wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 05:27 PM EDT

PDB ID	:	4V5K
Title	:	Structure of cytotoxic domain of colicin E3 bound to the 70S ribosome
Authors	:	Ng, C.L.; Lang, K.; Meenan, N.A.G.; Sharma, A.; Kelley, A.C.; Kleanthous, C.; Ramakrishnan, V.
Deposited on	:	2010-05-29
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

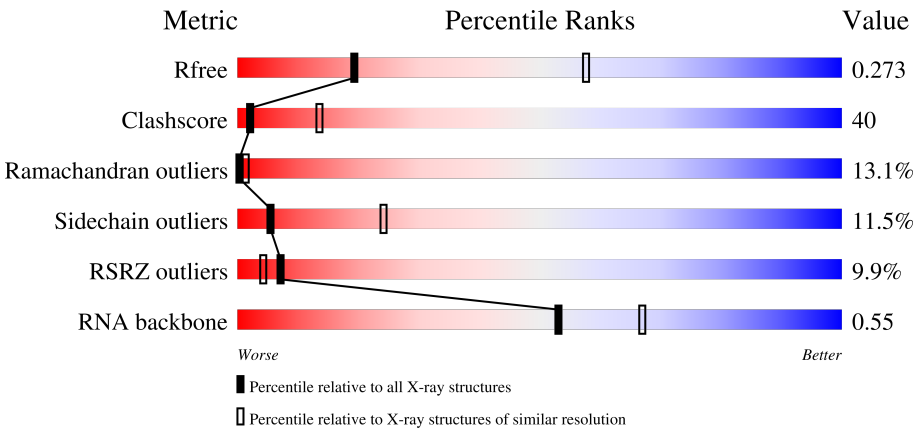
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	3% 29% 61% 9% •
1	CA	1522	12% 23% 63% 13% •
2	AB	256	7% 17% 61% 13% • 8%
2	CB	256	17% 18% 61% 12% • 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	8% 21% 56% 10% 13%
3	CC	239	21% 19% 57% 11% 13%
4	AD	209	28% 60% 11%
4	CD	209	27% 28% 58% 12%
5	AE	162	2% 20% 60% 12% 7%
5	CE	162	24% 17% 64% 12% 7%
6	AF	101	3% 35% 53% 10%
6	CF	101	% 34% 55% 9%
7	AG	156	9% 35% 59% 6%
7	CG	156	23% 32% 62% 6%
8	AH	138	% 22% 69% 8%
8	CH	138	18% 23% 68% 8%
9	AI	128	22% 18% 66% 14%
9	CI	128	48% 20% 66% 13%
10	AJ	105	33% 15% 68% 11% 6%
10	CJ	105	55% 17% 65% 12% 6%
11	AK	129	6% 26% 57% 9% 8%
11	CK	129	9% 28% 55% 9% 8%
12	AL	135	% 33% 46% 13% 7%
12	CL	135	21% 28% 52% 11% 7%
13	AM	126	14% 20% 58% 15% 6%
13	CM	126	21% 21% 56% 16% 6%
14	AN	61	16% 21% 67% 8%
14	CN	61	23% 23% 66% 10%
15	AO	89	% 21% 67% 10%

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Mol	Chain	Length	Quality of chain
15	CO	89	4% 28% 61% 10% •
16	AP	88	% 25% 58% 11% • 5%
16	CP	88	43% 24% 57% 14% • 5%
17	AQ	105	% 22% 65% 9% 5%
17	CQ	105	10% 25% 63% 8% 5%
18	AR	88	6% 11% 55% 14% 20%
18	CR	88	6% 13% 53% 14% 20%
19	AS	93	18% 17% 52% 20% • 9%
19	CS	93	33% 15% 56% 18% • 9%
20	AT	106	3% 31% 49% 13% 7%
20	CT	106	15% 31% 49% 13% 7%
21	AU	27	41% 30% 52% 11% 7%
21	CU	27	74% 30% 56% 7% 7%
22	AV	77	% 36% 44% 17% •
22	AW	77	68% 23% 61% 16%
22	CV	77	3% 14% 61% 25%
22	CW	77	73% 23% 69% 8%
23	AX	25	40% 12% 52% 36%
24	AY	97	27% 18% 42% 35% 5%
24	CY	97	9% • 9% 5% 84%
25	B0	85	8% 40% 48% 11% •
25	D0	85	14% 41% 47% 11% •
26	B1	98	3% 31% 51% 13% • •
26	D1	98	30% 52% 13% • •
27	B2	72	36% 47% 14% ••

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Mol	Chain	Length	Quality of chain
27	D2	72	4% 19% 62% 15%
28	B3	60	7% 42% 43% 15%
28	D3	60	5% 38% 48% 13%
29	B4	71	7% 10% 44% 25% 21%
29	D4	71	15% 13% 44% 23% 21%
30	B5	60	8% 47% 42% 7%
30	D5	60	8% 45% 43% 7%
31	B6	54	56% 13% 54% 11% 6% 17%
31	D6	54	48% 15% 48% 15% 6% 17%
32	B7	49	47% 49%
32	D7	49	45% 51%
33	B8	65	22% 52% 23%
33	D8	65	3% 23% 51% 23%
34	B9	37	43% 32% 57% 8%
34	D9	37	41% 27% 62% 8%
35	BA	2848	4% 35% 50% 12%
35	DA	2848	3% 34% 51% 12%
36	BB	122	% 30% 56% 11%
36	DB	122	3% 30% 56% 11%
37	BC	229	68% 41% 30% 11% 17%
37	DC	229	65% 41% 31% 10% 17%
38	BD	276	29% 52% 16%
38	DD	276	28% 53% 16%
39	BE	206	% 31% 50% 19%
39	DE	206	3% 30% 50% 20%

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Mol	Chain	Length	Quality of chain
40	BF	210	32% 49% 16%
40	DF	210	2% 31% 50% 16%
41	BG	182	9% 14% 65% 18%
41	DG	182	10% 14% 65% 16%
42	BH	180	27% 19% 52% 18% 8%
42	DH	180	6% 19% 52% 18% 8%
43	BI	148	37% 18% 60% 14% 6%
43	DI	148	14% 22% 55% 14% 7%
44	BJ	131	76% 23%
44	DJ	131	63% 37%
45	BN	140	% 30% 47% 19%
45	DN	140	31% 45% 20%
46	BO	122	36% 56% 8%
46	DO	122	% 34% 57% 10%
47	BP	150	2% 19% 37% 35% 6%
47	DP	150	5% 19% 38% 35% 5%
48	BQ	141	% 36% 56% 8%
48	DQ	141	4% 40% 53% 7%
49	BR	118	21% 57% 19%
49	DR	118	% 24% 53% 19%
50	BS	112	12% 18% 39% 27% 12%
50	DS	112	19% 21% 36% 28% 12%
51	BT	146	3% 18% 51% 22% 5%
51	DT	146	8% 17% 53% 21% 5%
52	BU	118	% 42% 42% 14%

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Mol	Chain	Length	Quality of chain
52	DU	118	45% 40% 13%
53	BV	101	5% 33% 43% 22%
53	DV	101	31% 46% 21%
54	BW	113	% 36% 52% 10%
54	DW	113	36% 50% 12%
55	BX	96	% 31% 53% 11%
55	DX	96	% 29% 57% 9%
56	BY	110	15% 15% 50% 21% 6% 8%
56	DY	110	7% 14% 51% 21% 6% 8%
57	BZ	206	4% 19% 54% 17% 9%
57	DZ	206	4% 20% 49% 20% 9%
58	CX	25	8% 32% 68%

