bd	209	
4	Ae	162	
4	Be	162	
5	Af	101	
5	Bf	101	
6	Ag	156	
6	Bg	156	
7	Ah	138	
7	Bh	138	
8	Ai	128	
8	Bi	128	
9	Aj	105	
9	Bj	105	
10	Ak	129	
10	Bk	129	
11	Al	132	
11	Bl	132	
12	Am	126	
12	Bm	126	
13	An	61	
13	Bn	61	
14	Ao	89	
14	Bo	89	
15	Ap	88	

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Mol	Chain	Length	Quality of chain
15	Bp	88	
16	Aq	105	
16	Bq	105	
17	Ar	88	
17	Br	88	
18	As	93	
18	Bs	93	
19	At	106	
19	Bt	106	
20	Au	27	
20	Bu	27	
21	Ay	95	
21	By	95	
22	Aa	1504	
22	Ba	1504	
23	Ax	25	
23	Bx	25	
24	Av	77	
24	Bv	77	
25	Aw	77	
25	Bw	77	
26	AC	229	
26	BC	229	
27	AD	276	
27	BD	276	

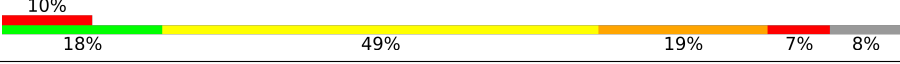
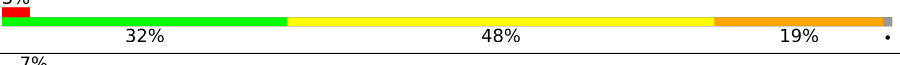
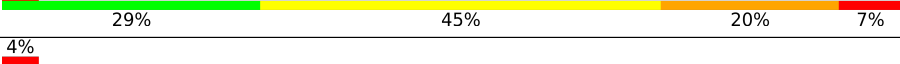
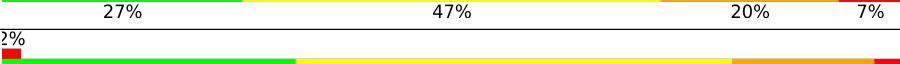
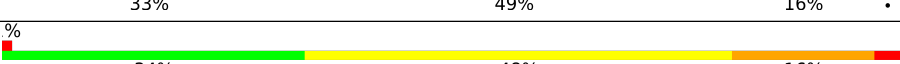
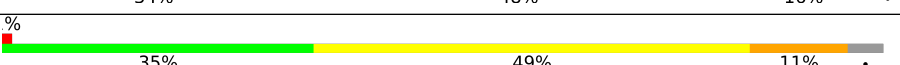
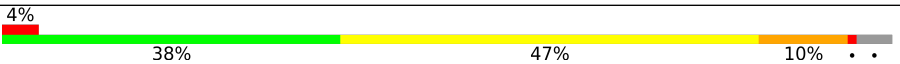
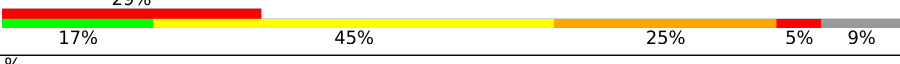
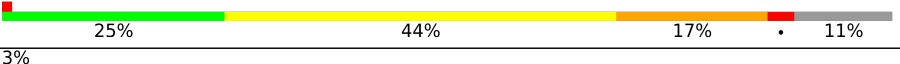
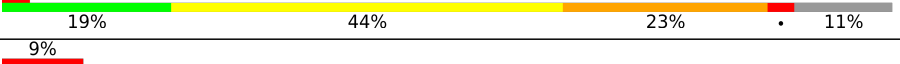
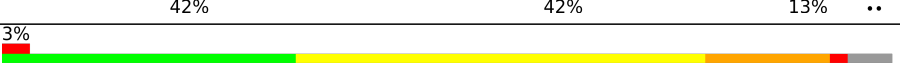
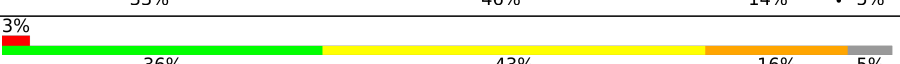
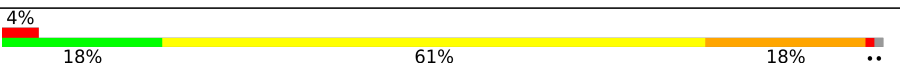
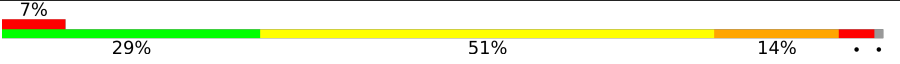
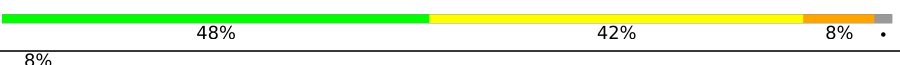
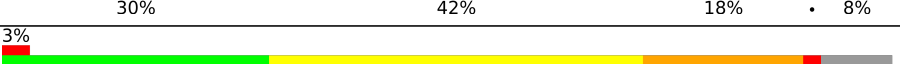
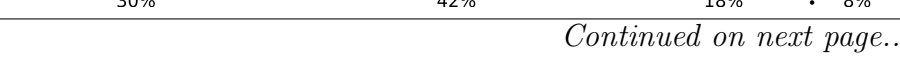
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Mol	Chain	Length	Quality of chain
28	AE	206	
28	BE	206	
29	AF	210	
29	BF	210	
30	AG	182	
30	BG	182	
31	AH	180	
31	BH	180	
32	AI	148	
32	BI	148	
33	AJ	173	
33	BJ	173	
34	AN	140	
34	BN	140	
35	AO	122	
35	BO	122	
36	AP	150	
36	BP	150	
37	AQ	141	
37	BQ	141	
38	AR	118	
38	BR	118	
39	AS	112	
39	BS	112	
40	AT	146	

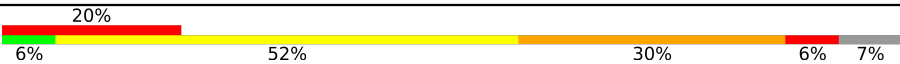
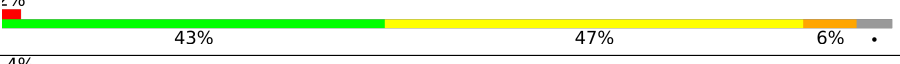
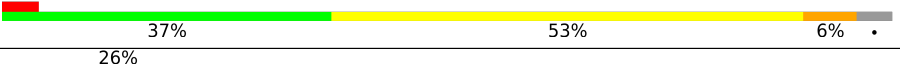
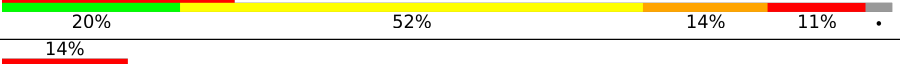
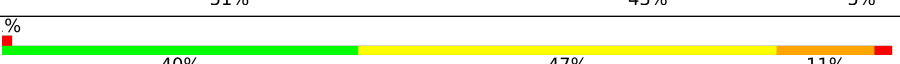
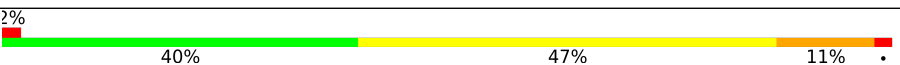
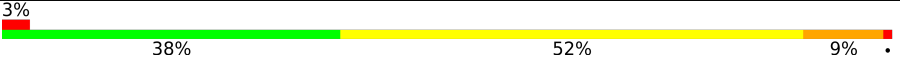
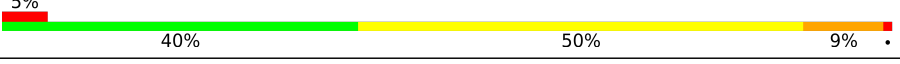
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Mol	Chain	Length	Quality of chain
40	BT	146	
41	AU	118	
41	BU	118	
42	AV	101	
42	BV	101	
43	AW	113	
43	BW	113	
44	AX	96	
44	BX	96	
45	AY	110	
45	BY	110	
46	AZ	206	
46	BZ	206	
47	A0	85	
47	B0	85	
48	A1	98	
48	B1	98	
49	A2	72	
49	B2	72	
50	A3	60	
50	B3	60	
51	A4	71	
51	B4	71	
52	A5	60	
52	B5	60	

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Mol	Chain	Length	Quality of chain
53	A6	54	
53	B6	54	
54	A7	49	
54	B7	49	
55	A8	65	
55	B8	65	
56	A9	37	
56	B9	37	
57	AA	2848	
57	BA	2848	
58	AB	119	
58	BB	119	

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
23	OMG	Ax	21	-	-	X	-
60	MG	AA	2928	-	-	-	X
60	MG	AA	2940	-	-	-	X
60	MG	AA	2967	-	-	-	X
60	MG	AA	2975	-	-	-	X
60	MG	AA	2980	-	-	-	X
60	MG	AA	3002	-	-	-	X
60	MG	AA	3015	-	-	-	X
60	MG	AA	3030	-	-	-	X
60	MG	AA	3036	-	-	-	X
60	MG	AA	3057	-	-	-	X
60	MG	AA	3069	-	-	-	X
60	MG	AA	3091	-	-	-	X
60	MG	AA	3103	-	-	-	X
60	MG	AA	3109	-	-	-	X
60	MG	AA	3112	-	-	-	X
60	MG	AA	3149	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3152	-	-	-	X
60	MG	AA	3215	-	-	-	X
60	MG	AA	3237	-	-	-	X
60	MG	AA	3239	-	-	-	X
60	MG	AA	3243	-	-	-	X
60	MG	AA	3249	-	-	-	X
60	MG	AB	202	-	-	-	X
60	MG	Aa	1616	-	-	-	X
60	MG	Aa	1637	-	-	-	X
60	MG	Aa	1647	-	-	-	X
60	MG	Aa	1651	-	-	-	X
60	MG	Aa	1664	-	-	-	X
60	MG	Aa	1678	-	-	-	X
60	MG	Aa	1694	-	-	-	X
60	MG	Aa	1705	-	-	-	X
60	MG	Aa	1730	-	-	-	X
60	MG	Aa	1741	-	-	-	X
60	MG	BA	2958	-	-	-	X
60	MG	BA	2970	-	-	-	X
60	MG	BA	3036	-	-	-	X
60	MG	BA	3053	-	-	-	X
60	MG	BA	3071	-	-	-	X
60	MG	BA	3081	-	-	-	X
60	MG	BA	3135	-	-	-	X
60	MG	BA	3149	-	-	-	X
60	MG	BA	3150	-	-	-	X
60	MG	BA	3162	-	-	-	X
60	MG	BA	3177	-	-	-	X
60	MG	BA	3200	-	-	-	X
60	MG	BA	3208	-	-	-	X
60	MG	BA	3210	-	-	-	X
60	MG	BA	3233	-	-	-	X
60	MG	BA	3234	-	-	-	X
60	MG	BA	3235	-	-	-	X
60	MG	BA	3265	-	-	-	X
60	MG	Ba	1625	-	-	-	X
60	MG	Ba	1635	-	-	-	X
60	MG	Ba	1636	-	-	-	X
60	MG	Ba	1646	-	-	-	X
60	MG	Ba	1676	-	-	-	X
60	MG	Ba	1677	-	-	-	X
60	MG	Ba	1680	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	Ba	1682	-	-	-	X
60	MG	Ba	1692	-	-	-	X
60	MG	Ba	1698	-	-	-	X
60	MG	Ba	1699	-	-	-	X
60	MG	Ba	1702	-	-	-	X
60	MG	Ba	1703	-	-	-	X
60	MG	Ba	1704	-	-	-	X
60	MG	Ba	1706	-	-	-	X
60	MG	Ba	1707	-	-	-	X
60	MG	Ba	1713	-	-	-	X
60	MG	Ba	1717	-	-	-	X
60	MG	Ba	1720	-	-	-	X
60	MG	Ba	1728	-	-	-	X
60	MG	Ba	1739	-	-	-	X
60	MG	Bv	103	-	-	-	X
60	MG	Bv	104	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 297206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ab	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
1	Bb	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Ac	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
2	Bc	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Ad	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
3	Bd	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Ae	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			
4	Be	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Af	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
5	Bf	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	Ag	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
6	Bg	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Ah	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
7	Bh	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Ai	127	Total	C	N	O		0	0	0
			1010	639	197	174				
8	Bi	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Aj	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
9	Bj	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Ak	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Bk	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Al	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
11	Bl	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Am	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			
12	Bm	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	An	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
13	Bn	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Ao	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
14	Bo	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	Ap	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
15	Bp	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Aq	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
16	Bq	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Ar	70	Total	C	N	O	0	0	0
			574	367	112	95			
17	Br	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	As	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
18	Bs	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	At	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
19	Bt	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Au	24	Total	C	N	O	0	0	0
			208	128	50	30			
20	Bu	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 21 is a protein called Toxin relE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Ay	94	Total	C	N	O	S	0	0	0
			770	496	133	139	2			
21	By	94	Total	C	N	O	S	0	0	0
			766	495	130	139	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ay	45	ALA	ARG	engineered mutation	UNP P0C077
Ay	81	ALA	ARG	engineered mutation	UNP P0C077
By	45	ALA	ARG	engineered mutation	UNP P0C077
By	81	ALA	ARG	engineered mutation	UNP P0C077

- Molecule 22 is a RNA chain called RNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Aa	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
22	Ba	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 23 is a RNA chain called RNA (5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*A*AP*AP*AP*AP*UP*GP*(OMU)P*(A2M)P*(OMG)P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Ax	12	Total	C	N	O	P	0	0	0
			262	121	54	76	11			
23	Bx	12	Total	C	N	O	P	0	0	0
			262	121	54	76	11			

- Molecule 24 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Av	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			
24	Bv	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 25 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Aw	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
25	Bw	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
26	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			
27	BD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
28	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			
29	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	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	AH	164	Total	C	N	O	S	0	0	0
			1259	800	233	225	1			
31	BH	164	Total	C	N	O	S	0	0	0
			1259	800	233	225	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
32	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AJ	130	Total	C	N	O		0	0	0
			641	381	130	130				
33	BJ	130	Total	C	N	O		0	0	0
			641	381	130	130				

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
34	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			
37	BQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	AR	117	Total	C	N	O	0	0	0
			960	599	202	159			
38	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	AS	98	Total	C	N	O	0	0	0
			770	486	154	130			
39	BS	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	AT	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			
40	BT	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
41	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
43	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	AX	92	Total	C	N	O	0	0	0
			725	471	131	123			
44	BX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	AY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
45	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	AZ	184	Total	C	N	O	S	0	0	0
			1467	936	261	268	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	184	Total	C	N	O	S	0	0	0
			1467	936	261	268	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	A0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
47	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	A1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			
48	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	A2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	A3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
50	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	A4	57	Total	C	N	O	S	0	0	0
			450	285	77	83	5			
51	B4	57	Total	C	N	O	S	0	0	0
			450	285	77	83	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	A5	55	Total	C	N	O	S	0	0	0
			427	267	86	69	5			
52	B5	55	Total	C	N	O	S	0	0	0
			427	267	86	69	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	A6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
53	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	A7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
54	B7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	A8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
55	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
56	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 57 is a RNA chain called RNA (2848-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	AA	2848	Total 61341	C 27300	N 11478	O 19716	P 2847	0	0	0
57	BA	2848	Total 61341	C 27300	N 11478	O 19716	P 2847	0	0	0

- Molecule 58 is a RNA chain called RNA (119-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	AB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0
58	BB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Ad	1	Total 1	Zn 1	0	0
59	An	1	Total 1	Zn 1	0	0
59	A4	1	Total 1	Zn 1	0	0
59	A9	1	Total 1	Zn 1	0	0
59	Bd	1	Total 1	Zn 1	0	0
59	Bn	1	Total 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	Am	1	Total 1	Mg 1	0	0
60	Aq	1	Total 1	Mg 1	0	0
60	Aa	145	Total 145	Mg 145	0	0

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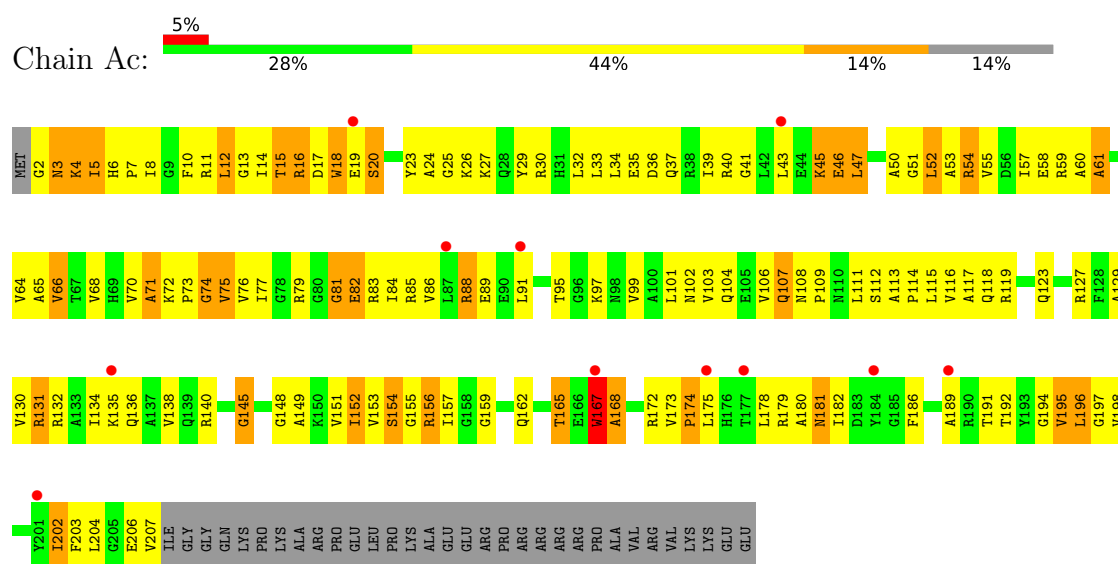
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	Av	4	Total 4	Mg 4	0	0
60	Aw	1	Total 1	Mg 1	0	0
60	AD	2	Total 2	Mg 2	0	0
60	AF	1	Total 1	Mg 1	0	0
60	AQ	1	Total 1	Mg 1	0	0
60	AX	1	Total 1	Mg 1	0	0
60	A1	1	Total 1	Mg 1	0	0
60	A5	1	Total 1	Mg 1	0	0
60	A7	2	Total 2	Mg 2	0	0
60	AA	368	Total 368	Mg 368	0	0
60	AB	3	Total 3	Mg 3	0	0
60	Bm	2	Total 2	Mg 2	0	0
60	Bq	1	Total 1	Mg 1	0	0
60	Ba	143	Total 143	Mg 143	0	0
60	Bx	1	Total 1	Mg 1	0	0
60	Bv	5	Total 5	Mg 5	0	0
60	Bw	1	Total 1	Mg 1	0	0
60	BD	2	Total 2	Mg 2	0	0
60	BF	1	Total 1	Mg 1	0	0
60	BQ	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0

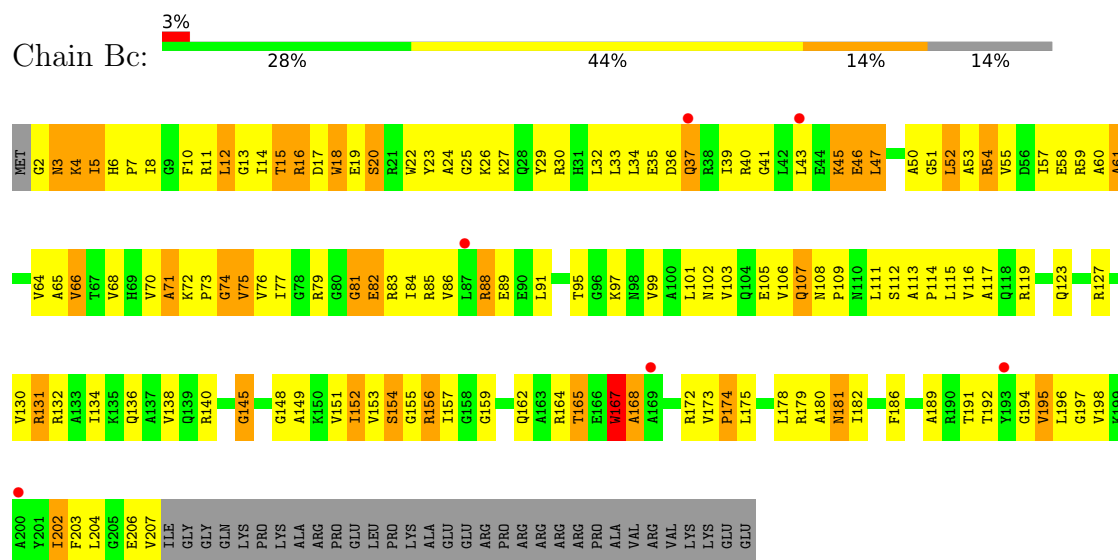
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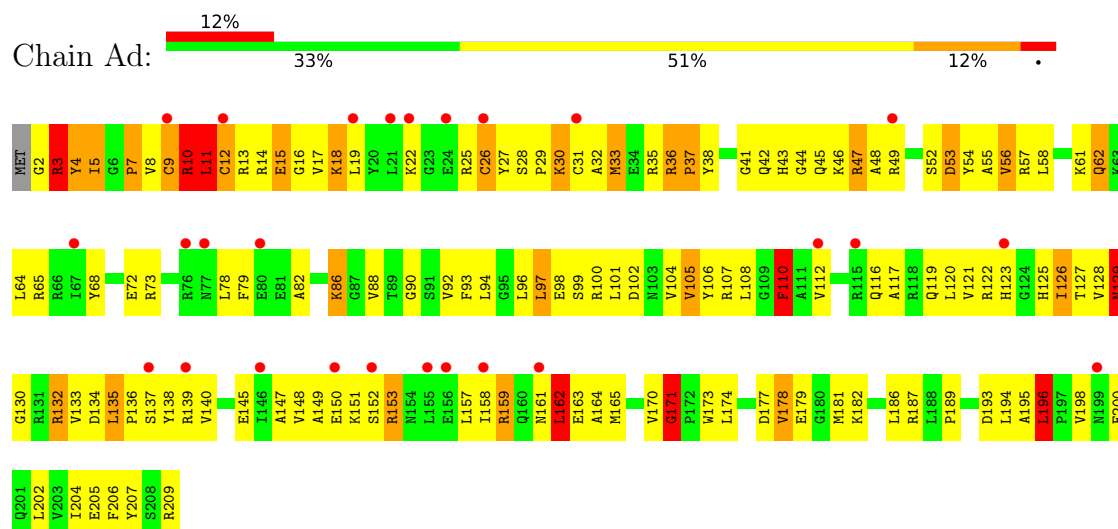
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B0	2	Total 2	Mg 2	0	0
60	B5	1	Total 1	Mg 1	0	0
60	B7	2	Total 2	Mg 2	0	0
60	BA	366	Total 366	Mg 366	0	0
60	BB	3	Total 3	Mg 3	0	0



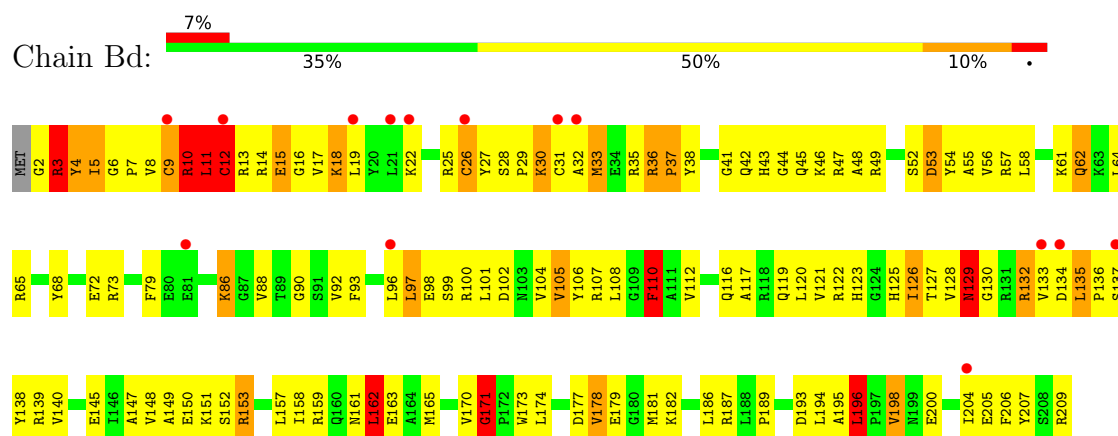
• Molecule 2: 30S ribosomal protein S3



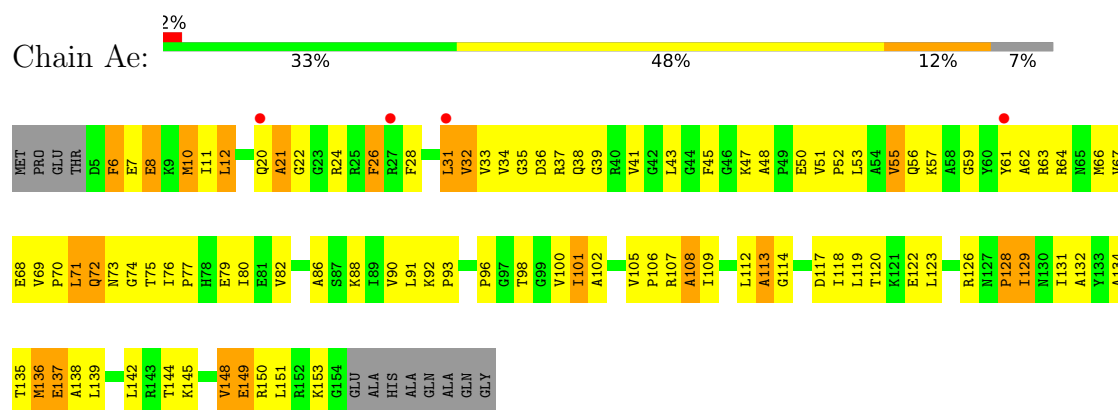
• Molecule 3: 30S ribosomal protein S4



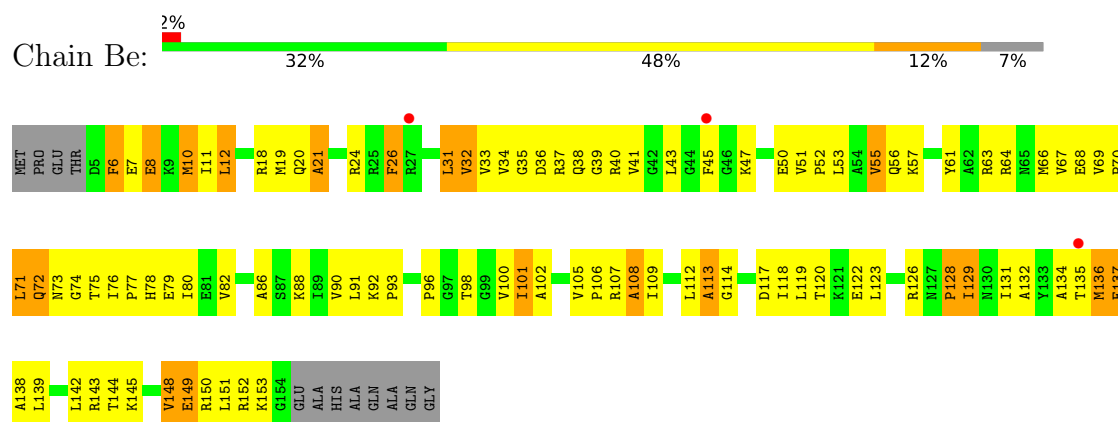
- Molecule 3: 30S ribosomal protein S4



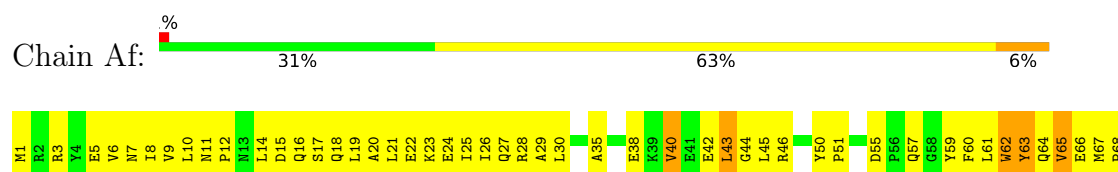
- Molecule 4: 30S ribosomal protein S5

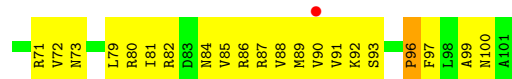


- Molecule 4: 30S ribosomal protein S5

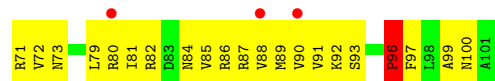


- Molecule 5: 30S ribosomal protein S6





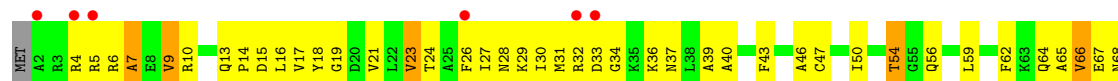
• Molecule 5: 30S ribosomal protein S6



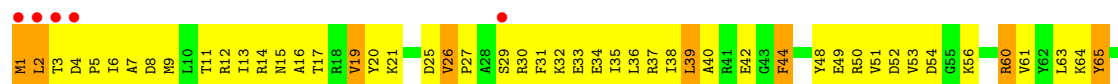
• Molecule 6: 30S ribosomal protein S7



• Molecule 6: 30S ribosomal protein S7

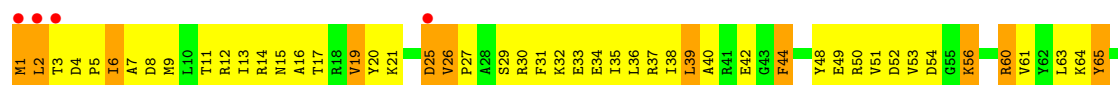


• Molecule 7: 30S ribosomal protein S8





• Molecule 7: 30S ribosomal protein S8



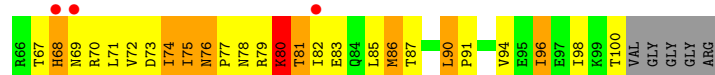
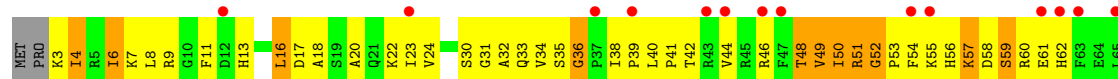
• Molecule 8: 30S ribosomal protein S9



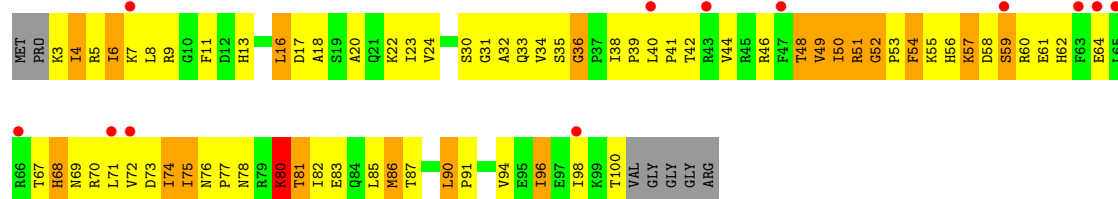
• Molecule 8: 30S ribosomal protein S9



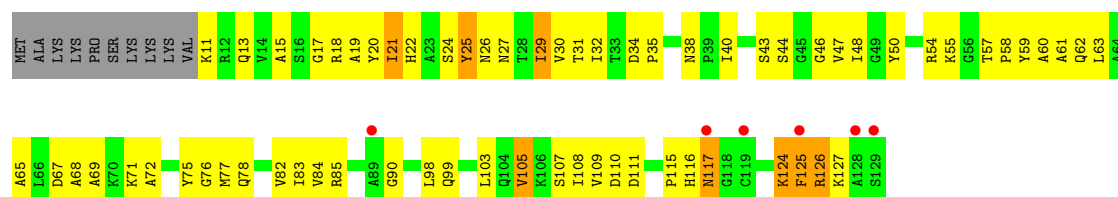
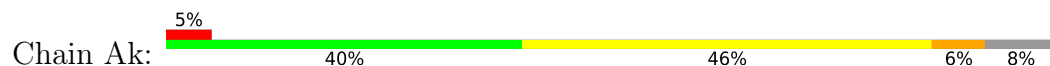
• Molecule 9: 30S ribosomal protein S10



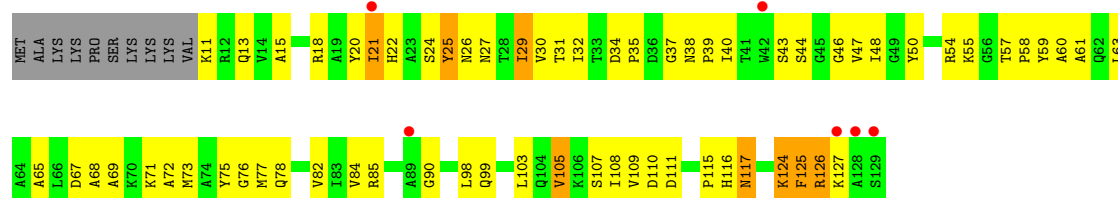
• Molecule 9: 30S ribosomal protein S10



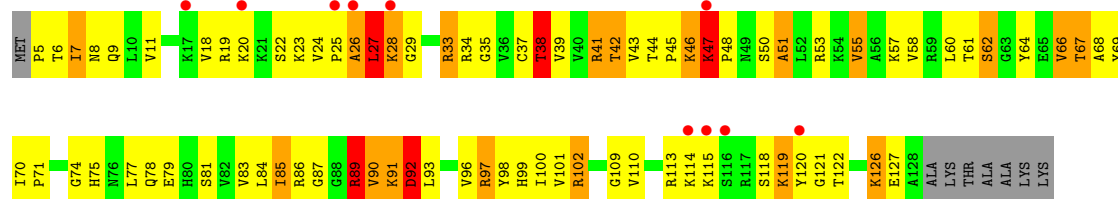
- Molecule 10: 30S ribosomal protein S11



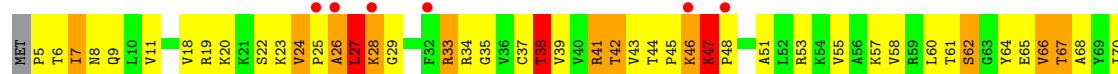
- Molecule 10: 30S ribosomal protein S11