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
1	A3P	AA	1493	-	-	X	-
1	A3P	CA	1493	-	-	-	X
59	MG	AA	1619	-	-	-	X
59	MG	AA	1620	-	-	-	X
59	MG	AA	1624	-	-	-	X
59	MG	AA	1625	-	-	-	X
59	MG	AA	1627	-	-	-	X
59	MG	AA	1635	-	-	-	X
59	MG	AA	1640	-	-	-	X
59	MG	AA	1648	-	-	-	X
59	MG	AA	1666	-	-	-	X
59	MG	AA	1671	-	-	-	X
59	MG	AA	1673	-	-	-	X
59	MG	AA	1682	-	-	-	X
59	MG	AA	1698	-	-	-	X
59	MG	AA	1722	-	-	-	X
59	MG	AA	1725	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	1735	-	-	-	X
59	MG	AA	1736	-	-	-	X
59	MG	AA	1738	-	-	-	X
59	MG	AA	1745	-	-	-	X
59	MG	AA	1757	-	-	-	X
59	MG	AA	1758	-	-	-	X
59	MG	AA	1764	-	-	-	X
59	MG	AA	1766	-	-	-	X
59	MG	AA	1768	-	-	-	X
59	MG	AA	1772	-	-	-	X
59	MG	AA	1776	-	-	-	X
59	MG	AA	1794	-	-	-	X
59	MG	AA	1798	-	-	-	X
59	MG	AA	1800	-	-	-	X
59	MG	AA	1803	-	-	-	X
59	MG	AA	1814	-	-	-	X
59	MG	AA	1829	-	-	-	X
59	MG	AA	1835	-	-	-	X
59	MG	AA	1838	-	-	-	X
59	MG	AA	1851	-	-	-	X
59	MG	AA	1861	-	-	-	X
59	MG	AA	1869	-	-	-	X
59	MG	AA	1872	-	-	-	X
59	MG	AA	1880	-	-	-	X
59	MG	AA	1883	-	-	-	X
59	MG	AA	1889	-	-	-	X
59	MG	AA	1904	-	-	-	X
59	MG	AA	1905	-	-	-	X
59	MG	AA	1915	-	-	-	X
59	MG	AA	1938	-	-	-	X
59	MG	AA	1943	-	-	-	X
59	MG	AA	1945	-	-	-	X
59	MG	AA	1948	-	-	-	X
59	MG	AA	1953	-	-	-	X
59	MG	AA	1956	-	-	-	X
59	MG	AA	1959	-	-	-	X
59	MG	AA	1962	-	-	-	X
59	MG	AA	1964	-	-	-	X
59	MG	AA	1968	-	-	-	X
59	MG	AA	1972	-	-	-	X
59	MG	AD	303	-	-	-	X
59	MG	AO	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AQ	202	-	-	-	X
59	MG	AX	103	-	-	-	X
59	MG	AY	103	-	-	-	X
59	MG	B5	101	-	-	-	X
59	MG	B6	101	-	-	-	X
59	MG	BA	2901	-	-	-	X
59	MG	BA	2904	-	-	-	X
59	MG	BA	2914	-	-	-	X
59	MG	BA	2923	-	-	-	X
59	MG	BA	2935	-	-	-	X
59	MG	BA	2949	-	-	-	X
59	MG	BA	2951	-	-	-	X
59	MG	BA	2953	-	-	-	X
59	MG	BA	2965	-	-	-	X
59	MG	BA	2970	-	-	-	X
59	MG	BA	2971	-	-	-	X
59	MG	BA	2973	-	-	-	X
59	MG	BA	2991	-	-	-	X
59	MG	BA	2993	-	-	-	X
59	MG	BA	3004	-	-	-	X
59	MG	BA	3006	-	-	-	X
59	MG	BA	3017	-	-	-	X
59	MG	BA	3019	-	-	-	X
59	MG	BA	3030	-	-	-	X
59	MG	BA	3037	-	-	-	X
59	MG	BA	3039	-	-	-	X
59	MG	BA	3052	-	-	-	X
59	MG	BA	3071	-	-	-	X
59	MG	BA	3085	-	-	-	X
59	MG	BA	3087	-	-	-	X
59	MG	BA	3097	-	-	-	X
59	MG	BA	3102	-	-	-	X
59	MG	BA	3104	-	-	-	X
59	MG	BA	3111	-	-	-	X
59	MG	BA	3112	-	-	-	X
59	MG	BA	3115	-	-	-	X
59	MG	BA	3116	-	-	-	X
59	MG	BA	3121	-	-	-	X
59	MG	BA	3122	-	-	-	X
59	MG	BA	3132	-	-	-	X
59	MG	BA	3140	-	-	-	X
59	MG	BA	3141	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3146	-	-	-	X
59	MG	BA	3190	-	-	-	X
59	MG	BA	3193	-	-	-	X
59	MG	BA	3196	-	-	-	X
59	MG	BA	3199	-	-	-	X
59	MG	BA	3205	-	-	-	X
59	MG	BA	3210	-	-	-	X
59	MG	BA	3213	-	-	-	X
59	MG	BA	3215	-	-	-	X
59	MG	BA	3222	-	-	-	X
59	MG	BA	3234	-	-	-	X
59	MG	BA	3251	-	-	-	X
59	MG	BA	3272	-	-	-	X
59	MG	BA	3276	-	-	-	X
59	MG	BA	3281	-	-	-	X
59	MG	BA	3284	-	-	-	X
59	MG	BA	3301	-	-	-	X
59	MG	BA	3304	-	-	-	X
59	MG	BA	3316	-	-	-	X
59	MG	BA	3317	-	-	-	X
59	MG	BA	3326	-	-	-	X
59	MG	BA	3327	-	-	-	X
59	MG	BA	3331	-	-	-	X
59	MG	BA	3335	-	-	-	X
59	MG	BA	3338	-	-	-	X
59	MG	BA	3340	-	-	-	X
59	MG	BA	3342	-	-	-	X
59	MG	BA	3346	-	-	-	X
59	MG	BA	3350	-	-	-	X
59	MG	BA	3354	-	-	-	X
59	MG	BA	3359	-	-	-	X
59	MG	BA	3361	-	-	-	X
59	MG	BA	3367	-	-	-	X
59	MG	BA	3374	-	-	-	X
59	MG	BA	3375	-	-	-	X
59	MG	BA	3379	-	-	-	X
59	MG	BA	3380	-	-	-	X
59	MG	BA	3384	-	-	-	X
59	MG	BA	3387	-	-	-	X
59	MG	BA	3391	-	-	-	X
59	MG	BA	3395	-	-	-	X
59	MG	BA	3417	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3445	-	-	-	X
59	MG	BA	3458	-	-	-	X
59	MG	BA	3460	-	-	-	X
59	MG	BA	3479	-	-	-	X
59	MG	BA	3493	-	-	-	X
59	MG	BA	3505	-	-	-	X
59	MG	BA	3528	-	-	-	X
59	MG	BA	3529	-	-	-	X
59	MG	BA	3532	-	-	-	X
59	MG	BA	3536	-	-	-	X
59	MG	BA	3560	-	-	-	X
59	MG	BA	3568	-	-	-	X
59	MG	BA	3569	-	-	-	X
59	MG	BA	3570	-	-	-	X
59	MG	BA	3571	-	-	-	X
59	MG	BA	3581	-	-	-	X
59	MG	BA	3583	-	-	-	X
59	MG	BA	3585	-	-	-	X
59	MG	BA	3587	-	-	-	X
59	MG	BA	3588	-	-	-	X
59	MG	BA	3596	-	-	-	X
59	MG	BA	3600	-	-	-	X
59	MG	BA	3601	-	-	-	X
59	MG	BA	3602	-	-	-	X
59	MG	BA	3604	-	-	-	X
59	MG	BB	206	-	-	-	X
59	MG	BE	304	-	-	-	X
59	MG	BN	201	-	-	-	X
59	MG	BP	202	-	-	X	-
59	MG	BP	203	-	-	X	-
59	MG	BR	201	-	-	-	X
59	MG	CA	1608	-	-	-	X
59	MG	CA	1609	-	-	-	X
59	MG	CA	1610	-	-	-	X
59	MG	CA	1611	-	-	-	X
59	MG	CA	1615	-	-	-	X
59	MG	CA	1622	-	-	-	X
59	MG	CA	1626	-	-	-	X
59	MG	CA	1640	-	-	-	X
59	MG	CA	1646	-	-	-	X
59	MG	CA	1647	-	-	-	X
59	MG	CA	1649	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	1650	-	-	-	X
59	MG	CA	1654	-	-	-	X
59	MG	CA	1657	-	-	-	X
59	MG	CA	1658	-	-	-	X
59	MG	CA	1659	-	-	-	X
59	MG	CA	1671	-	-	-	X
59	MG	CA	1677	-	-	-	X
59	MG	CA	1680	-	-	-	X
59	MG	CA	1681	-	-	-	X
59	MG	CA	1684	-	-	-	X
59	MG	CA	1695	-	-	-	X
59	MG	CA	1696	-	-	-	X
59	MG	CA	1697	-	-	-	X
59	MG	CA	1698	-	-	-	X
59	MG	CA	1700	-	-	-	X
59	MG	CA	1712	-	-	-	X
59	MG	CA	1716	-	-	-	X
59	MG	CA	1723	-	-	-	X
59	MG	CA	1726	-	-	-	X
59	MG	CA	1735	-	-	-	X
59	MG	CA	1739	-	-	-	X
59	MG	CA	1741	-	-	-	X
59	MG	CA	1743	-	-	-	X
59	MG	CA	1746	-	-	-	X
59	MG	CA	1749	-	-	-	X
59	MG	CA	1750	-	-	-	X
59	MG	CA	1752	-	-	-	X
59	MG	CA	1756	-	-	-	X
59	MG	CA	1758	-	-	-	X
59	MG	CA	1763	-	-	-	X
59	MG	CA	1765	-	-	-	X
59	MG	CA	1767	-	-	-	X
59	MG	CA	1770	-	-	-	X
59	MG	CA	1773	-	-	-	X
59	MG	CA	1776	-	-	-	X
59	MG	CA	1779	-	-	-	X
59	MG	CC	301	-	-	-	X
59	MG	CJ	201	-	-	-	X
59	MG	CV	110	-	-	-	X
59	MG	D0	104	-	-	-	X
59	MG	D6	101	-	-	-	X
59	MG	D6	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	2908	-	-	-	X
59	MG	DA	2909	-	-	-	X
59	MG	DA	2911	-	-	-	X
59	MG	DA	2914	-	-	-	X
59	MG	DA	2925	-	-	-	X
59	MG	DA	2931	-	-	-	X
59	MG	DA	2936	-	-	-	X
59	MG	DA	2942	-	-	-	X
59	MG	DA	2944	-	-	-	X
59	MG	DA	2951	-	-	-	X
59	MG	DA	2953	-	-	-	X
59	MG	DA	2961	-	-	-	X
59	MG	DA	2972	-	-	-	X
59	MG	DA	2976	-	-	-	X
59	MG	DA	2983	-	-	-	X
59	MG	DA	2984	-	-	-	X
59	MG	DA	2988	-	-	-	X
59	MG	DA	2990	-	-	-	X
59	MG	DA	3004	-	-	-	X
59	MG	DA	3009	-	-	-	X
59	MG	DA	3014	-	-	-	X
59	MG	DA	3017	-	-	-	X
59	MG	DA	3021	-	-	-	X
59	MG	DA	3022	-	-	-	X
59	MG	DA	3027	-	-	-	X
59	MG	DA	3042	-	-	-	X
59	MG	DA	3060	-	-	-	X
59	MG	DA	3065	-	-	-	X
59	MG	DA	3072	-	-	-	X
59	MG	DA	3074	-	-	-	X
59	MG	DA	3094	-	-	-	X
59	MG	DA	3096	-	-	-	X
59	MG	DA	3105	-	-	-	X
59	MG	DA	3107	-	-	-	X
59	MG	DA	3109	-	-	-	X
59	MG	DA	3113	-	-	-	X
59	MG	DA	3123	-	-	-	X
59	MG	DA	3124	-	-	-	X
59	MG	DA	3131	-	-	-	X
59	MG	DA	3133	-	-	-	X
59	MG	DA	3138	-	-	-	X
59	MG	DA	3143	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3145	-	-	-	X
59	MG	DA	3146	-	-	-	X
59	MG	DA	3155	-	-	-	X
59	MG	DA	3158	-	-	-	X
59	MG	DA	3165	-	-	-	X
59	MG	DA	3168	-	-	-	X
59	MG	DA	3172	-	-	-	X
59	MG	DA	3192	-	-	-	X
59	MG	DA	3195	-	-	-	X
59	MG	DA	3200	-	-	-	X
59	MG	DA	3203	-	-	-	X
59	MG	DA	3208	-	-	-	X
59	MG	DA	3214	-	-	-	X
59	MG	DA	3220	-	-	-	X
59	MG	DA	3231	-	-	-	X
59	MG	DA	3235	-	-	-	X
59	MG	DA	3241	-	-	-	X
59	MG	DA	3253	-	-	-	X
59	MG	DA	3271	-	-	-	X
59	MG	DA	3289	-	-	-	X
59	MG	DA	3316	-	-	-	X
59	MG	DA	3326	-	-	-	X
59	MG	DA	3329	-	-	-	X
59	MG	DA	3341	-	-	-	X
59	MG	DA	3345	-	-	-	X
59	MG	DA	3349	-	-	-	X
59	MG	DA	3366	-	-	-	X
59	MG	DA	3384	-	-	-	X
59	MG	DA	3389	-	-	-	X
59	MG	DA	3390	-	-	-	X
59	MG	DA	3391	-	-	-	X
59	MG	DA	3400	-	-	-	X
59	MG	DA	3404	-	-	-	X
59	MG	DA	3414	-	-	-	X
59	MG	DA	3417	-	-	-	X
59	MG	DA	3419	-	-	-	X
59	MG	DA	3420	-	-	-	X
59	MG	DA	3423	-	-	-	X
59	MG	DA	3432	-	-	-	X
59	MG	DA	3443	-	-	-	X
59	MG	DA	3449	-	-	-	X
59	MG	DA	3459	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3464	-	-	-	X
59	MG	DA	3468	-	-	-	X
59	MG	DA	3470	-	-	-	X
59	MG	DA	3476	-	-	-	X
59	MG	DA	3485	-	-	-	X
59	MG	DA	3489	-	-	-	X
59	MG	DA	3491	-	-	-	X
59	MG	DA	3495	-	-	-	X
59	MG	DA	3505	-	-	-	X
59	MG	DA	3511	-	-	-	X
59	MG	DA	3515	-	-	-	X
59	MG	DA	3524	-	-	-	X
59	MG	DA	3525	-	-	-	X
59	MG	DA	3537	-	-	-	X
59	MG	DA	3538	-	-	-	X
59	MG	DA	3539	-	-	-	X
59	MG	DA	3546	-	-	-	X
59	MG	DA	3547	-	-	-	X
59	MG	DA	3549	-	-	-	X
59	MG	DA	3552	-	-	-	X
59	MG	DA	3553	-	-	-	X
59	MG	DA	3556	-	-	-	X
59	MG	DA	3561	-	-	-	X
59	MG	DA	3563	-	-	-	X
59	MG	DA	3571	-	-	-	X
59	MG	DA	3582	-	-	-	X
59	MG	DA	3584	-	-	-	X
59	MG	DA	3590	-	-	-	X
59	MG	DA	3617	-	-	-	X
59	MG	DA	3628	-	-	-	X
59	MG	DA	3637	-	-	-	X
59	MG	DA	3640	-	-	-	X
59	MG	DA	3649	-	-	-	X
59	MG	DA	3665	-	-	-	X
59	MG	DA	3666	-	-	-	X
59	MG	DA	3670	-	-	-	X
59	MG	DA	3671	-	-	-	X
59	MG	DA	3673	-	-	-	X
59	MG	DA	3676	-	-	-	X
59	MG	DA	3680	-	-	-	X
59	MG	DA	3693	-	-	-	X
59	MG	DA	3695	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3702	-	-	-	X
59	MG	DA	3710	-	-	-	X
59	MG	DA	3718	-	-	-	X
59	MG	DA	3727	-	-	-	X
59	MG	DA	3730	-	-	-	X
59	MG	DA	3737	-	-	-	X
59	MG	DA	3747	-	-	-	X
59	MG	DA	3751	-	-	-	X
59	MG	DA	3761	-	-	-	X
59	MG	DA	3763	-	-	-	X
59	MG	DA	3779	-	-	-	X
59	MG	DA	3780	-	-	-	X
59	MG	DA	3781	-	-	-	X
59	MG	DA	3785	-	-	-	X
59	MG	DB	207	-	-	-	X
59	MG	DF	302	-	-	-	X
59	MG	DN	202	-	-	-	X
59	MG	DN	203	-	-	-	X
59	MG	DP	202	-	-	-	X
59	MG	DP	206	-	-	-	X
59	MG	DY	201	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 296762 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1508	32412	14427	6003	10475	1507	0	0	0
1	CA	1508	32413	14427	6004	10475	1507	0	0	0

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	235	1901	1213	342	341	5	0	0	1
2	CB	235	1901	1213	342	341	5	0	0	1

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	207	1613	1016	315	281	1	0	0	1
3	CC	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	208	1692	1060	336	289	7	0	0	1
4	CD	208	1692	1060	336	289	7	0	0	1

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AE	151	1147	724	218	201	4	0	0	1
5	CE	151	1147	724	218	201	4	0	0	1

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	AI	127	1011	639	198	174	0	0	0
9	CI	127	1011	639	198	174	0	0	0

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	AJ	99	795	499	157	138	1	0	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	CJ	99	795	499	157	138	1	0	0	1

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AK	119	885	549	168	165	3	0	0	0
11	CK	119	885	549	168	165	3	0	0	0

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AL	125	971	611	196	163	1	0	0	1
12	CL	125	971	611	196	163	1	0	0	1

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AM	118	934	577	193	162	2	0	0	1
13	CM	118	934	577	193	162	2	0	0	1

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AP	84	701	443	140	117	1	0	0	1
16	CP	84	701	443	140	117	1	0	0	1

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	AQ	100	824	528	152	142	2	0	0	1
17	CQ	100	824	528	152	142	2	0	0	1

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AS	85	671	427	124	118	2	0	0	1
19	CS	85	671	427	124	118	2	0	0	1

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	AU	25	209	128	51	30	0	0	1
21	CU	25	209	128	51	30	0	0	1

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	AV	77	1640	732	297	535	76	0	0	0
22	AW	77	1640	732	297	535	76	0	0	0
22	CV	77	1640	732	297	535	76	0	0	0
22	CW	77	1640	732	297	535	76	0	0	0

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	AX	16	341	155	66	105	15	0	0	0

- Molecule 24 is a protein called COLICIN-E3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
24	AY	97	769	483	144	142	0	0	0
24	CY	16	126	82	23	21	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	58	ALA	HIS	engineered mutation	UNP P06646
CY	58	ALA	HIS	engineered mutation	UNP P00646

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	D0	84	662	410	140	111	1	0	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	B1	94	734	460	148	125	1	0	0	1
26	D1	94	734	460	148	125	1	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	conflict	UNP P60494
D1	81	ARG	LYS	conflict	UNP P60494

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	B2	71	598	370	121	106	1	0	0	0
27	D2	71	598	370	121	106	1	0	0	0

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	B3	60	468	298	91	78	1	0	0	1
28	D3	60	468	298	91	78	1	0	0	1

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	B4	56	434	274	75	81	4	0	0	1
29	D4	56	434	274	75	81	4	0	0	1

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	B5	59	459	288	90	76	5	0	0	0
30	D5	59	459	288	90	76	5	0	0	0

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	B6	45	381	235	78	64	4	0	0	1
31	D6	45	381	235	78	64	4	0	0	1

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	B7	49	419	257	105	55	2	0	0	1
32	D7	49	419	257	105	55	2	0	0	1

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	B8	64	508	326	102	78	2	0	0	1
33	D8	64	508	326	102	78	2	0	0	1

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	B9	36	299	183	67	46	3	0	0	0
34	D9	36	299	183	67	46	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	BA	2807	60459	26907	11311	19435	2806	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	DA	2807	60459	26907	11311	19435	2806	0	0	0

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

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
37	BC	191	1142	691	221	230	0	0	1
37	DC	191	1142	691	221	230	0	0	1

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	BD	272	2105	1329	417	356	3	0	0	1
38	DD	272	2105	1329	417	356	3	0	0	1

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	BE	205	1564	988	300	270	6	0	0	1
39	DE	205	1564	988	300	270	6	0	0	1

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	BF	208	1624	1035	304	282	3	0	0	1
40	DF	208	1624	1035	304	282	3	0	0	1

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	BG	181	1474	942	268	260	4	0	0	0
41	DG	181	1474	942	268	260	4	0	0	0

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BH	165	1260	800	234	225	1	0	0	1
42	DH	165	1260	800	234	225	1	0	0	1