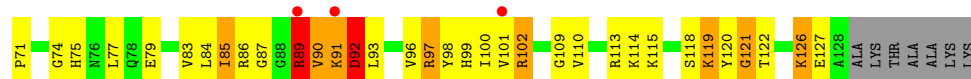


- Molecule 11: 30S ribosomal protein S12

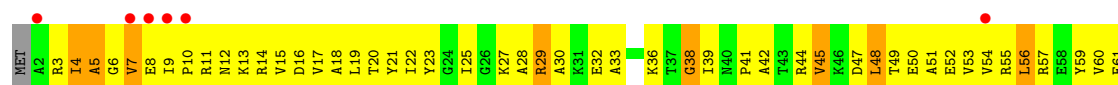
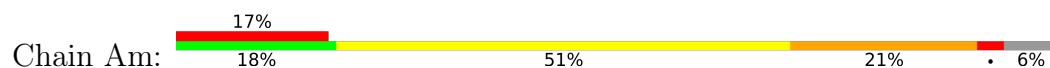


- Molecule 11: 30S ribosomal protein S12



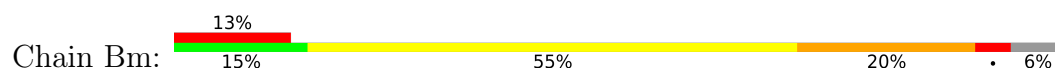


• Molecule 12: 30S ribosomal protein S13



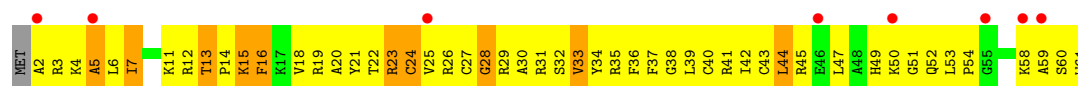
ALA
PRO
ARG
LYS

• Molecule 12: 30S ribosomal protein S13

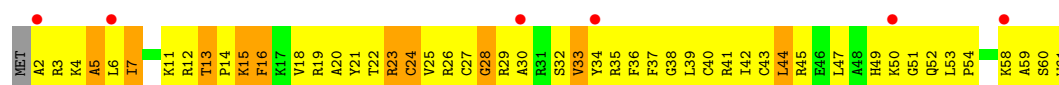


LYS
ALA
PRO
ARG
LYS

• Molecule 13: 30S ribosomal protein S14 type Z

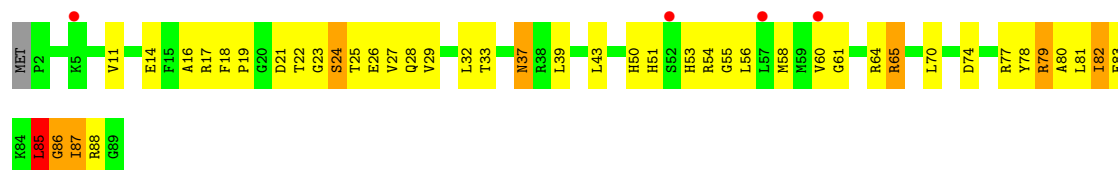


• Molecule 13: 30S ribosomal protein S14 type Z

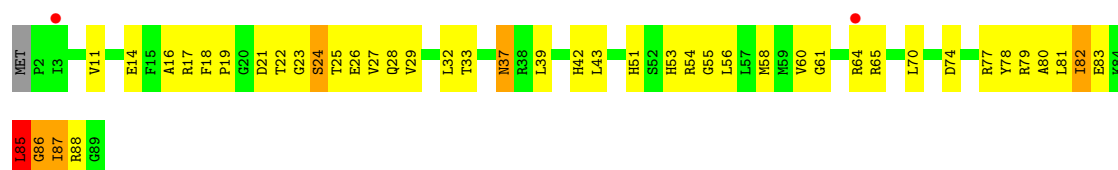


• Molecule 14: 30S ribosomal protein S15

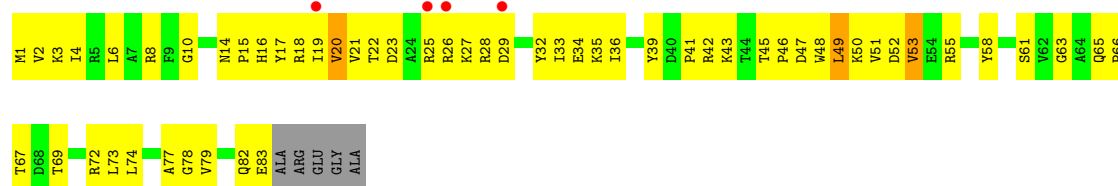




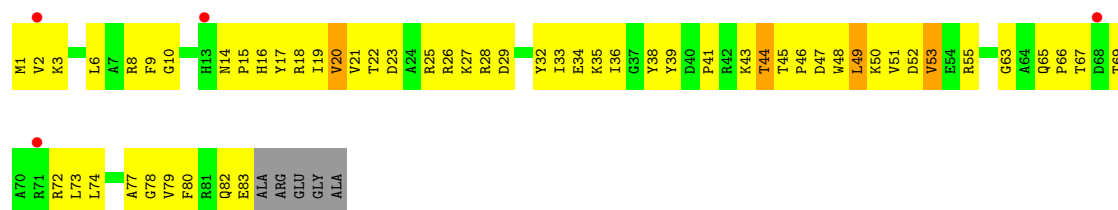
- Molecule 14: 30S ribosomal protein S15



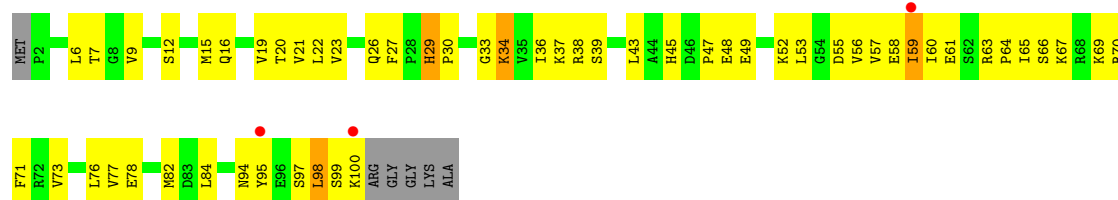
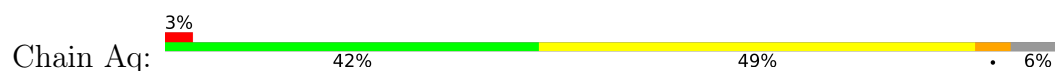
- Molecule 15: 30S ribosomal protein S16



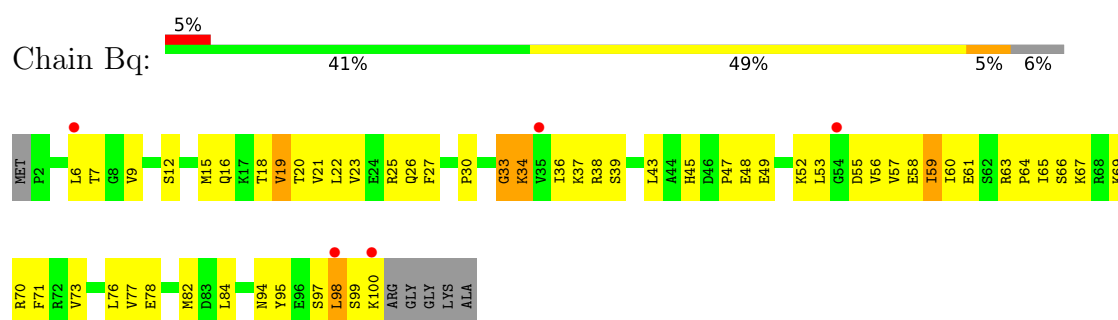
- Molecule 15: 30S ribosomal protein S16



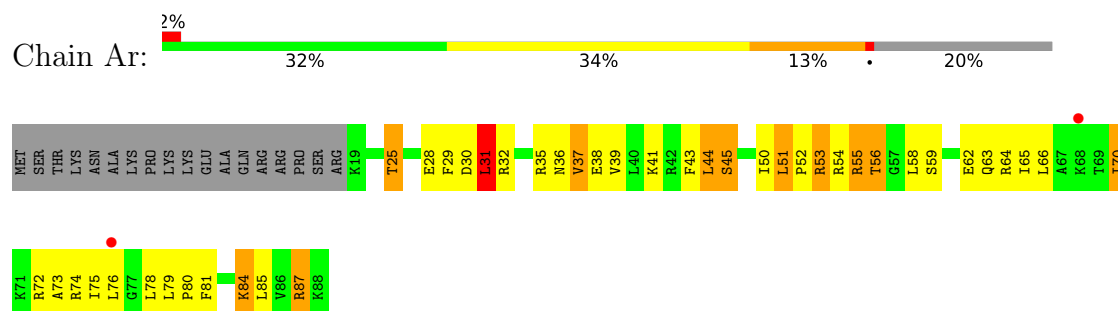
- Molecule 16: 30S ribosomal protein S17



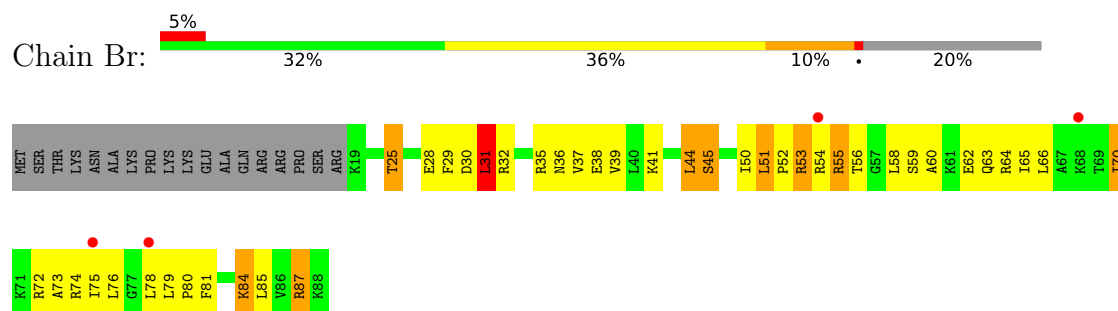
- Molecule 16: 30S ribosomal protein S17



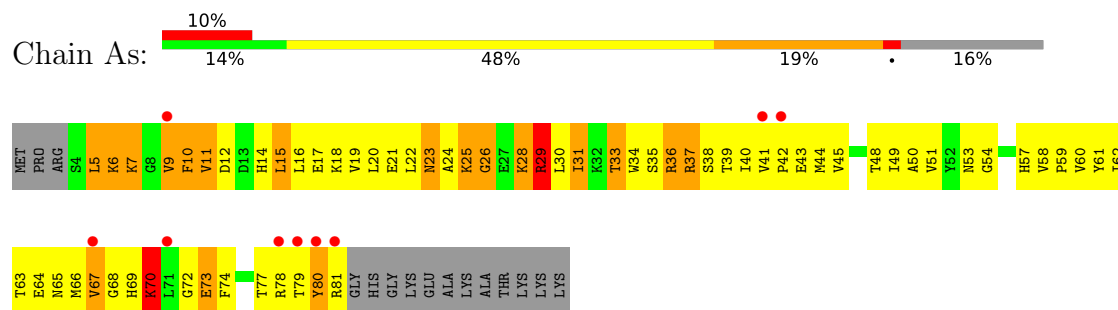
- Molecule 17: 30S ribosomal protein S18



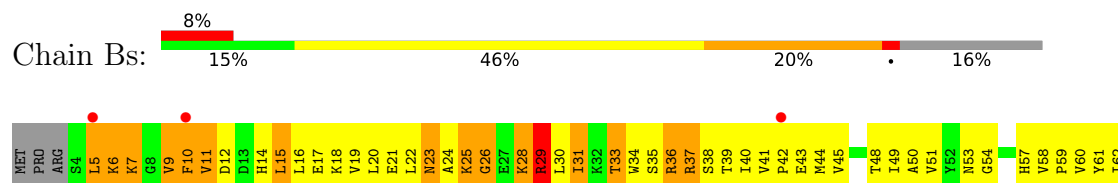
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19

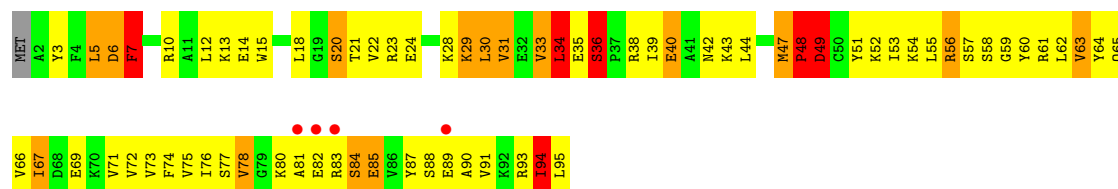
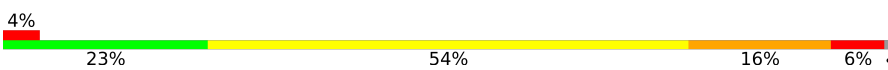


- Molecule 18: 30S ribosomal protein S19

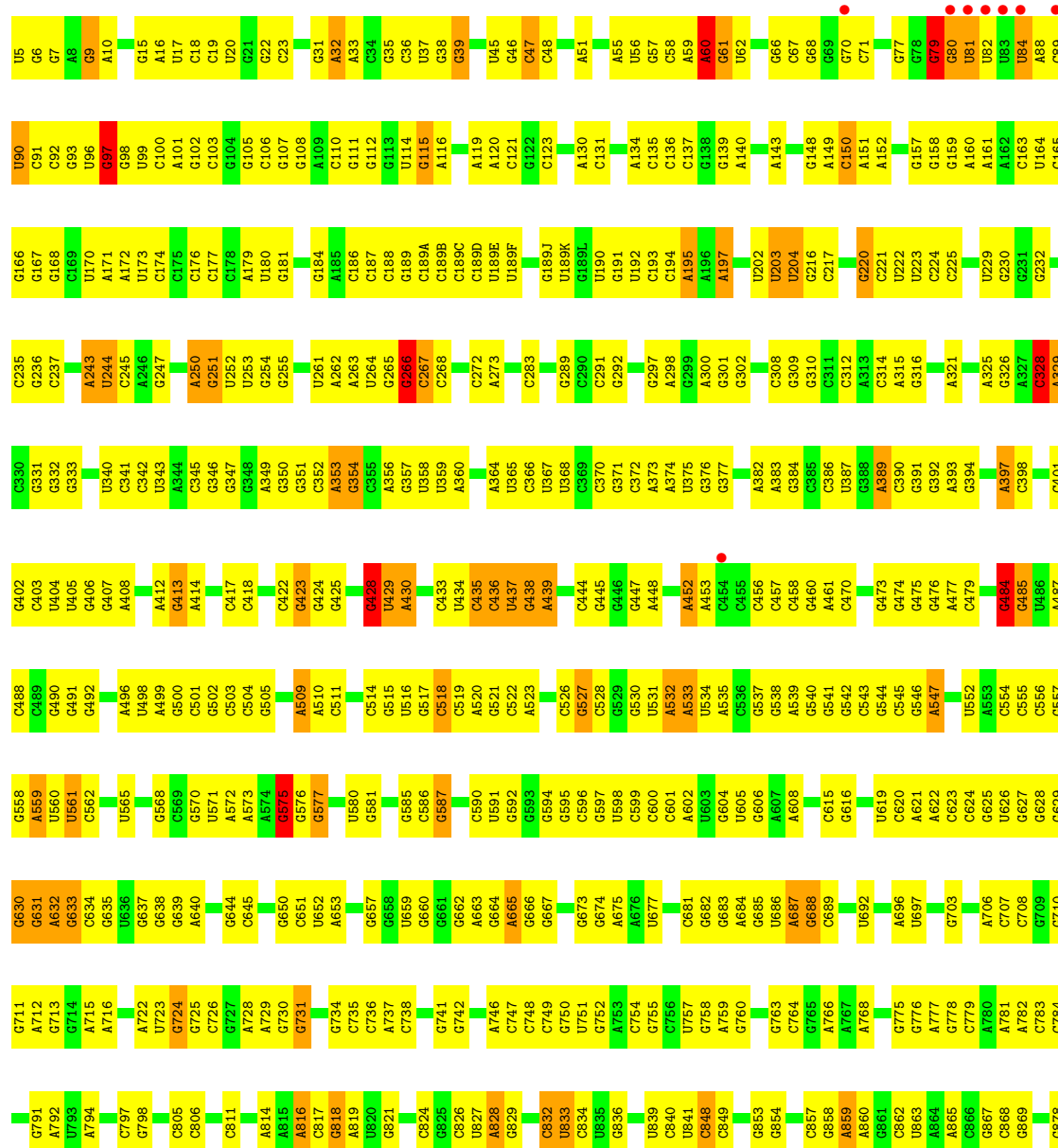


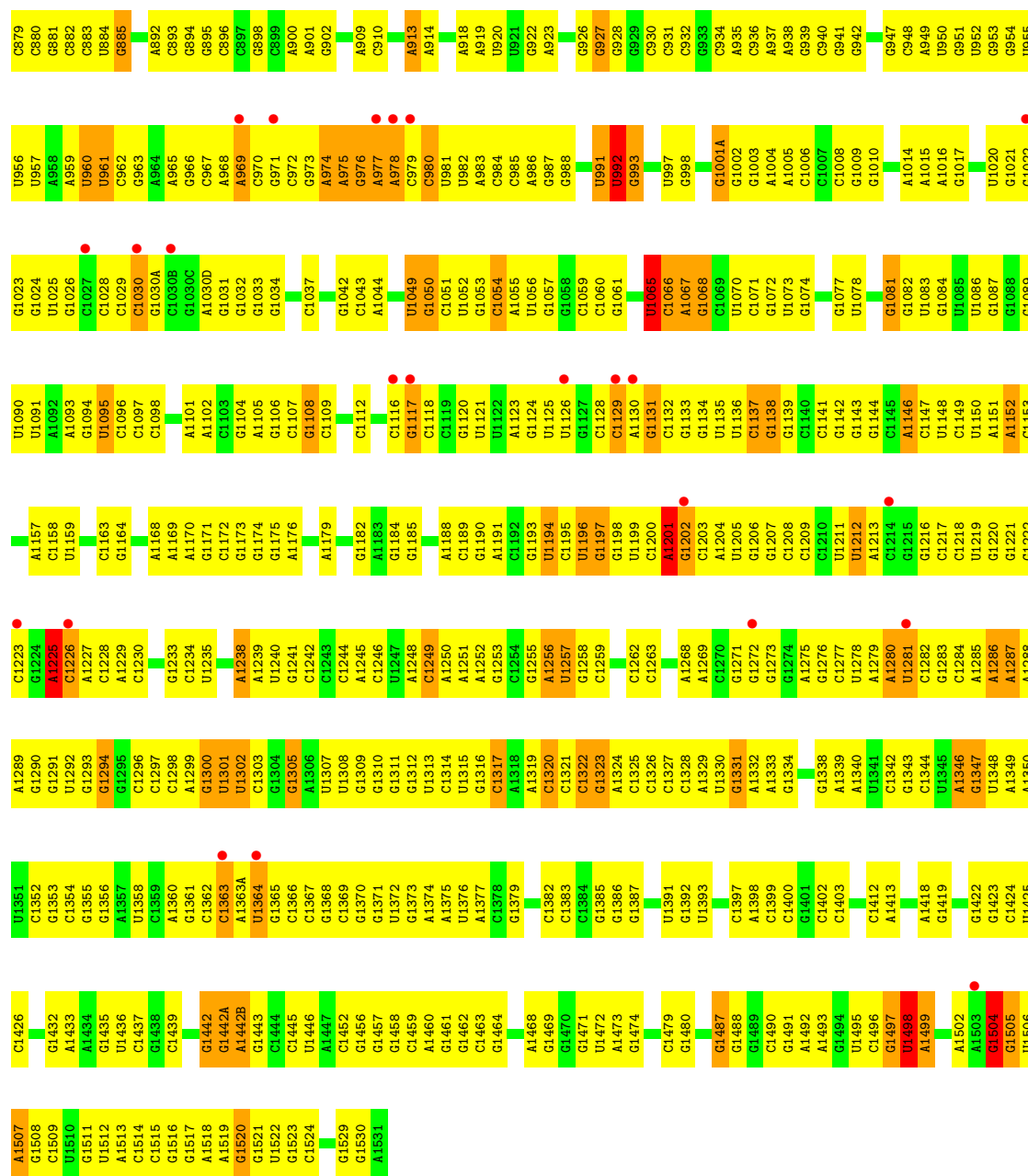


● Molecule 21: Toxin relE

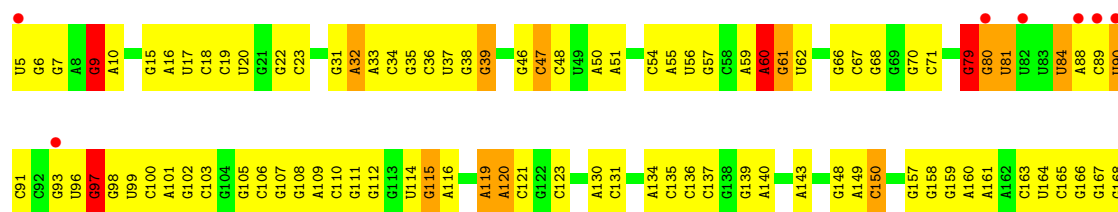
Chain By: 

● Molecule 22: RNA (1504-MER)

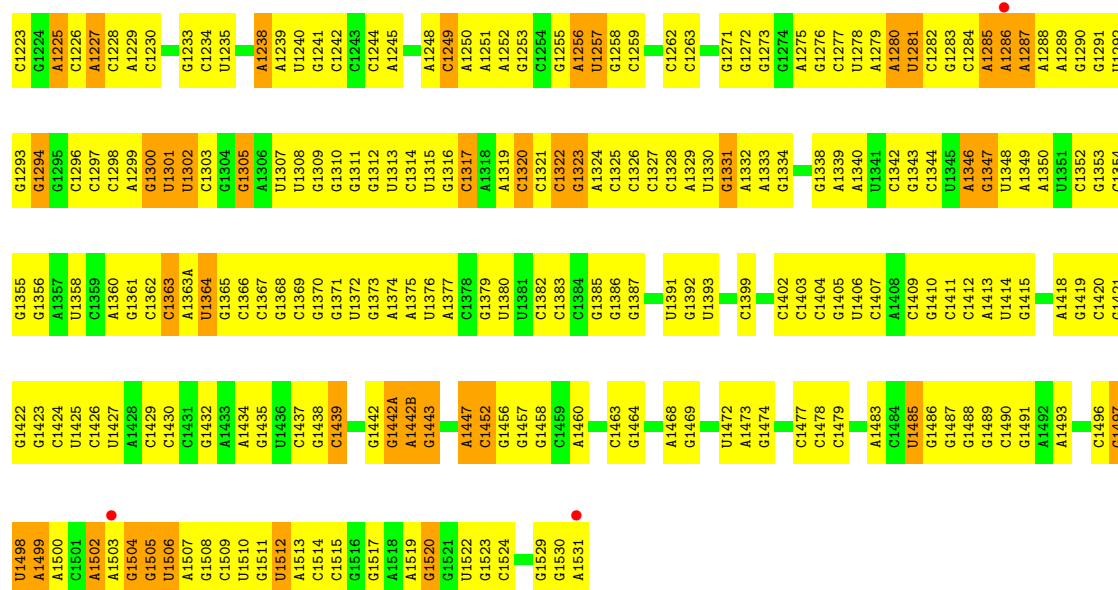
Chain Aa: 



• Molecule 22: RNA (1504-MER)



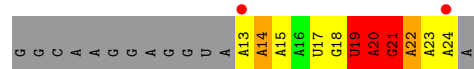
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C1158	A1092	U1025	A958	C880	U793	A715	U636	C562	A495	U244	C341	U244	A171
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C1163	G1094	C1027	U960	C882	C797	A722	G638	U666	U498	G413	U343	A246	U173
U1095	C1028	G1028	U961	C883	G798	U723	G639	G568	A499	A414	A344	G247	C175
C1096	C1029	G1029	C962	U884	G798	U724	A640	C589	G500	C417	C345	C247	C176
C1097	G1030	U1030A	G963	G885	C805	G725	G644	U570	C501	C418	G346	A250	C177
C1098	A1030A	G1030A	A965	C886	C806	C726	C645	U571	C502	G347	G347	A251	C178
A1101	A1030B	A1030B	G966	C887	C811	G727	G650	A573	G505	C422	G351	U252	U179
A1102	G1031	G1031	C967	A892	G728	A728	C651	A574	G506	G423	C352	G254	U180
G1103	G1032	G1032	A968	C893	A729	G730	U652	G575	C507	G425	A353	G255	G181
G1104	G1033	G1033	A969	C894	G730	G731	A653	G576	C508	G426	G354		
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G1107	C1037	C1037	C972	C818	A816	G735	G659	U580	A511	U429	G357	A262	C186
G1108	G1042	G1042	A974	A901	A819	C736	U659	G581	C511	A430	U358	A263	C187
C1109	C1043	C1043	A975	G902	U830	A737	G660	U582	U612		U359	C266	C188
C1112	A1044	A1044	G976	C909	G821	C738	G661	G577	C513	C433	A360	C267	C189
C1116	U1049	U1049	A977	C910	C824	G740	G662	U585	U516	U434	C364	C268	C189A
G1117	G1050	G1050	C978	C910	C825	G741	A663	C586	G517	U435	A364	C269	C189B
C1118	C1051	C1051	C979	A913	C826	G742	A664	G587	C518	C436	U365	C272	C189C
G1119	U1052	U1052	U981	A914	U827	G746	A665	C588	C519	U437	C366	A273	C189D
G1120	G1053	G1053	U982	A915	A828	A747	G666	C589	G521	G438	U367		U189E
C1121	U1054	U1054	C980	A916	U828	C747	G667	G590	C522	A439	C368	C283	U189F
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G1125	U1058	U1058	C987	G922	C834	U751	A676	G595	G447	G447	A373	G292	U191
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C1060	G1061	G1061	U991	G926	G836	G755	C681	C599	G530	A452	U375	C297	C193
C1061	U1062	U1062	C992	G927	C840	C756	G682	C600	U531	A453	G376	A298	C194
U1065	C1066	C1066	G993	G928	U841	U757	G683	C601	A532	C456	A382	G299	A195
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G1068	G1068	G1068	C931	G932	C849	G760	U686	A608	U534	C458	G384	G301	A197
C1069	C1069	C1069	C932	G933	G854	G761	C689	G615	G537	G460	C385	G302	U202
U1070	U1070	U1070	C934	C934	G855	G762	U692	G616	A539	A461	U387	C308	U203
C1071	C1071	C1071	A935	A935	C857	A766	G693	G617	G541	C470	C386	G309	U204
G1072	G1072	G1072	C936	C936	G858	A767	A694	C620	G542	G474	C390	G310	G216
U1073	U1073	U1073	A1005	A937	A859	A768	G695	C621	C543	G475	C391	C312	G220
G1074	G1074	G1074	C1006	A938	C860	G765	A696	A622	G544	G476	C392	C313	C221
C1140	C1007	C1007	C1007	G939	A880	G766	A697	C623	G545	A477	A393	G316	U222
C1008	G1077	G1077	C940	C940	G861	G775	U697	C624	G546	C479	G394		U223
G1078	U1078	U1078	G941	G941	U863	G776	G703	G625	A547	C484	A397	A321	C224
G1079	G1079	G1079	G942	G942	A864	G777	G704	G626	U552	G485	C398	G326	C225
A1080	A1080	A1080	C948	C948	A865	C779	A706	U626	A553	U486	C399	A327	U229
G1081	A1014	A1014	A949	A949	C866	A780	G707	G627	G554	C401	C402	C328	G230
U1082	A1015	A1015	U950	U950	C867	A781	C708	G628	C555	A487	G402	C329	G231
G1083	A1016	A1016	G951	G951	C868	A782	G709	G629	C556	C488	C403	G330	G232
U1085	G1017	G1017	U952	U952	C869	C783	G710	G630	G557	C489	U404	G331	C235
U1086	U1020	U1020	G953	G953	A872	C784	G711	A632	G558	G490	U405	G332	G236
U1087	G1021	G1021	G954	G954						G491	G333		C237
G1088	G1022	G1022	U955	U955		A790	A712	G633	A559	G492	G406		



- Molecule 23: RNA (5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*A*AP*AP*AP*AP*UP*GP*(OMU)P*(A2M)P*(OMG)P*AP*AP*AP*A)-3')



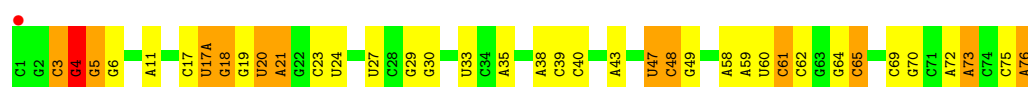
- Molecule 23: RNA (5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*A*AP*AP*AP*AP*UP*GP*(OMU)P*(A2M)P*(OMG)P*AP*AP*AP*A)-3')



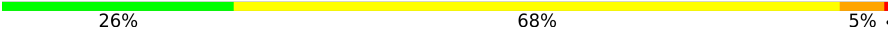
- Molecule 24: RNA (77-MER)



- Molecule 24: RNA (77-MER)



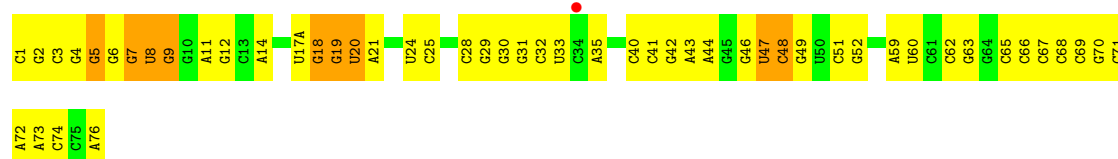
- Molecule 25: RNA (77-MER)

Chain Aw: 



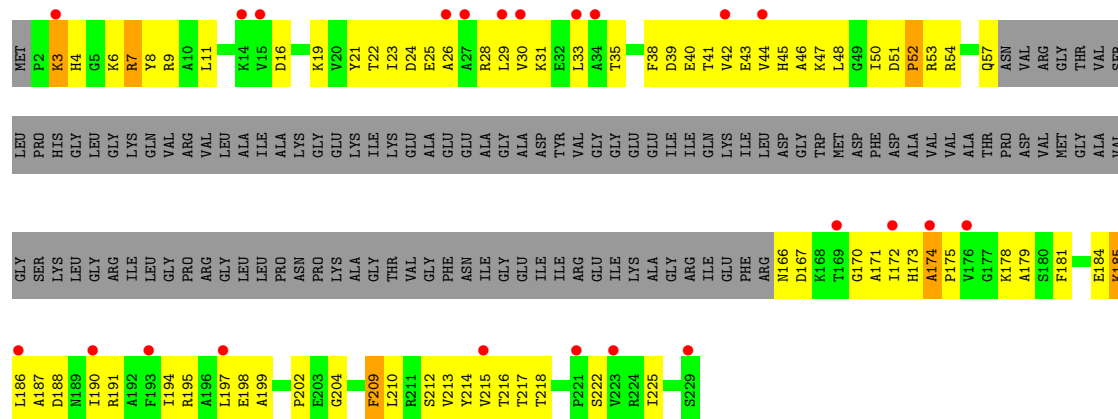
• Molecule 25: RNA (77-MER)

Chain Bw: 



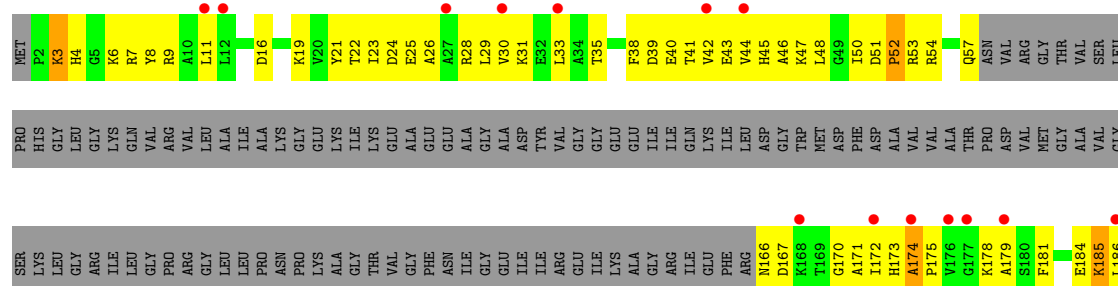
• Molecule 26: 50S ribosomal protein L1

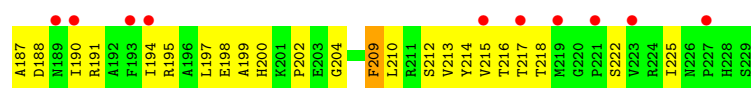
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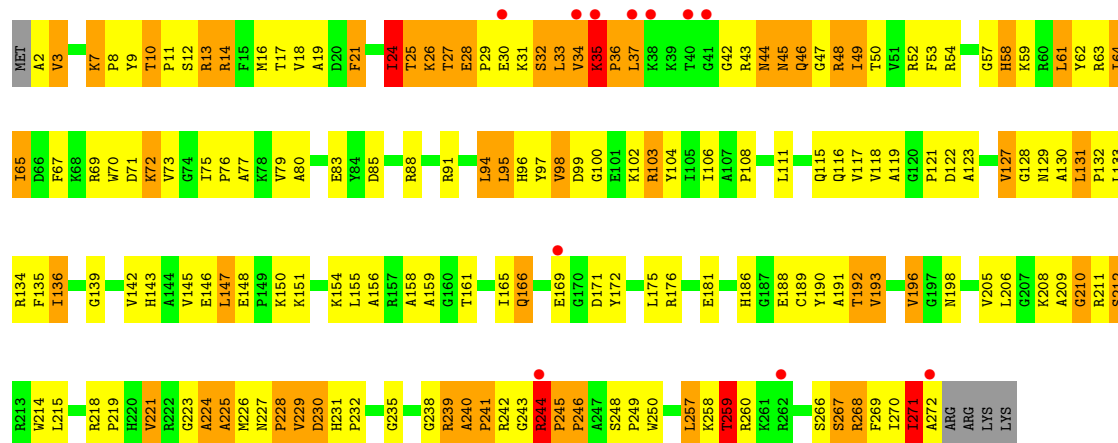
• Molecule 26: 50S ribosomal protein L1

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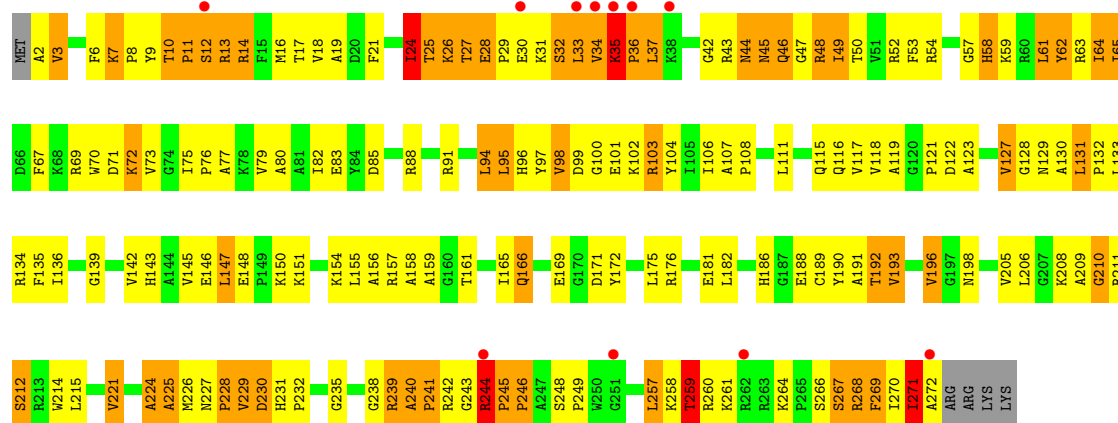




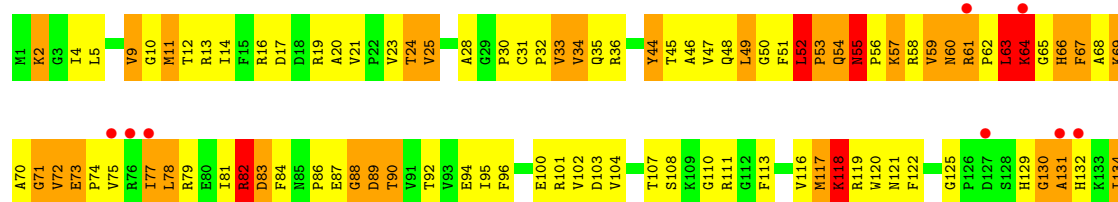
• Molecule 27: 50S ribosomal protein L2

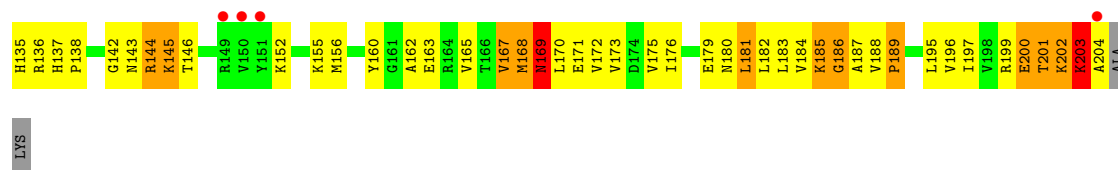


• Molecule 27: 50S ribosomal protein L2

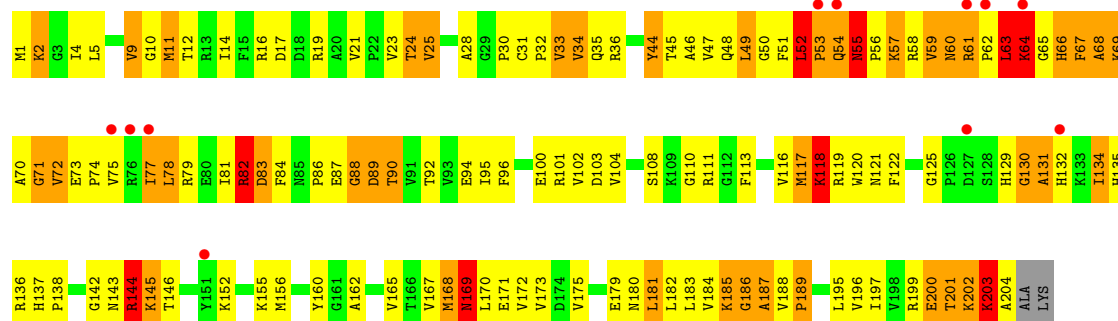


• Molecule 28: 50S ribosomal protein L3

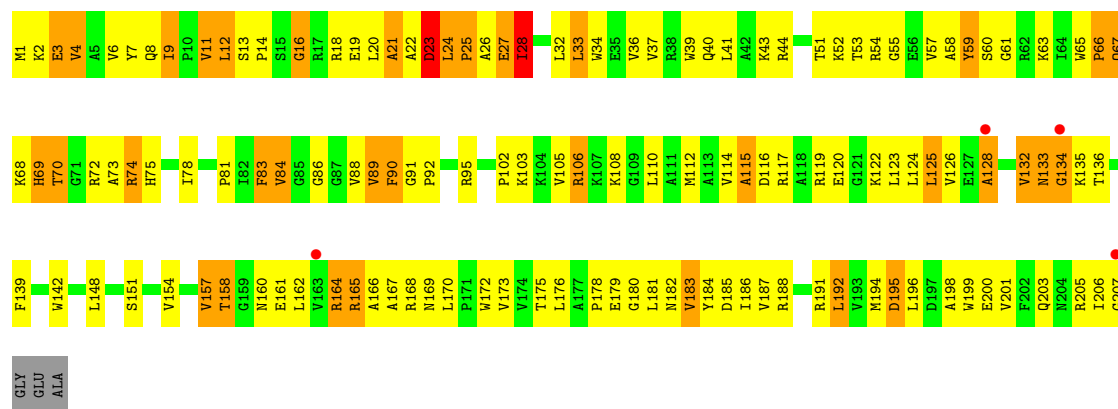




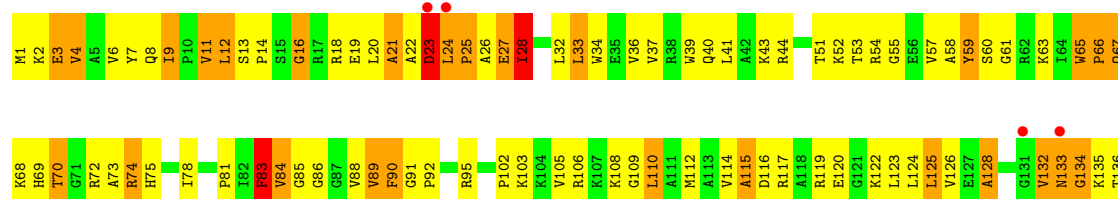
• Molecule 28: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L4

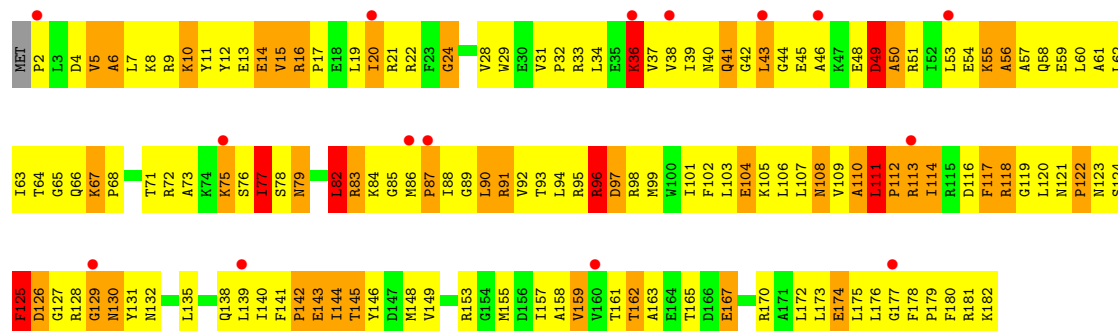
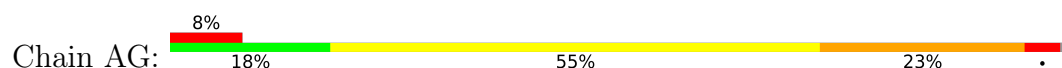


• Molecule 29: 50S ribosomal protein L4

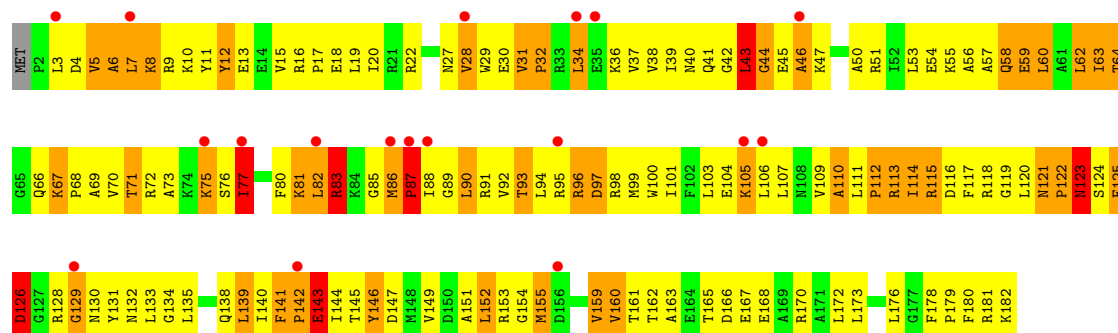
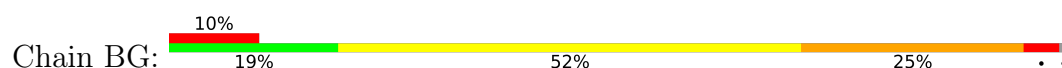




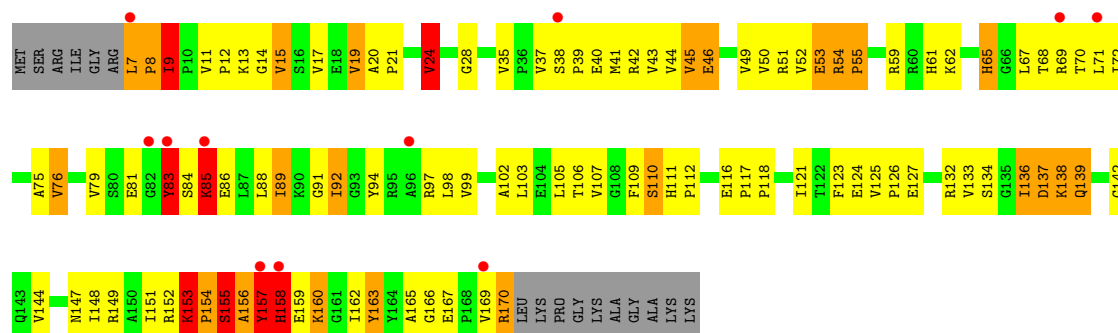
• Molecule 30: 50S ribosomal protein L5



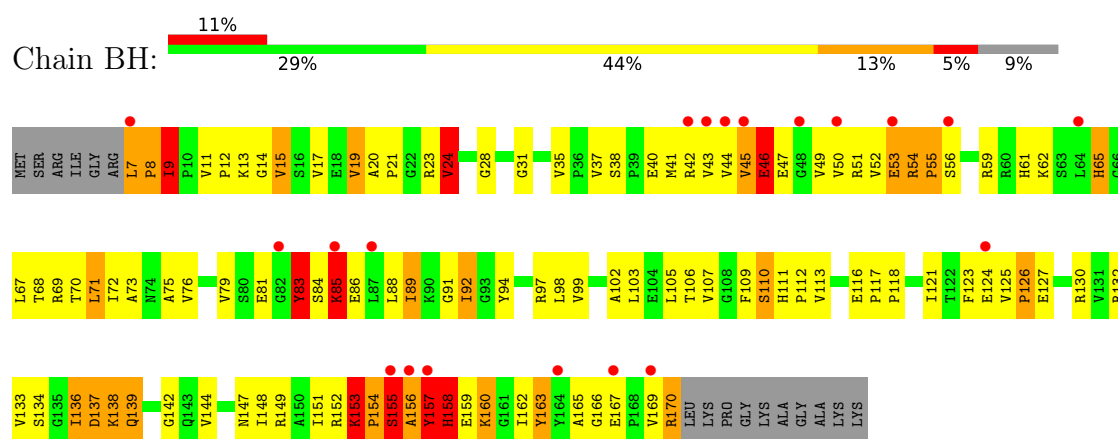
• Molecule 30: 50S ribosomal protein L5



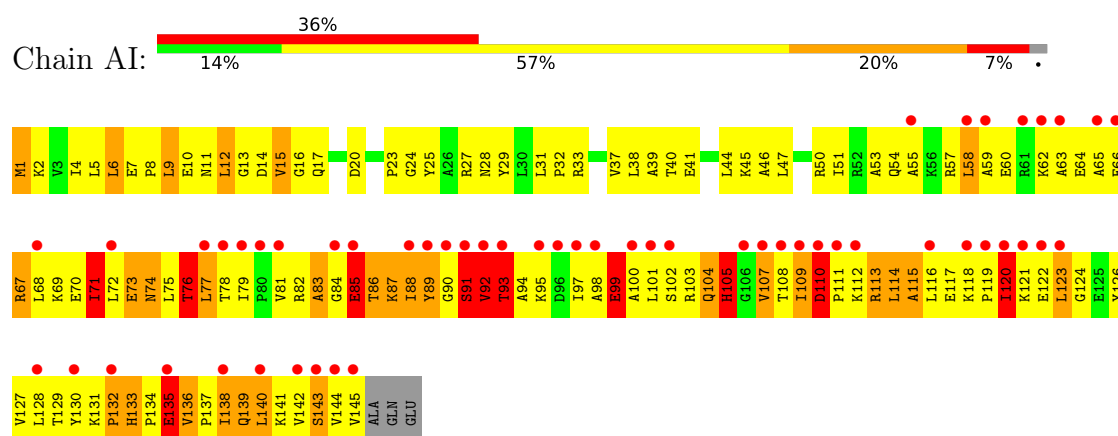
• Molecule 31: 50S ribosomal protein L6



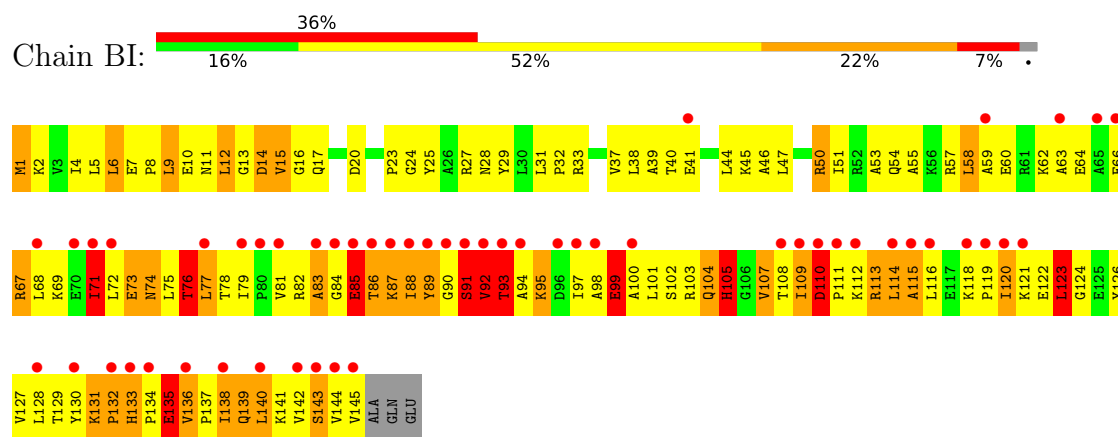
• Molecule 31: 50S ribosomal protein L6



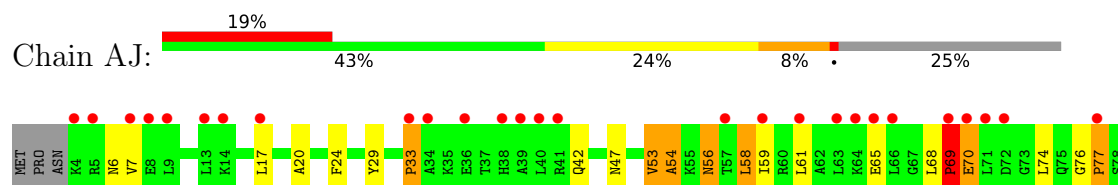
• Molecule 32: 50S ribosomal protein L9

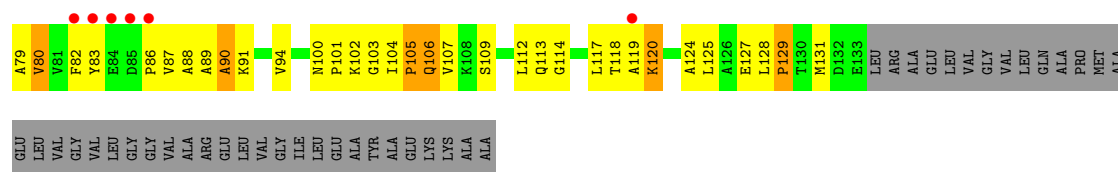


• Molecule 32: 50S ribosomal protein L9

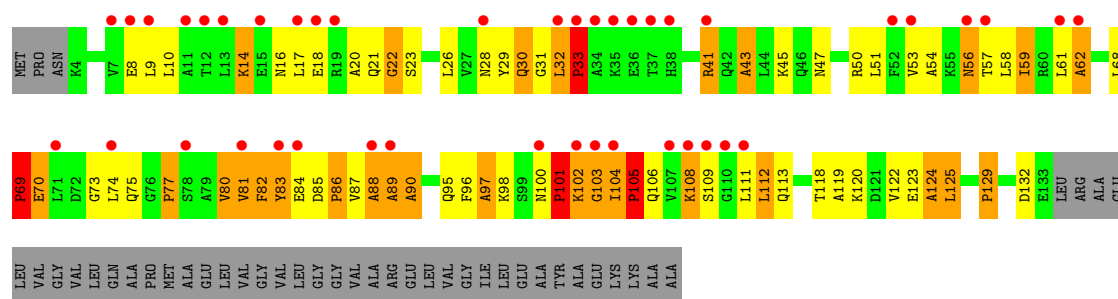
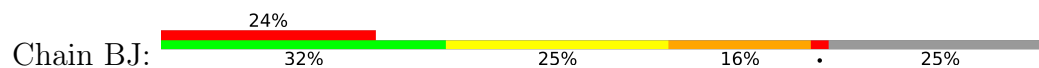


• Molecule 33: 50S ribosomal protein L10

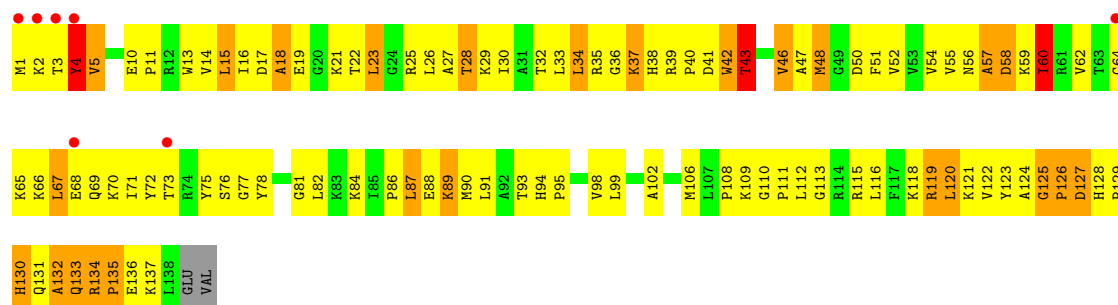




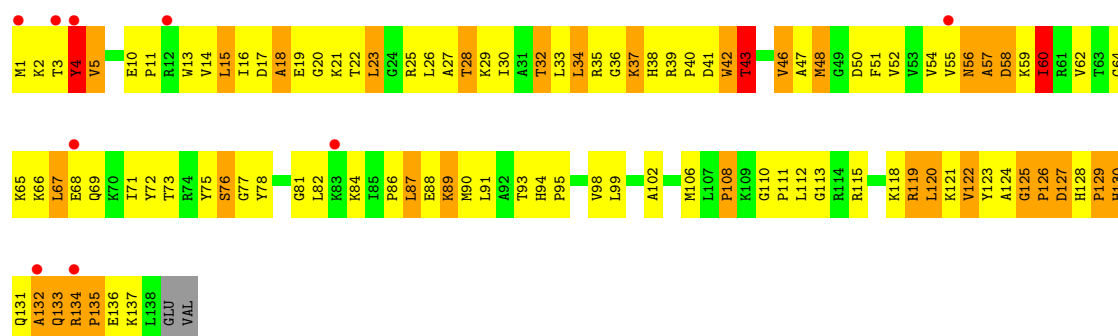
• Molecule 33: 50S ribosomal protein L10



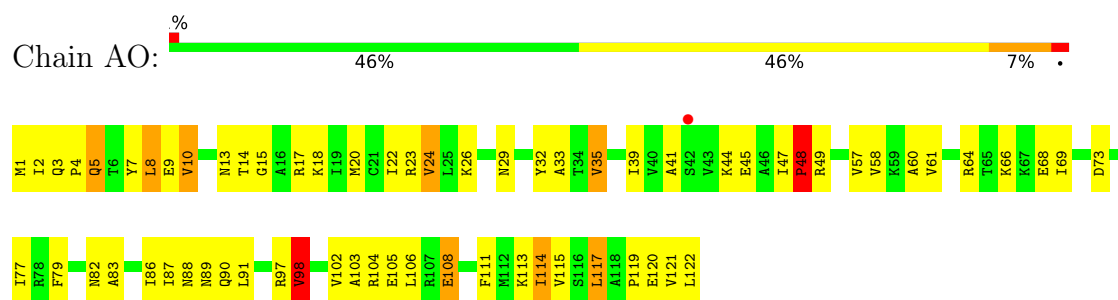
• Molecule 34: 50S ribosomal protein L13



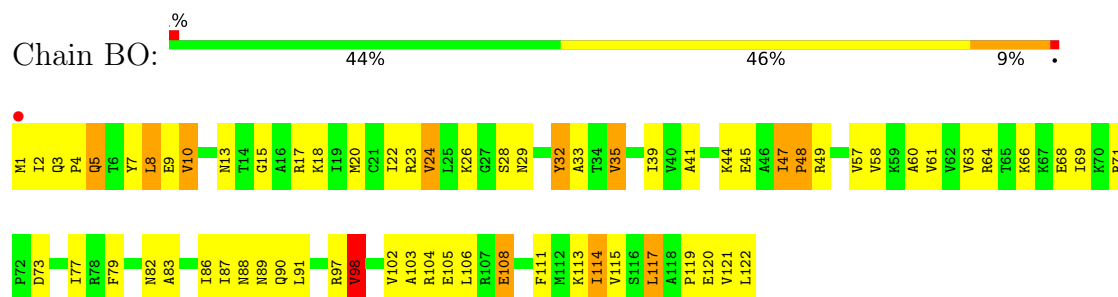
• Molecule 34: 50S ribosomal protein L13



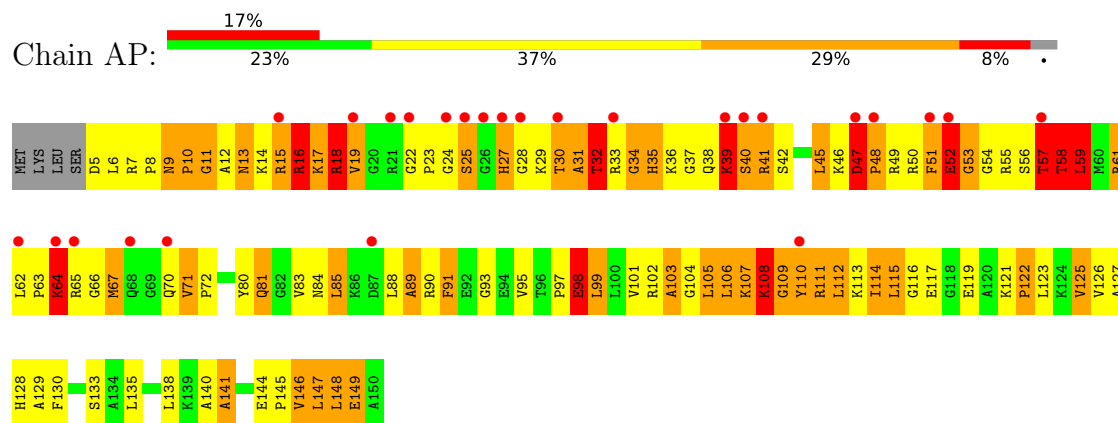
• Molecule 35: 50S ribosomal protein L14



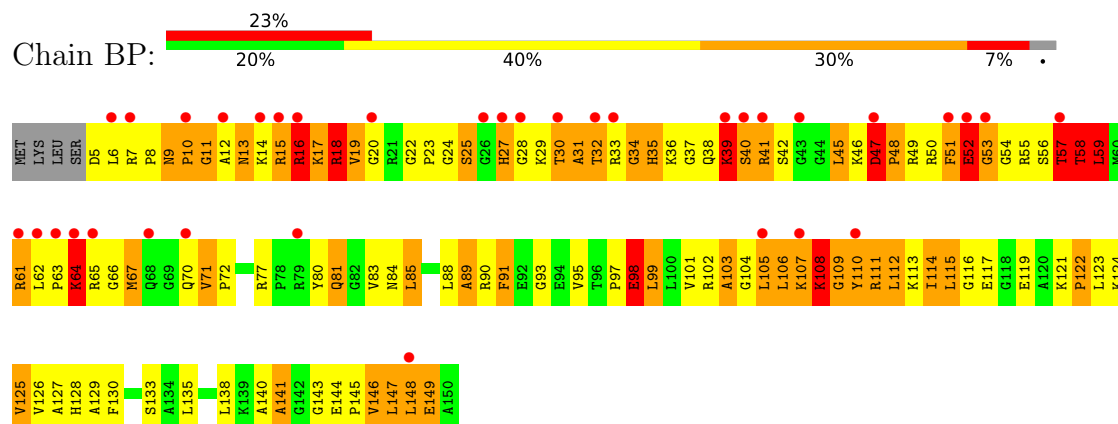
• Molecule 35: 50S ribosomal protein L14



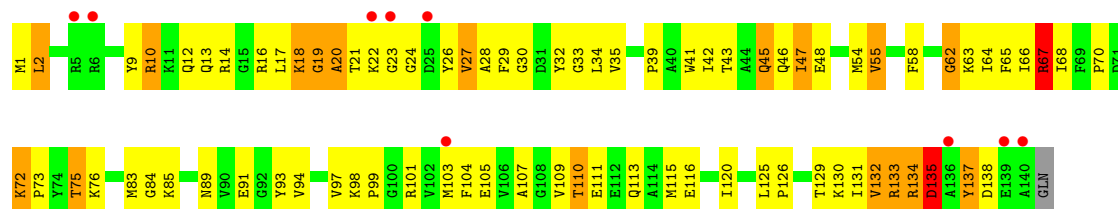
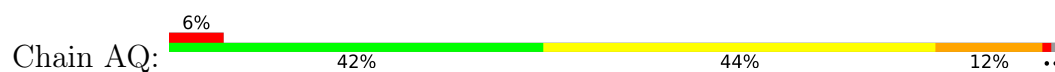
• Molecule 36: 50S ribosomal protein L15



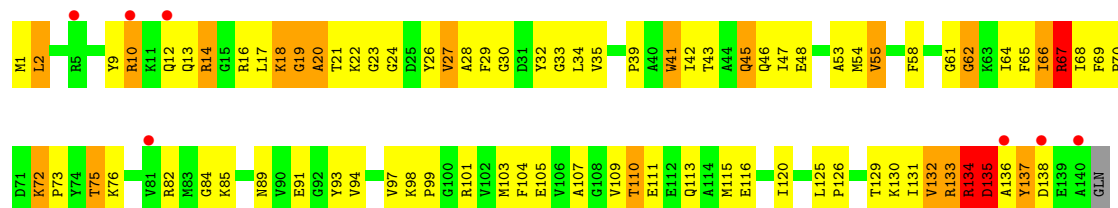
• Molecule 36: 50S ribosomal protein L15



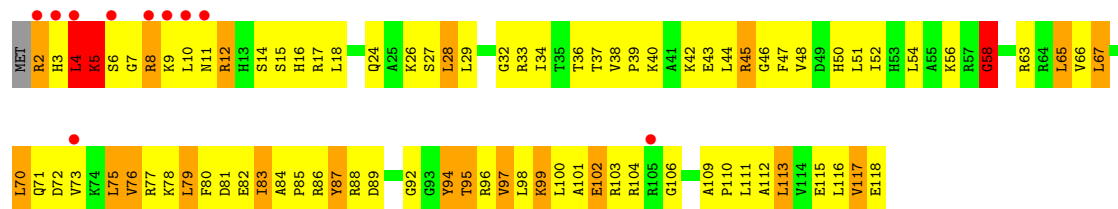
• Molecule 37: 50S ribosomal protein L16



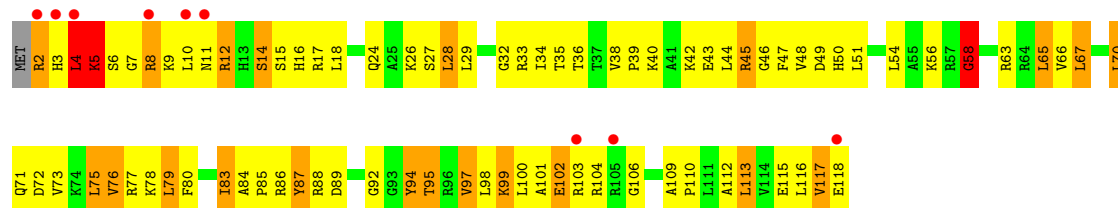
• Molecule 37: 50S ribosomal protein L16



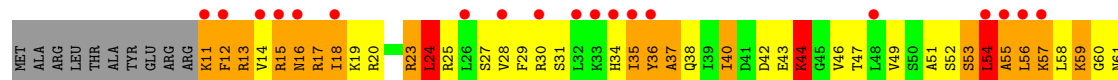
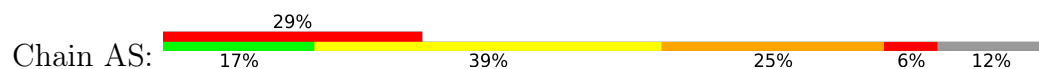
• Molecule 38: 50S ribosomal protein L17

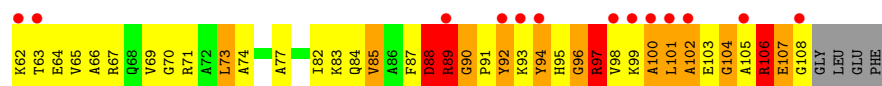


• Molecule 38: 50S ribosomal protein L17

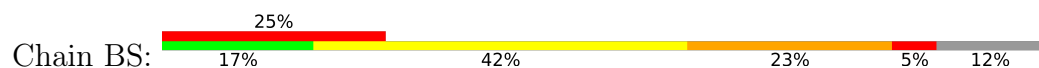


• Molecule 39: 50S ribosomal protein L18

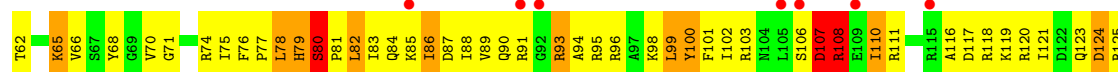
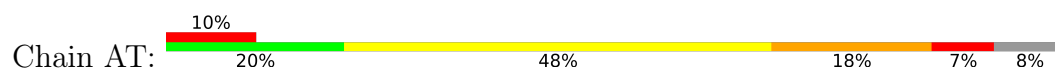




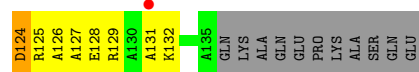
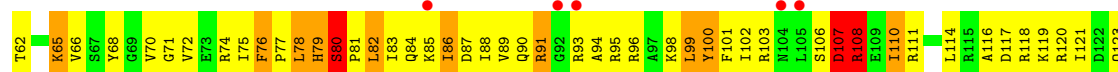
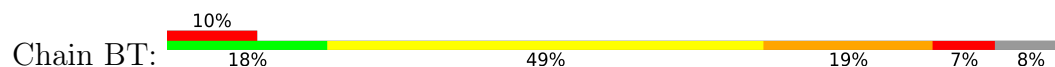
• Molecule 39: 50S ribosomal protein L18



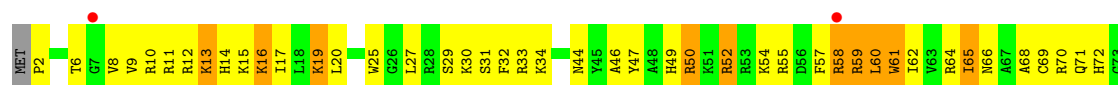
• Molecule 40: 50S ribosomal protein L19

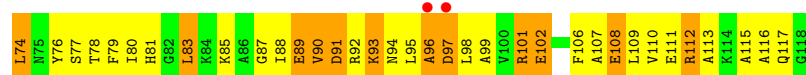


• Molecule 40: 50S ribosomal protein L19

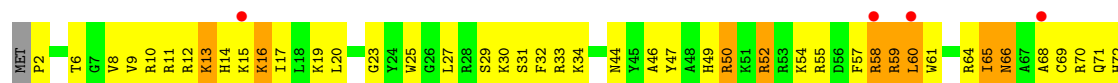


• Molecule 41: 50S ribosomal protein L20

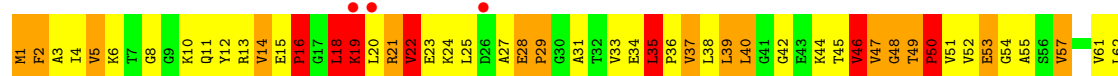




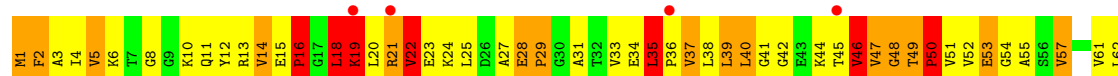
- Molecule 41: 50S ribosomal protein L20



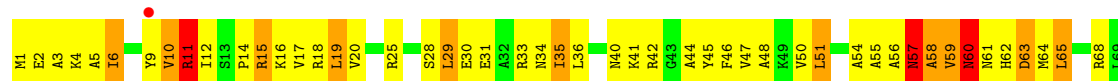
- Molecule 42: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L21