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	BI	145	1125	718	200	206	1	0	0	1
43	DI	145	1125	718	200	206	1	0	0	1

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
44	BJ	130	651	390	130	131	0	0	0
44	DJ	131	651	390	131	130	0	0	1

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BN	139	1105	712	207	182	4	0	0	1
45	DN	139	1105	712	207	182	4	0	0	1

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	BQ	141	1122	715	212	188	7	0	0	0
48	DQ	141	1122	715	212	188	7	0	0	0

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
50	BS	99	771	486	155	130	0	0	1
50	DS	99	771	486	155	130	0	0	1

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	BT	138	1142	710	235	196	1	0	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	DT	138	1142	710	235	196	1	0	0	1

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
55	BX	93	726	471	132	123	0	0	1
55	DX	93	726	471	132	123	0	0	1

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	BY	101	776	500	149	123	4	0	0	1
56	DY	101	776	500	149	123	4	0	0	1

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	BZ	187	1482	944	264	272	2	0	0	1
57	DZ	187	1482	944	264	272	2	0	0	1

- Molecule 58 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
58	CX	8	173	79	37	50	7	0	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
59	AA	373	373	373	0	0
59	AC	2	2	2	0	0
59	AD	3	3	3	0	0
59	AH	1	1	1	0	0
59	AI	3	3	3	0	0
59	AL	6	6	6	0	0
59	AN	2	2	2	0	0
59	AO	2	2	2	0	0
59	AP	1	1	1	0	0
59	AQ	3	3	3	0	0
59	AT	1	1	1	0	0
59	AV	7	7	7	0	0
59	AX	4	4	4	0	0
59	AY	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
59	B0	2	2	2	0	0
59	B1	1	1	1	0	0
59	B5	3	3	3	0	0
59	B6	1	1	1	0	0
59	B7	1	1	1	0	0
59	BA	709	709	709	0	0
59	BB	6	6	6	0	0
59	BD	5	5	5	0	0
59	BE	4	4	4	0	0
59	BF	1	1	1	0	0
59	BH	4	4	4	0	0
59	BN	1	1	1	0	0
59	BO	1	1	1	0	0
59	BP	4	4	4	0	0
59	BQ	1	1	1	0	0
59	BR	5	5	5	0	0
59	BT	1	1	1	0	0
59	BU	2	2	2	0	0
59	BY	1	1	1	0	0
59	CA	184	184	184	0	0
59	CC	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
59	CD	1	1	1	0	0
59	CH	1	1	1	0	0
59	CJ	2	2	2	0	0
59	CM	3	3	3	0	0
59	CP	1	1	1	0	0
59	CQ	1	1	1	0	0
59	CS	2	2	2	0	0
59	CV	12	12	12	0	0
59	CY	1	1	1	0	0
59	D0	4	4	4	0	0
59	D1	2	2	2	0	0
59	D2	1	1	1	0	0
59	D3	1	1	1	0	0
59	D5	3	3	3	0	0
59	D6	2	2	2	0	0
59	D7	4	4	4	0	0
59	D8	1	1	1	0	0
59	D9	1	1	1	0	0
59	DA	897	897	897	0	0
59	DB	11	11	11	0	0
59	DD	6	6	6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
59	DE	4	4	4	0	0
59	DF	3	3	3	0	0
59	DN	3	3	3	0	0
59	DO	1	1	1	0	0
59	DP	6	6	6	0	0
59	DR	2	2	2	0	0
59	DT	1	1	1	0	0
59	DU	4	4	4	0	0
59	DW	1	1	1	0	0
59	DY	1	1	1	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
60	AD	2	2	2	0	0
60	AN	1	1	1	0	0
60	CD	1	1	1	0	0

- Molecule 61 is water.

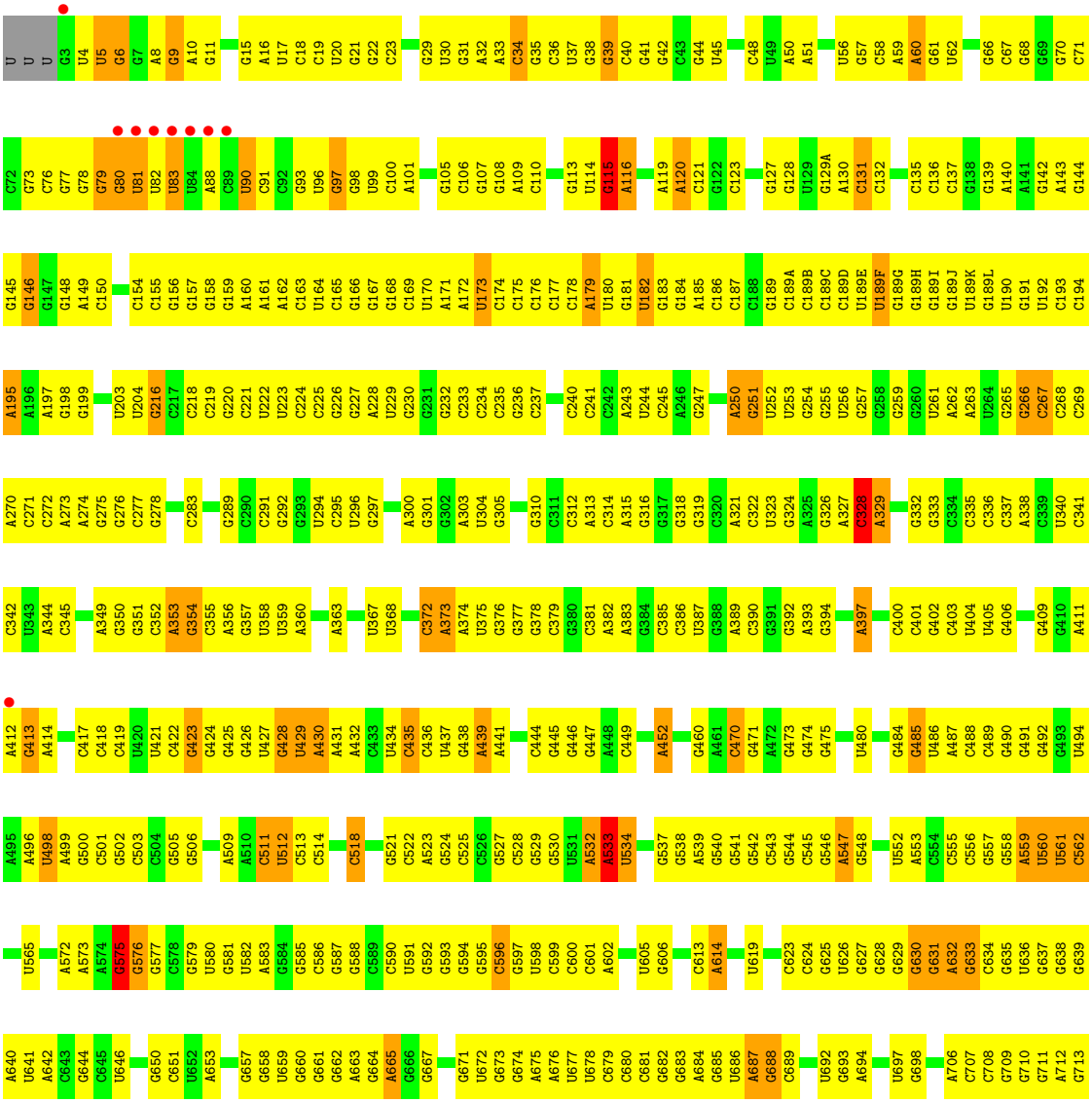
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
61	AA	2	2	2	0	0

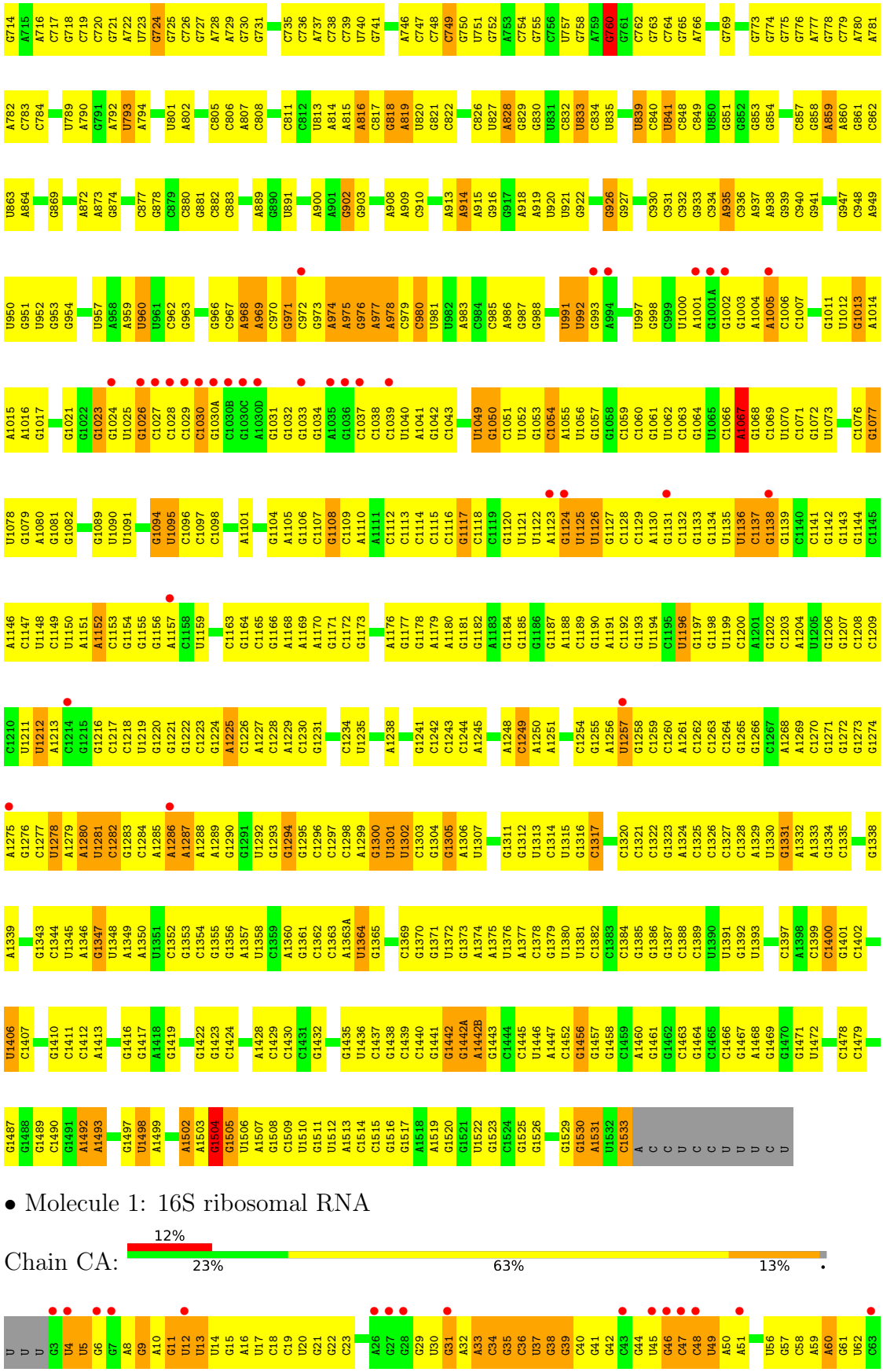
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