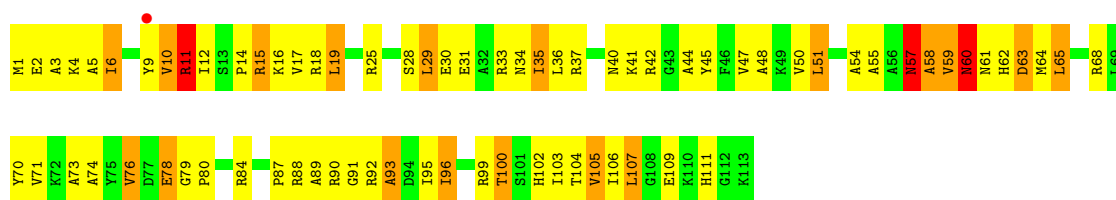


- Molecule 43: 50S ribosomal protein L22

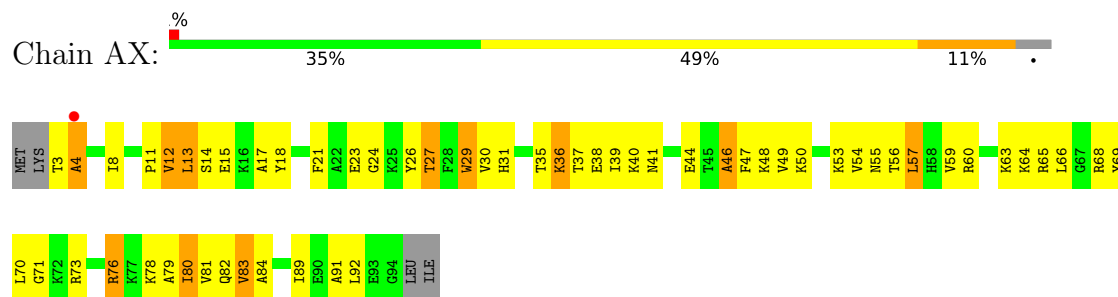


- Molecule 43: 50S ribosomal protein L22

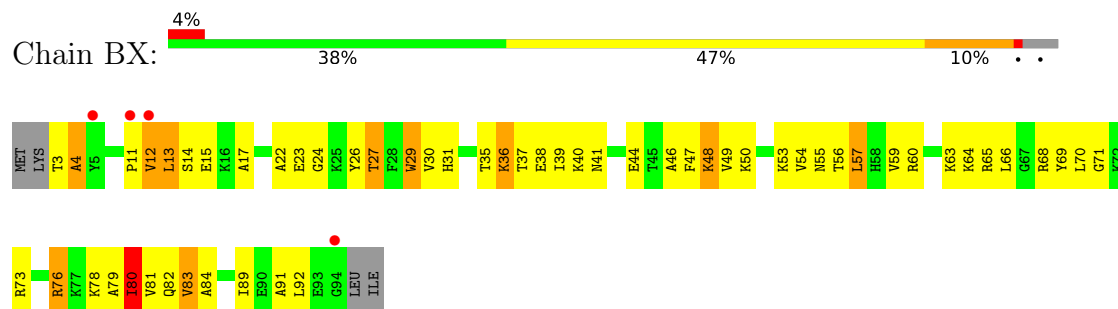




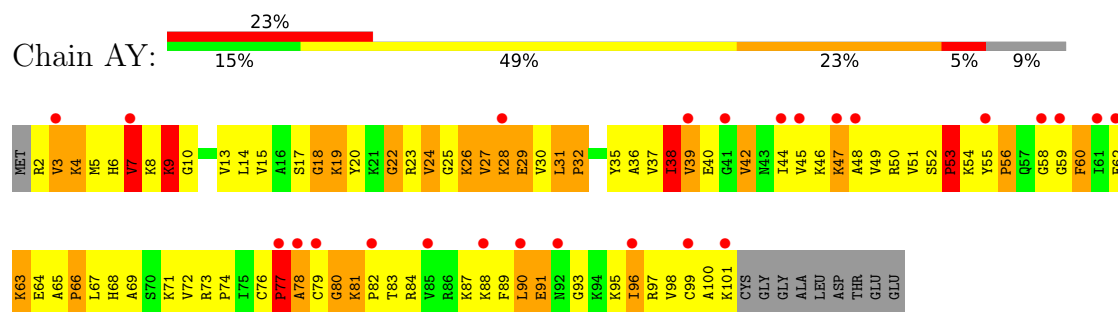
• Molecule 44: 50S ribosomal protein L23



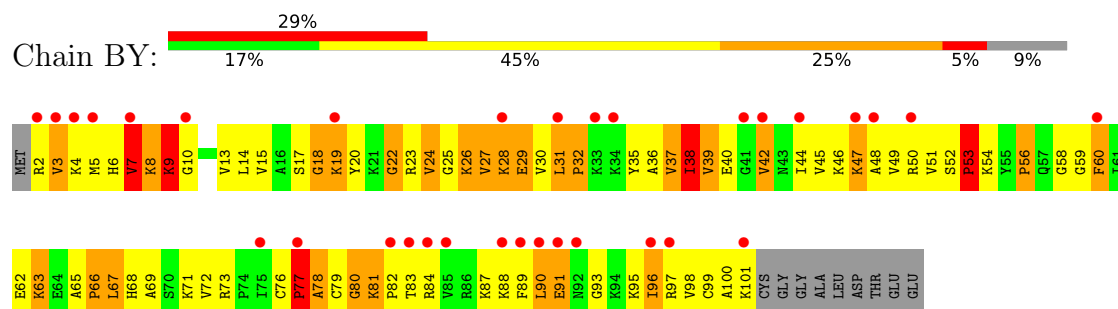
• Molecule 44: 50S ribosomal protein L23



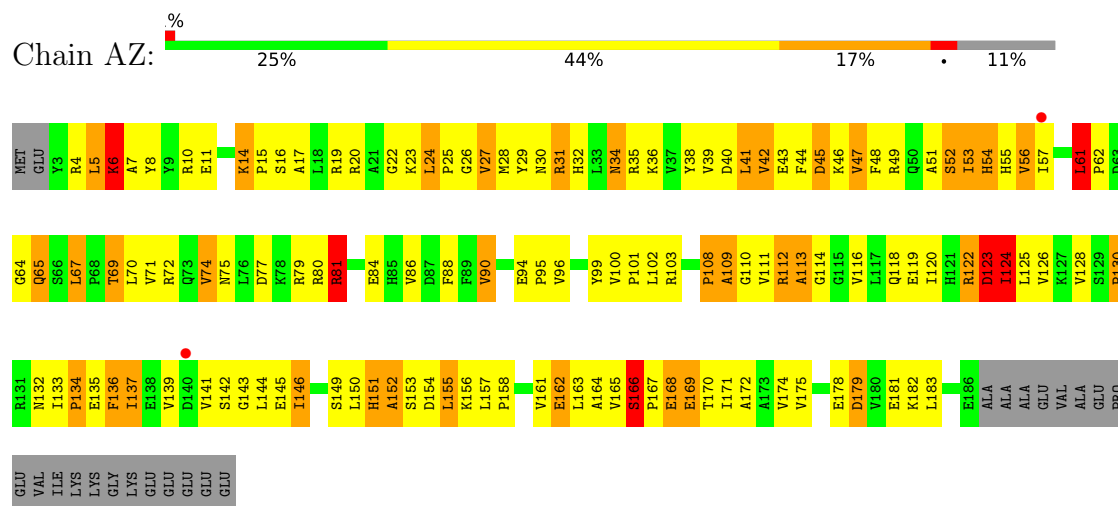
• Molecule 45: 50S ribosomal protein L24



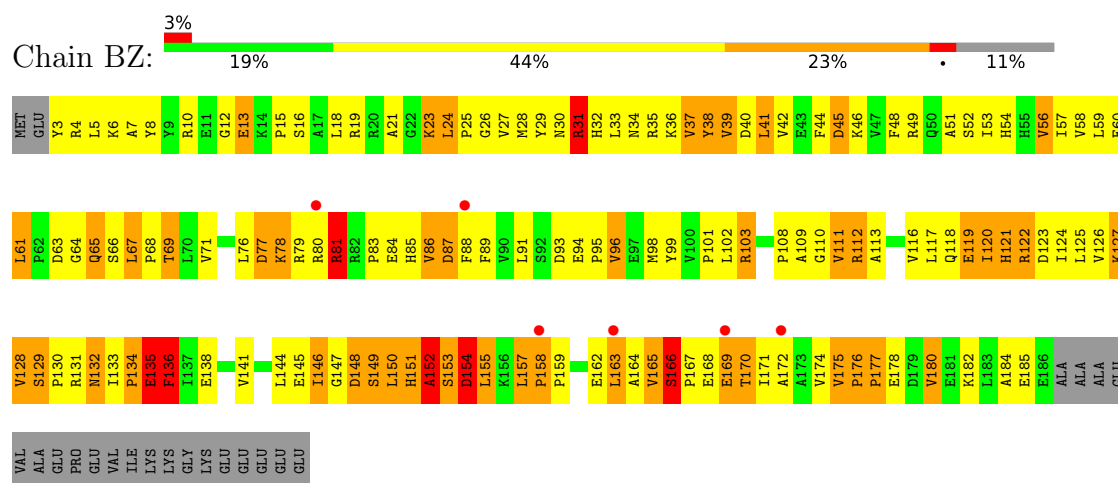
• Molecule 45: 50S ribosomal protein L24



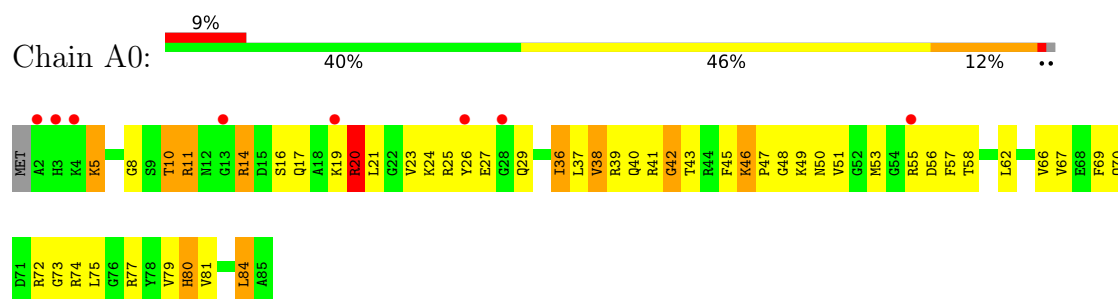
• Molecule 46: 50S ribosomal protein L25



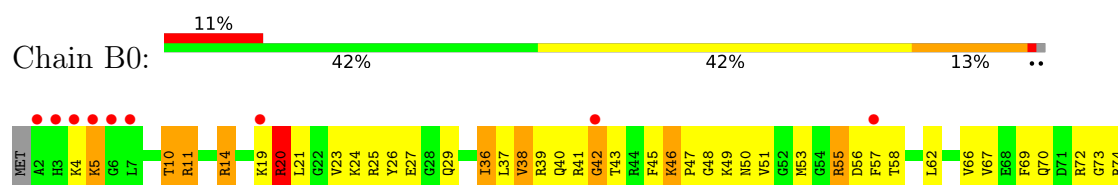
• Molecule 46: 50S ribosomal protein L25

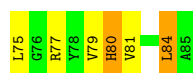


• Molecule 47: 50S ribosomal protein L27

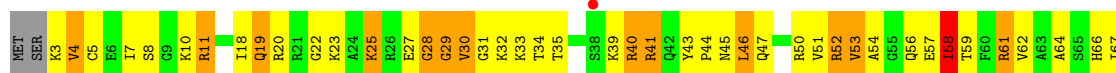


• Molecule 47: 50S ribosomal protein L27

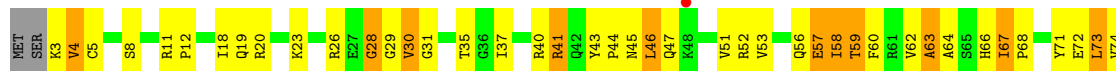




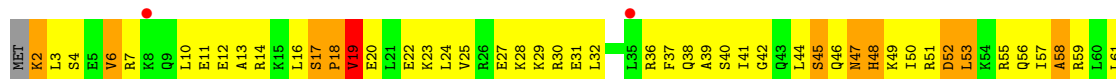
- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29

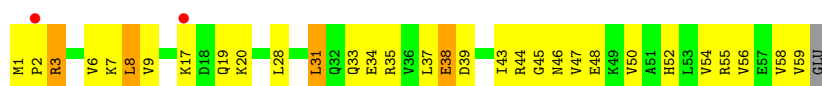


- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30

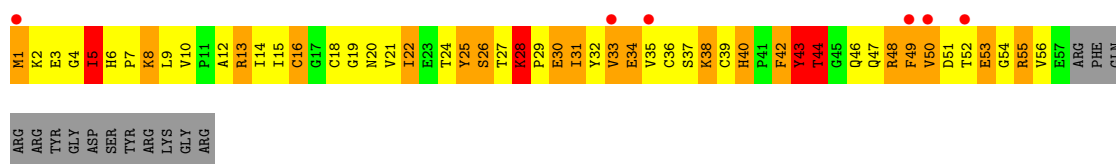




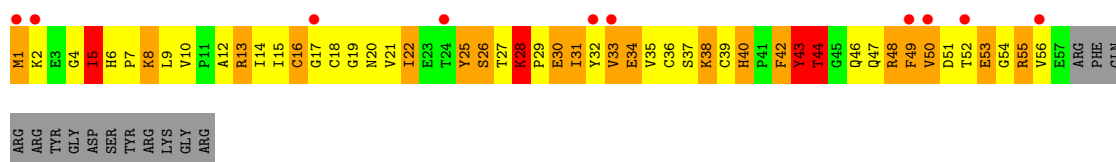
- Molecule 50: 50S ribosomal protein L30



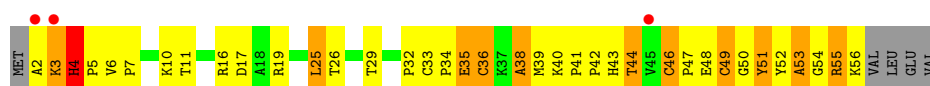
- Molecule 51: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32

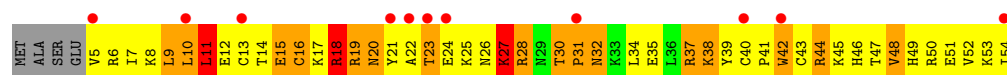


- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33





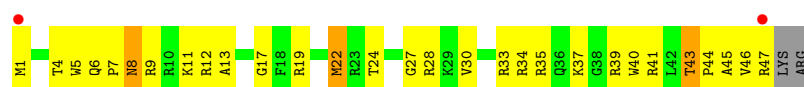
- Molecule 53: 50S ribosomal protein L33



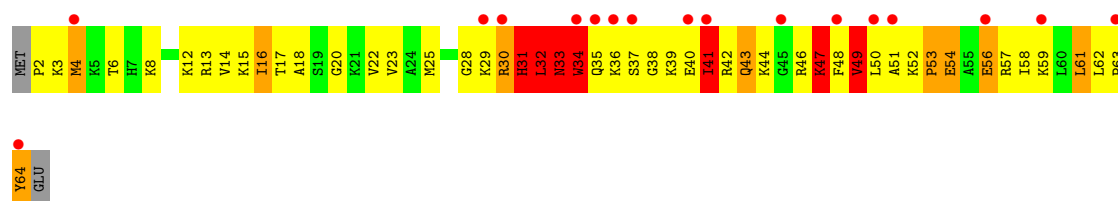
- Molecule 54: 50S ribosomal protein L34



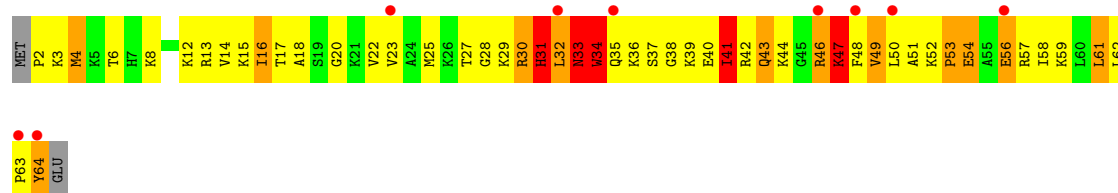
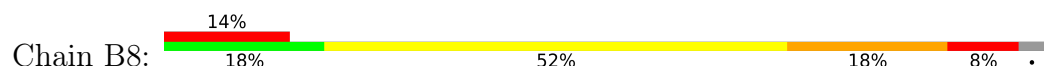
- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35

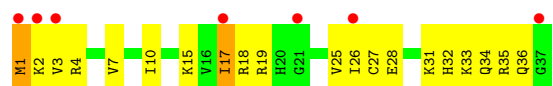


- Molecule 55: 50S ribosomal protein L35

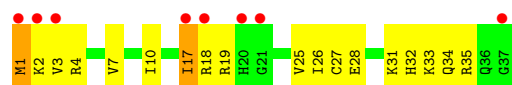


- Molecule 56: 50S ribosomal protein L36

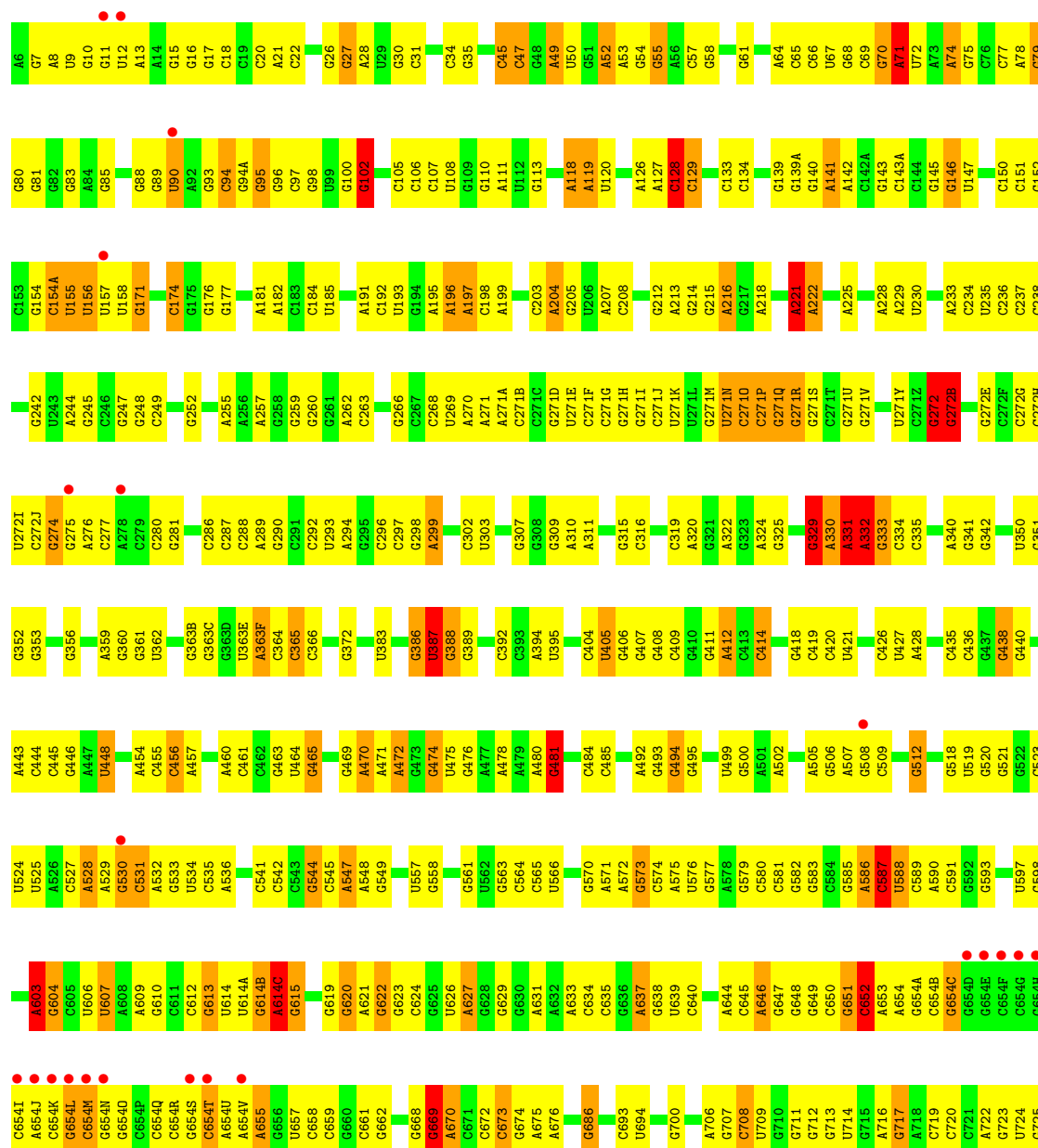




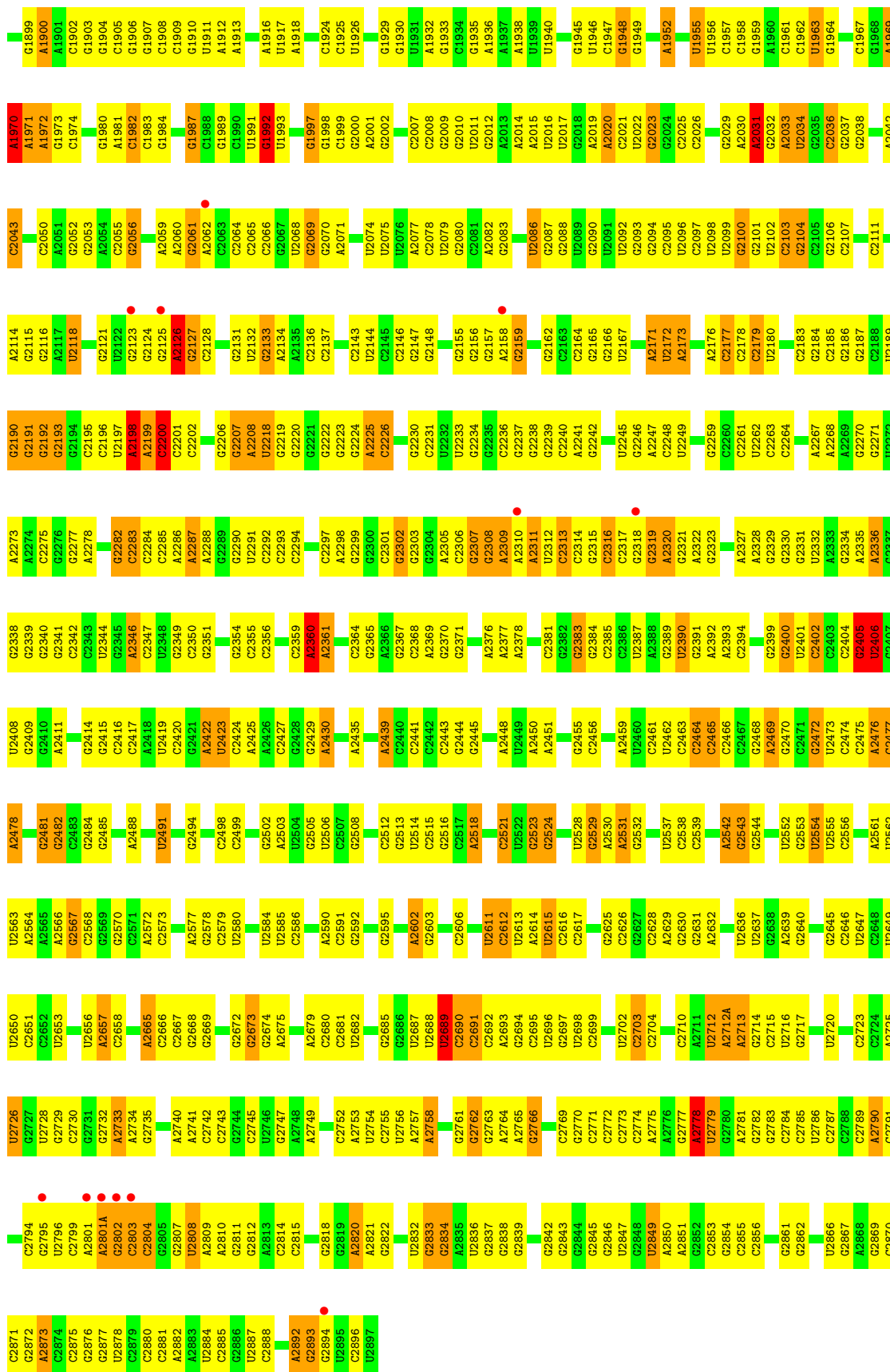
- Molecule 56: 50S ribosomal protein L36



- Molecule 57: RNA (2848-MER)



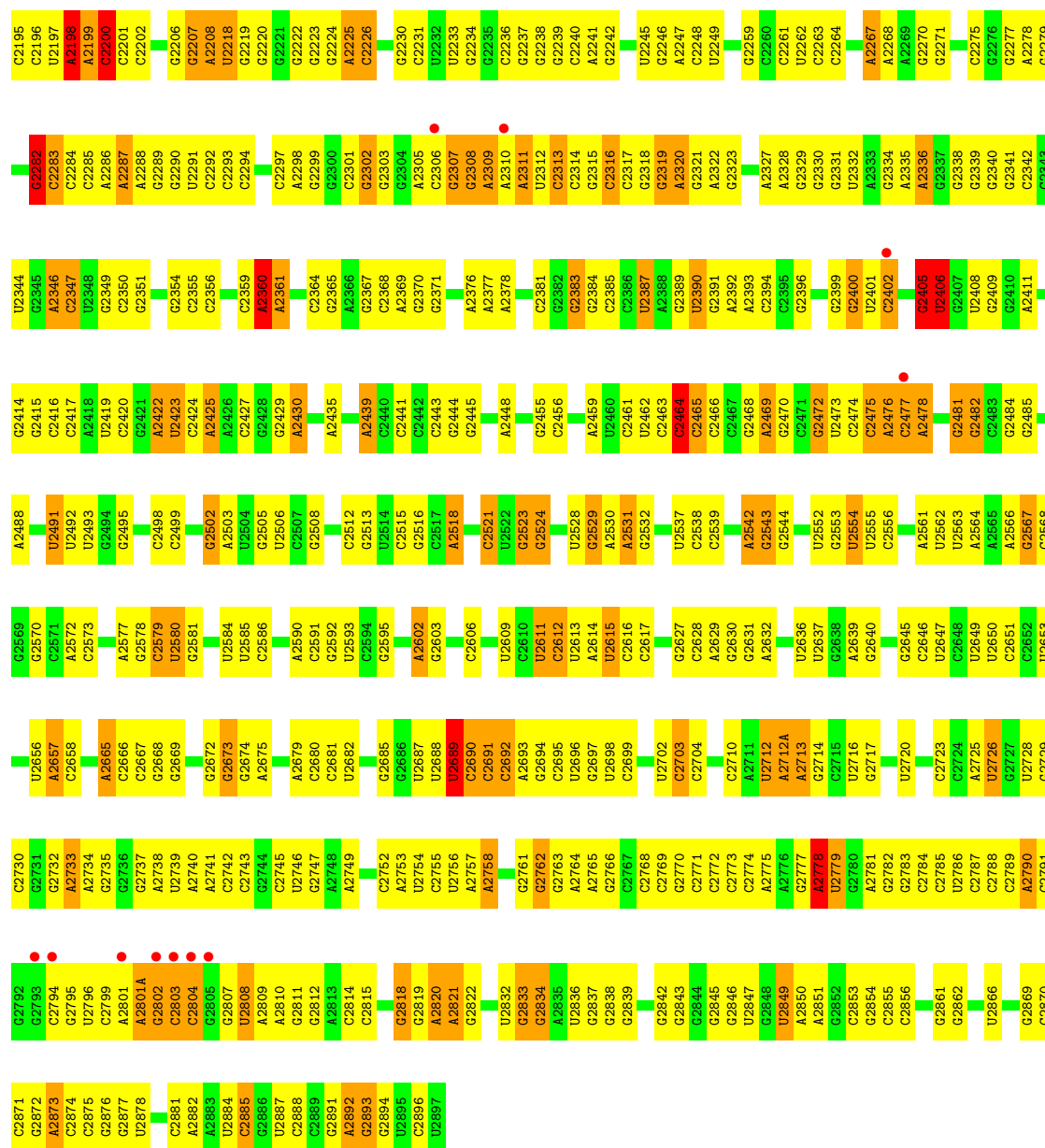
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U1808	C1809	G1625	G1625	G1538	A1469	G1385	U1312	C1233	U1159	G1037	A959	G880	U811	A728
A1809	C1810	G1626	G1626	U1540	C1470	C1386	U1313	U1234	G1160	C1038	A960	G881	C812	G729
A1810	C1811	G1627	G1627	U1541	A1471	C1387	U1314	U1240	C1161	G1039	C961	G882	U813	C730
U1811	C1812	U1629	G1628	A1542	A1472	U1396	C1315	U1240	G1162	C1040	U963	G883	C814	G744
G1816	C1813	G1714	G1633	C1543	C1473	U1396	U1316	A1241	G1163	C1041	C964	C888	C815	G744
G1817	C1814	G1717	G1634	A1544	C1474	U1396	U1317	A1242	G1164	A1045	C965	C889	A819	U747
U1818	C1815	G1718	G1635	A1545	G1475	C1403	C1318	G1243	C1165	A1046	U969	G892	U822	G748
A1819	C1816	U1720	C1636	C1546	G1476	C1404	G1319	G1243	U1167	G1047	C970	G893	G823	A752
U1820	C1817	G1721	A1637	C1547	G1477	U1405	C1320	A1247	G1168	A1048	C971	C894	U826	C753
A1821	C1818	A1722	U1639	C1548	C1480	U1406	A1321	G1250	G1169	C1049	G972	U895	U827	C754
G1826	C1819	U1739	C1640	A1554	U1481	C1407	G1324	C1251	G1170	A1050	A973	A896	U828	C755
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U1833	C1822	C1743	G1643	G1560	A1486	C1411	G1328	G1256	U1175	C1053	G977	G831	G832	C758
U1834	C1823	G1746	C1648	A1566	G1487	G1413	A1331	C1257	G1176	A1106	G978	G832	G760	G759
G1835	C1824	G1747	G1649	A1567	C1488	G1416	G1332	C1261	A1177	G1107	G979	G833	A761	A761
U1839	C1825	G1748	G1651	U1568	U1489	C1417	A1336	A1262	C1178	G1108	A980	C904	A764	A764
G1845	C1826	G1749	A1652	A1569	A1490	G1418	G1337	A1263	C1181	G1109	A983	U905	G765	G765
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G1853	C1829	G1750	G1655	A1572	C1493	G1422	U1340	A1266	G1191	C1117	C992	U907	G843	U773
G1854	C1830	C1751	G1656	G1573	A1494	A1428	U1341	A1267	G1192	C1118	C995	C908	C844	A774
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G1878	C1844	A1791	C1685	A1603	U1518	A1449	G1361	C1289	G1209	U1142	U1012	A933	A861	G792
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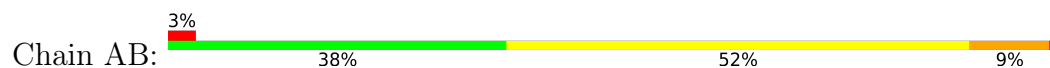
- Molecule 57: RNA (2848-MER)



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G2124	C1983	C1905	C1906	U1818	G1714	A1638	C1547	G1473	U1397	G1312	C1231	U1159	G1037
G2125	G1984	A1819	G1907	A1820	G1718	U1639	C1548	G1475	C1403	C1313	G1232	G1160	C1038
A2126	A2061	G1987	G1908	A1821	G1719	C1640	A1549	G1478	G1404	C1314	G1233	G1161	G1039
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G2133	C2065	A1912	U1912	G1829	G1739	U1643	A1568	U1482	C1408	G1318	U1242	U1165	A1046
A2134	G1992	G1922	A1913	U1834	U1740	C1648	G1559	G1483	C1409	G1319	A1243	G1166	G1047
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C2136	G2068	U1915	U1915	G1836	A1743	G1652	A1567	G1485	A1411	A1321	U1247	G1168	A1049
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G2147	G2010	A1932	A1932	G1852	C1752	A1665	C1577	U1496	A1427	U1339	G1257	G1181	A1111
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G2012	C2012	U1936	U1936	A1854	G1763	G1667	A1580	C1498	G1429	U1341	A1262	U1113	U1113
A2013	A2013	A1937	A1937	G1855	G1764	G1668	G1591	U1500	C1430	A1942	G1263	G1188	G1115
G2156	U2086	G1938	G1938	G1856	C1771	A1669	C1582	C1501	G1431	G1943	G1264	U1188	G1116
A2158	G2087	U1939	U1939	G1857	G1772	C1670	A1583	U1502	C1432	C1344	G1265	A1189	G1117
G2159	U2088	U1940	U1940	A1858	A1773	U1673	C1584	U1503	G1433	C1345	G1266	G1190	G1117
G2162	G2089	U1941	U1941	G1859	C1773	A1687	A1586	C1504	A1434	G1346	G1267	G1191	C1118
C2163	C2090	G2018	G2018	G1860	G1774	G1674	A1587	C1505	U1437	G1347	G1270	G1192	C1124
C2164	U2091	G1945	G1945	G1861	U1779	A1674	C1588	C1506	U1438	G1348	G1271	G1193	G1125
G2165	A2020	U1946	U1946	G1862	A1780	A1677	C1589	C1509	A1439	A1349	U1272	A1194	U1130
C2166	C2021	C1947	C1947	G1863	G1785	G1678	U1590	A1509A	G1440	U1352	A1274	G1196	G1131
G2167	U2022	G1948	G1948	U1864	A1786	C1683	G1591	A1509B	G1441	A1353	A1275	G1197	G1132
G2023	G2023	G1949	G1949	C1865	A1786	C1684	G1596	C1510	G1442	A1354	U1278	U1198	A1132
G2024	G2024	A1952	A1952	C1866	C1786	C1685	C1598	C1511	A1445	G1355	G1279	G1200	U1133
C2025	C2025	U1876	U1876	A1877	A1789	U1688	U1602	G1517	U1448	G1356	G1279	G1201	C1135
C2026	G1878	G1878	G1878	C1881	C1790	A1689	A1603	U1518	G1449	C1358	G1281	G1137	G1136
G2029	C1882	C1882	C1882	G1883	A1791	U1693	G1607	G1519	G1450	A1359	U1282	U1204	G1138
A2030	G1883	G1883	G1883	A1884	U1796	C1694	A1608	C1528	C1450A	A1360	G1283	U1205	G1139
G2032	A2031	C1957	C1957	A1885	C1797	C1695	A1609	A1528	G1451	G1361	G1284	G1206	C1140
A2033	G2032	G1958	G1958	G1886	U1798	G1696	A1609	A1528A	C1452	C1362	G1285	U1207	U1141
U2034	U2034	C1961	C1961	C1887	G1799	G1697	A1610	G1529	A1453	C1363	A1286	G1209	G1142
G2035	G2035	U1962	U1962	C1888	C1800	G1697	G1610	G1529	U1453	G1364	A1287	A1210	A142A
C2036	C2036	U1963	U1963	G1889	G1801	A1698	A1614	G1532	U1459	A1365	U1288	U1211	A1143
G2037	G1888	A1802	A1802	A1889	A1802	A1701	G1615	G1533	G1459	C1368	C1289	G1212	G1144
G2038	A1890	A1803	A1803	A1890	A1803	G1702	C1616	U1534	A1460	G1369	C1290	G1215	G1145
A2042	G1968	C1804	C1804	A1891	U1805	G1703	C1617	A1535	G1461	U1369	U1291	G1216	C1146
C2043	C1894	C1806	C1806	C1894	C1806	G1705	A1618	C1536	C1462	U1292	U1292	C1217	C1147
G2050	C1895	G1707	G1707	C1895	U1706	U1706	G1627	G1537	C1464	A1378	U1294	C1217	A1148
A2051	G1899	U1808	U1808	G1899	G1708	C1708	G1628	G1538	U1467	G1380	C1221	G1221	G1149
G2052	A1900	A1810	A1810	A1900	U1709	U1709	G1629	G1539	C1468	A1384	U1300	C1221A	G1151
C2120	A1901	G1811	G1811	A1901	U1710	C1710	G1633	U1540	A1469	G1385	A1301	C1222	C1152
A2054	C1902	C1902	C1902	C1902	C1711	C1711		A1542	G1470	C1386	A1308	G1223	G1154