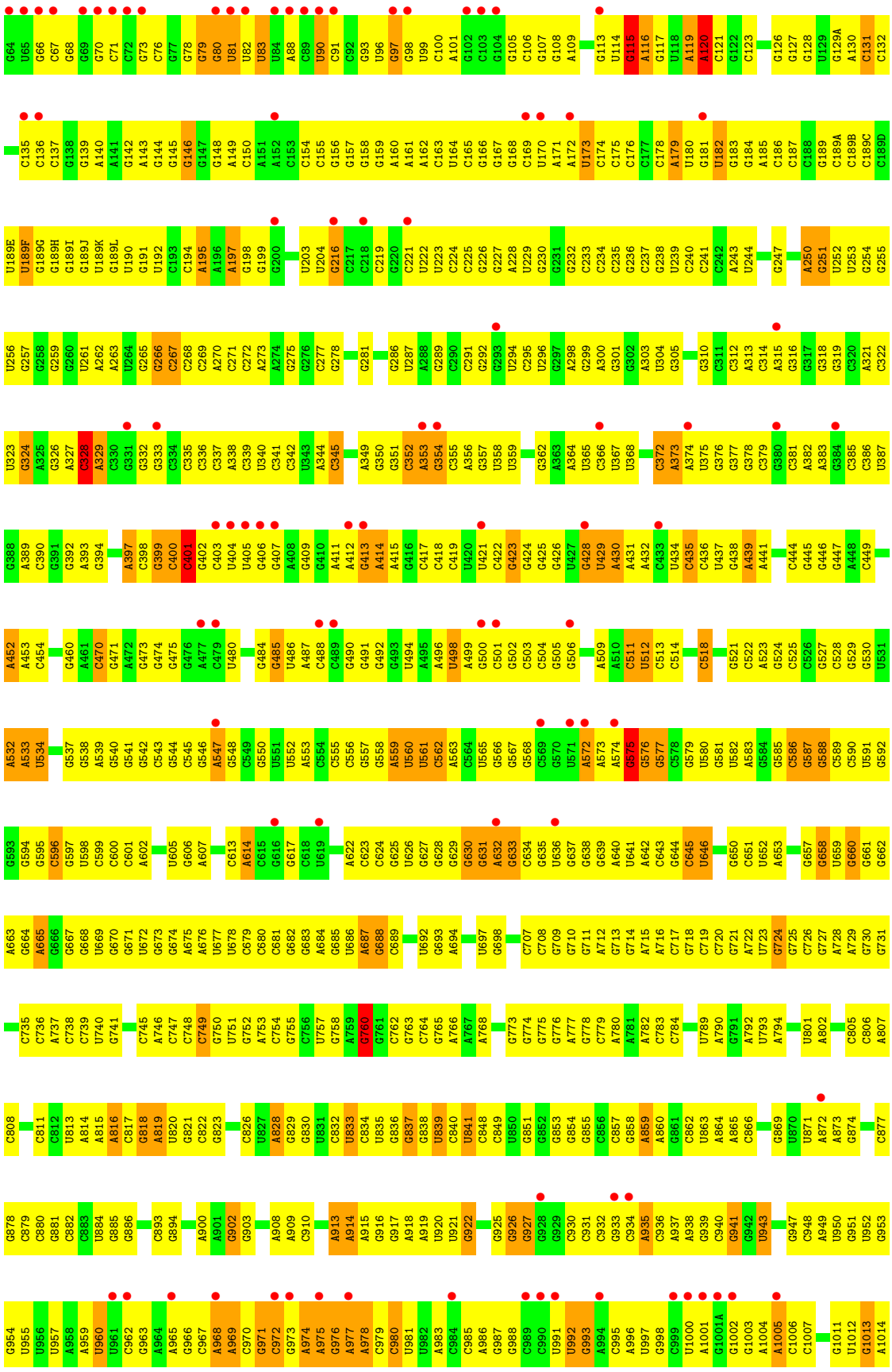
Chain AA: 3% 29% 61% 9%

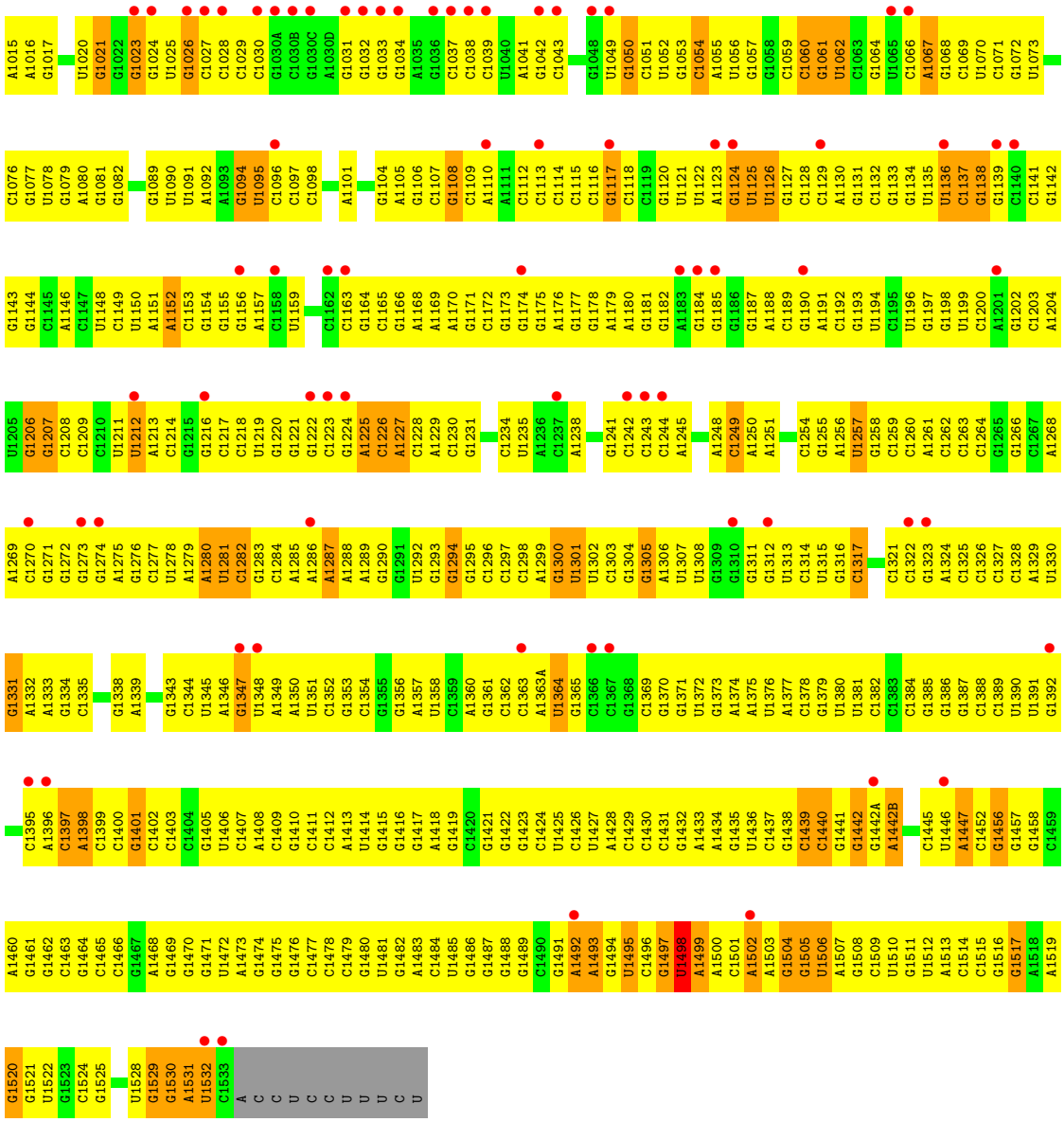




• Molecule 1: 16S ribosomal RNA

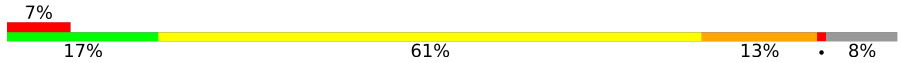
Chain CA:

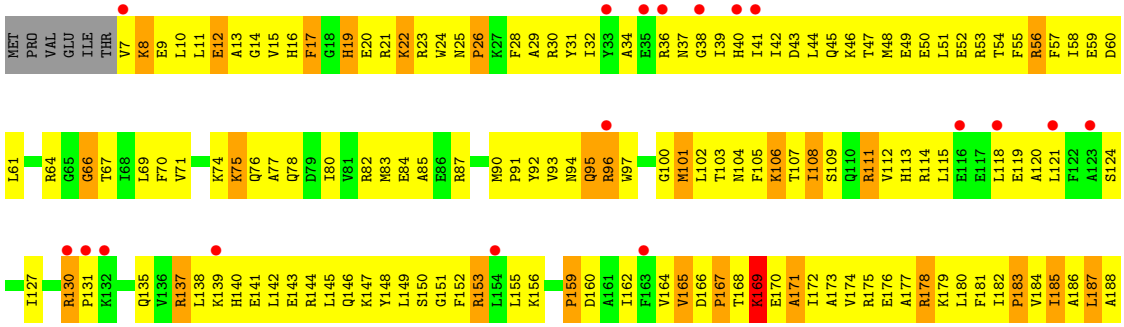

G64 U65 G66 C67 G68 G69 G70 C71 C72 G73 C76 G77 G78 G79 G80 U81 U82 U83 U84 A88 C89 U90 C91 C92 G93 U96 G97 G98 U99 C100 A101 G102 C103 G104 G105 C106 G107 G108 A109 G113 U114 G115 A116 G117 U118 A119 A120 C121 G122 C123 G126 G127 G128 U129 G129A A130 C131 C132
C135 C136 C137 G138 G139 A140 A141 G142 A143 G144 G145 G146 G147 G148 A149 C150 A151 A152 C153 C154 C155 G156 G157 G158 G159 A160 A161 A162 C163 U164 C165 G166 G167 G168 C169 U170 A171 A172 U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 G183 G184 A185 C186 C187 C188 G189 C189A C189B C189C C189D
U189E U189F G189G G189H G189I G189J U189K G189L U190 G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 U203 U204 G216 C217 C218 C219 G220 C221 U222 U223 C224 C225 G226 G227 A228 U229 G230 G231 G232 C233 C234 C235 G236 C237 G238 U239 C240 C241 C242 A243 U244 G247 A250 G251 U252 U253 G254 G255
U256 C257 C258 G259 G260 U261 A262 A263 U264 G265 G266 C267 C268 C269 A270 C271 C272 A273 A274 C275 C276 C277 G278 G281 G286 U287 A288 G289 C290 C291 G292 G293 U294 C295 U296 G297 A298 C299 A300 G301 G302 A303 U304 G305 G310 C311 C312 A313 C314 A315 G316 G317 G318 G319 C320 A321 C322
U323 G324 A325 G326 A327 C328 A329 G330 G331 G332 G333 C334 C335 C336 C337 A338 C339 U340 C341 C342 U343 A344 C345 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 U359 G362 A363 A364 U365 C366 U367 U368 C372 A373 A374 U375 G376 G377 G378 G379 G380 C381 A382 A383 G384 C385 C386 U387
G388 A389 C390 G391 G392 A393 G394 A397 C398 G399 C400 C401 G402 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 C417 C418 C419 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A441 C444 G445 G446 G447 A448 C449
A452 A453 C454 G460 A461 C470 G471 A472 G473 G474 G475 G476 A477 C479 U480 G484 G485 U486 A487 C488 C489 G490 G491 G492 G493 U494 A495 A496 U498 A499 G500 C501 C502 C503 C504 G505 G506 A509 A510 C511 U512 C513 C514 C518 G521 C522 A523 G524 C525 C526 G527 C528 G529 G530 U531
A532 A533 U534 G537 G538 A539 G540 G541 G542 G543 G544 C545 G546 A547 G548 C549 G550 U551 U552 A553 C554 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G567 G568 C569 G570 U571 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 U582 A583 G584 G585 C586 G587 G588 C589 C590 U591 G592
G593 G594 G595 C596 G597 U598 C599 C600 C601 A602 U605 G606 A607 C613 A614 C615 G616 G617 C618 U619 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G635 U636 G637 G638 G639 A640 U641 A642 C643 G644 C645 U646 G650 C651 U652 A653 G657 G658 U659 G660 G661 G662
A663 G664 A665 G666 G667 G668 U669 G670 G671 U672 G673 G674 A675 A676 U677 U678 C679 C680 C681 G682 G683 A684 U685 U686 A687 G688 C689 U692 G693 A694 U697 G698 C707 C708 G709 G710 G711 A712 G713 G714 A715 A716 C717 G718 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731
C735 C736 A737 C738 C739 U740 G741 C745 A746 C747 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A759 C760 G761 C762 G763 C764 G765 A766 A767 A768 G773 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783 C784 U789 A790 G791 A792 U793 A794 U801 A802 C805 C806 A807
C808 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C822 G823 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 C849 U850 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 G869 U870 U871 A872 A873 G874 C877
G878 C879 C880 G881 C882 C883 U884 G885 G886 C893 G894 A900 A901 G902 G903 A908 A909 C910 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 G925 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G947 C948 A949 U950 G951 U952 G953
G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 G1011 U1012 G1013 A1014

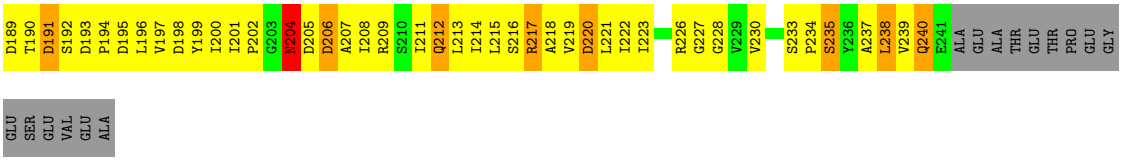


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

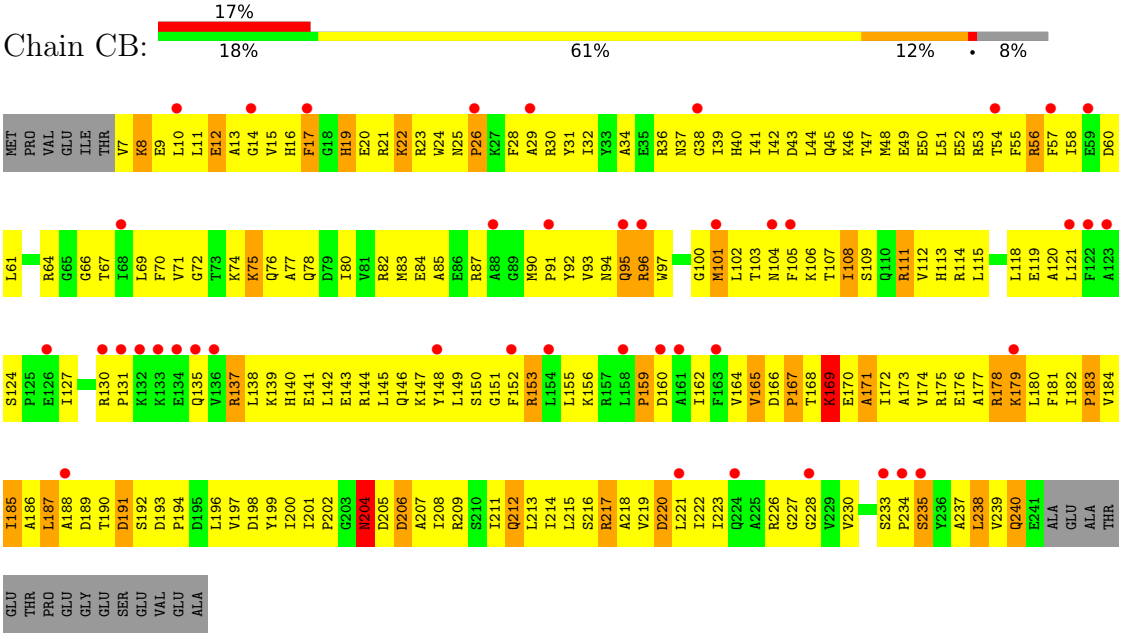
Chain AB:



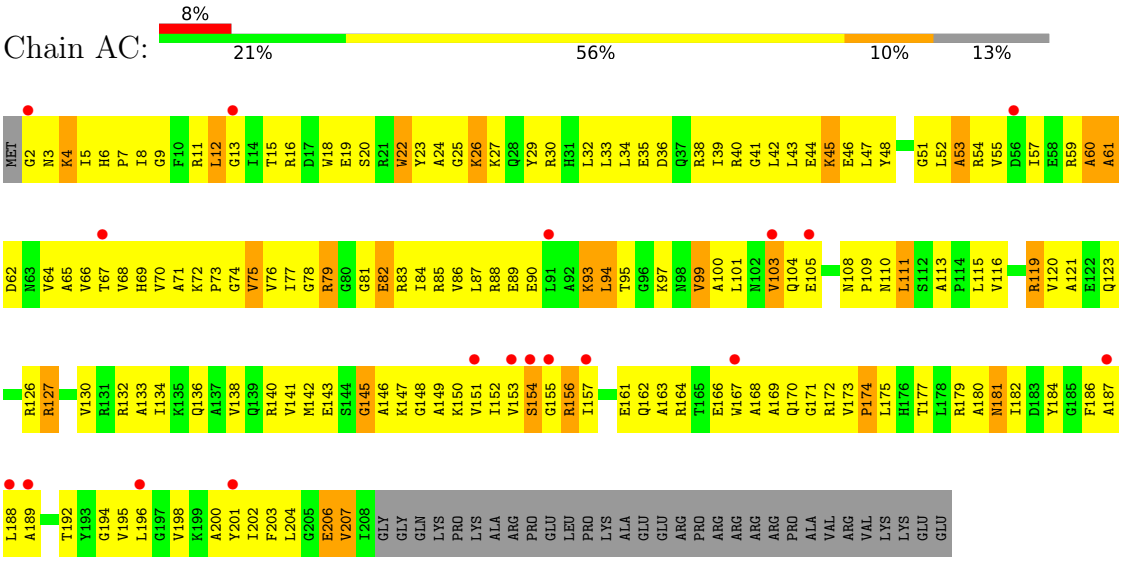




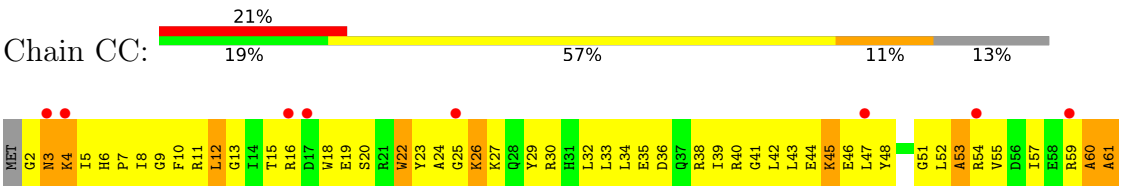
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

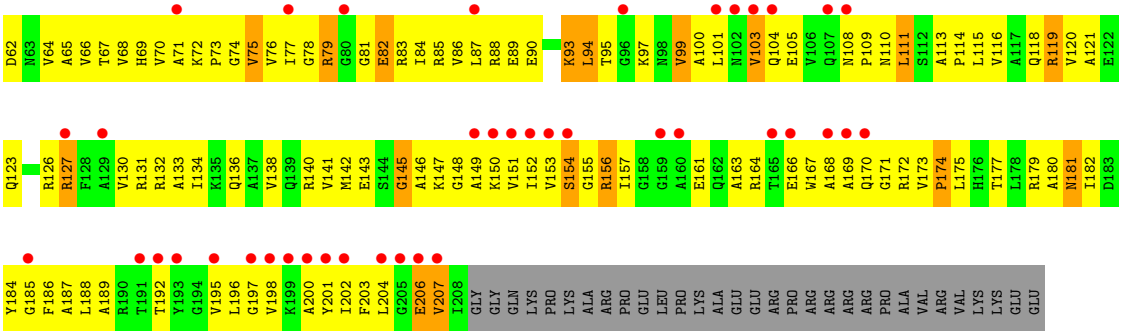


• Molecule 3: 30S RIBOSOMAL PROTEIN S3



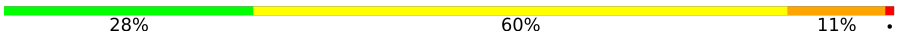
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

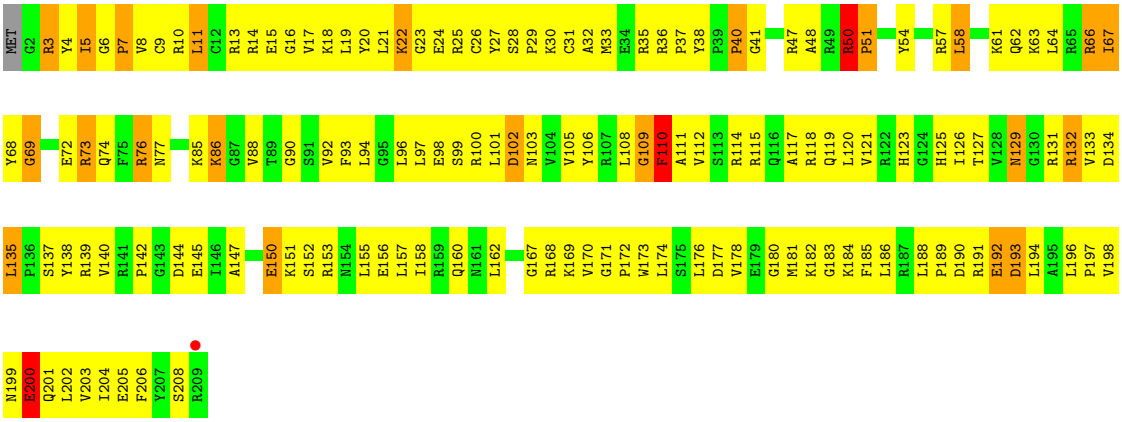




- Molecule 4: 30S RIBOSOMAL PROTEIN S4

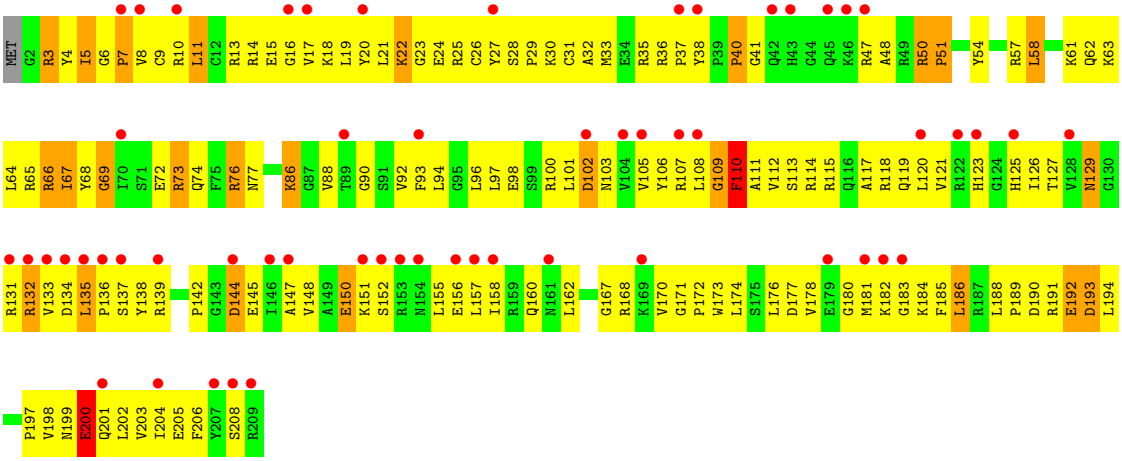
Chain AD:





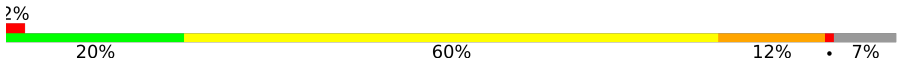
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

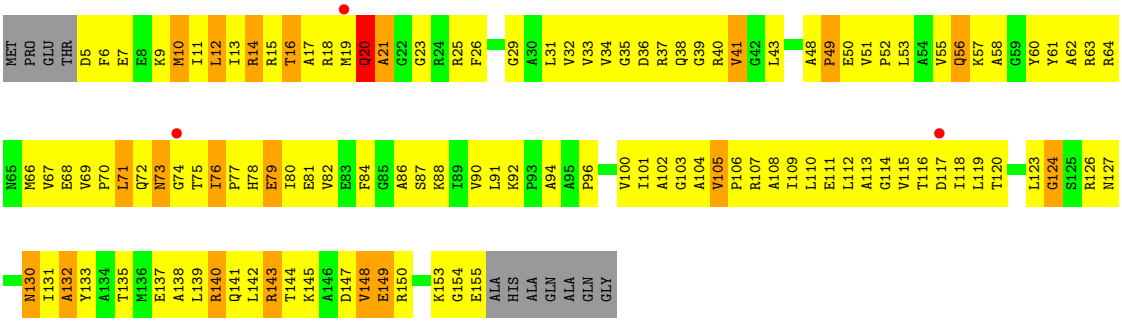
Chain CD:



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

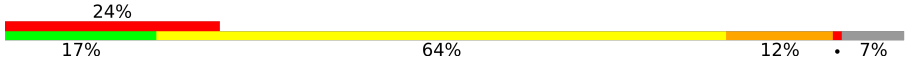
Chain AE:

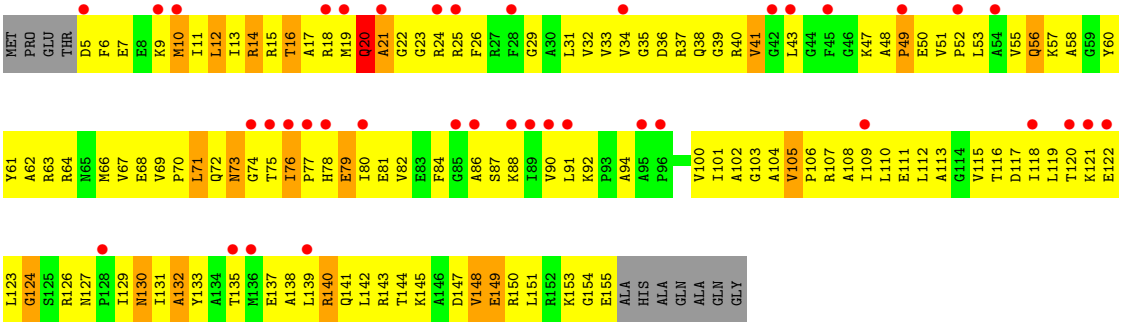




- Molecule 5: 30S RIBOSOMAL PROTEIN S5

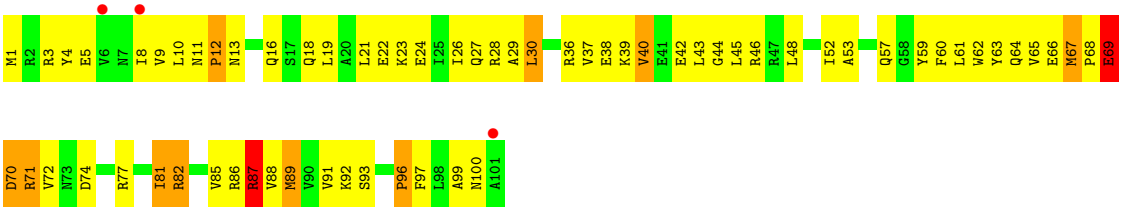
Chain CE:





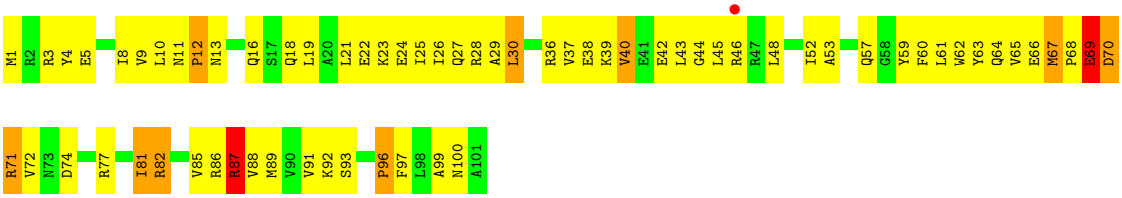
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:

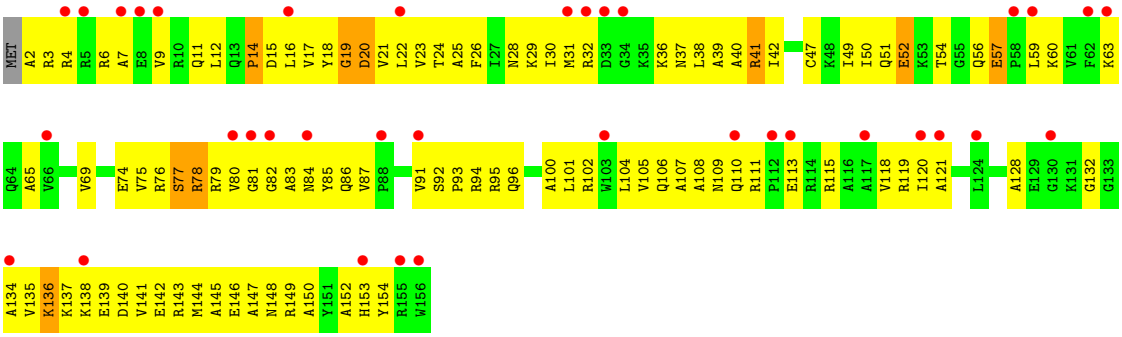


- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:

- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG: 23% 32% 62% 6%

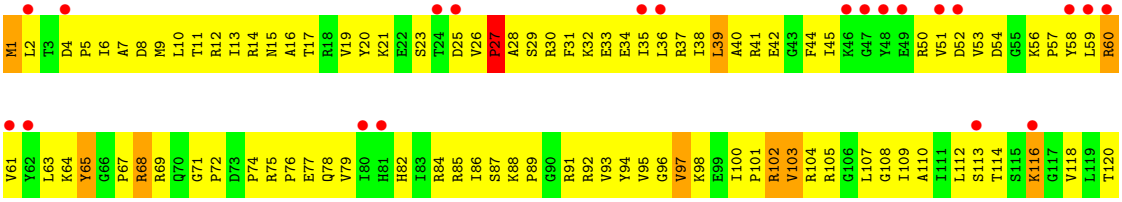


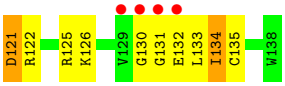
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH: % 22% 69% 8%

- Molecule 8: 30S RIBOSOMAL PROTEIN S8

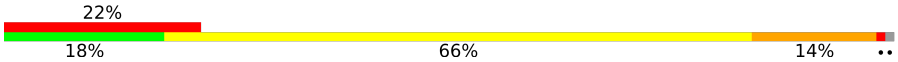
Chain CH: 18% 23% 68% 8%

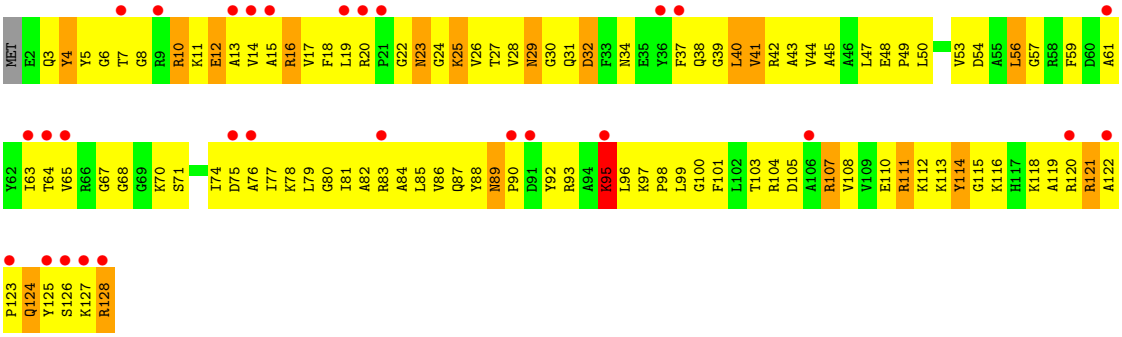




• Molecule 9: 30S RIBOSOMAL PROTEIN S9

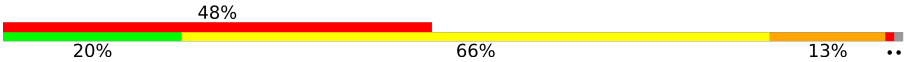
Chain AI:

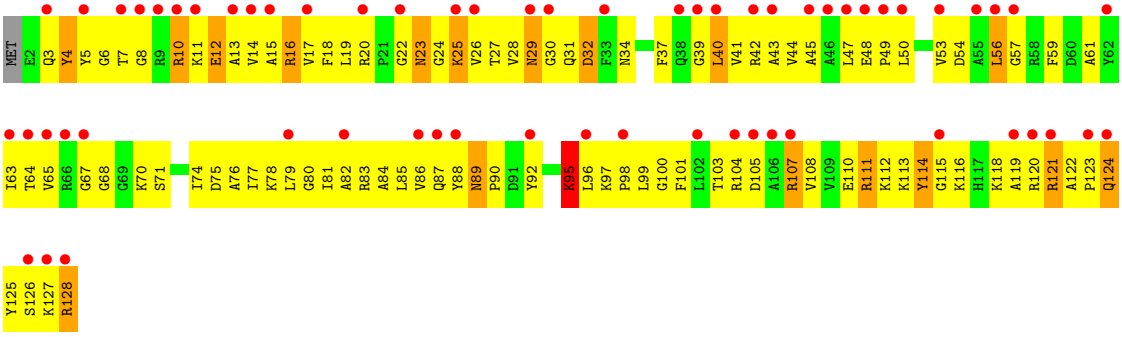




• Molecule 9: 30S RIBOSOMAL PROTEIN S9

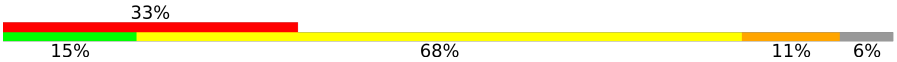
Chain CI:

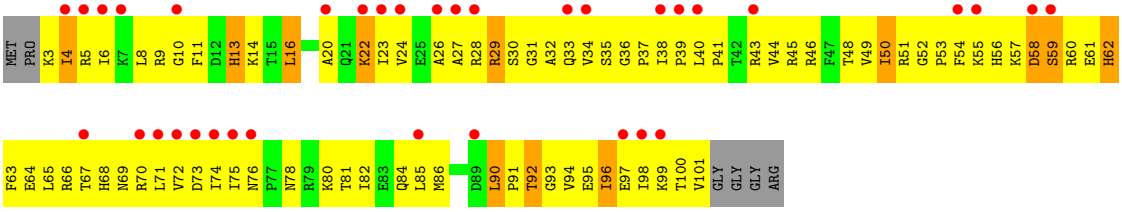




• Molecule 10: 30S RIBOSOMAL PROTEIN S10

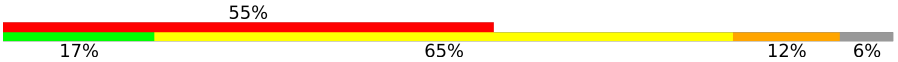
Chain AJ:

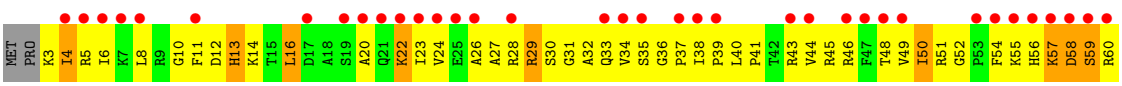


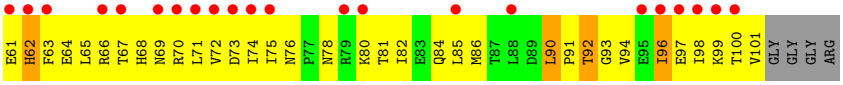


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:

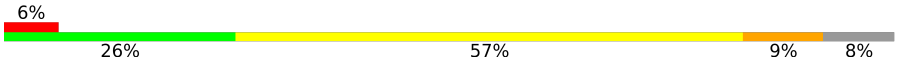


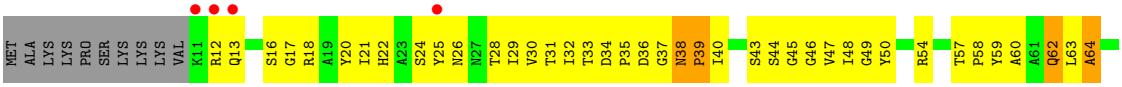


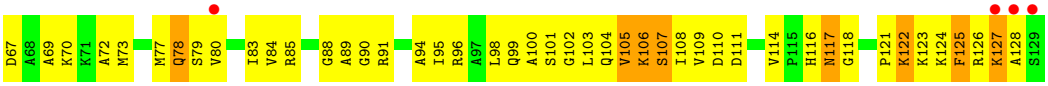


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:

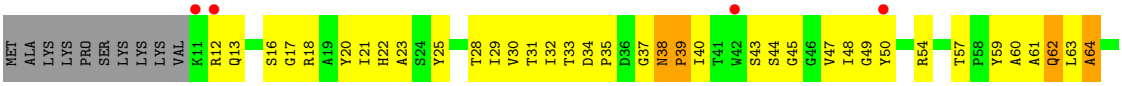


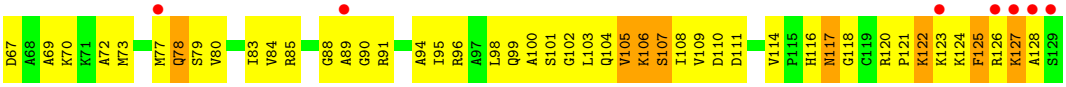




• Molecule 11: 30S RIBOSOMAL PROTEIN S11

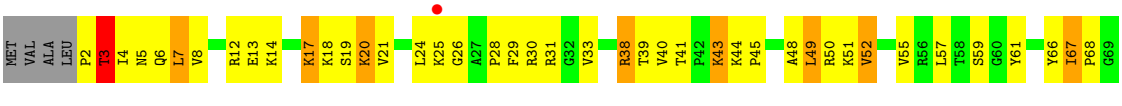
Chain CK:





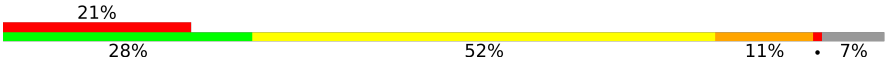
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

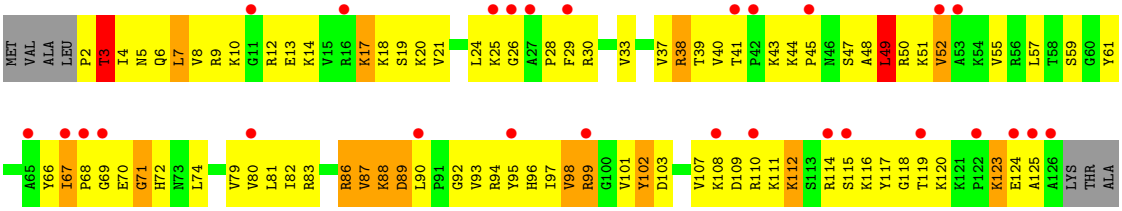
Chain AL:

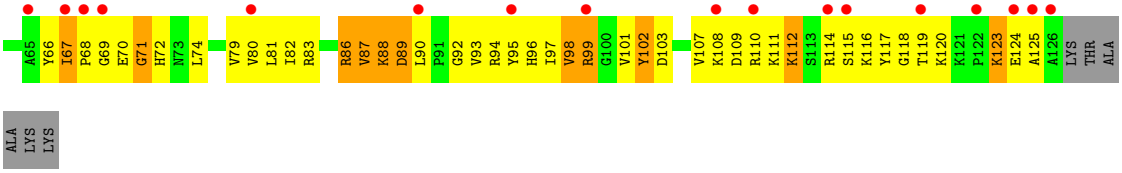


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:

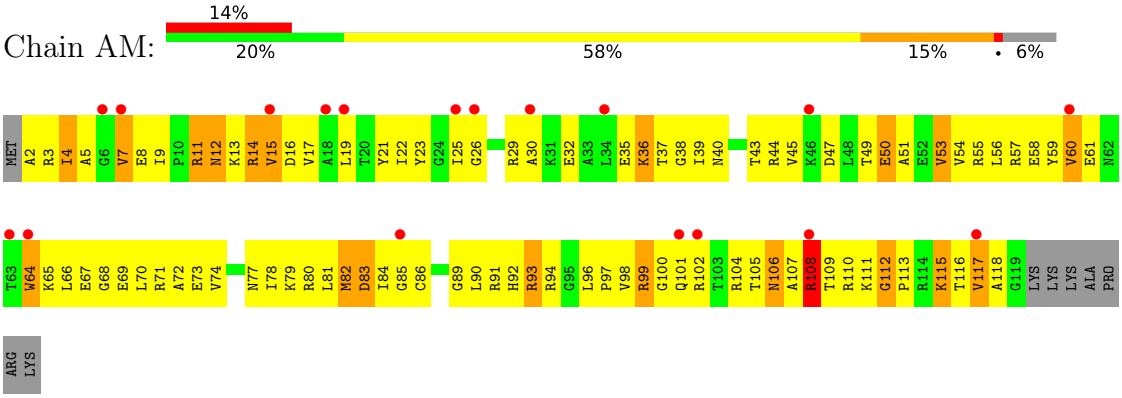






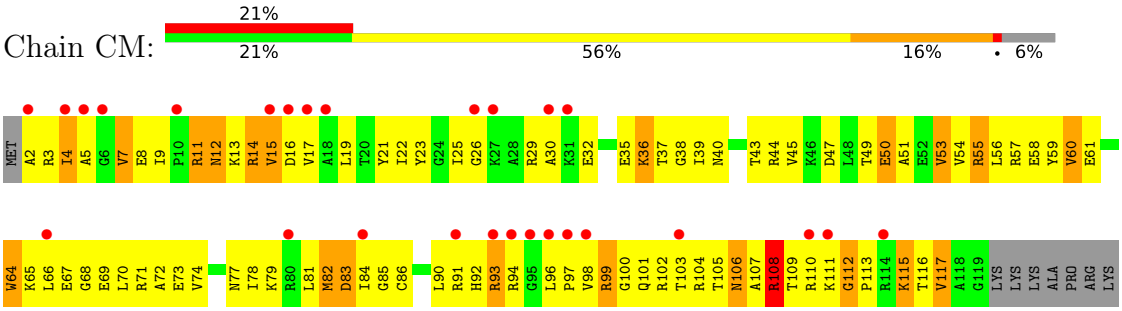
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



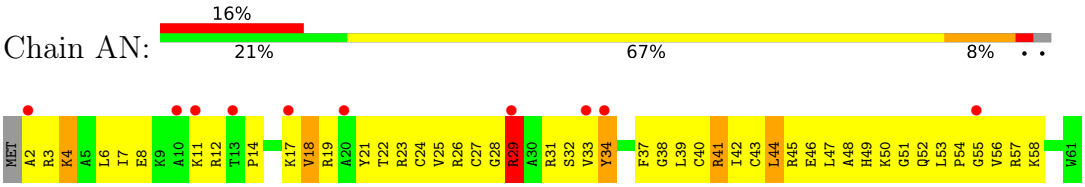
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



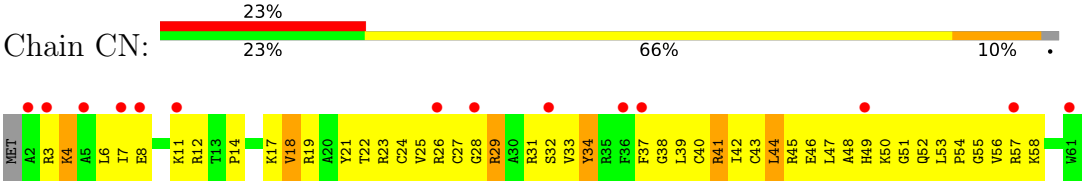
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



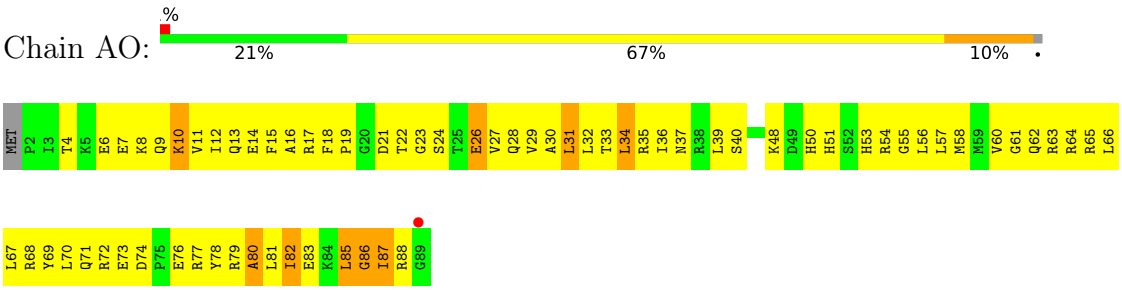
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