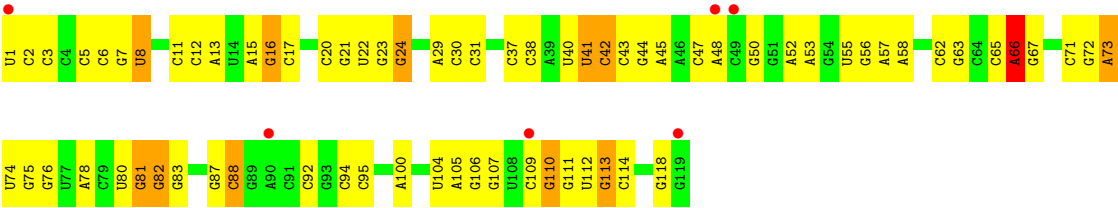


• Molecule 58: RNA (119-MER)



• Molecule 58: RNA (119-MER)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.57Å 451.96Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.30) 99.8 (50.00-3.30)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	0.02	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.247 0.220 , 0.248	Depositor DCC
R_{free} test set	40918 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	99.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297206	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: OMU, 5MU, A2M, OMG, 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	Ab	0.40	0/1935	1.01	11/2609 (0.4%)
1	Bb	0.40	0/1935	1.00	11/2609 (0.4%)
2	Ac	0.41	0/1636	0.87	4/2205 (0.2%)
2	Bc	0.40	0/1636	0.87	3/2205 (0.1%)
3	Ad	0.44	0/1733	0.99	8/2318 (0.3%)
3	Bd	0.45	0/1733	0.99	9/2318 (0.4%)
4	Ae	0.42	0/1162	0.98	4/1564 (0.3%)
4	Be	0.45	0/1162	0.98	4/1564 (0.3%)
5	Af	0.40	0/856	0.97	1/1154 (0.1%)
5	Bf	0.42	0/856	0.98	1/1154 (0.1%)
6	Ag	0.37	0/1276	0.87	1/1709 (0.1%)
6	Bg	0.37	0/1276	0.88	1/1709 (0.1%)
7	Ah	0.41	0/1136	1.06	9/1527 (0.6%)
7	Bh	0.41	0/1136	1.06	9/1527 (0.6%)
8	Ai	0.38	0/1029	0.90	5/1379 (0.4%)
8	Bi	0.39	0/1029	0.89	4/1379 (0.3%)
9	Aj	0.44	0/807	1.02	8/1085 (0.7%)
9	Bj	0.45	0/807	1.03	7/1085 (0.6%)
10	Ak	0.42	0/900	0.96	4/1213 (0.3%)
10	Bk	0.42	0/900	0.97	4/1213 (0.3%)
11	Al	0.51	0/986	1.09	6/1320 (0.5%)
11	Bl	0.50	0/986	1.08	6/1320 (0.5%)
12	Am	0.38	0/947	1.03	5/1270 (0.4%)
12	Bm	0.38	0/947	1.00	6/1270 (0.5%)
13	An	0.37	0/501	0.85	1/664 (0.2%)
13	Bn	0.38	0/501	0.85	1/664 (0.2%)
14	Ao	0.41	0/745	0.89	1/992 (0.1%)
14	Bo	0.42	0/745	0.89	1/992 (0.1%)
15	Ap	0.45	0/716	0.94	2/963 (0.2%)
15	Bp	0.40	0/716	0.93	2/963 (0.2%)
16	Aq	0.39	0/836	0.93	2/1117 (0.2%)
16	Bq	0.40	0/836	0.94	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Ar	0.42	0/579	1.07	7/768 (0.9%)
17	Br	0.43	0/579	1.07	6/768 (0.8%)
18	As	0.42	0/642	1.06	4/865 (0.5%)
18	Bs	0.44	0/642	1.06	4/865 (0.5%)
19	At	0.41	0/765	0.98	4/1007 (0.4%)
19	Bt	0.38	0/765	0.98	5/1007 (0.5%)
20	Au	0.42	0/212	0.85	0/277
20	Bu	0.41	0/212	0.84	0/277
21	Ay	0.36	0/781	0.95	7/1045 (0.7%)
21	By	0.46	0/777	1.06	5/1040 (0.5%)
22	Aa	0.42	0/36190	0.62	34/56486 (0.1%)
22	Ba	0.42	0/36190	0.63	34/56486 (0.1%)
23	Ax	0.45	0/219	0.80	0/340
23	Bx	0.47	0/219	0.80	0/340
24	Av	0.41	0/1810	0.67	1/2821 (0.0%)
24	Bv	0.43	0/1810	0.70	2/2821 (0.1%)
25	Aw	0.47	0/1832	0.56	1/2855 (0.0%)
25	Bw	0.49	0/1832	0.55	0/2855
26	AC	0.45	0/956	0.91	3/1288 (0.2%)
26	BC	0.46	0/956	0.91	2/1288 (0.2%)
27	AD	0.60	0/2154	1.20	22/2905 (0.8%)
27	BD	0.62	0/2154	1.21	20/2905 (0.7%)
28	AE	0.58	0/1596	1.21	15/2153 (0.7%)
28	BE	0.60	0/1596	1.23	16/2153 (0.7%)
29	AF	0.53	0/1658	1.12	11/2244 (0.5%)
29	BF	0.57	0/1658	1.14	13/2244 (0.6%)
30	AG	0.45	1/1499 (0.1%)	1.07	11/2016 (0.5%)
30	BG	0.48	1/1499 (0.1%)	1.14	18/2016 (0.9%)
31	AH	0.48	0/1284	1.17	18/1739 (1.0%)
31	BH	0.52	0/1284	1.19	18/1739 (1.0%)
32	AI	0.59	0/1146	1.27	22/1551 (1.4%)
32	BI	0.58	0/1146	1.25	23/1551 (1.5%)
33	AJ	0.60	0/640	1.35	12/889 (1.3%)
33	BJ	0.62	0/640	1.32	13/889 (1.5%)
34	AN	0.48	0/1131	1.15	11/1525 (0.7%)
34	BN	0.53	0/1131	1.18	11/1525 (0.7%)
35	AO	0.54	0/943	0.99	0/1269
35	BO	0.55	0/943	1.00	2/1269 (0.2%)
36	AP	0.60	0/1131	1.51	20/1504 (1.3%)
36	BP	0.67	0/1131	1.54	21/1504 (1.4%)
37	AQ	0.50	0/1133	1.03	8/1515 (0.5%)
37	BQ	0.52	0/1133	1.06	10/1515 (0.7%)
38	AR	0.54	0/974	1.04	3/1302 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BR	0.57	0/974	1.06	4/1302 (0.3%)
39	AS	0.45	0/778	1.04	9/1036 (0.9%)
39	BS	0.49	0/778	1.05	7/1036 (0.7%)
40	AT	0.54	0/1137	1.32	21/1519 (1.4%)
40	BT	0.56	0/1137	1.33	19/1519 (1.3%)
41	AU	0.54	0/975	1.10	7/1297 (0.5%)
41	BU	0.62	0/975	1.13	6/1297 (0.5%)
42	AV	0.47	0/790	0.99	1/1057 (0.1%)
42	BV	0.52	0/790	1.01	1/1057 (0.1%)
43	AW	0.52	0/907	1.07	5/1216 (0.4%)
43	BW	0.56	0/907	1.06	5/1216 (0.4%)
44	AX	0.54	0/739	1.04	3/993 (0.3%)
44	BX	0.59	1/739 (0.1%)	1.06	3/993 (0.3%)
45	AY	0.61	0/788	1.19	5/1051 (0.5%)
45	BY	0.66	0/788	1.21	5/1051 (0.5%)
46	AZ	0.42	0/1499	1.02	11/2035 (0.5%)
46	BZ	0.49	0/1499	1.13	16/2035 (0.8%)
47	A0	0.47	0/671	1.04	5/892 (0.6%)
47	B0	0.51	0/671	1.03	3/892 (0.3%)
48	A1	0.50	0/738	1.13	6/981 (0.6%)
48	B1	0.57	0/738	1.15	7/981 (0.7%)
49	A2	0.40	0/600	0.92	0/793
49	B2	0.53	0/600	0.96	1/793 (0.1%)
50	A3	0.46	0/472	1.03	1/634 (0.2%)
50	B3	0.48	0/472	1.02	1/634 (0.2%)
51	A4	0.55	0/460	1.02	3/621 (0.5%)
51	B4	0.56	0/460	1.02	3/621 (0.5%)
52	A5	0.56	0/441	1.22	6/596 (1.0%)
52	B5	0.61	0/441	1.27	6/596 (1.0%)
53	A6	0.59	0/440	1.22	6/586 (1.0%)
53	B6	0.58	0/440	1.21	5/586 (0.9%)
54	A7	0.54	0/417	1.10	3/550 (0.5%)
54	B7	0.61	0/417	1.11	3/550 (0.5%)
55	A8	0.64	0/515	1.26	5/679 (0.7%)
55	B8	0.64	0/515	1.24	4/679 (0.6%)
56	A9	0.42	0/310	0.92	1/407 (0.2%)
56	B9	0.44	0/310	0.92	1/407 (0.2%)
57	AA	0.43	0/68704	0.70	77/107260 (0.1%)
57	BA	0.45	0/68704	0.72	88/107260 (0.1%)
58	AB	0.41	0/2853	0.65	0/4451
58	BB	0.42	0/2853	0.66	0/4451
All	All	0.45	3/321416 (0.0%)	0.81	941/480209 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	Ay	0	1
22	Aa	0	11
22	Ba	1	11
24	Av	0	1
24	Bv	0	1
38	AR	0	1
38	BR	0	1
52	A5	0	1
52	B5	0	1
57	AA	2	50
57	BA	2	68
58	AB	0	1
58	BB	0	1
All	All	5	149

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BG	77	ILE	CA-CB	6.33	1.61	1.53
30	AG	77	ILE	CA-CB	5.73	1.62	1.54
44	BX	80	ILE	CA-CB	5.24	1.60	1.53

The worst 5 of 941 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	1992	G	C2'-C3'-O3'	15.16	132.24	109.50
57	BA	1992	G	C2'-C3'-O3'	15.06	132.09	109.50
22	Ba	1498	U	C2'-C3'-O3'	14.98	131.97	109.50
30	BG	125	PHE	N-CA-C	-13.88	94.47	111.40
57	BA	1653	G	C2'-C3'-O3'	13.46	129.69	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	AA	1799	G	C3'
57	AA	1819	A	C3'
22	Ba	1498	U	C3'
57	BA	1799	G	C3'

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Mol	Chain	Res	Type	Atom
57	BA	1819	A	C3'

5 of 149 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	Aa	265	G	Sidechain
22	Aa	436	C	Sidechain
22	Aa	484	G	Sidechain
22	Aa	97	G	Sidechain
21	Ay	83	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ab	1900	0	1951	222	0
1	Bb	1900	0	1951	218	0
2	Ac	1612	0	1677	174	0
2	Bc	1612	0	1677	177	0
3	Ad	1703	0	1763	192	0
3	Bd	1703	0	1764	180	0
4	Ae	1146	0	1207	122	0
4	Be	1146	0	1207	128	0
5	Af	843	0	857	82	0
5	Bf	843	0	857	80	0
6	Ag	1257	0	1296	113	0
6	Bg	1257	0	1296	113	0
7	Ah	1116	0	1177	118	0
7	Bh	1116	0	1177	119	0
8	Ai	1010	0	1037	159	0
8	Bi	1010	0	1037	153	0
9	Aj	794	0	840	159	0
9	Bj	794	0	840	158	0
10	Ak	885	0	904	80	0
10	Bk	885	0	904	81	0
11	Al	970	0	1057	112	0
11	Bl	970	0	1057	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Am	937	0	995	203	0
12	Bm	937	0	995	184	0
13	An	492	0	529	79	0
13	Bn	492	0	529	77	0
14	Ao	734	0	771	61	0
14	Bo	734	0	771	59	0
15	Ap	700	0	720	57	0
15	Bp	700	0	720	60	0
16	Aq	823	0	891	58	0
16	Bq	823	0	891	60	0
17	Ar	574	0	644	71	0
17	Br	574	0	644	69	0
18	As	629	0	652	97	0
18	Bs	629	0	652	97	0
19	At	763	0	861	80	0
19	Bt	763	0	861	82	0
20	Au	208	0	221	11	0
20	Bu	208	0	221	9	0
21	Ay	770	0	811	168	0
21	By	766	0	804	106	0
22	Aa	32329	0	16317	1054	0
22	Ba	32329	0	16318	1048	0
23	Ax	262	0	138	44	0
23	Bx	262	0	138	22	0
24	Av	1641	0	839	35	0
24	Bv	1641	0	839	40	0
25	Aw	1640	0	837	53	0
25	Bw	1640	0	837	49	0
26	AC	937	0	957	101	0
26	BC	937	0	957	107	0
27	AD	2104	0	2182	283	0
27	BD	2104	0	2182	292	0
28	AE	1563	0	1629	221	0
28	BE	1563	0	1629	220	0
29	AF	1623	0	1677	174	0
29	BF	1623	0	1677	174	0
30	AG	1474	0	1535	294	0
30	BG	1474	0	1535	264	0
31	AH	1259	0	1326	139	0
31	BH	1259	0	1326	151	0
32	AI	1131	0	1218	217	0
32	BI	1131	0	1218	218	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	AJ	641	0	309	20	0
33	BJ	641	0	309	39	0
34	AN	1104	0	1180	142	0
34	BN	1104	0	1180	149	0
35	AO	933	0	996	92	0
35	BO	933	0	996	98	0
36	AP	1114	0	1187	277	0
36	BP	1114	0	1187	283	0
37	AQ	1112	0	1171	114	0
37	BQ	1112	0	1171	108	0
38	AR	960	0	1021	128	0
38	BR	960	0	1021	118	0
39	AS	770	0	832	132	0
39	BS	770	0	832	122	0
40	AT	1123	0	1181	211	0
40	BT	1123	0	1181	224	0
41	AU	958	0	1015	142	0
41	BU	958	0	1015	143	0
42	AV	779	0	852	156	0
42	BV	779	0	852	159	0
43	AW	896	0	953	84	0
43	BW	896	0	953	86	0
44	AX	725	0	778	66	0
44	BX	725	0	778	65	0
45	AY	775	0	870	159	0
45	BY	775	0	870	157	0
46	AZ	1467	0	1492	195	0
46	BZ	1467	0	1492	193	0
47	A0	662	0	688	71	0
47	B0	662	0	688	82	0
48	A1	731	0	808	69	0
48	B1	731	0	808	78	0
49	A2	598	0	653	82	0
49	B2	598	0	653	59	0
50	A3	467	0	523	36	0
50	B3	467	0	523	37	0
51	A4	450	0	449	115	0
51	B4	450	0	449	81	0
52	A5	427	0	445	72	0
52	B5	427	0	445	73	0
53	A6	433	0	461	102	0
53	B6	433	0	461	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	A7	409	0	454	32	0
54	B7	409	0	454	32	0
55	A8	507	0	576	119	0
55	B8	507	0	576	113	0
56	A9	307	0	336	25	0
56	B9	307	0	335	22	0
57	AA	61341	0	30926	1758	0
57	BA	61341	0	30928	1744	0
58	AB	2551	0	1295	102	0
58	BB	2551	0	1295	84	0
59	A4	1	0	0	0	0
59	A9	1	0	0	0	0
59	Ad	1	0	0	0	0
59	An	1	0	0	0	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	Bd	1	0	0	0	0
59	Bn	1	0	0	0	0
60	A1	1	0	0	0	0
60	A5	1	0	0	0	0
60	A7	2	0	0	0	0
60	AA	368	0	0	0	0
60	AB	3	0	0	0	0
60	AD	2	0	0	0	0
60	AF	1	0	0	0	0
60	AQ	1	0	0	0	0
60	AX	1	0	0	0	0
60	Aa	145	0	0	0	0
60	Am	1	0	0	0	0
60	Aq	1	0	0	0	0
60	Av	4	0	0	0	0
60	Aw	1	0	0	0	0
60	B0	2	0	0	0	0
60	B5	1	0	0	0	0
60	B7	2	0	0	0	0
60	BA	366	0	0	0	0
60	BB	3	0	0	0	0
60	BD	2	0	0	0	0
60	BF	1	0	0	0	0
60	BQ	1	0	0	0	0
60	BX	1	0	0	0	0
60	Ba	143	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	Bm	2	0	0	0	0
60	Bq	1	0	0	0	0
60	Bv	5	0	0	0	0
60	Bw	1	0	0	0	0
60	Bx	1	0	0	0	0
All	All	297206	0	201930	17107	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 34.

The worst 5 of 17107 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)
12:Am:69:GLU:HB2	12:Am:72:ALA:CB	1.35	1.53
12:Am:65:LYS:CB	12:Am:66:LEU:HB2	1.40	1.51
12:Bm:65:LYS:CB	12:Bm:66:LEU:HB2	1.42	1.49
30:AG:110:ALA:C	30:AG:112:PRO:HD2	1.47	1.39
21:Ay:43:LYS:NZ	22:Aa:1493:A:H1'	1.33	1.38

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ab	232/256 (91%)	160 (69%)	45 (19%)	27 (12%)	0	2
1	Bb	232/256 (91%)	160 (69%)	46 (20%)	26 (11%)	0	2
2	Ac	204/239 (85%)	128 (63%)	51 (25%)	25 (12%)	0	1
2	Bc	204/239 (85%)	131 (64%)	49 (24%)	24 (12%)	0	1
3	Ad	206/209 (99%)	142 (69%)	45 (22%)	19 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Bd	206/209 (99%)	142 (69%)	46 (22%)	18 (9%)	0	4
4	Ae	148/162 (91%)	112 (76%)	24 (16%)	12 (8%)	1	5
4	Be	148/162 (91%)	111 (75%)	25 (17%)	12 (8%)	1	5
5	Af	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	5
5	Bf	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	5
6	Ag	153/156 (98%)	119 (78%)	24 (16%)	10 (6%)	1	8
6	Bg	153/156 (98%)	121 (79%)	22 (14%)	10 (6%)	1	8
7	Ah	136/138 (99%)	106 (78%)	27 (20%)	3 (2%)	5	26
7	Bh	136/138 (99%)	107 (79%)	26 (19%)	3 (2%)	5	26
8	Ai	125/128 (98%)	92 (74%)	22 (18%)	11 (9%)	0	4
8	Bi	125/128 (98%)	90 (72%)	23 (18%)	12 (10%)	0	3
9	Aj	96/105 (91%)	71 (74%)	18 (19%)	7 (7%)	1	6
9	Bj	96/105 (91%)	69 (72%)	20 (21%)	7 (7%)	1	6
10	Ak	117/129 (91%)	98 (84%)	16 (14%)	3 (3%)	4	23
10	Bk	117/129 (91%)	98 (84%)	16 (14%)	3 (3%)	4	23
11	Al	122/132 (92%)	93 (76%)	17 (14%)	12 (10%)	0	3
11	Bl	122/132 (92%)	93 (76%)	17 (14%)	12 (10%)	0	3
12	Am	116/126 (92%)	76 (66%)	21 (18%)	19 (16%)	0	1
12	Bm	116/126 (92%)	74 (64%)	23 (20%)	19 (16%)	0	1
13	An	58/61 (95%)	39 (67%)	10 (17%)	9 (16%)	0	1
13	Bn	58/61 (95%)	39 (67%)	10 (17%)	9 (16%)	0	1
14	Ao	86/89 (97%)	66 (77%)	16 (19%)	4 (5%)	2	12
14	Bo	86/89 (97%)	66 (77%)	16 (19%)	4 (5%)	2	12
15	Ap	81/88 (92%)	55 (68%)	21 (26%)	5 (6%)	1	9
15	Bp	81/88 (92%)	56 (69%)	20 (25%)	5 (6%)	1	9
16	Aq	97/105 (92%)	82 (84%)	13 (13%)	2 (2%)	5	26
16	Bq	97/105 (92%)	83 (86%)	11 (11%)	3 (3%)	3	20
17	Ar	68/88 (77%)	47 (69%)	14 (21%)	7 (10%)	0	2
17	Br	68/88 (77%)	47 (69%)	15 (22%)	6 (9%)	0	4
18	As	76/93 (82%)	50 (66%)	14 (18%)	12 (16%)	0	1
18	Bs	76/93 (82%)	49 (64%)	15 (20%)	12 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	At	97/106 (92%)	70 (72%)	15 (16%)	12 (12%)	0	1
19	Bt	97/106 (92%)	70 (72%)	15 (16%)	12 (12%)	0	1
20	Au	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	13
20	Bu	22/27 (82%)	15 (68%)	6 (27%)	1 (4%)	2	13
21	Ay	92/95 (97%)	55 (60%)	12 (13%)	25 (27%)	0	0
21	By	92/95 (97%)	58 (63%)	21 (23%)	13 (14%)	0	1
26	AC	116/229 (51%)	93 (80%)	20 (17%)	3 (3%)	4	23
26	BC	116/229 (51%)	93 (80%)	20 (17%)	3 (3%)	4	23
27	AD	269/276 (98%)	203 (76%)	37 (14%)	29 (11%)	0	2
27	BD	269/276 (98%)	203 (76%)	36 (13%)	30 (11%)	0	2
28	AE	202/206 (98%)	138 (68%)	32 (16%)	32 (16%)	0	1
28	BE	202/206 (98%)	138 (68%)	31 (15%)	33 (16%)	0	1
29	AF	205/210 (98%)	154 (75%)	31 (15%)	20 (10%)	0	3
29	BF	205/210 (98%)	155 (76%)	30 (15%)	20 (10%)	0	3
30	AG	179/182 (98%)	106 (59%)	44 (25%)	29 (16%)	0	1
30	BG	179/182 (98%)	119 (66%)	31 (17%)	29 (16%)	0	1
31	AH	162/180 (90%)	109 (67%)	27 (17%)	26 (16%)	0	1
31	BH	162/180 (90%)	109 (67%)	27 (17%)	26 (16%)	0	1
32	AI	143/148 (97%)	84 (59%)	38 (27%)	21 (15%)	0	1
32	BI	143/148 (97%)	85 (59%)	36 (25%)	22 (15%)	0	1
33	AJ	128/173 (74%)	56 (44%)	43 (34%)	29 (23%)	0	0
33	BJ	128/173 (74%)	44 (34%)	38 (30%)	46 (36%)	0	0
34	AN	136/140 (97%)	101 (74%)	20 (15%)	15 (11%)	0	2
34	BN	136/140 (97%)	100 (74%)	20 (15%)	16 (12%)	0	1
35	AO	120/122 (98%)	104 (87%)	10 (8%)	6 (5%)	1	11
35	BO	120/122 (98%)	102 (85%)	13 (11%)	5 (4%)	2	14
36	AP	144/150 (96%)	76 (53%)	35 (24%)	33 (23%)	0	0
36	BP	144/150 (96%)	79 (55%)	32 (22%)	33 (23%)	0	0
37	AQ	138/141 (98%)	109 (79%)	21 (15%)	8 (6%)	1	9
37	BQ	138/141 (98%)	109 (79%)	21 (15%)	8 (6%)	1	9
38	AR	115/118 (98%)	85 (74%)	20 (17%)	10 (9%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BR	115/118 (98%)	84 (73%)	21 (18%)	10 (9%)	0	4
39	AS	96/112 (86%)	60 (62%)	13 (14%)	23 (24%)	0	0
39	BS	96/112 (86%)	60 (62%)	13 (14%)	23 (24%)	0	0
40	AT	133/146 (91%)	90 (68%)	24 (18%)	19 (14%)	0	1
40	BT	133/146 (91%)	90 (68%)	23 (17%)	20 (15%)	0	1
41	AU	115/118 (98%)	88 (76%)	21 (18%)	6 (5%)	1	11
41	BU	115/118 (98%)	90 (78%)	20 (17%)	5 (4%)	2	14
42	AV	99/101 (98%)	65 (66%)	17 (17%)	17 (17%)	0	1
42	BV	99/101 (98%)	64 (65%)	18 (18%)	17 (17%)	0	1
43	AW	111/113 (98%)	89 (80%)	11 (10%)	11 (10%)	0	3
43	BW	111/113 (98%)	90 (81%)	11 (10%)	10 (9%)	0	4
44	AX	90/96 (94%)	72 (80%)	13 (14%)	5 (6%)	1	9
44	BX	90/96 (94%)	72 (80%)	11 (12%)	7 (8%)	1	5
45	AY	98/110 (89%)	51 (52%)	18 (18%)	29 (30%)	0	0
45	BY	98/110 (89%)	52 (53%)	16 (16%)	30 (31%)	0	0
46	AZ	182/206 (88%)	115 (63%)	40 (22%)	27 (15%)	0	1
46	BZ	182/206 (88%)	118 (65%)	37 (20%)	27 (15%)	0	1
47	A0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	1	12
47	B0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	1	12
48	A1	91/98 (93%)	74 (81%)	10 (11%)	7 (8%)	1	5
48	B1	91/98 (93%)	71 (78%)	14 (15%)	6 (7%)	1	7
49	A2	69/72 (96%)	44 (64%)	16 (23%)	9 (13%)	0	1
49	B2	69/72 (96%)	50 (72%)	13 (19%)	6 (9%)	0	4
50	A3	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	1	10
50	B3	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	1	10
51	A4	55/71 (78%)	23 (42%)	18 (33%)	14 (26%)	0	0
51	B4	55/71 (78%)	23 (42%)	18 (33%)	14 (26%)	0	0
52	A5	53/60 (88%)	40 (76%)	7 (13%)	6 (11%)	0	2
52	B5	53/60 (88%)	40 (76%)	7 (13%)	6 (11%)	0	2
53	A6	48/54 (89%)	24 (50%)	14 (29%)	10 (21%)	0	0
53	B6	48/54 (89%)	24 (50%)	14 (29%)	10 (21%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	A7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
54	B7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
55	A8	61/65 (94%)	41 (67%)	14 (23%)	6 (10%)	0	3
55	B8	61/65 (94%)	41 (67%)	14 (23%)	6 (10%)	0	3
56	A9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
56	B9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	12016/13122 (92%)	8475 (70%)	2157 (18%)	1384 (12%)	0	2

5 of 1384 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ab	15	VAL
1	Ab	18	GLY
1	Ab	26	PRO
1	Ab	63	MET
1	Ab	80	ILE

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	
1	Ab	202/220 (92%)	186 (92%)	16 (8%)	11	36
1	Bb	202/220 (92%)	187 (93%)	15 (7%)	13	38
2	Ac	160/188 (85%)	147 (92%)	13 (8%)	11	36
2	Bc	160/188 (85%)	148 (92%)	12 (8%)	12	38
3	Ad	180/181 (99%)	160 (89%)	20 (11%)	6	22
3	Bd	180/181 (99%)	160 (89%)	20 (11%)	6	22
4	Ae	115/123 (94%)	106 (92%)	9 (8%)	11	36
4	Be	115/123 (94%)	106 (92%)	9 (8%)	11	36
5	Af	90/90 (100%)	86 (96%)	4 (4%)	25	54
5	Bf	90/90 (100%)	85 (94%)	5 (6%)	19	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Ag	126/127 (99%)	117 (93%)	9 (7%)	13	40
6	Bg	126/127 (99%)	117 (93%)	9 (7%)	13	40
7	Ah	119/119 (100%)	110 (92%)	9 (8%)	12	37
7	Bh	119/119 (100%)	110 (92%)	9 (8%)	12	37
8	Ai	98/99 (99%)	89 (91%)	9 (9%)	8	30
8	Bi	98/99 (99%)	89 (91%)	9 (9%)	8	30
9	Aj	88/92 (96%)	80 (91%)	8 (9%)	9	31
9	Bj	88/92 (96%)	80 (91%)	8 (9%)	9	31
10	Ak	90/99 (91%)	85 (94%)	5 (6%)	19	47
10	Bk	90/99 (91%)	85 (94%)	5 (6%)	19	47
11	Al	104/109 (95%)	86 (83%)	18 (17%)	2	9
11	Bl	104/109 (95%)	85 (82%)	19 (18%)	2	7
12	Am	94/101 (93%)	79 (84%)	15 (16%)	2	11
12	Bm	94/101 (93%)	79 (84%)	15 (16%)	2	11
13	An	49/50 (98%)	47 (96%)	2 (4%)	27	55
13	Bn	49/50 (98%)	47 (96%)	2 (4%)	27	55
14	Ao	79/80 (99%)	74 (94%)	5 (6%)	16	44
14	Bo	79/80 (99%)	75 (95%)	4 (5%)	21	50
15	Ap	72/74 (97%)	69 (96%)	3 (4%)	26	55
15	Bp	72/74 (97%)	68 (94%)	4 (6%)	19	47
16	Aq	94/97 (97%)	89 (95%)	5 (5%)	20	49
16	Bq	94/97 (97%)	89 (95%)	5 (5%)	20	49
17	Ar	61/77 (79%)	58 (95%)	3 (5%)	22	51
17	Br	61/77 (79%)	58 (95%)	3 (5%)	22	51
18	As	69/80 (86%)	61 (88%)	8 (12%)	5	21
18	Bs	69/80 (86%)	60 (87%)	9 (13%)	4	17
19	At	76/82 (93%)	67 (88%)	9 (12%)	5	20
19	Bt	76/82 (93%)	67 (88%)	9 (12%)	5	20
20	Au	19/22 (86%)	19 (100%)	0	100	100
20	Bu	19/22 (86%)	19 (100%)	0	100	100
21	Ay	84/85 (99%)	65 (77%)	19 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	By	83/85 (98%)	72 (87%)	11 (13%)	4	17
26	AC	99/181 (55%)	97 (98%)	2 (2%)	48	68
26	BC	99/181 (55%)	97 (98%)	2 (2%)	48	68
27	AD	213/218 (98%)	184 (86%)	29 (14%)	3	16
27	BD	213/218 (98%)	184 (86%)	29 (14%)	3	16
28	AE	165/166 (99%)	141 (86%)	24 (14%)	3	14
28	BE	165/166 (99%)	142 (86%)	23 (14%)	3	15
29	AF	165/166 (99%)	146 (88%)	19 (12%)	5	21
29	BF	165/166 (99%)	146 (88%)	19 (12%)	5	21
30	AG	155/156 (99%)	134 (86%)	21 (14%)	4	16
30	BG	155/156 (99%)	133 (86%)	22 (14%)	3	14
31	AH	137/148 (93%)	123 (90%)	14 (10%)	7	26
31	BH	137/148 (93%)	123 (90%)	14 (10%)	7	26
32	AI	122/124 (98%)	98 (80%)	24 (20%)	1	6
32	BI	122/124 (98%)	99 (81%)	23 (19%)	1	7
34	AN	117/119 (98%)	100 (86%)	17 (14%)	3	14
34	BN	117/119 (98%)	99 (85%)	18 (15%)	2	12
35	AO	100/100 (100%)	89 (89%)	11 (11%)	6	23
35	BO	100/100 (100%)	89 (89%)	11 (11%)	6	23
36	AP	112/116 (97%)	86 (77%)	26 (23%)	1	4
36	BP	112/116 (97%)	86 (77%)	26 (23%)	1	4
37	AQ	110/111 (99%)	101 (92%)	9 (8%)	10	35
37	BQ	110/111 (99%)	99 (90%)	11 (10%)	7	27
38	AR	100/101 (99%)	83 (83%)	17 (17%)	2	10
38	BR	100/101 (99%)	84 (84%)	16 (16%)	2	11
39	AS	77/88 (88%)	65 (84%)	12 (16%)	2	12
39	BS	77/88 (88%)	65 (84%)	12 (16%)	2	12
40	AT	118/127 (93%)	97 (82%)	21 (18%)	2	8
40	BT	118/127 (93%)	96 (81%)	22 (19%)	1	7
41	AU	92/94 (98%)	79 (86%)	13 (14%)	3	14
41	BU	92/94 (98%)	78 (85%)	14 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	AV	82/82 (100%)	61 (74%)	21 (26%)	0	2
42	BV	82/82 (100%)	61 (74%)	21 (26%)	0	2
43	AW	91/92 (99%)	78 (86%)	13 (14%)	3	14
43	BW	91/92 (99%)	79 (87%)	12 (13%)	4	17
44	AX	74/78 (95%)	63 (85%)	11 (15%)	3	13
44	BX	74/78 (95%)	63 (85%)	11 (15%)	3	13
45	AY	84/91 (92%)	76 (90%)	8 (10%)	8	29
45	BY	84/91 (92%)	76 (90%)	8 (10%)	8	29
46	AZ	162/179 (90%)	142 (88%)	20 (12%)	4	19
46	BZ	162/179 (90%)	129 (80%)	33 (20%)	1	6
47	A0	66/67 (98%)	58 (88%)	8 (12%)	5	20
47	B0	66/67 (98%)	58 (88%)	8 (12%)	5	20
48	A1	78/83 (94%)	65 (83%)	13 (17%)	2	11
48	B1	78/83 (94%)	72 (92%)	6 (8%)	12	37
49	A2	66/67 (98%)	60 (91%)	6 (9%)	9	31
49	B2	66/67 (98%)	55 (83%)	11 (17%)	2	11
50	A3	51/52 (98%)	47 (92%)	4 (8%)	11	36
50	B3	51/52 (98%)	47 (92%)	4 (8%)	11	36
51	A4	51/63 (81%)	38 (74%)	13 (26%)	0	3
51	B4	51/63 (81%)	38 (74%)	13 (26%)	0	3
52	A5	47/52 (90%)	43 (92%)	4 (8%)	10	33
52	B5	47/52 (90%)	43 (92%)	4 (8%)	10	33
53	A6	49/52 (94%)	40 (82%)	9 (18%)	1	7
53	B6	49/52 (94%)	39 (80%)	10 (20%)	1	6
54	A7	40/42 (95%)	35 (88%)	5 (12%)	4	19
54	B7	40/42 (95%)	35 (88%)	5 (12%)	4	19
55	A8	53/55 (96%)	40 (76%)	13 (24%)	1	3
55	B8	53/55 (96%)	39 (74%)	14 (26%)	0	2
56	A9	34/34 (100%)	32 (94%)	2 (6%)	18	46
56	B9	34/34 (100%)	32 (94%)	2 (6%)	18	46
All	All	9957/10598 (94%)	8753 (88%)	1204 (12%)	5	20

5 of 1204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	BN	108	PRO
49	B2	34	GLU
36	BP	64	LYS
34	BN	89	LYS
41	BU	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 359 such sidechains are listed below:

Mol	Chain	Res	Type
10	Bk	117	ASN
32	BI	104	GLN
12	Bm	101	GLN
27	BD	164	GLN
36	BP	68	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	Aa	1503/1504 (99%)	208 (13%)	0
22	Ba	1503/1504 (99%)	209 (13%)	0
23	Ax	11/25 (44%)	5 (45%)	0
23	Bx	11/25 (44%)	5 (45%)	0
24	Av	76/77 (98%)	18 (23%)	0
24	Bv	76/77 (98%)	14 (18%)	0
25	Aw	76/77 (98%)	9 (11%)	0
25	Bw	76/77 (98%)	10 (13%)	0
57	AA	2847/2848 (99%)	493 (17%)	61 (2%)
57	BA	2847/2848 (99%)	494 (17%)	64 (2%)
58	AB	118/119 (99%)	18 (15%)	1 (0%)
58	BB	118/119 (99%)	18 (15%)	1 (0%)
All	All	9262/9300 (99%)	1501 (16%)	127 (1%)

5 of 1501 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	Aa	9	G
22	Aa	31	G
22	Aa	32	A
22	Aa	39	G
22	Aa	47	C

5 of 127 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	AA	2481	G
57	BA	1992	G
57	BA	266	G
57	BA	1970	A
57	BA	2311	A

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

8 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	Ax	20	23	22,25,26	0.36	0	30,36,39	0.85	1 (3%)
24	5MU	Av	54	24	19,22,23	0.23	0	27,32,35	0.38	0
23	OMU	Ax	19	23	19,22,23	0.45	0	25,31,34	0.82	1 (4%)
23	A2M	Bx	20	23	22,25,26	0.28	0	30,36,39	0.81	2 (6%)
24	5MU	Bv	54	24	19,22,23	0.31	0	27,32,35	0.33	0
23	OMG	Ax	21	23	23,26,27	0.39	0	32,38,41	0.70	0
23	OMG	Bx	21	23	23,26,27	0.35	0	32,38,41	0.55	1 (3%)
23	OMU	Bx	19	23	19,22,23	0.60	1 (5%)	25,31,34	0.74	0

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	Ax	20	23	-	1/9/27/28	0/3/3/3
24	5MU	Av	54	24	-	0/7/25/26	0/2/2/2
23	OMU	Ax	19	23	-	3/9/27/28	0/2/2/2
23	A2M	Bx	20	23	-	0/9/27/28	0/3/3/3
24	5MU	Bv	54	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMG	Ax	21	23	-	2/9/27/28	0/3/3/3
23	OMG	Bx	21	23	-	0/9/27/28	0/3/3/3
23	OMU	Bx	19	23	-	5/9/27/28	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Bx	19	OMU	C2-N1	2.17	1.41	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Ax	20	A2M	C2'-C1'-N9	2.64	118.09	113.75
23	Bx	20	A2M	O3'-C3'-C2'	2.60	118.46	111.19
23	Ax	19	OMU	C2'-C1'-N1	2.35	118.70	114.24
23	Bx	21	OMG	CM2-O2'-C2'	-2.30	108.57	114.47
23	Bx	20	A2M	CM'-O2'-C2'	-2.12	109.02	114.47

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Bx	19	OMU	C2'-C1'-N1-C2
23	Ax	19	OMU	C2'-C1'-N1-C2
23	Ax	19	OMU	C2'-C1'-N1-C6
23	Bx	19	OMU	C2'-C1'-N1-C6
23	Ax	21	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Ax	20	A2M	5	0
23	Ax	19	OMU	5	0
23	Bx	20	A2M	3	0
23	Ax	21	OMG	13	0
23	Bx	21	OMG	6	0
23	Bx	19	OMU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1072 ligands modelled in this entry, 1072 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	Ab	234/256 (91%)	0.45	11 (4%) 36 24	119, 151, 187, 193	0
1	Bb	234/256 (91%)	0.57	10 (4%) 40 25	117, 151, 186, 193	0
2	Ac	206/239 (86%)	0.51	11 (5%) 32 22	116, 147, 171, 173	0
2	Bc	206/239 (86%)	0.39	6 (2%) 53 35	115, 147, 171, 174	0
3	Ad	208/209 (99%)	0.62	26 (12%) 8 6	94, 123, 145, 154	0
3	Bd	208/209 (99%)	0.74	14 (6%) 24 16	94, 124, 146, 155	0
4	Ae	150/162 (92%)	0.27	4 (2%) 56 37	90, 114, 142, 160	0
4	Be	150/162 (92%)	0.29	3 (2%) 65 46	91, 114, 143, 161	0
5	Af	101/101 (100%)	0.36	1 (0%) 79 63	103, 127, 143, 167	0
5	Bf	101/101 (100%)	0.54	6 (5%) 28 19	100, 126, 143, 167	0
6	Ag	155/156 (99%)	0.57	12 (7%) 19 14	119, 141, 173, 189	0
6	Bg	155/156 (99%)	0.50	11 (7%) 22 15	120, 141, 173, 189	0
7	Ah	138/138 (100%)	0.33	8 (5%) 29 19	99, 118, 133, 143	0
7	Bh	138/138 (100%)	0.45	11 (7%) 18 14	100, 118, 133, 144	0
8	Ai	127/128 (99%)	1.03	16 (12%) 8 6	121, 162, 182, 190	0
8	Bi	127/128 (99%)	0.82	14 (11%) 10 9	121, 162, 182, 189	0
9	Aj	98/105 (93%)	1.11	17 (17%) 4 4	118, 165, 185, 187	0
9	Bj	98/105 (93%)	1.06	12 (12%) 8 7	116, 164, 184, 188	0
10	Ak	119/129 (92%)	0.48	6 (5%) 34 23	89, 121, 156, 176	0
10	Bk	119/129 (92%)	0.28	6 (5%) 34 23	91, 120, 155, 175	0
11	Al	124/132 (93%)	0.58	10 (8%) 18 13	81, 101, 133, 169	0
11	Bl	124/132 (93%)	0.56	9 (7%) 21 15	83, 102, 134, 169	0
12	Am	118/126 (93%)	1.01	22 (18%) 3 3	115, 147, 161, 169	0
12	Bm	118/126 (93%)	0.92	16 (13%) 7 6	115, 146, 161, 168	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	An	60/61 (98%)	1.26	8 (13%) 7 6	127, 140, 158, 161	0
13	Bn	60/61 (98%)	0.94	6 (10%) 12 10	125, 140, 157, 160	0
14	Ao	88/89 (98%)	0.30	4 (4%) 38 25	87, 114, 138, 146	0
14	Bo	88/89 (98%)	0.31	2 (2%) 61 42	88, 114, 138, 146	0
15	Ap	83/88 (94%)	0.70	4 (4%) 35 24	96, 114, 135, 162	0
15	Bp	83/88 (94%)	0.49	4 (4%) 35 24	97, 116, 136, 163	0
16	Aq	99/105 (94%)	0.18	3 (3%) 52 35	89, 112, 125, 133	0
16	Bq	99/105 (94%)	0.37	5 (5%) 33 22	92, 112, 125, 133	0
17	Ar	70/88 (79%)	0.60	2 (2%) 53 35	98, 125, 147, 153	0
17	Br	70/88 (79%)	0.49	4 (5%) 29 20	98, 123, 147, 153	0
18	As	78/93 (83%)	0.84	9 (11%) 9 8	135, 151, 180, 185	0
18	Bs	78/93 (83%)	0.71	7 (8%) 15 11	135, 151, 180, 185	0
19	At	99/106 (93%)	0.84	16 (16%) 4 4	105, 123, 157, 161	0
19	Bt	99/106 (93%)	0.59	7 (7%) 22 15	107, 124, 158, 162	0
20	Au	24/27 (88%)	1.50	9 (37%) 1 1	113, 141, 162, 175	0
20	Bu	24/27 (88%)	1.80	8 (33%) 1 1	113, 141, 162, 174	0
21	Ay	94/95 (98%)	0.74	10 (10%) 11 9	67, 133, 155, 159	0
21	By	94/95 (98%)	0.28	4 (4%) 40 25	112, 136, 154, 169	0
22	Aa	1504/1504 (100%)	0.17	31 (2%) 63 44	70, 123, 196, 208	0
22	Ba	1504/1504 (100%)	0.17	24 (1%) 70 52	70, 124, 196, 208	0
23	Ax	9/25 (36%)	1.12	2 (22%) 2 2	102, 161, 194, 201	0
23	Bx	9/25 (36%)	0.98	2 (22%) 2 2	100, 159, 202, 204	0
24	Av	76/77 (98%)	-0.05	0 100 100	93, 120, 159, 176	0
24	Bv	76/77 (98%)	-0.23	1 (1%) 75 56	82, 113, 154, 168	0
25	Aw	77/77 (100%)	0.17	0 100 100	135, 202, 204, 205	0
25	Bw	77/77 (100%)	0.22	1 (1%) 75 56	134, 203, 205, 207	0
26	AC	120/229 (52%)	0.81	23 (19%) 3 3	167, 186, 194, 195	0
26	BC	120/229 (52%)	1.04	24 (20%) 3 2	166, 186, 194, 195	0
27	AD	271/276 (98%)	0.27	11 (4%) 41 27	58, 81, 109, 137	0
27	BD	271/276 (98%)	0.15	11 (4%) 41 27	55, 79, 108, 137	0
28	AE	204/206 (99%)	0.31	12 (5%) 28 19	62, 88, 143, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	BE	204/206 (99%)	0.39	11 (5%) 31 21	59, 87, 143, 160	0
29	AF	207/210 (98%)	0.26	4 (1%) 66 48	61, 93, 150, 182	0
29	BF	207/210 (98%)	0.23	8 (3%) 43 29	55, 90, 150, 182	0
30	AG	181/182 (99%)	0.63	15 (8%) 17 13	113, 140, 165, 181	0
30	BG	181/182 (99%)	0.72	18 (9%) 13 10	102, 133, 164, 183	0
31	AH	164/180 (91%)	0.54	11 (6%) 24 16	103, 134, 154, 175	0
31	BH	164/180 (91%)	1.02	20 (12%) 8 7	96, 131, 151, 176	0
32	AI	145/148 (97%)	1.89	54 (37%) 1 1	91, 163, 180, 185	0
32	BI	145/148 (97%)	1.66	53 (36%) 1 1	90, 163, 181, 186	0
33	AJ	130/173 (75%)	1.41	33 (25%) 1 1	180, 195, 199, 201	0
33	BJ	130/173 (75%)	1.61	42 (32%) 1 1	167, 185, 194, 197	0
34	AN	138/140 (98%)	0.29	7 (5%) 33 22	76, 98, 133, 153	0
34	BN	138/140 (98%)	0.52	9 (6%) 25 17	73, 95, 132, 152	0
35	AO	122/122 (100%)	-0.08	1 (0%) 82 68	65, 84, 106, 133	0
35	BO	122/122 (100%)	-0.10	1 (0%) 82 68	64, 83, 106, 131	0
36	AP	146/150 (97%)	0.98	26 (17%) 4 3	63, 112, 139, 175	0
36	BP	146/150 (97%)	1.29	35 (23%) 2 1	62, 111, 139, 173	0
37	AQ	140/141 (99%)	0.42	9 (6%) 25 17	76, 99, 132, 153	0
37	BQ	140/141 (99%)	0.43	7 (5%) 34 23	74, 99, 131, 153	0
38	AR	117/118 (99%)	0.36	10 (8%) 16 13	70, 90, 119, 144	0
38	BR	117/118 (99%)	0.40	9 (7%) 19 14	67, 89, 119, 143	0
39	AS	98/112 (87%)	1.36	32 (32%) 1 1	115, 139, 161, 162	0
39	BS	98/112 (87%)	1.44	28 (28%) 1 1	112, 138, 161, 163	0
40	AT	135/146 (92%)	0.62	15 (11%) 10 9	78, 103, 154, 185	0
40	BT	135/146 (92%)	0.63	15 (11%) 10 9	78, 103, 154, 185	0
41	AU	117/118 (99%)	0.27	4 (3%) 48 32	67, 88, 124, 155	0
41	BU	117/118 (99%)	0.45	8 (6%) 23 16	63, 84, 123, 156	0
42	AV	101/101 (100%)	0.41	4 (3%) 42 28	62, 114, 136, 151	0
42	BV	101/101 (100%)	0.50	4 (3%) 42 28	59, 110, 135, 151	0
43	AW	113/113 (100%)	-0.01	2 (1%) 67 49	67, 83, 110, 183	0
43	BW	113/113 (100%)	0.10	1 (0%) 81 65	65, 81, 108, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AX	92/96 (95%)	0.32	1 (1%) 78 60	74, 93, 115, 124	0
44	BX	92/96 (95%)	0.59	4 (4%) 40 25	66, 90, 113, 125	0
45	AY	100/110 (90%)	1.32	25 (25%) 2 1	85, 122, 162, 169	0
45	BY	100/110 (90%)	1.52	32 (32%) 1 1	84, 120, 162, 168	0
46	AZ	184/206 (89%)	0.29	2 (1%) 78 60	109, 138, 158, 192	0
46	BZ	184/206 (89%)	0.42	6 (3%) 49 33	96, 128, 152, 187	0
47	A0	84/85 (98%)	0.55	8 (9%) 14 11	87, 104, 152, 185	0
47	B0	84/85 (98%)	0.87	9 (10%) 11 9	86, 102, 153, 185	0
48	A1	93/98 (94%)	0.31	3 (3%) 50 34	68, 93, 132, 144	0
48	B1	93/98 (94%)	0.45	3 (3%) 50 34	60, 87, 133, 146	0
49	A2	71/72 (98%)	0.57	3 (4%) 40 26	89, 124, 144, 163	0
49	B2	71/72 (98%)	0.23	5 (7%) 22 15	60, 90, 134, 169	0
50	A3	59/60 (98%)	0.38	2 (3%) 48 32	79, 100, 124, 169	0
50	B3	59/60 (98%)	0.47	0 100 100	75, 98, 121, 169	0
51	A4	57/71 (80%)	0.73	6 (10%) 11 9	153, 167, 183, 186	0
51	B4	57/71 (80%)	1.14	10 (17%) 4 4	154, 167, 182, 187	0
52	A5	55/60 (91%)	0.56	3 (5%) 30 21	55, 91, 137, 144	0
52	B5	55/60 (91%)	0.31	2 (3%) 46 31	54, 89, 137, 145	0
53	A6	50/54 (92%)	1.14	11 (22%) 2 2	128, 155, 169, 182	0
53	B6	50/54 (92%)	0.92	4 (8%) 18 14	128, 154, 169, 182	0
54	A7	47/49 (95%)	0.23	1 (2%) 63 44	58, 70, 95, 144	0
54	B7	47/49 (95%)	0.17	2 (4%) 40 25	53, 66, 91, 144	0
55	A8	63/65 (96%)	1.24	17 (26%) 1 1	70, 91, 118, 155	0
55	B8	63/65 (96%)	1.03	9 (14%) 6 5	70, 89, 117, 155	0
56	A9	37/37 (100%)	1.13	7 (18%) 3 3	109, 121, 141, 144	0
56	B9	37/37 (100%)	1.09	8 (21%) 2 2	105, 120, 141, 144	0
57	AA	2848/2848 (100%)	-0.22	41 (1%) 73 55	56, 90, 194, 209	0
57	BA	2848/2848 (100%)	-0.13	50 (1%) 67 49	53, 87, 195, 208	0
58	AB	119/119 (100%)	0.26	3 (2%) 58 39	96, 140, 176, 197	0
58	BB	119/119 (100%)	0.58	6 (5%) 34 23	94, 139, 175, 197	0
All	All	21494/22422 (95%)	0.33	1295 (6%) 27 19	53, 114, 186, 209	0

The worst 5 of 1295 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	BI	88	ILE	12.7
52	A5	2	ALA	11.2
32	AI	97	ILE	10.0
10	Bk	129	SER	9.9
57	BA	277	C	9.7

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($\text{\AA}^2$)	Q<0.9
23	A2M	Ax	20	23/24	0.75	0.14	160,168,169,173	0
23	OMG	Ax	21	24/25	0.78	0.16	174,180,182,184	0
23	OMU	Bx	19	21/22	0.84	0.15	129,157,162,162	0
23	OMG	Bx	21	24/25	0.86	0.17	177,182,184,186	0
23	A2M	Bx	20	23/24	0.87	0.13	161,170,172,175	0
24	5MU	Bv	54	21/22	0.88	0.12	121,125,138,138	0
24	5MU	Av	54	21/22	0.89	0.12	139,140,144,145	0
23	OMU	Ax	19	21/22	0.90	0.11	133,158,162,164	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($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1727	1/1	-0.15	0.38	90,90,90,90	1
60	MG	Ba	1728	1/1	-0.01	0.51	113,113,113,113	0
60	MG	Ba	1647	1/1	0.01	0.32	148,148,148,148	0
60	MG	Ba	1695	1/1	0.02	0.40	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Bw	101	1/1	0.03	0.28	140,140,140,140	1
60	MG	Ba	1713	1/1	0.05	0.43	105,105,105,105	0
60	MG	Aa	1713	1/1	0.16	0.24	149,149,149,149	0
60	MG	BA	3126	1/1	0.17	0.31	154,154,154,154	0
60	MG	Aa	1736	1/1	0.19	0.17	126,126,126,126	0
60	MG	AA	2954	1/1	0.25	0.28	103,103,103,103	0
60	MG	BA	3191	1/1	0.25	0.35	116,116,116,116	0
60	MG	AA	3260	1/1	0.33	0.33	104,104,104,104	0
60	MG	Aa	1714	1/1	0.35	0.34	111,111,111,111	0
60	MG	Ba	1625	1/1	0.37	0.50	113,113,113,113	0
60	MG	BA	3088	1/1	0.40	0.31	113,113,113,113	0
60	MG	Ba	1708	1/1	0.41	0.16	139,139,139,139	0
60	MG	Aa	1690	1/1	0.42	0.32	96,96,96,96	1
60	MG	AA	3261	1/1	0.42	0.39	110,110,110,110	0
60	MG	AA	3248	1/1	0.43	0.37	141,141,141,141	0
60	MG	AA	3194	1/1	0.43	0.34	108,108,108,108	0
60	MG	Ba	1645	1/1	0.43	0.35	89,89,89,89	0
60	MG	BA	3258	1/1	0.43	0.34	110,110,110,110	0
60	MG	Ba	1677	1/1	0.45	0.48	152,152,152,152	1
60	MG	Aa	1622	1/1	0.45	0.22	101,101,101,101	0
60	MG	BA	3162	1/1	0.46	0.41	86,86,86,86	0
60	MG	AA	3249	1/1	0.46	0.43	109,109,109,109	0
60	MG	Aa	1730	1/1	0.46	0.46	104,104,104,104	0
60	MG	BA	2965	1/1	0.47	0.26	74,74,74,74	0
60	MG	Aa	1614	1/1	0.47	0.29	88,88,88,88	0
60	MG	Ba	1676	1/1	0.47	0.55	113,113,113,113	0
60	MG	AA	3086	1/1	0.47	0.28	94,94,94,94	0
60	MG	Aa	1623	1/1	0.47	0.33	107,107,107,107	0
60	MG	BA	2945	1/1	0.47	0.22	149,149,149,149	0
60	MG	Ba	1715	1/1	0.48	0.25	121,121,121,121	0
60	MG	Aa	1674	1/1	0.49	0.22	108,108,108,108	0
60	MG	Ba	1613	1/1	0.49	0.28	101,101,101,101	0
60	MG	AA	3165	1/1	0.49	0.28	83,83,83,83	0
60	MG	AA	3069	1/1	0.49	0.41	87,87,87,87	0
60	MG	AA	3078	1/1	0.50	0.36	94,94,94,94	0
60	MG	Ba	1646	1/1	0.50	0.56	122,122,122,122	0
60	MG	AA	3207	1/1	0.50	0.28	122,122,122,122	0
60	MG	Aa	1697	1/1	0.51	0.28	129,129,129,129	0
60	MG	BA	3113	1/1	0.51	0.32	55,55,55,55	1
60	MG	Ba	1712	1/1	0.51	0.38	96,96,96,96	0
60	MG	Aa	1681	1/1	0.51	0.24	86,86,86,86	0
60	MG	BA	2953	1/1	0.51	0.31	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3149	1/1	0.51	0.45	109,109,109,109	0
60	MG	Ba	1606	1/1	0.52	0.36	101,101,101,101	0
60	MG	AA	2975	1/1	0.52	0.49	97,97,97,97	0
60	MG	AA	3030	1/1	0.53	0.53	94,94,94,94	0
60	MG	Ba	1723	1/1	0.53	0.28	89,89,89,89	0
60	MG	BA	3131	1/1	0.53	0.25	89,89,89,89	0
60	MG	BA	3182	1/1	0.54	0.25	140,140,140,140	0
60	MG	Aa	1722	1/1	0.54	0.34	110,110,110,110	0
60	MG	Ba	1678	1/1	0.54	0.26	131,131,131,131	0
60	MG	Ba	1699	1/1	0.55	0.60	113,113,113,113	0
60	MG	BA	3119	1/1	0.55	0.23	79,79,79,79	0
60	MG	Ba	1706	1/1	0.56	0.61	131,131,131,131	0
60	MG	AA	3241	1/1	0.56	0.36	100,100,100,100	0
60	MG	Aa	1611	1/1	0.56	0.40	82,82,82,82	0
60	MG	Ba	1648	1/1	0.56	0.38	145,145,145,145	0
60	MG	AA	3115	1/1	0.56	0.27	108,108,108,108	0
60	MG	Aa	1665	1/1	0.57	0.26	88,88,88,88	0
60	MG	Ba	1688	1/1	0.57	0.33	90,90,90,90	1
60	MG	Aa	1671	1/1	0.57	0.35	113,113,113,113	0
60	MG	Aa	1606	1/1	0.57	0.31	105,105,105,105	0
60	MG	Aw	101	1/1	0.57	0.15	95,95,95,95	1
60	MG	AA	2946	1/1	0.57	0.13	116,116,116,116	0
60	MG	Ba	1704	1/1	0.58	0.53	108,108,108,108	0
60	MG	Ba	1725	1/1	0.58	0.40	72,72,72,72	1
60	MG	Ba	1680	1/1	0.58	0.49	134,134,134,134	0
60	MG	Bv	104	1/1	0.58	0.59	118,118,118,118	1
60	MG	Aa	1725	1/1	0.58	0.33	88,88,88,88	0
60	MG	Ba	1692	1/1	0.58	0.49	99,99,99,99	0
60	MG	BA	2947	1/1	0.58	0.24	68,68,68,68	0
60	MG	Ba	1636	1/1	0.58	0.53	91,91,91,91	0
60	MG	BA	3204	1/1	0.58	0.34	92,92,92,92	0
60	MG	AA	3264	1/1	0.58	0.24	101,101,101,101	0
60	MG	Ba	1617	1/1	0.59	0.25	69,69,69,69	1
60	MG	AA	3002	1/1	0.59	0.47	84,84,84,84	0
60	MG	Ba	1660	1/1	0.59	0.32	127,127,127,127	0
60	MG	Aa	1699	1/1	0.59	0.40	125,125,125,125	1
60	MG	AA	3103	1/1	0.59	0.43	103,103,103,103	0
60	MG	Aa	1641	1/1	0.59	0.37	87,87,87,87	0
60	MG	AA	3036	1/1	0.60	0.48	99,99,99,99	0
60	MG	AA	3057	1/1	0.60	0.43	73,73,73,73	0
60	MG	Aa	1678	1/1	0.60	0.42	111,111,111,111	1
60	MG	AA	3111	1/1	0.60	0.28	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	BA	3205	1/1	0.60	0.29	113,113,113,113	0
60	MG	BA	3071	1/1	0.60	0.56	113,113,113,113	0
60	MG	BA	3154	1/1	0.61	0.08	164,164,164,164	0
60	MG	Aa	1744	1/1	0.61	0.34	114,114,114,114	0
60	MG	AA	3146	1/1	0.61	0.30	87,87,87,87	0
60	MG	AB	202	1/1	0.61	0.43	103,103,103,103	0
60	MG	AA	2968	1/1	0.61	0.29	73,73,73,73	0
60	MG	Aa	1618	1/1	0.61	0.22	73,73,73,73	1
60	MG	Aa	1637	1/1	0.61	0.43	99,99,99,99	0
60	MG	Aa	1734	1/1	0.62	0.39	125,125,125,125	0
60	MG	Aa	1610	1/1	0.62	0.27	117,117,117,117	0
60	MG	AA	3134	1/1	0.62	0.21	98,98,98,98	0
60	MG	Bm	202	1/1	0.62	0.38	97,97,97,97	0
60	MG	BA	3150	1/1	0.62	0.51	104,104,104,104	0
60	MG	Ba	1605	1/1	0.62	0.34	99,99,99,99	0
60	MG	Ba	1721	1/1	0.63	0.25	108,108,108,108	0
60	MG	AX	101	1/1	0.63	0.37	96,96,96,96	1
60	MG	AA	3255	1/1	0.63	0.24	70,70,70,70	0
60	MG	Aa	1654	1/1	0.64	0.19	93,93,93,93	0
60	MG	Ba	1655	1/1	0.64	0.23	66,66,66,66	0
60	MG	Ba	1700	1/1	0.64	0.29	113,113,113,113	0
60	MG	AA	3168	1/1	0.64	0.27	84,84,84,84	0
60	MG	Am	201	1/1	0.64	0.33	88,88,88,88	0
60	MG	Aa	1721	1/1	0.64	0.38	97,97,97,97	0
60	MG	AA	3268	1/1	0.64	0.39	102,102,102,102	0
60	MG	AA	3090	1/1	0.64	0.35	86,86,86,86	0
60	MG	Ba	1687	1/1	0.64	0.23	69,69,69,69	1
60	MG	Aa	1633	1/1	0.64	0.32	71,71,71,71	0
60	MG	BA	3233	1/1	0.64	0.42	109,109,109,109	0
60	MG	AA	3150	1/1	0.64	0.24	81,81,81,81	0
60	MG	BA	3262	1/1	0.64	0.29	100,100,100,100	0
60	MG	AA	3211	1/1	0.65	0.20	97,97,97,97	0
60	MG	Ba	1714	1/1	0.65	0.11	90,90,90,90	0
60	MG	AA	3262	1/1	0.65	0.33	94,94,94,94	0
60	MG	AA	3219	1/1	0.65	0.30	94,94,94,94	0
60	MG	AA	3132	1/1	0.65	0.39	93,93,93,93	0
60	MG	AA	3038	1/1	0.65	0.39	95,95,95,95	0
60	MG	AA	3136	1/1	0.65	0.22	88,88,88,88	0
60	MG	BA	3231	1/1	0.65	0.32	105,105,105,105	0
60	MG	Ba	1732	1/1	0.65	0.34	135,135,135,135	0
60	MG	AA	2925	1/1	0.65	0.30	92,92,92,92	0
60	MG	Aa	1616	1/1	0.65	0.45	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Ba	1664	1/1	0.66	0.24	88,88,88,88	0
60	MG	AA	3266	1/1	0.66	0.26	73,73,73,73	0
60	MG	Ba	1737	1/1	0.66	0.14	101,101,101,101	0
60	MG	BA	3099	1/1	0.66	0.39	97,97,97,97	0
60	MG	AA	3210	1/1	0.66	0.39	99,99,99,99	0
60	MG	AA	3080	1/1	0.66	0.26	120,120,120,120	0
60	MG	Ba	1621	1/1	0.66	0.27	84,84,84,84	0
60	MG	AA	3209	1/1	0.66	0.30	108,108,108,108	0
60	MG	BA	3138	1/1	0.66	0.13	61,61,61,61	0
60	MG	AA	3239	1/1	0.66	0.41	113,113,113,113	0
60	MG	Ba	1616	1/1	0.67	0.21	99,99,99,99	0
60	MG	Ba	1707	1/1	0.67	0.51	100,100,100,100	0
60	MG	AA	3187	1/1	0.67	0.31	98,98,98,98	0
60	MG	AQ	201	1/1	0.67	0.34	105,105,105,105	0
60	MG	AA	3164	1/1	0.67	0.24	81,81,81,81	0
60	MG	Ba	1626	1/1	0.67	0.25	92,92,92,92	0
60	MG	BA	2902	1/1	0.67	0.30	129,129,129,129	0
60	MG	AA	3208	1/1	0.67	0.28	72,72,72,72	0
60	MG	AA	2943	1/1	0.67	0.31	77,77,77,77	0
60	MG	Aa	1664	1/1	0.67	0.48	114,114,114,114	0
60	MG	BA	3074	1/1	0.68	0.38	97,97,97,97	0
60	MG	AA	3202	1/1	0.68	0.28	85,85,85,85	1
60	MG	AA	3152	1/1	0.68	0.47	113,113,113,113	0
60	MG	Aa	1689	1/1	0.68	0.16	57,57,57,57	1
60	MG	AA	3191	1/1	0.68	0.31	102,102,102,102	0
60	MG	Ba	1698	1/1	0.68	0.44	123,123,123,123	1
60	MG	BA	3209	1/1	0.68	0.12	107,107,107,107	0
60	MG	AA	3247	1/1	0.68	0.24	92,92,92,92	0
60	MG	Ba	1734	1/1	0.68	0.15	138,138,138,138	0
60	MG	BA	3149	1/1	0.68	0.42	126,126,126,126	0
60	MG	Av	104	1/1	0.68	0.37	88,88,88,88	1
60	MG	AA	3240	1/1	0.69	0.31	104,104,104,104	0
60	MG	BA	3081	1/1	0.69	0.50	106,106,106,106	0
60	MG	Ba	1738	1/1	0.69	0.34	77,77,77,77	0
60	MG	AA	3102	1/1	0.69	0.35	92,92,92,92	0
60	MG	BA	3210	1/1	0.69	0.60	93,93,93,93	0
60	MG	Ba	1635	1/1	0.69	0.50	86,86,86,86	0
60	MG	BA	3049	1/1	0.69	0.22	82,82,82,82	0
60	MG	Ba	1736	1/1	0.69	0.35	88,88,88,88	0
60	MG	BA	3188	1/1	0.69	0.29	90,90,90,90	0
60	MG	AA	3091	1/1	0.70	0.46	104,104,104,104	0
60	MG	AA	3157	1/1	0.70	0.11	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3141	1/1	0.70	0.24	82,82,82,82	0
60	MG	Ba	1711	1/1	0.70	0.12	117,117,117,117	0
60	MG	BA	2901	1/1	0.70	0.34	122,122,122,122	0
60	MG	BA	2958	1/1	0.70	0.43	100,100,100,100	0
60	MG	Aq	201	1/1	0.71	0.31	91,91,91,91	0
60	MG	AA	3162	1/1	0.71	0.27	126,126,126,126	0
60	MG	AA	3258	1/1	0.71	0.27	103,103,103,103	0
60	MG	AA	3029	1/1	0.71	0.28	74,74,74,74	0
60	MG	AA	3243	1/1	0.71	0.46	117,117,117,117	0
60	MG	Ba	1739	1/1	0.71	0.44	82,82,82,82	0
60	MG	BA	3206	1/1	0.71	0.37	78,78,78,78	0
60	MG	BA	3136	1/1	0.71	0.28	109,109,109,109	0
60	MG	BA	3048	1/1	0.71	0.38	95,95,95,95	0
60	MG	BA	3229	1/1	0.71	0.24	101,101,101,101	0
60	MG	Bv	103	1/1	0.71	0.45	110,110,110,110	0
60	MG	AA	3108	1/1	0.71	0.26	69,69,69,69	0
60	MG	Aa	1719	1/1	0.71	0.27	92,92,92,92	0
60	MG	Ba	1672	1/1	0.71	0.34	106,106,106,106	0
60	MG	Aa	1723	1/1	0.72	0.35	98,98,98,98	0
60	MG	Aa	1686	1/1	0.72	0.29	74,74,74,74	0
60	MG	BA	3036	1/1	0.72	0.46	73,73,73,73	0
60	MG	AA	3203	1/1	0.72	0.30	79,79,79,79	0
60	MG	AA	2931	1/1	0.72	0.36	63,63,63,63	0
60	MG	AA	3166	1/1	0.72	0.32	94,94,94,94	0
60	MG	BA	3072	1/1	0.72	0.34	75,75,75,75	0
60	MG	AA	3040	1/1	0.72	0.25	82,82,82,82	0
60	MG	AA	3007	1/1	0.72	0.24	83,83,83,83	0
60	MG	BA	3082	1/1	0.72	0.28	71,71,71,71	0
60	MG	AA	2959	1/1	0.72	0.25	77,77,77,77	0
60	MG	BA	3259	1/1	0.72	0.35	99,99,99,99	0
60	MG	Ba	1717	1/1	0.72	0.43	99,99,99,99	0
60	MG	Aa	1620	1/1	0.73	0.26	79,79,79,79	0
60	MG	AA	3119	1/1	0.73	0.35	143,143,143,143	0
60	MG	AA	3092	1/1	0.73	0.35	112,112,112,112	0
60	MG	Ba	1720	1/1	0.73	0.43	123,123,123,123	0
60	MG	BA	3190	1/1	0.73	0.35	98,98,98,98	0
60	MG	AA	3101	1/1	0.73	0.18	92,92,92,92	0
60	MG	BA	2942	1/1	0.73	0.38	78,78,78,78	0
60	MG	Aa	1656	1/1	0.73	0.14	67,67,67,67	0
60	MG	AA	2967	1/1	0.73	0.55	96,96,96,96	0
60	MG	AA	3257	1/1	0.73	0.25	75,75,75,75	0
60	MG	AA	3185	1/1	0.73	0.16	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3212	1/1	0.73	0.33	79,79,79,79	0
60	MG	AA	3218	1/1	0.73	0.35	104,104,104,104	0
60	MG	AA	3015	1/1	0.73	0.48	103,103,103,103	0
60	MG	BA	3143	1/1	0.73	0.34	90,90,90,90	0
60	MG	AA	3109	1/1	0.73	0.42	73,73,73,73	0
60	MG	Aa	1617	1/1	0.73	0.15	66,66,66,66	0
60	MG	Aa	1648	1/1	0.74	0.26	118,118,118,118	0
60	MG	AA	3193	1/1	0.74	0.26	85,85,85,85	0
60	MG	Aa	1742	1/1	0.74	0.30	91,91,91,91	0
60	MG	AA	3122	1/1	0.74	0.26	101,101,101,101	0
60	MG	AA	3215	1/1	0.74	0.48	89,89,89,89	0
60	MG	BA	2946	1/1	0.74	0.11	74,74,74,74	0
60	MG	Aa	1667	1/1	0.74	0.23	100,100,100,100	0
60	MG	Ba	1702	1/1	0.74	0.52	110,110,110,110	0
60	MG	Aa	1601	1/1	0.74	0.20	93,93,93,93	0
60	MG	BA	3234	1/1	0.74	0.59	116,116,116,116	0
60	MG	Ba	1684	1/1	0.74	0.28	76,76,76,76	0
60	MG	BA	3034	1/1	0.74	0.35	78,78,78,78	0
60	MG	AA	3081	1/1	0.74	0.14	89,89,89,89	0
60	MG	BA	3264	1/1	0.74	0.30	68,68,68,68	0
60	MG	BA	3265	1/1	0.74	0.41	104,104,104,104	0
60	MG	BA	3183	1/1	0.75	0.15	67,67,67,67	0
60	MG	AA	3048	1/1	0.75	0.23	69,69,69,69	0
60	MG	BA	3102	1/1	0.75	0.16	81,81,81,81	0
60	MG	Aa	1705	1/1	0.75	0.55	50,50,50,50	1
60	MG	BA	2970	1/1	0.75	0.50	104,104,104,104	0
60	MG	BA	3011	1/1	0.75	0.29	81,81,81,81	0
60	MG	Aa	1706	1/1	0.75	0.23	91,91,91,91	0
60	MG	BA	3208	1/1	0.75	0.42	97,97,97,97	0
60	MG	BA	3135	1/1	0.75	0.50	146,146,146,146	0
60	MG	AA	3167	1/1	0.75	0.09	84,84,84,84	0
60	MG	Ba	1703	1/1	0.75	0.68	69,69,69,69	1
60	MG	AA	3237	1/1	0.75	0.41	88,88,88,88	0
60	MG	AA	2970	1/1	0.75	0.16	67,67,67,67	0
60	MG	Ba	1686	1/1	0.75	0.20	79,79,79,79	0
60	MG	BA	3239	1/1	0.75	0.24	88,88,88,88	0
60	MG	AA	3169	1/1	0.75	0.24	78,78,78,78	0
60	MG	Aa	1695	1/1	0.75	0.18	97,97,97,97	0
60	MG	Aa	1677	1/1	0.75	0.37	82,82,82,82	0
60	MG	BA	3167	1/1	0.75	0.21	74,74,74,74	0
60	MG	Aa	1672	1/1	0.75	0.20	77,77,77,77	0
60	MG	Aa	1688	1/1	0.76	0.22	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1647	1/1	0.76	0.46	105,105,105,105	0
60	MG	AA	2980	1/1	0.76	0.42	97,97,97,97	0
60	MG	AA	2947	1/1	0.76	0.33	103,103,103,103	0
60	MG	Aa	1735	1/1	0.76	0.25	80,80,80,80	1
60	MG	Aa	1624	1/1	0.76	0.19	86,86,86,86	0
60	MG	BA	3129	1/1	0.76	0.30	75,75,75,75	0
60	MG	AA	3076	1/1	0.76	0.38	92,92,92,92	0
60	MG	BA	3255	1/1	0.76	0.40	74,74,74,74	0
60	MG	Ba	1657	1/1	0.76	0.28	109,109,109,109	0
60	MG	Aa	1651	1/1	0.76	0.47	84,84,84,84	0
60	MG	Aa	1728	1/1	0.76	0.19	81,81,81,81	0
60	MG	BA	3084	1/1	0.76	0.30	64,64,64,64	0
60	MG	BA	3087	1/1	0.76	0.39	74,74,74,74	0
60	MG	Ba	1658	1/1	0.77	0.20	84,84,84,84	0
60	MG	Ba	1693	1/1	0.77	0.11	108,108,108,108	0
60	MG	BA	3200	1/1	0.77	0.57	98,98,98,98	0
60	MG	Aa	1692	1/1	0.77	0.22	62,62,62,62	0
60	MG	AA	3267	1/1	0.77	0.30	89,89,89,89	0
60	MG	BA	3063	1/1	0.77	0.14	59,59,59,59	0
60	MG	BA	3207	1/1	0.77	0.18	90,90,90,90	0
60	MG	Ba	1718	1/1	0.77	0.15	75,75,75,75	0
60	MG	AA	3254	1/1	0.77	0.32	84,84,84,84	0
60	MG	AA	3053	1/1	0.77	0.15	79,79,79,79	0
60	MG	AA	2999	1/1	0.77	0.25	61,61,61,61	0
60	MG	Aa	1676	1/1	0.77	0.12	120,120,120,120	0
60	MG	AA	3138	1/1	0.77	0.29	115,115,115,115	0
60	MG	Ba	1682	1/1	0.77	0.49	113,113,113,113	0
60	MG	Ba	1609	1/1	0.77	0.30	104,104,104,104	0
60	MG	AA	3075	1/1	0.77	0.27	104,104,104,104	0
60	MG	BA	3177	1/1	0.77	0.41	66,66,66,66	0
60	MG	BA	3180	1/1	0.77	0.23	92,92,92,92	0
60	MG	BA	3261	1/1	0.77	0.28	95,95,95,95	0
60	MG	AA	2939	1/1	0.77	0.17	53,53,53,53	0
60	MG	Aa	1733	1/1	0.77	0.24	79,79,79,79	0
60	MG	BA	3118	1/1	0.77	0.22	82,82,82,82	0
60	MG	AA	2995	1/1	0.78	0.22	82,82,82,82	0
60	MG	Aa	1715	1/1	0.78	0.10	84,84,84,84	0
60	MG	AA	3112	1/1	0.78	0.50	114,114,114,114	0
60	MG	Aa	1687	1/1	0.78	0.12	51,51,51,51	1
60	MG	Aa	1663	1/1	0.78	0.26	68,68,68,68	0
60	MG	Aa	1626	1/1	0.78	0.37	85,85,85,85	0
60	MG	AA	2956	1/1	0.78	0.34	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3182	1/1	0.78	0.11	82,82,82,82	0
60	MG	Ba	1694	1/1	0.78	0.27	112,112,112,112	0
60	MG	AA	3227	1/1	0.78	0.34	110,110,110,110	0
60	MG	Ba	1697	1/1	0.78	0.19	98,98,98,98	1
60	MG	BA	2998	1/1	0.78	0.38	59,59,59,59	0
60	MG	AA	2957	1/1	0.78	0.18	83,83,83,83	0
60	MG	Ba	1730	1/1	0.78	0.33	64,64,64,64	0
60	MG	Aa	1680	1/1	0.78	0.18	115,115,115,115	0
60	MG	Ba	1733	1/1	0.78	0.14	100,100,100,100	1
60	MG	AA	2902	1/1	0.78	0.29	131,131,131,131	0
60	MG	BA	3245	1/1	0.78	0.22	80,80,80,80	0
60	MG	BA	3053	1/1	0.78	0.41	70,70,70,70	0
60	MG	AA	2903	1/1	0.78	0.18	98,98,98,98	0
60	MG	Aa	1640	1/1	0.78	0.29	82,82,82,82	0
60	MG	BA	3260	1/1	0.78	0.17	93,93,93,93	0
60	MG	Aa	1658	1/1	0.78	0.23	105,105,105,105	0
60	MG	Aa	1743	1/1	0.78	0.38	80,80,80,80	0
60	MG	AA	3204	1/1	0.78	0.17	84,84,84,84	0
60	MG	AA	3062	1/1	0.78	0.23	62,62,62,62	0
60	MG	AA	3087	1/1	0.79	0.33	81,81,81,81	0
60	MG	BA	3147	1/1	0.79	0.24	67,67,67,67	0
60	MG	BA	3235	1/1	0.79	0.42	90,90,90,90	0
60	MG	BX	101	1/1	0.79	0.21	59,59,59,59	1
60	MG	AA	2928	1/1	0.79	0.47	89,89,89,89	0
60	MG	AA	2940	1/1	0.79	0.56	102,102,102,102	0
60	MG	BA	3076	1/1	0.79	0.16	91,91,91,91	0
60	MG	AA	3129	1/1	0.79	0.17	112,112,112,112	0
60	MG	BA	2944	1/1	0.79	0.10	86,86,86,86	0
60	MG	AA	2942	1/1	0.79	0.19	65,65,65,65	0
60	MG	AA	3093	1/1	0.79	0.25	73,73,73,73	0
60	MG	Ba	1634	1/1	0.79	0.22	83,83,83,83	0
60	MG	Aa	1741	1/1	0.79	0.41	88,88,88,88	0
60	MG	Aa	1704	1/1	0.80	0.36	86,86,86,86	0
60	MG	BA	3091	1/1	0.80	0.35	66,66,66,66	0
60	MG	Aa	1636	1/1	0.80	0.39	62,62,62,62	0
60	MG	AA	2929	1/1	0.80	0.26	68,68,68,68	0
60	MG	BA	3201	1/1	0.80	0.25	62,62,62,62	0
60	MG	Ba	1610	1/1	0.80	0.27	87,87,87,87	0
60	MG	Ba	1612	1/1	0.80	0.21	100,100,100,100	0
60	MG	Ba	1663	1/1	0.80	0.26	86,86,86,86	0
60	MG	AA	2982	1/1	0.80	0.39	83,83,83,83	0
60	MG	Ba	1668	1/1	0.80	0.33	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3226	1/1	0.80	0.27	91,91,91,91	0
60	MG	BA	3134	1/1	0.80	0.31	98,98,98,98	0
60	MG	BA	3219	1/1	0.80	0.35	88,88,88,88	0
60	MG	AA	2944	1/1	0.80	0.41	82,82,82,82	0
60	MG	AA	3232	1/1	0.80	0.29	70,70,70,70	0
60	MG	AA	2961	1/1	0.80	0.43	99,99,99,99	0
60	MG	Ba	1740	1/1	0.80	0.34	93,93,93,93	0
60	MG	Ba	1741	1/1	0.80	0.36	81,81,81,81	0
60	MG	AA	3135	1/1	0.80	0.45	89,89,89,89	0
60	MG	AA	3001	1/1	0.80	0.28	68,68,68,68	0
60	MG	BA	3253	1/1	0.80	0.24	72,72,72,72	0
60	MG	Bv	105	1/1	0.80	0.33	95,95,95,95	1
60	MG	AA	3052	1/1	0.80	0.37	98,98,98,98	0
60	MG	AA	3144	1/1	0.80	0.23	85,85,85,85	0
60	MG	Ba	1642	1/1	0.80	0.29	83,83,83,83	0
60	MG	Aa	1679	1/1	0.80	0.32	131,131,131,131	0
60	MG	Aa	1694	1/1	0.80	0.44	107,107,107,107	0
60	MG	BA	3086	1/1	0.80	0.29	65,65,65,65	0
60	MG	Ba	1601	1/1	0.80	0.24	77,77,77,77	0
60	MG	AA	3077	1/1	0.81	0.37	60,60,60,60	0
60	MG	Aa	1602	1/1	0.81	0.26	108,108,108,108	0
60	MG	Aa	1737	1/1	0.81	0.21	107,107,107,107	0
60	MG	AA	2923	1/1	0.81	0.31	75,75,75,75	0
60	MG	Ba	1653	1/1	0.81	0.15	91,91,91,91	0
60	MG	AA	3058	1/1	0.81	0.41	54,54,54,54	0
60	MG	BA	3065	1/1	0.81	0.39	66,66,66,66	0
60	MG	AA	3037	1/1	0.81	0.25	52,52,52,52	0
60	MG	AA	3230	1/1	0.81	0.42	94,94,94,94	0
60	MG	Aa	1642	1/1	0.81	0.37	102,102,102,102	0
60	MG	AA	3233	1/1	0.81	0.24	90,90,90,90	0
60	MG	Av	102	1/1	0.81	0.12	107,107,107,107	0
60	MG	AA	3140	1/1	0.81	0.26	107,107,107,107	0
60	MG	AA	2988	1/1	0.81	0.31	89,89,89,89	0
60	MG	BA	3155	1/1	0.81	0.11	77,77,77,77	1
60	MG	BA	2951	1/1	0.81	0.50	90,90,90,90	0
60	MG	AA	3116	1/1	0.81	0.26	39,39,39,39	1
60	MG	AB	201	1/1	0.81	0.22	69,69,69,69	0
60	MG	AA	3175	1/1	0.81	0.29	54,54,54,54	0
60	MG	Ba	1640	1/1	0.81	0.39	105,105,105,105	0
60	MG	Ba	1641	1/1	0.81	0.32	92,92,92,92	0
60	MG	BA	3106	1/1	0.81	0.21	58,58,58,58	0
60	MG	AA	3148	1/1	0.81	0.36	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3116	1/1	0.81	0.31	99,99,99,99	0
60	MG	BA	3031	1/1	0.81	0.26	46,46,46,46	0
60	MG	AA	3011	1/1	0.82	0.22	55,55,55,55	0
60	MG	BA	3202	1/1	0.82	0.15	65,65,65,65	0
60	MG	AA	2934	1/1	0.82	0.32	53,53,53,53	1
60	MG	AA	3265	1/1	0.82	0.42	83,83,83,83	0
60	MG	B0	101	1/1	0.82	0.41	104,104,104,104	0
60	MG	AA	3113	1/1	0.82	0.32	55,55,55,55	0
60	MG	Aa	1645	1/1	0.82	0.32	83,83,83,83	0
60	MG	Ba	1627	1/1	0.82	0.21	71,71,71,71	0
60	MG	Ba	1726	1/1	0.82	0.25	65,65,65,65	0
60	MG	BA	3211	1/1	0.82	0.28	81,81,81,81	0
60	MG	BA	3216	1/1	0.82	0.25	89,89,89,89	0
60	MG	Aa	1717	1/1	0.82	0.25	90,90,90,90	0
60	MG	BA	3146	1/1	0.82	0.21	112,112,112,112	0
60	MG	AA	3176	1/1	0.82	0.21	84,84,84,84	0
60	MG	Ba	1673	1/1	0.82	0.10	83,83,83,83	0
60	MG	AA	3179	1/1	0.82	0.31	76,76,76,76	0
60	MG	AA	3096	1/1	0.82	0.39	109,109,109,109	0
60	MG	BA	3238	1/1	0.82	0.19	89,89,89,89	0
60	MG	AA	3099	1/1	0.82	0.55	78,78,78,78	0
60	MG	AA	3035	1/1	0.82	0.26	74,74,74,74	0
60	MG	BA	3252	1/1	0.82	0.26	72,72,72,72	0
60	MG	AA	3188	1/1	0.82	0.22	91,91,91,91	0
60	MG	BA	2985	1/1	0.82	0.22	64,64,64,64	0
60	MG	AA	2909	1/1	0.82	0.27	46,46,46,46	0
60	MG	AA	3085	1/1	0.82	0.39	86,86,86,86	0
60	MG	AA	3004	1/1	0.82	0.13	84,84,84,84	0
60	MG	Aa	1698	1/1	0.82	0.33	86,86,86,86	0
60	MG	BA	3117	1/1	0.82	0.42	106,106,106,106	0
60	MG	Ba	1690	1/1	0.82	0.26	67,67,67,67	0
60	MG	BA	3047	1/1	0.82	0.24	57,57,57,57	0
60	MG	BA	2921	1/1	0.83	0.28	77,77,77,77	0
60	MG	BA	3168	1/1	0.83	0.18	87,87,87,87	0
60	MG	BA	3174	1/1	0.83	0.43	63,63,63,63	0
60	MG	BA	2923	1/1	0.83	0.21	60,60,60,60	0
60	MG	BA	2926	1/1	0.83	0.23	58,58,58,58	0
60	MG	BA	2931	1/1	0.83	0.34	52,52,52,52	0
60	MG	BA	2937	1/1	0.83	0.13	70,70,70,70	0
60	MG	BA	2938	1/1	0.83	0.77	104,104,104,104	0
60	MG	AA	3223	1/1	0.83	0.28	75,75,75,75	0
60	MG	BA	2943	1/1	0.83	0.26	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3089	1/1	0.83	0.23	74,74,74,74	0
60	MG	AA	3196	1/1	0.83	0.26	59,59,59,59	0
60	MG	AA	3200	1/1	0.83	0.29	82,82,82,82	0
60	MG	Aa	1643	1/1	0.83	0.17	117,117,117,117	0
60	MG	Ba	1667	1/1	0.83	0.20	91,91,91,91	0
60	MG	BA	2952	1/1	0.83	0.14	87,87,87,87	0
60	MG	AA	3173	1/1	0.83	0.13	72,72,72,72	0
60	MG	BA	2956	1/1	0.83	0.24	89,89,89,89	0
60	MG	Aa	1720	1/1	0.83	0.26	90,90,90,90	0
60	MG	BA	2962	1/1	0.83	0.23	71,71,71,71	0
60	MG	Ba	1631	1/1	0.83	0.31	101,101,101,101	0
60	MG	AA	3206	1/1	0.83	0.22	75,75,75,75	0
60	MG	BA	3127	1/1	0.83	0.33	38,38,38,38	0
60	MG	AA	3151	1/1	0.83	0.15	88,88,88,88	0
60	MG	AA	3079	1/1	0.83	0.19	95,95,95,95	0
60	MG	AA	3242	1/1	0.83	0.37	78,78,78,78	0
60	MG	BA	3023	1/1	0.83	0.34	54,54,54,54	0
60	MG	BA	3026	1/1	0.83	0.27	59,59,59,59	0
60	MG	BA	3236	1/1	0.83	0.12	64,64,64,64	0
60	MG	BA	3237	1/1	0.83	0.40	98,98,98,98	0
60	MG	AA	3064	1/1	0.83	0.19	59,59,59,59	0
60	MG	AA	3183	1/1	0.83	0.16	79,79,79,79	0
60	MG	AA	3065	1/1	0.83	0.33	82,82,82,82	0
60	MG	BA	3251	1/1	0.83	0.35	78,78,78,78	0
60	MG	BA	3044	1/1	0.83	0.24	52,52,52,52	0
60	MG	AA	3114	1/1	0.83	0.30	84,84,84,84	0
60	MG	BA	3148	1/1	0.83	0.16	82,82,82,82	0
60	MG	AA	3012	1/1	0.83	0.33	46,46,46,46	0
60	MG	Aa	1652	1/1	0.83	0.43	91,91,91,91	0
60	MG	BA	3152	1/1	0.83	0.39	92,92,92,92	0
60	MG	Ba	1719	1/1	0.83	0.35	85,85,85,85	0
60	MG	Ba	1611	1/1	0.83	0.17	81,81,81,81	0
60	MG	Aa	1693	1/1	0.83	0.39	65,65,65,65	0
60	MG	BA	3163	1/1	0.83	0.29	87,87,87,87	0
60	MG	Ba	1661	1/1	0.84	0.27	98,98,98,98	0
60	MG	Aa	1657	1/1	0.84	0.25	93,93,93,93	0
60	MG	BA	3222	1/1	0.84	0.27	109,109,109,109	0
60	MG	AA	3131	1/1	0.84	0.16	75,75,75,75	0
60	MG	Ba	1709	1/1	0.84	0.15	63,63,63,63	0
60	MG	Aa	1739	1/1	0.84	0.33	100,100,100,100	0
60	MG	BA	3179	1/1	0.84	0.32	90,90,90,90	0
60	MG	AA	3238	1/1	0.84	0.31	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	2959	1/1	0.84	0.20	62,62,62,62	0
60	MG	AF	301	1/1	0.84	0.18	87,87,87,87	0
60	MG	Ba	1622	1/1	0.84	0.26	88,88,88,88	0
60	MG	BA	2927	1/1	0.84	0.24	45,45,45,45	0
60	MG	BA	3243	1/1	0.84	0.39	75,75,75,75	0
60	MG	Ba	1623	1/1	0.84	0.11	75,75,75,75	0
60	MG	BA	2932	1/1	0.84	0.40	87,87,87,87	0
60	MG	BA	2934	1/1	0.84	0.42	65,65,65,65	1
60	MG	Ba	1716	1/1	0.84	0.44	102,102,102,102	0
60	MG	Aa	1604	1/1	0.84	0.09	82,82,82,82	0
60	MG	Aa	1605	1/1	0.84	0.14	70,70,70,70	0
60	MG	Aa	1724	1/1	0.84	0.09	100,100,100,100	0
60	MG	Aa	1707	1/1	0.84	0.39	79,79,79,79	0
60	MG	BA	3043	1/1	0.84	0.28	49,49,49,49	0
60	MG	BA	3108	1/1	0.84	0.17	71,71,71,71	0
60	MG	AA	3229	1/1	0.84	0.25	87,87,87,87	0
60	MG	Aa	1703	1/1	0.84	0.20	70,70,70,70	0
60	MG	Ba	1608	1/1	0.85	0.13	91,91,91,91	0
60	MG	AA	2963	1/1	0.85	0.33	65,65,65,65	0
60	MG	Ba	1644	1/1	0.85	0.33	109,109,109,109	0
60	MG	AA	3224	1/1	0.85	0.54	86,86,86,86	0
60	MG	AA	3084	1/1	0.85	0.23	84,84,84,84	0
60	MG	Aa	1700	1/1	0.85	0.19	84,84,84,84	1
60	MG	AA	3005	1/1	0.85	0.23	64,64,64,64	0
60	MG	AA	2986	1/1	0.85	0.21	86,86,86,86	0
60	MG	BA	3098	1/1	0.85	0.28	77,77,77,77	0
60	MG	AA	3088	1/1	0.85	0.19	64,64,64,64	0
60	MG	BA	3226	1/1	0.85	0.22	50,50,50,50	0
60	MG	AA	3039	1/1	0.85	0.23	50,50,50,50	0
60	MG	AA	3142	1/1	0.85	0.10	65,65,65,65	0
60	MG	BA	3164	1/1	0.85	0.31	78,78,78,78	0
60	MG	BA	3165	1/1	0.85	0.26	73,73,73,73	0
60	MG	Ba	1696	1/1	0.85	0.31	99,99,99,99	0
60	MG	BA	3111	1/1	0.85	0.41	99,99,99,99	0
60	MG	BA	3170	1/1	0.85	0.10	58,58,58,58	0
60	MG	AA	2987	1/1	0.85	0.29	41,41,41,41	0
60	MG	BA	3175	1/1	0.85	0.26	91,91,91,91	0
60	MG	Aa	1669	1/1	0.85	0.22	71,71,71,71	0
60	MG	AA	3147	1/1	0.85	0.36	66,66,66,66	0
60	MG	AA	3050	1/1	0.85	0.27	87,87,87,87	0
60	MG	Ba	1629	1/1	0.85	0.26	69,69,69,69	0
60	MG	Aa	1646	1/1	0.85	0.29	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3118	1/1	0.85	0.28	59,59,59,59	0
60	MG	BA	3256	1/1	0.85	0.27	84,84,84,84	0
60	MG	BA	3189	1/1	0.85	0.44	62,62,62,62	0
60	MG	Ba	1705	1/1	0.85	0.31	80,80,80,80	0
60	MG	AA	3094	1/1	0.85	0.25	65,65,65,65	0
60	MG	AA	2962	1/1	0.85	0.20	53,53,53,53	0
60	MG	Ba	1639	1/1	0.85	0.24	68,68,68,68	0
60	MG	AA	2976	1/1	0.85	0.25	85,85,85,85	0
60	MG	Ba	1679	1/1	0.85	0.28	67,67,67,67	0
60	MG	BA	3073	1/1	0.86	0.28	54,54,54,54	0
60	MG	BA	3144	1/1	0.86	0.26	59,59,59,59	0
60	MG	BA	2963	1/1	0.86	0.48	91,91,91,91	0
60	MG	Aa	1668	1/1	0.86	0.33	84,84,84,84	0
60	MG	Aa	1630	1/1	0.86	0.33	89,89,89,89	0
60	MG	BA	2972	1/1	0.86	0.29	79,79,79,79	0
60	MG	BA	2976	1/1	0.86	0.45	93,93,93,93	0
60	MG	AA	2952	1/1	0.86	0.25	81,81,81,81	0
60	MG	BA	2990	1/1	0.86	0.32	56,56,56,56	0
60	MG	BA	3221	1/1	0.86	0.27	66,66,66,66	0
60	MG	Aa	1738	1/1	0.86	0.22	78,78,78,78	0
60	MG	BA	3225	1/1	0.86	0.28	99,99,99,99	0
60	MG	BA	2999	1/1	0.86	0.23	41,41,41,41	0
60	MG	Aa	1670	1/1	0.86	0.25	70,70,70,70	0
60	MG	BA	3018	1/1	0.86	0.26	51,51,51,51	0
60	MG	Aa	1716	1/1	0.86	0.08	79,79,79,79	0
60	MG	AA	3105	1/1	0.86	0.57	92,92,92,92	0
60	MG	AA	3027	1/1	0.86	0.29	57,57,57,57	0
60	MG	BA	3033	1/1	0.86	0.22	42,42,42,42	0
60	MG	Ba	1670	1/1	0.86	0.19	132,132,132,132	0
60	MG	Ba	1643	1/1	0.86	0.26	95,95,95,95	0
60	MG	BA	3038	1/1	0.86	0.23	52,52,52,52	0
60	MG	BA	3178	1/1	0.86	0.30	71,71,71,71	0
60	MG	Aa	1655	1/1	0.86	0.35	88,88,88,88	0
59	ZN	B4	101	1/1	0.86	0.09	203,203,203,203	0
60	MG	AA	3031	1/1	0.86	0.20	56,56,56,56	0
60	MG	Ba	1701	1/1	0.86	0.26	71,71,71,71	0
60	MG	BA	3185	1/1	0.86	0.16	66,66,66,66	0
60	MG	Bq	201	1/1	0.86	0.29	116,116,116,116	0
60	MG	BA	3130	1/1	0.86	0.37	63,63,63,63	0
60	MG	AA	3033	1/1	0.86	0.32	68,68,68,68	0
60	MG	BA	3058	1/1	0.86	0.22	60,60,60,60	0
60	MG	Ba	1652	1/1	0.86	0.36	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3137	1/1	0.86	0.33	95,95,95,95	0
60	MG	AA	3186	1/1	0.86	0.13	74,74,74,74	0
60	MG	BA	2925	1/1	0.86	0.09	82,82,82,82	0
60	MG	AA	2908	1/1	0.87	0.15	53,53,53,53	0
60	MG	BA	3184	1/1	0.87	0.24	83,83,83,83	0
60	MG	BA	2981	1/1	0.87	0.29	45,45,45,45	0
60	MG	BA	3186	1/1	0.87	0.14	70,70,70,70	0
60	MG	Ba	1618	1/1	0.87	0.29	56,56,56,56	0
60	MG	AA	3067	1/1	0.87	0.16	66,66,66,66	0
60	MG	AA	2978	1/1	0.87	0.39	100,100,100,100	0
60	MG	B0	102	1/1	0.87	0.18	77,77,77,77	0
60	MG	Aa	1682	1/1	0.87	0.33	97,97,97,97	0
60	MG	Ba	1710	1/1	0.87	0.13	81,81,81,81	0
60	MG	BA	3022	1/1	0.87	0.19	33,33,33,33	0
60	MG	BA	2907	1/1	0.87	0.24	51,51,51,51	0
60	MG	BA	3125	1/1	0.87	0.19	68,68,68,68	0
60	MG	AA	2948	1/1	0.87	0.18	80,80,80,80	0
60	MG	AA	3213	1/1	0.87	0.36	98,98,98,98	0
60	MG	Aa	1661	1/1	0.87	0.21	91,91,91,91	0
60	MG	AA	3216	1/1	0.87	0.21	74,74,74,74	0
60	MG	AA	3178	1/1	0.87	0.42	86,86,86,86	0
60	MG	BA	3133	1/1	0.87	0.10	83,83,83,83	0
60	MG	Ba	1632	1/1	0.87	0.14	81,81,81,81	0
60	MG	BA	3039	1/1	0.87	0.15	44,44,44,44	0
60	MG	AA	3263	1/1	0.87	0.20	94,94,94,94	0
60	MG	Aa	1662	1/1	0.87	0.26	76,76,76,76	0
60	MG	BA	3224	1/1	0.87	0.19	89,89,89,89	0
60	MG	AA	3220	1/1	0.87	0.24	47,47,47,47	0
60	MG	AA	2955	1/1	0.87	0.19	60,60,60,60	0
60	MG	AA	3143	1/1	0.87	0.39	72,72,72,72	0
60	MG	AA	3225	1/1	0.87	0.14	71,71,71,71	0
60	MG	Ba	1689	1/1	0.87	0.35	82,82,82,82	0
60	MG	Aa	1696	1/1	0.87	0.17	93,93,93,93	0
60	MG	Aa	1639	1/1	0.87	0.30	83,83,83,83	0
60	MG	Aa	1710	1/1	0.87	0.07	128,128,128,128	0
60	MG	BA	2948	1/1	0.87	0.48	93,93,93,93	0
60	MG	AA	3047	1/1	0.87	0.26	62,62,62,62	0
60	MG	Aa	1711	1/1	0.87	0.19	61,61,61,61	0
60	MG	Aa	1635	1/1	0.87	0.13	61,61,61,61	0
60	MG	BA	3077	1/1	0.87	0.18	69,69,69,69	0
60	MG	BA	3246	1/1	0.87	0.33	107,107,107,107	0
60	MG	BA	3247	1/1	0.87	0.23	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3080	1/1	0.87	0.21	79,79,79,79	0
60	MG	Aa	1609	1/1	0.87	0.09	82,82,82,82	0
60	MG	AA	2901	1/1	0.87	0.10	77,77,77,77	0
60	MG	AA	3156	1/1	0.87	0.27	83,83,83,83	0
60	MG	Aa	1740	1/1	0.87	0.26	65,65,65,65	0
60	MG	Aa	1607	1/1	0.87	0.27	95,95,95,95	0
60	MG	AA	2971	1/1	0.87	0.08	77,77,77,77	0
60	MG	BA	3090	1/1	0.87	0.16	47,47,47,47	0
60	MG	AA	3130	1/1	0.87	0.31	42,42,42,42	0
60	MG	BA	3092	1/1	0.87	0.21	83,83,83,83	0
60	MG	BA	3097	1/1	0.87	0.15	65,65,65,65	0
60	MG	AA	2945	1/1	0.87	0.11	73,73,73,73	0
60	MG	Ba	1649	1/1	0.88	0.17	52,52,52,52	0
60	MG	BA	2978	1/1	0.88	0.26	72,72,72,72	0
60	MG	Aa	1619	1/1	0.88	0.31	62,62,62,62	0
60	MG	AA	3198	1/1	0.88	0.24	73,73,73,73	0
60	MG	BD	301	1/1	0.88	0.25	39,39,39,39	0
60	MG	AA	2926	1/1	0.88	0.29	62,62,62,62	0
60	MG	AA	3125	1/1	0.88	0.23	49,49,49,49	0
60	MG	BA	3004	1/1	0.88	0.26	45,45,45,45	0
60	MG	BA	3007	1/1	0.88	0.19	56,56,56,56	0
60	MG	Aa	1632	1/1	0.88	0.40	86,86,86,86	0
60	MG	BA	3112	1/1	0.88	0.07	81,81,81,81	0
60	MG	BA	3014	1/1	0.88	0.20	38,38,38,38	0
60	MG	AA	2907	1/1	0.88	0.20	58,58,58,58	0
60	MG	BA	3019	1/1	0.88	0.25	72,72,72,72	0
60	MG	Ba	1615	1/1	0.88	0.31	86,86,86,86	0
60	MG	AA	2964	1/1	0.88	0.31	76,76,76,76	0
60	MG	AA	3245	1/1	0.88	0.39	71,71,71,71	0
60	MG	BA	3027	1/1	0.88	0.23	53,53,53,53	0
60	MG	AA	3095	1/1	0.88	0.24	67,67,67,67	0
60	MG	Ba	1620	1/1	0.88	0.15	102,102,102,102	0
60	MG	AA	3070	1/1	0.88	0.20	47,47,47,47	0
60	MG	AA	3073	1/1	0.88	0.36	84,84,84,84	0
60	MG	AA	2991	1/1	0.88	0.23	62,62,62,62	0
60	MG	AA	3171	1/1	0.88	0.23	68,68,68,68	0
60	MG	Aa	1644	1/1	0.88	0.37	100,100,100,100	0
60	MG	A7	101	1/1	0.88	0.20	73,73,73,73	0
60	MG	Ba	1628	1/1	0.88	0.23	79,79,79,79	0
60	MG	AA	3139	1/1	0.88	0.18	90,90,90,90	0
60	MG	AA	3177	1/1	0.88	0.32	54,54,54,54	0
60	MG	BA	3230	1/1	0.88	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Ba	1683	1/1	0.88	0.11	93,93,93,93	0
60	MG	AA	3217	1/1	0.88	0.40	70,70,70,70	0
60	MG	BA	3061	1/1	0.88	0.15	64,64,64,64	0
60	MG	Ba	1685	1/1	0.88	0.21	42,42,42,42	1
60	MG	AA	2935	1/1	0.88	0.39	90,90,90,90	0
60	MG	AA	3141	1/1	0.88	0.11	54,54,54,54	0
60	MG	BA	3151	1/1	0.88	0.34	105,105,105,105	0
60	MG	AA	2938	1/1	0.88	0.51	95,95,95,95	0
60	MG	BA	3242	1/1	0.88	0.39	73,73,73,73	0
60	MG	AA	3003	1/1	0.88	0.23	43,43,43,43	0
60	MG	AA	3184	1/1	0.88	0.35	69,69,69,69	0
60	MG	BA	3075	1/1	0.88	0.20	56,56,56,56	0
60	MG	AA	2972	1/1	0.88	0.28	75,75,75,75	0
60	MG	AA	2974	1/1	0.88	0.51	85,85,85,85	0
60	MG	BA	3079	1/1	0.88	0.21	79,79,79,79	0
60	MG	AA	2911	1/1	0.88	0.35	39,39,39,39	0
60	MG	AA	3228	1/1	0.88	0.13	57,57,57,57	0
60	MG	AA	2917	1/1	0.88	0.32	99,99,99,99	0
60	MG	BA	3173	1/1	0.88	0.33	91,91,91,91	0
60	MG	AA	2977	1/1	0.88	0.31	69,69,69,69	0
60	MG	Aa	1613	1/1	0.88	0.13	85,85,85,85	0
60	MG	BA	3176	1/1	0.88	0.24	66,66,66,66	0
60	MG	AA	3016	1/1	0.88	0.69	82,82,82,82	0
60	MG	BA	3263	1/1	0.88	0.27	66,66,66,66	0
60	MG	BA	2975	1/1	0.88	0.30	93,93,93,93	0
60	MG	BA	3089	1/1	0.88	0.18	61,61,61,61	0
60	MG	AA	3256	1/1	0.89	0.33	74,74,74,74	0
60	MG	BA	3197	1/1	0.89	0.18	58,58,58,58	0
60	MG	BA	3128	1/1	0.89	0.15	40,40,40,40	0
60	MG	AA	3145	1/1	0.89	0.28	68,68,68,68	0
60	MG	Aa	1660	1/1	0.89	0.34	88,88,88,88	0
60	MG	AA	2958	1/1	0.89	0.25	77,77,77,77	0
60	MG	BA	3132	1/1	0.89	0.38	73,73,73,73	0
60	MG	Ba	1742	1/1	0.89	0.20	105,105,105,105	0
60	MG	BA	3066	1/1	0.89	0.17	28,28,28,28	0
60	MG	BA	3070	1/1	0.89	0.31	96,96,96,96	0
60	MG	AA	2979	1/1	0.89	0.29	71,71,71,71	0
60	MG	AA	2904	1/1	0.89	0.10	142,142,142,142	0
60	MG	AA	3063	1/1	0.89	0.28	47,47,47,47	0
60	MG	Aa	1603	1/1	0.89	0.22	112,112,112,112	1
60	MG	Aa	1732	1/1	0.89	0.27	58,58,58,58	0
60	MG	AA	3155	1/1	0.89	0.35	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3126	1/1	0.89	0.40	49,49,49,49	0
60	MG	Aa	1701	1/1	0.89	0.30	96,96,96,96	0
60	MG	BA	2986	1/1	0.89	0.27	42,42,42,42	0
60	MG	Ba	1633	1/1	0.89	0.27	71,71,71,71	0
60	MG	AA	3231	1/1	0.89	0.29	107,107,107,107	0
60	MG	A7	102	1/1	0.89	0.24	98,98,98,98	0
60	MG	Bm	201	1/1	0.89	0.25	103,103,103,103	0
60	MG	BA	3232	1/1	0.89	0.10	82,82,82,82	0
60	MG	AA	2966	1/1	0.89	0.28	74,74,74,74	0
60	MG	Aa	1685	1/1	0.89	0.13	85,85,85,85	0
60	MG	AA	3133	1/1	0.89	0.43	78,78,78,78	0
60	MG	AA	3097	1/1	0.89	0.35	69,69,69,69	0
60	MG	AA	2950	1/1	0.89	0.18	59,59,59,59	0
60	MG	BA	3166	1/1	0.89	0.22	54,54,54,54	0
60	MG	AA	2951	1/1	0.89	0.11	61,61,61,61	0
60	MG	BA	3093	1/1	0.89	0.27	71,71,71,71	0
60	MG	BA	2933	1/1	0.89	0.39	84,84,84,84	0
60	MG	BA	3025	1/1	0.89	0.16	69,69,69,69	0
60	MG	AA	2937	1/1	0.89	0.14	63,63,63,63	0
60	MG	AA	2953	1/1	0.89	0.10	81,81,81,81	0
60	MG	AA	2973	1/1	0.89	0.20	82,82,82,82	0
60	MG	BA	3107	1/1	0.89	0.18	58,58,58,58	0
60	MG	Ba	1691	1/1	0.89	0.27	61,61,61,61	0
60	MG	AA	2919	1/1	0.89	0.19	49,49,49,49	0
60	MG	Ba	1729	1/1	0.89	0.35	84,84,84,84	0
60	MG	AA	2920	1/1	0.89	0.26	45,45,45,45	0
60	MG	Ba	1731	1/1	0.89	0.26	103,103,103,103	0
60	MG	Ba	1650	1/1	0.89	0.44	82,82,82,82	0
60	MG	AA	3082	1/1	0.89	0.29	69,69,69,69	0
60	MG	AA	3051	1/1	0.89	0.25	66,66,66,66	0
60	MG	BA	3121	1/1	0.89	0.42	82,82,82,82	0
60	MG	Ba	1654	1/1	0.89	0.33	97,97,97,97	0
60	MG	Aa	1708	1/1	0.89	0.26	89,89,89,89	0
60	MG	BB	203	1/1	0.89	0.38	79,79,79,79	0
60	MG	BA	3035	1/1	0.90	0.18	43,43,43,43	0
60	MG	AA	3041	1/1	0.90	0.27	49,49,49,49	0
60	MG	AA	3098	1/1	0.90	0.27	47,47,47,47	0
60	MG	AA	2941	1/1	0.90	0.24	68,68,68,68	0
60	MG	BA	3123	1/1	0.90	0.32	37,37,37,37	0
60	MG	AA	3205	1/1	0.90	0.17	58,58,58,58	0
60	MG	BA	3199	1/1	0.90	0.24	89,89,89,89	1
60	MG	Aa	1691	1/1	0.90	0.33	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	2949	1/1	0.90	0.10	63,63,63,63	0
60	MG	BA	2950	1/1	0.90	0.16	69,69,69,69	0
60	MG	AA	3017	1/1	0.90	0.23	59,59,59,59	0
60	MG	AA	3022	1/1	0.90	0.17	43,43,43,43	0
60	MG	BA	3056	1/1	0.90	0.22	53,53,53,53	0
60	MG	AA	3024	1/1	0.90	0.21	51,51,51,51	0
60	MG	BA	3060	1/1	0.90	0.17	51,51,51,51	0
60	MG	AA	2996	1/1	0.90	0.40	62,62,62,62	0
60	MG	AA	3174	1/1	0.90	0.17	50,50,50,50	0
60	MG	Ba	1656	1/1	0.90	0.34	80,80,80,80	0
60	MG	AA	3055	1/1	0.90	0.23	59,59,59,59	0
60	MG	BA	3139	1/1	0.90	0.19	67,67,67,67	0
60	MG	Bx	101	1/1	0.90	0.12	92,92,92,92	0
60	MG	BA	2964	1/1	0.90	0.32	84,84,84,84	0
60	MG	AA	3083	1/1	0.90	0.28	74,74,74,74	0
60	MG	Ba	1619	1/1	0.90	0.18	70,70,70,70	0
60	MG	AA	3056	1/1	0.90	0.16	48,48,48,48	0
60	MG	Aa	1709	1/1	0.90	0.12	92,92,92,92	0
60	MG	AA	2916	1/1	0.90	0.16	35,35,35,35	0
60	MG	AA	3180	1/1	0.90	0.17	58,58,58,58	0
60	MG	Ba	1624	1/1	0.90	0.10	73,73,73,73	0
60	MG	BA	2983	1/1	0.90	0.27	37,37,37,37	0
60	MG	AA	3059	1/1	0.90	0.29	90,90,90,90	0
60	MG	AA	3061	1/1	0.90	0.55	89,89,89,89	0
60	MG	BA	3158	1/1	0.90	0.29	61,61,61,61	0
60	MG	Aa	1659	1/1	0.90	0.14	70,70,70,70	0
60	MG	Aa	1653	1/1	0.90	0.32	71,71,71,71	0
60	MG	BA	2908	1/1	0.90	0.22	49,49,49,49	0
60	MG	BA	3240	1/1	0.90	0.17	73,73,73,73	0
60	MG	Aa	1731	1/1	0.90	0.46	82,82,82,82	0
60	MG	BA	3005	1/1	0.90	0.22	57,57,57,57	0
60	MG	BA	3244	1/1	0.90	0.20	89,89,89,89	0
60	MG	Aa	1621	1/1	0.90	0.14	91,91,91,91	0
60	MG	BA	2924	1/1	0.90	0.19	43,43,43,43	0
60	MG	A1	101	1/1	0.90	0.26	70,70,70,70	0
60	MG	BA	3250	1/1	0.90	0.55	97,97,97,97	0
60	MG	BA	3172	1/1	0.90	0.16	45,45,45,45	0
60	MG	BA	3015	1/1	0.90	0.25	39,39,39,39	0
60	MG	AA	3127	1/1	0.90	0.21	44,44,44,44	0
60	MG	AA	3154	1/1	0.90	0.10	86,86,86,86	0
60	MG	AA	3128	1/1	0.90	0.24	71,71,71,71	0
60	MG	AB	203	1/1	0.90	0.45	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3195	1/1	0.90	0.17	41,41,41,41	0
60	MG	A5	101	1/1	0.90	0.28	62,62,62,62	0
60	MG	AA	2990	1/1	0.90	0.28	51,51,51,51	0
60	MG	BA	3181	1/1	0.90	0.27	51,51,51,51	0
60	MG	BA	3029	1/1	0.90	0.23	49,49,49,49	0
60	MG	AA	3013	1/1	0.90	0.33	49,49,49,49	0
60	MG	Ba	1602	1/1	0.90	0.09	73,73,73,73	0
60	MG	Ba	1604	1/1	0.90	0.10	78,78,78,78	0
60	MG	AA	3161	1/1	0.91	0.32	75,75,75,75	0
60	MG	AA	3028	1/1	0.91	0.18	53,53,53,53	0
60	MG	AA	3044	1/1	0.91	0.23	46,46,46,46	0
60	MG	AA	2965	1/1	0.91	0.24	80,80,80,80	0
60	MG	BA	3068	1/1	0.91	0.13	91,91,91,91	0
60	MG	AA	3124	1/1	0.91	0.27	63,63,63,63	0
60	MG	BA	2935	1/1	0.91	0.70	124,124,124,124	0
60	MG	BA	3001	1/1	0.91	0.21	45,45,45,45	0
60	MG	BA	3003	1/1	0.91	0.16	73,73,73,73	0
60	MG	AA	3189	1/1	0.91	0.32	73,73,73,73	0
60	MG	AA	3010	1/1	0.91	0.16	94,94,94,94	0
60	MG	AA	2989	1/1	0.91	0.09	50,50,50,50	0
60	MG	Ba	1743	1/1	0.91	0.49	90,90,90,90	0
60	MG	BA	3214	1/1	0.91	0.12	52,52,52,52	0
60	MG	BA	3013	1/1	0.91	0.19	41,41,41,41	0
60	MG	AA	3032	1/1	0.91	0.15	64,64,64,64	0
60	MG	Bv	101	1/1	0.91	0.35	71,71,71,71	1
60	MG	BA	3016	1/1	0.91	0.14	50,50,50,50	0
60	MG	BA	3223	1/1	0.91	0.35	74,74,74,74	0
60	MG	BA	3083	1/1	0.91	0.39	73,73,73,73	0
60	MG	AA	3246	1/1	0.91	0.23	103,103,103,103	0
60	MG	AA	3068	1/1	0.91	0.25	50,50,50,50	0
60	MG	BA	3021	1/1	0.91	0.29	45,45,45,45	0
60	MG	AA	3018	1/1	0.91	0.18	46,46,46,46	0
60	MG	AA	3221	1/1	0.91	0.09	59,59,59,59	0
60	MG	BA	3160	1/1	0.91	0.16	73,73,73,73	0
60	MG	AA	3252	1/1	0.91	0.48	85,85,85,85	0
60	MG	AA	3106	1/1	0.91	0.33	75,75,75,75	0
60	MG	AA	3199	1/1	0.91	0.30	44,44,44,44	0
60	MG	BA	3028	1/1	0.91	0.17	44,44,44,44	0
60	MG	BA	3094	1/1	0.91	0.34	39,39,39,39	0
60	MG	AA	3020	1/1	0.91	0.23	63,63,63,63	0
60	MG	BA	2954	1/1	0.91	0.17	37,37,37,37	0
60	MG	B7	101	1/1	0.91	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	B7	102	1/1	0.91	0.18	80,80,80,80	0
60	MG	BA	3105	1/1	0.91	0.15	55,55,55,55	0
59	ZN	A4	101	1/1	0.91	0.06	195,195,195,195	0
60	MG	AA	3074	1/1	0.91	0.32	87,87,87,87	0
60	MG	BA	2903	1/1	0.91	0.33	91,91,91,91	0
60	MG	BA	3109	1/1	0.91	0.36	83,83,83,83	0
60	MG	Ba	1669	1/1	0.91	0.21	55,55,55,55	0
60	MG	BA	3042	1/1	0.91	0.42	48,48,48,48	0
60	MG	AA	3023	1/1	0.91	0.18	96,96,96,96	0
60	MG	BA	2967	1/1	0.91	0.14	58,58,58,58	0
60	MG	BA	2968	1/1	0.91	0.09	63,63,63,63	0
60	MG	BA	2911	1/1	0.91	0.29	36,36,36,36	0
60	MG	BA	3257	1/1	0.91	0.29	63,63,63,63	0
60	MG	AA	2933	1/1	0.91	0.29	84,84,84,84	0
60	MG	BA	3051	1/1	0.91	0.17	38,38,38,38	0
60	MG	AA	3026	1/1	0.91	0.26	43,43,43,43	0
60	MG	Ba	1674	1/1	0.91	0.07	57,57,57,57	0
60	MG	AA	3014	1/1	0.91	0.23	51,51,51,51	0
60	MG	BA	3059	1/1	0.91	0.30	52,52,52,52	0
60	MG	AA	3060	1/1	0.91	0.31	55,55,55,55	0
60	MG	BA	3192	1/1	0.91	0.15	43,43,43,43	0
60	MG	BB	201	1/1	0.91	0.12	50,50,50,50	0
60	MG	BA	3195	1/1	0.91	0.17	57,57,57,57	0
60	MG	AA	2960	1/1	0.92	0.31	37,37,37,37	0
60	MG	Aa	1675	1/1	0.92	0.11	58,58,58,58	0
60	MG	AA	3153	1/1	0.92	0.27	92,92,92,92	0
60	MG	Aa	1638	1/1	0.92	0.31	84,84,84,84	0
60	MG	BA	3122	1/1	0.92	0.20	51,51,51,51	0
60	MG	BA	2966	1/1	0.92	0.24	39,39,39,39	0
60	MG	AA	3025	1/1	0.92	0.28	39,39,39,39	0
60	MG	AA	3234	1/1	0.92	0.14	59,59,59,59	0
60	MG	AA	2912	1/1	0.92	0.12	56,56,56,56	0
60	MG	Aa	1684	1/1	0.92	0.23	71,71,71,71	0
60	MG	BA	3032	1/1	0.92	0.36	88,88,88,88	0
60	MG	AA	3159	1/1	0.92	0.08	75,75,75,75	0
60	MG	AA	3117	1/1	0.92	0.18	43,43,43,43	0
60	MG	AA	2993	1/1	0.92	0.23	57,57,57,57	0
60	MG	AA	2994	1/1	0.92	0.27	69,69,69,69	0
60	MG	AA	3121	1/1	0.92	0.29	83,83,83,83	0
60	MG	Av	101	1/1	0.92	0.22	65,65,65,65	1
60	MG	AA	3192	1/1	0.92	0.25	59,59,59,59	0
60	MG	BA	3137	1/1	0.92	0.13	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3100	1/1	0.92	0.12	64,64,64,64	0
60	MG	BA	2997	1/1	0.92	0.20	49,49,49,49	0
60	MG	BA	3046	1/1	0.92	0.38	76,76,76,76	0
60	MG	Aa	1650	1/1	0.92	0.21	53,53,53,53	0
60	MG	BQ	201	1/1	0.92	0.30	79,79,79,79	0
60	MG	AA	2905	1/1	0.92	0.25	45,45,45,45	0
60	MG	BA	3198	1/1	0.92	0.09	70,70,70,70	0
60	MG	BA	3096	1/1	0.92	0.06	49,49,49,49	0
60	MG	Ba	1659	1/1	0.92	0.28	77,77,77,77	0
60	MG	BA	3052	1/1	0.92	0.15	30,30,30,30	0
60	MG	AA	3170	1/1	0.92	0.14	82,82,82,82	0
60	MG	AA	2936	1/1	0.92	0.32	33,33,33,33	0
60	MG	AA	3054	1/1	0.92	0.17	43,43,43,43	0
60	MG	AA	3072	1/1	0.92	0.20	79,79,79,79	0
60	MG	Ba	1665	1/1	0.92	0.46	80,80,80,80	0
60	MG	Av	103	1/1	0.92	0.36	69,69,69,69	1
60	MG	BA	2955	1/1	0.92	0.13	67,67,67,67	0
60	MG	Ba	1637	1/1	0.92	0.27	103,103,103,103	0
60	MG	Ba	1638	1/1	0.92	0.26	79,79,79,79	0
60	MG	Aa	1702	1/1	0.92	0.29	65,65,65,65	0
60	MG	BA	3266	1/1	0.92	0.16	80,80,80,80	0
60	MG	BA	3114	1/1	0.92	0.25	36,36,36,36	0
60	MG	BA	3069	1/1	0.92	0.13	72,72,72,72	0
60	MG	AA	3201	1/1	0.93	0.12	70,70,70,70	0
60	MG	BA	2929	1/1	0.93	0.10	43,43,43,43	0
60	MG	BA	2984	1/1	0.93	0.23	69,69,69,69	0
60	MG	BA	3054	1/1	0.93	0.27	37,37,37,37	0
60	MG	BA	2930	1/1	0.93	0.05	34,34,34,34	0
60	MG	BA	3057	1/1	0.93	0.30	58,58,58,58	0
60	MG	AA	3163	1/1	0.93	0.40	89,89,89,89	0
60	MG	BA	3124	1/1	0.93	0.13	45,45,45,45	0
60	MG	Ba	1675	1/1	0.93	0.07	69,69,69,69	0
60	MG	BA	2995	1/1	0.93	0.23	45,45,45,45	0
60	MG	Aa	1729	1/1	0.93	0.34	60,60,60,60	0
60	MG	BA	3062	1/1	0.93	0.14	45,45,45,45	0
60	MG	Aa	1608	1/1	0.93	0.18	48,48,48,48	0
60	MG	AA	2930	1/1	0.93	0.10	38,38,38,38	0
60	MG	AA	3066	1/1	0.93	0.14	55,55,55,55	0
60	MG	Ba	1651	1/1	0.93	0.28	51,51,51,51	0
60	MG	BA	2940	1/1	0.93	0.18	76,76,76,76	0
60	MG	BA	2941	1/1	0.93	0.29	98,98,98,98	0
60	MG	Ba	1681	1/1	0.93	0.06	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3008	1/1	0.93	0.22	34,34,34,34	0
60	MG	BA	3213	1/1	0.93	0.41	81,81,81,81	0
60	MG	BA	3010	1/1	0.93	0.17	28,28,28,28	0
60	MG	Bv	102	1/1	0.93	0.11	54,54,54,54	0
60	MG	BA	3218	1/1	0.93	0.18	38,38,38,38	0
60	MG	AA	3251	1/1	0.93	0.33	68,68,68,68	0
60	MG	BA	3220	1/1	0.93	0.28	59,59,59,59	0
60	MG	BA	3140	1/1	0.93	0.39	60,60,60,60	0
60	MG	AA	2921	1/1	0.93	0.22	59,59,59,59	0
60	MG	BA	3142	1/1	0.93	0.24	61,61,61,61	0
60	MG	AA	3009	1/1	0.93	0.12	61,61,61,61	0
60	MG	AA	2932	1/1	0.93	0.25	79,79,79,79	0
60	MG	BA	3145	1/1	0.93	0.31	62,62,62,62	0
60	MG	AA	3190	1/1	0.93	0.27	52,52,52,52	0
60	MG	BD	302	1/1	0.93	0.17	53,53,53,53	0
60	MG	BA	3020	1/1	0.93	0.19	47,47,47,47	0
60	MG	Ba	1607	1/1	0.93	0.08	67,67,67,67	0
60	MG	Aa	1726	1/1	0.93	0.20	57,57,57,57	0
60	MG	BA	3085	1/1	0.93	0.10	72,72,72,72	0
60	MG	AA	3120	1/1	0.93	0.31	90,90,90,90	0
60	MG	Aa	1625	1/1	0.93	0.21	61,61,61,61	0
60	MG	AA	3235	1/1	0.93	0.20	102,102,102,102	0
60	MG	BA	3156	1/1	0.93	0.09	64,64,64,64	0
60	MG	Ba	1662	1/1	0.93	0.15	68,68,68,68	0
60	MG	AA	3236	1/1	0.93	0.36	90,90,90,90	0
60	MG	BA	3241	1/1	0.93	0.24	106,106,106,106	0
60	MG	AA	2984	1/1	0.93	0.35	79,79,79,79	0
60	MG	Ba	1614	1/1	0.93	0.37	60,60,60,60	0
60	MG	BA	2904	1/1	0.93	0.06	138,138,138,138	0
60	MG	Ba	1666	1/1	0.93	0.27	84,84,84,84	0
60	MG	BA	3095	1/1	0.93	0.23	61,61,61,61	0
60	MG	AA	2985	1/1	0.93	0.24	44,44,44,44	0
60	MG	BA	3249	1/1	0.93	0.27	55,55,55,55	0
60	MG	AA	3043	1/1	0.93	0.14	63,63,63,63	0
60	MG	BA	2914	1/1	0.93	0.20	32,32,32,32	0
60	MG	BA	3171	1/1	0.93	0.11	38,38,38,38	0
60	MG	BA	2917	1/1	0.93	0.19	75,75,75,75	0
60	MG	BA	3100	1/1	0.93	0.06	63,63,63,63	0
60	MG	BA	3101	1/1	0.93	0.45	64,64,64,64	0
60	MG	BA	2919	1/1	0.93	0.12	40,40,40,40	0
60	MG	BA	3104	1/1	0.93	0.08	36,36,36,36	0
60	MG	BA	3040	1/1	0.93	0.23	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3041	1/1	0.93	0.13	42,42,42,42	0
60	MG	Aa	1615	1/1	0.93	0.32	58,58,58,58	0
60	MG	AA	3045	1/1	0.93	0.12	55,55,55,55	0
60	MG	BA	2973	1/1	0.93	0.35	61,61,61,61	0
60	MG	BA	2974	1/1	0.93	0.34	118,118,118,118	0
60	MG	Ba	1671	1/1	0.93	0.13	75,75,75,75	0
60	MG	Ba	1735	1/1	0.93	0.11	79,79,79,79	0
60	MG	AA	2927	1/1	0.93	0.21	50,50,50,50	0
60	MG	BB	202	1/1	0.93	0.22	55,55,55,55	0
60	MG	BA	3115	1/1	0.93	0.28	50,50,50,50	0
60	MG	AA	3021	1/1	0.94	0.16	42,42,42,42	0
60	MG	BA	2939	1/1	0.94	0.14	44,44,44,44	0
60	MG	Aa	1627	1/1	0.94	0.11	84,84,84,84	0
60	MG	AA	2913	1/1	0.94	0.26	44,44,44,44	0
60	MG	AA	3008	1/1	0.94	0.15	44,44,44,44	0
60	MG	BA	3187	1/1	0.94	0.37	68,68,68,68	0
60	MG	AA	2914	1/1	0.94	0.15	37,37,37,37	0
60	MG	BA	2905	1/1	0.94	0.20	31,31,31,31	0
60	MG	AA	2915	1/1	0.94	0.22	50,50,50,50	0
60	MG	Aa	1718	1/1	0.94	0.33	78,78,78,78	0
60	MG	BA	2909	1/1	0.94	0.19	36,36,36,36	0
60	MG	AA	3046	1/1	0.94	0.57	59,59,59,59	0
60	MG	BA	2913	1/1	0.94	0.31	47,47,47,47	0
60	MG	Aa	1712	1/1	0.94	0.26	86,86,86,86	0
60	MG	BA	3037	1/1	0.94	0.18	41,41,41,41	0
60	MG	AA	3107	1/1	0.94	0.07	58,58,58,58	0
60	MG	BA	3157	1/1	0.94	0.20	78,78,78,78	0
60	MG	Aa	1649	1/1	0.94	0.13	88,88,88,88	0
60	MG	AA	3049	1/1	0.94	0.24	64,64,64,64	0
60	MG	BA	3000	1/1	0.94	0.12	61,61,61,61	0
60	MG	AA	3244	1/1	0.94	0.78	98,98,98,98	0
60	MG	AA	2998	1/1	0.94	0.37	51,51,51,51	0
60	MG	AA	3222	1/1	0.94	0.27	67,67,67,67	0
60	MG	BA	2957	1/1	0.94	0.32	38,38,38,38	0
60	MG	BA	3006	1/1	0.94	0.44	107,107,107,107	0
60	MG	Aa	1628	1/1	0.94	0.16	72,72,72,72	0
60	MG	Aa	1634	1/1	0.94	0.22	56,56,56,56	0
60	MG	BA	2960	1/1	0.94	0.19	45,45,45,45	0
60	MG	AA	2922	1/1	0.94	0.09	52,52,52,52	0
60	MG	BA	3217	1/1	0.94	0.24	76,76,76,76	0
60	MG	BA	3012	1/1	0.94	0.66	69,69,69,69	0
60	MG	AA	3034	1/1	0.94	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BF	301	1/1	0.94	0.05	87,87,87,87	0
60	MG	Aa	1612	1/1	0.94	0.19	58,58,58,58	0
60	MG	AA	3181	1/1	0.94	0.14	65,65,65,65	0
60	MG	AA	3019	1/1	0.94	0.21	48,48,48,48	0
60	MG	AA	3160	1/1	0.94	0.19	65,65,65,65	0
60	MG	AA	2924	1/1	0.94	0.14	54,54,54,54	0
60	MG	BA	2971	1/1	0.94	0.41	63,63,63,63	0
60	MG	BA	3203	1/1	0.95	0.20	67,67,67,67	0
60	MG	BA	3103	1/1	0.95	0.25	63,63,63,63	0
60	MG	Ba	1727	1/1	0.95	0.31	44,44,44,44	0
60	MG	AA	3214	1/1	0.95	0.26	57,57,57,57	0
60	MG	BA	3064	1/1	0.95	0.21	44,44,44,44	0
60	MG	BA	2906	1/1	0.95	0.19	35,35,35,35	0
60	MG	BA	3153	1/1	0.95	0.35	73,73,73,73	0
60	MG	AA	3123	1/1	0.95	0.41	54,54,54,54	0
60	MG	BA	3067	1/1	0.95	0.32	78,78,78,78	0
60	MG	BA	3212	1/1	0.95	0.08	36,36,36,36	0
60	MG	BA	3110	1/1	0.95	0.20	46,46,46,46	0
60	MG	BA	2980	1/1	0.95	0.31	80,80,80,80	0
60	MG	AA	3172	1/1	0.95	0.21	58,58,58,58	0
60	MG	BA	3159	1/1	0.95	0.11	110,110,110,110	0
60	MG	AA	2969	1/1	0.95	0.15	36,36,36,36	0
60	MG	BA	3161	1/1	0.95	0.16	51,51,51,51	0
60	MG	BA	2910	1/1	0.95	0.30	70,70,70,70	0
60	MG	BA	3254	1/1	0.95	0.26	56,56,56,56	0
60	MG	AA	3250	1/1	0.95	0.19	65,65,65,65	0
60	MG	AD	302	1/1	0.95	0.33	64,64,64,64	0
60	MG	B5	101	1/1	0.95	0.21	43,43,43,43	0
60	MG	BA	2991	1/1	0.95	0.22	48,48,48,48	0
60	MG	BA	3193	1/1	0.95	0.13	44,44,44,44	0
60	MG	AD	301	1/1	0.95	0.19	38,38,38,38	0
60	MG	BA	3227	1/1	0.95	0.15	73,73,73,73	0
60	MG	BA	3228	1/1	0.95	0.34	82,82,82,82	0
60	MG	BA	3196	1/1	0.95	0.27	45,45,45,45	0
60	MG	Ba	1722	1/1	0.95	0.07	106,106,106,106	0
60	MG	BA	3169	1/1	0.95	0.29	58,58,58,58	0
60	MG	BA	3017	1/1	0.95	0.16	40,40,40,40	0
60	MG	AA	3253	1/1	0.95	0.26	87,87,87,87	0
60	MG	AA	3110	1/1	0.95	0.08	59,59,59,59	0
60	MG	AA	3158	1/1	0.95	0.08	104,104,104,104	1
60	MG	BA	2961	1/1	0.96	0.16	60,60,60,60	0
60	MG	BA	3050	1/1	0.96	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3104	1/1	0.96	0.06	64,64,64,64	0
60	MG	Ba	1603	1/1	0.96	0.11	73,73,73,73	1
60	MG	BA	2977	1/1	0.96	0.09	74,74,74,74	0
60	MG	Aa	1629	1/1	0.96	0.06	76,76,76,76	0
60	MG	AA	2906	1/1	0.96	0.14	38,38,38,38	0
60	MG	AA	3042	1/1	0.96	0.09	49,49,49,49	0
60	MG	BA	2982	1/1	0.96	0.12	53,53,53,53	0
60	MG	AA	2992	1/1	0.96	0.34	61,61,61,61	0
60	MG	BA	3078	1/1	0.96	0.32	61,61,61,61	0
60	MG	AA	2949	1/1	0.96	0.37	63,63,63,63	0
60	MG	Aa	1683	1/1	0.96	0.04	59,59,59,59	0
60	MG	BA	3024	1/1	0.96	0.14	46,46,46,46	0
60	MG	BA	3120	1/1	0.96	0.32	39,39,39,39	0
60	MG	Aa	1673	1/1	0.96	0.22	91,91,91,91	0
60	MG	BA	3009	1/1	0.96	0.29	38,38,38,38	0
60	MG	BA	2989	1/1	0.96	0.16	49,49,49,49	0
60	MG	AA	2983	1/1	0.96	0.30	43,43,43,43	0
60	MG	AA	2997	1/1	0.96	0.31	44,44,44,44	0
60	MG	BA	3248	1/1	0.96	0.17	64,64,64,64	0
60	MG	Ba	1724	1/1	0.97	0.32	74,74,74,74	0
60	MG	AA	3259	1/1	0.97	0.36	65,65,65,65	0
60	MG	BA	2915	1/1	0.97	0.13	32,32,32,32	0
60	MG	BA	3030	1/1	0.97	0.09	37,37,37,37	0
60	MG	BA	2936	1/1	0.97	0.25	40,40,40,40	0
60	MG	BA	2916	1/1	0.97	0.23	28,28,28,28	0
60	MG	BA	3002	1/1	0.97	0.11	38,38,38,38	0
60	MG	Ba	1630	1/1	0.97	0.05	53,53,53,53	0
60	MG	BA	2988	1/1	0.97	0.35	45,45,45,45	0
60	MG	AA	3000	1/1	0.97	0.05	49,49,49,49	0
60	MG	Aa	1666	1/1	0.97	0.37	66,66,66,66	0
60	MG	BA	3055	1/1	0.97	0.14	64,64,64,64	0
60	MG	AA	3071	1/1	0.97	0.35	87,87,87,87	0
60	MG	BA	2992	1/1	0.97	0.28	40,40,40,40	0
60	MG	BA	2993	1/1	0.97	0.32	40,40,40,40	0
60	MG	BA	2969	1/1	0.97	0.28	58,58,58,58	0
60	MG	BA	2996	1/1	0.97	0.07	35,35,35,35	0
60	MG	BA	3215	1/1	0.97	0.32	61,61,61,61	0
59	ZN	B9	101	1/1	0.98	0.06	124,124,124,124	0
60	MG	AA	2910	1/1	0.98	0.46	71,71,71,71	0
60	MG	BA	2987	1/1	0.98	0.12	43,43,43,43	0
59	ZN	Ad	301	1/1	0.98	0.22	94,94,94,94	0
60	MG	BA	3045	1/1	0.98	0.24	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1745	1/1	0.98	0.27	70,70,70,70	0
60	MG	BA	2928	1/1	0.98	0.35	77,77,77,77	0
59	ZN	Bd	301	1/1	0.98	0.22	103,103,103,103	0
60	MG	AA	3006	1/1	0.98	0.12	39,39,39,39	0
60	MG	BA	2920	1/1	0.98	0.06	31,31,31,31	0
59	ZN	An	101	1/1	0.98	0.07	171,171,171,171	0
60	MG	AA	3197	1/1	0.98	0.06	34,34,34,34	0
60	MG	BA	2912	1/1	0.99	0.11	39,39,39,39	0
60	MG	BA	3194	1/1	0.99	0.05	28,28,28,28	0
60	MG	BA	2994	1/1	0.99	0.36	44,44,44,44	0
60	MG	AA	2981	1/1	0.99	0.06	54,54,54,54	0
59	ZN	A9	101	1/1	0.99	0.07	143,143,143,143	0
60	MG	BA	2922	1/1	0.99	0.07	45,45,45,45	0
60	MG	BA	2979	1/1	0.99	0.27	36,36,36,36	0
60	MG	AA	2918	1/1	0.99	0.41	42,42,42,42	0
59	ZN	Bn	101	1/1	0.99	0.04	142,142,142,142	0
60	MG	Aa	1631	1/1	0.99	0.06	52,52,52,52	0
60	MG	BA	2918	1/1	0.99	0.31	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.