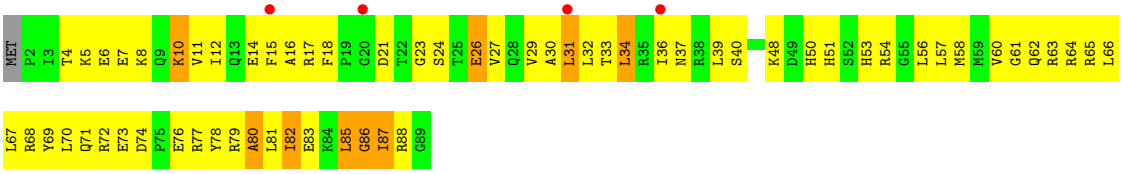
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



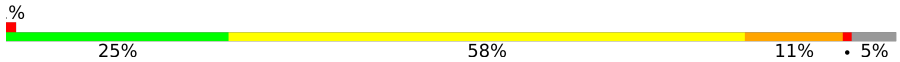
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

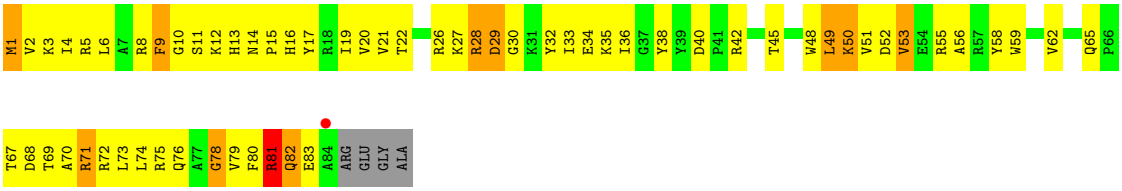
Chain CO:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

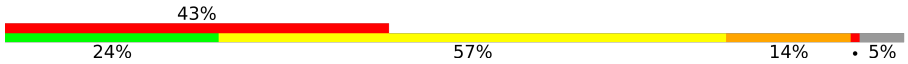
Chain AP:

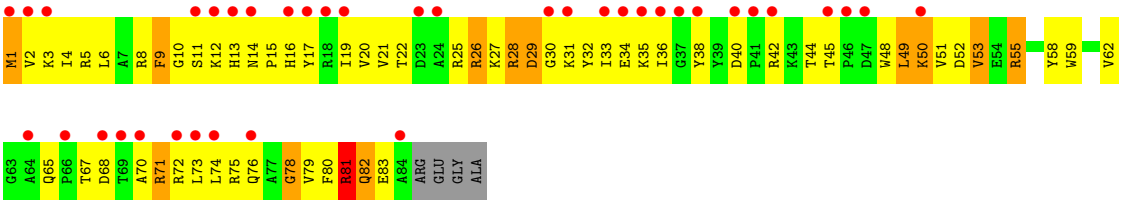




• Molecule 16: 30S RIBOSOMAL PROTEIN S16

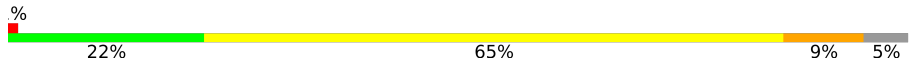
Chain CP:

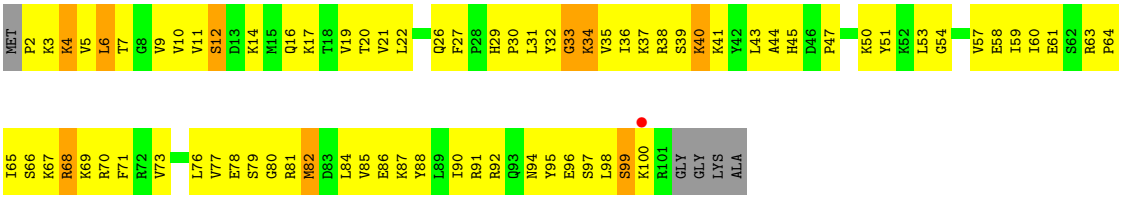




• Molecule 17: 30S RIBOSOMAL PROTEIN S17

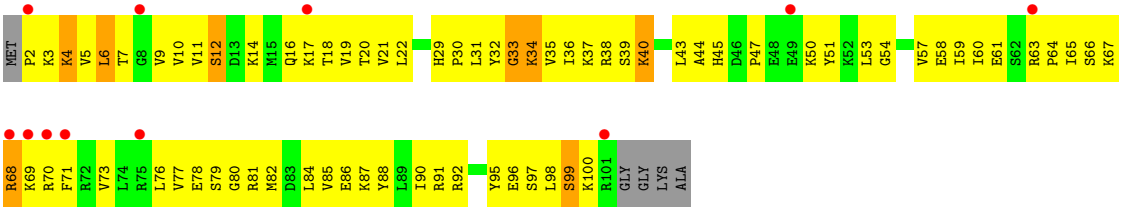
Chain AQ:





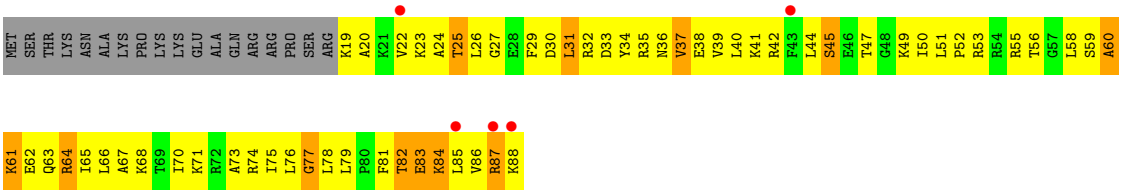
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



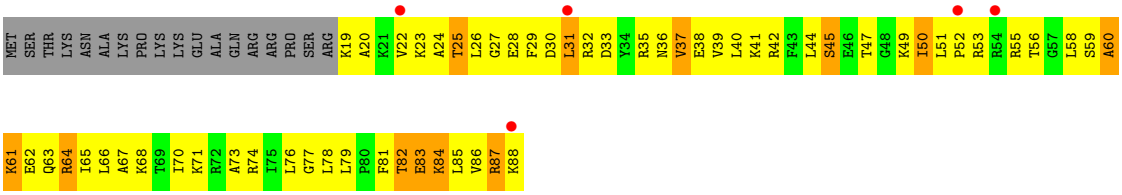
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



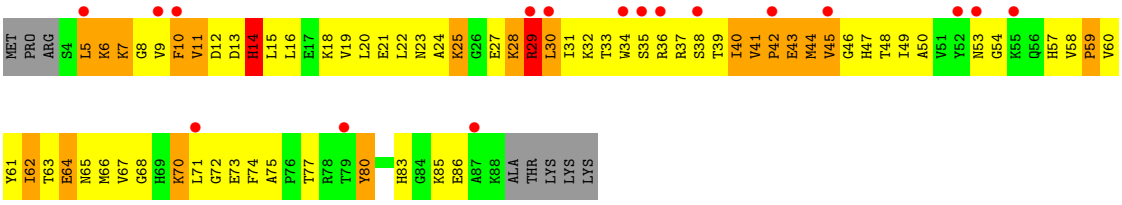
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



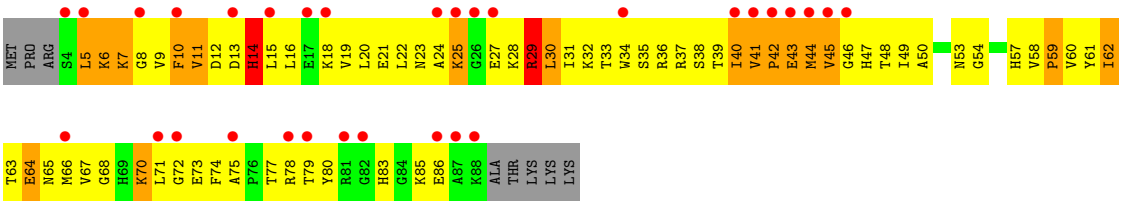
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



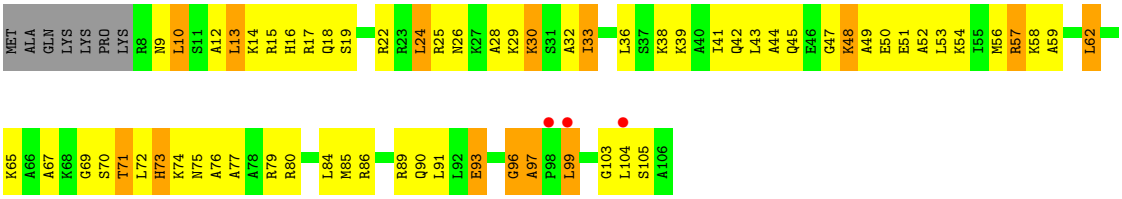
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



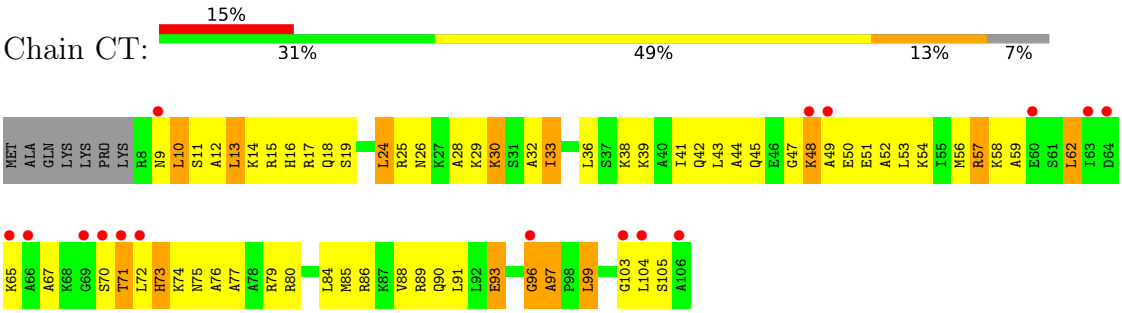
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



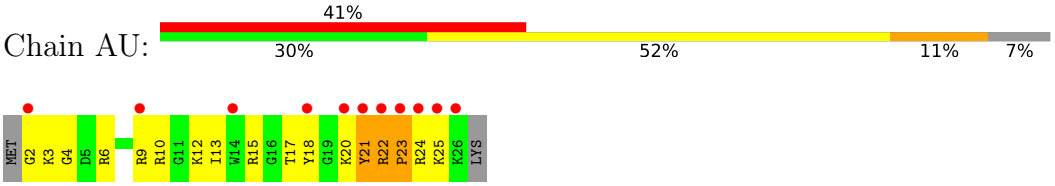
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



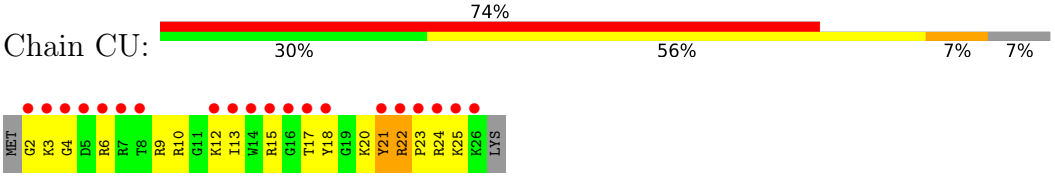
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



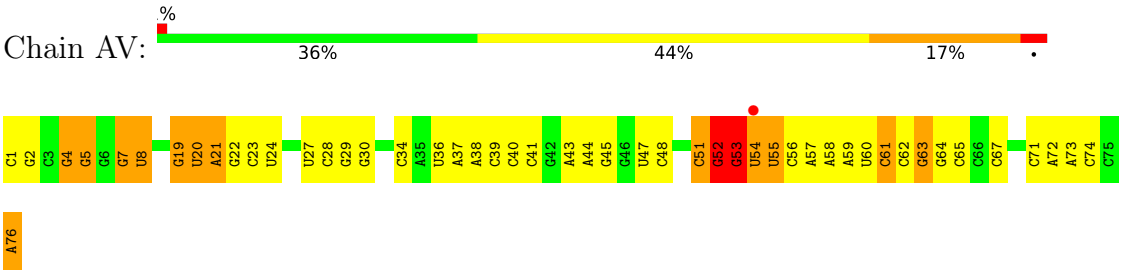
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



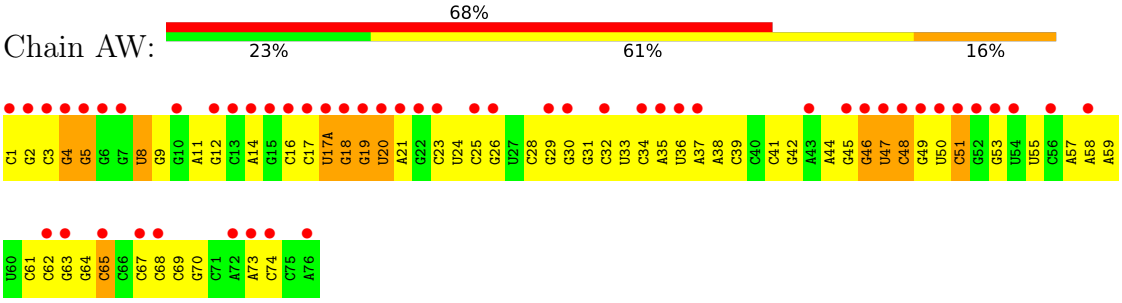
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV:



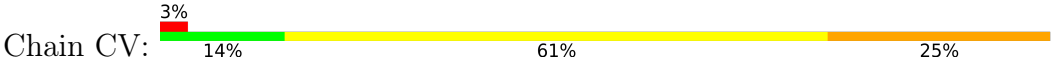
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

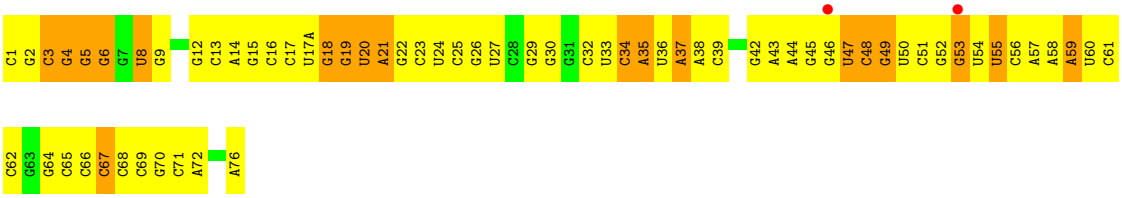
Chain AW:



• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

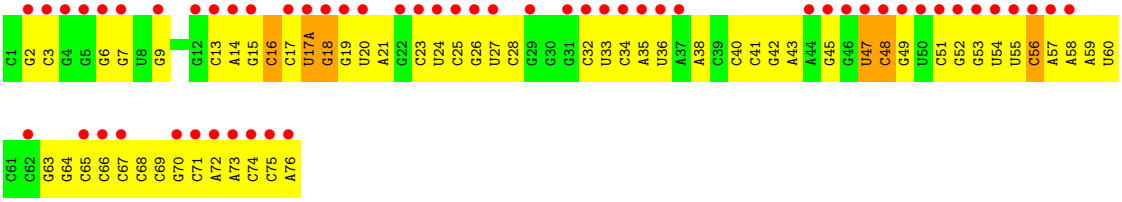
Chain CV:





• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CW:

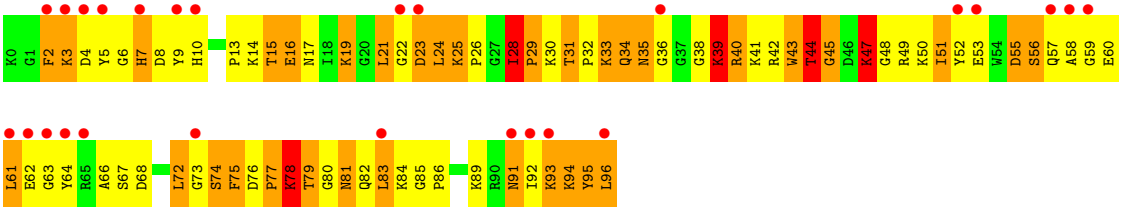


• Molecule 23: MRNA

Chain AX:

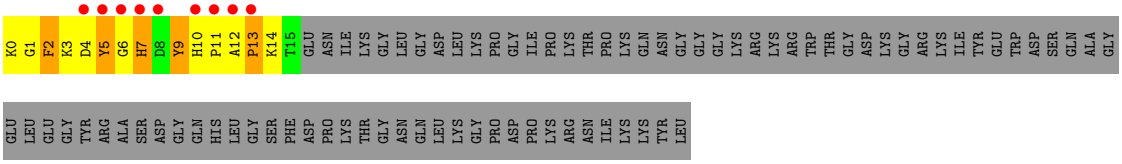
• Molecule 24: COLICIN-E3

Chain AY:



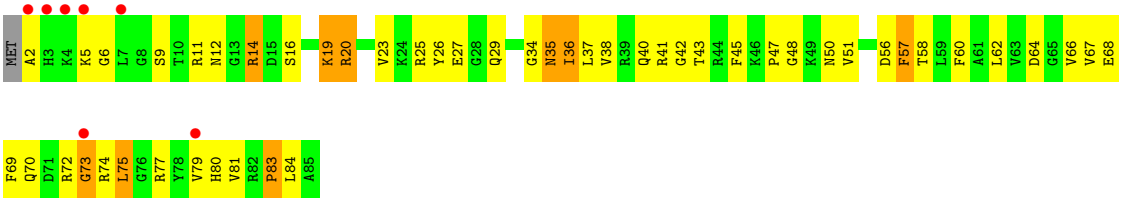
• Molecule 24: COLICIN-E3

Chain CY:



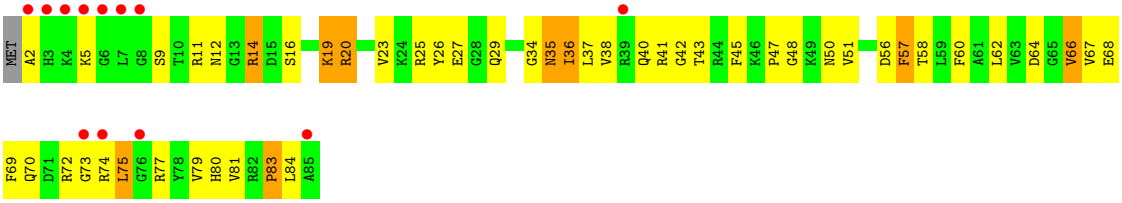
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



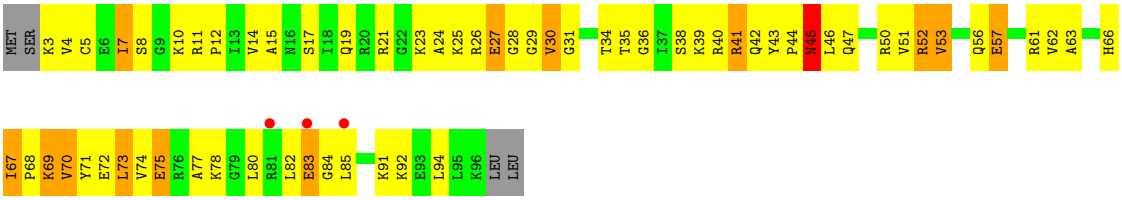
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain D0:



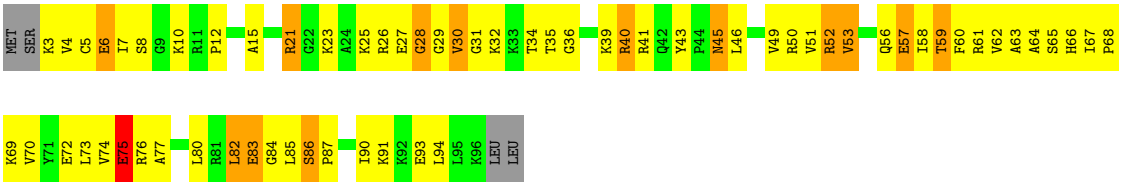
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



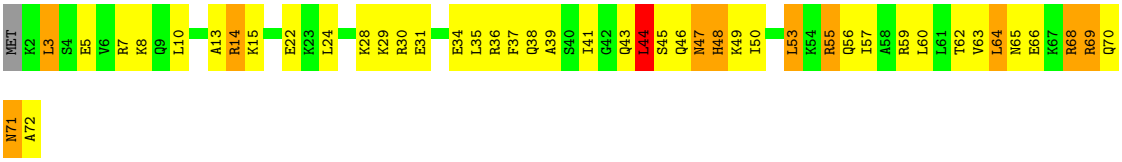
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



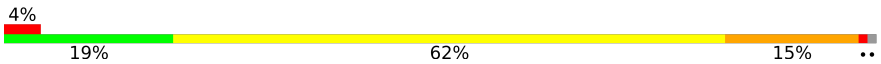
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

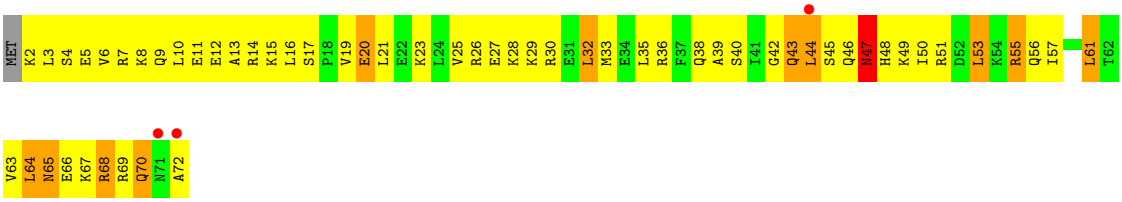
Chain B2:



• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:



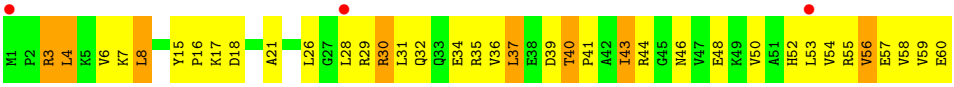


• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:

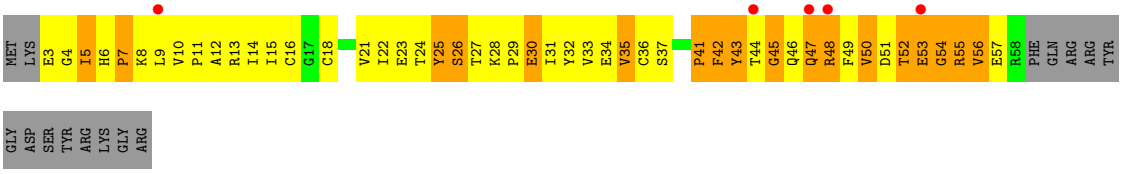
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:



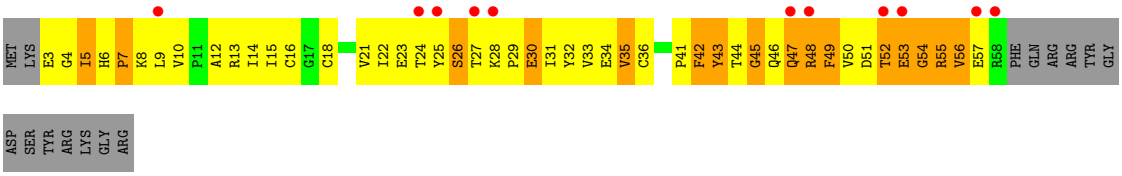
• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



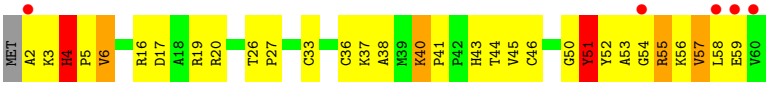
• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain D4:



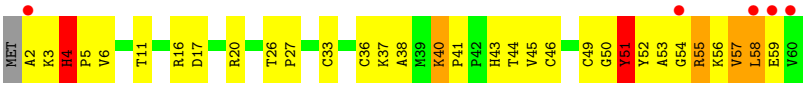
• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



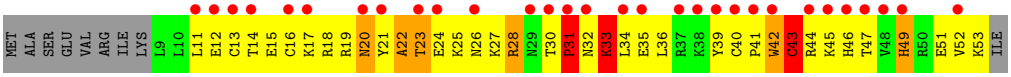
• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5:



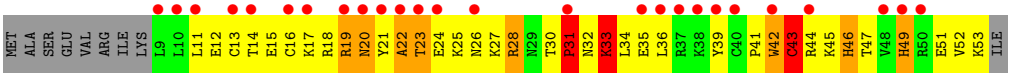
• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:



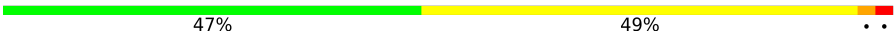
• Molecule 31: 50S RIBOSOMAL PROTEIN L33

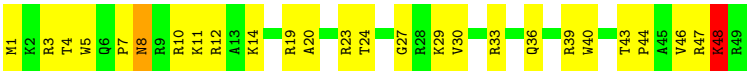
Chain D6:



• Molecule 32: 50S RIBOSOMAL PROTEIN L34

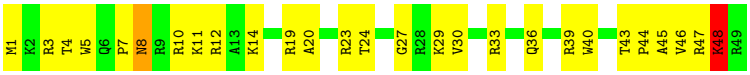
Chain B7:





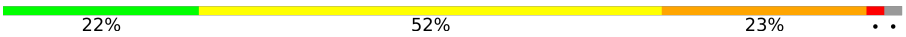
• Molecule 32: 50S RIBOSOMAL PROTEIN L34

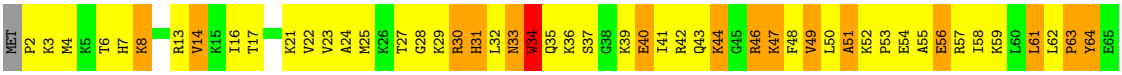
Chain D7:



• Molecule 33: 50S RIBOSOMAL PROTEIN L35

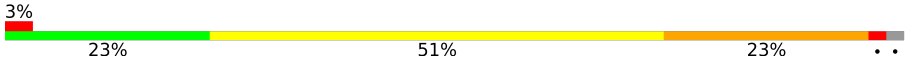
Chain B8:

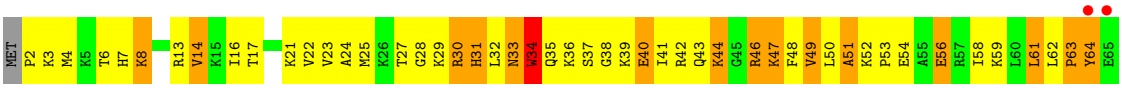




• Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8:





• Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9: 43% 32% 57% 8%

MET K2 V3 R4 A5 S6 V7 K8 R9 I10 C11 D12 K13 C14 K15 V16 I17 R18 R19 H20 G21 R22 V23 Y24 V25 I26 C27 E28 N29 P30 K31 H32 K33 Q34 R35 Q36 G37

• Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9: 41% 27% 62% 8%

MET K2 V3 R4 A5 S6 V7 K8 R9 I10 C11 D12 K13 C14 K15 V16 I17 R18 R19 H20 G21 R22 V23 Y24 V25 I26 C27 E28 N29 P30 K31 H32 K33 Q34 R35 Q36 G37

• Molecule 35: 23S ribosomal RNA

Chain BA: 4% 35% 50% 12%

A6 G7 A8 U9 G10 G11 U12 A13 A14 G15 G16 G17 C18 C19 C20 A21 C22 G26 G27 A28 U29 G30 C31 C32 U33 C34 G35 A38 C39 C40 C41 G42 C45 A49 U50 G51 C57 G58 A64 C65 C66 C69 G70 A71 U72 A73 A74 G75 C76 C77 G80 G81

G82 G83 A84 G88 G89 U90 A92 G93 C94 G94A G98 U99 G100 G102 C105 C106 C107 U108 G109 G110 A111 U112 G113 U114 C115 C116 G117 A118 A119 U120 G121 A127 C128 C129 G136 C137 G139 G139A G140 A141 A142 C142A G143 C143A C144 G145 G146 U147 C148 A149 C150 C151 G152 C153 G154

C154A U U U157 U158 G171 C172 G175 A181 A182 C183 C184 U185 G186 G187 C192 U193 G194 A195 A196 A197 C198 C201 U202 C203 A204 G205 U206 A207 C208 C209 G212 A213 G214 G215 A216 G217 A218 A221 A222 A223 G224 A225 G226 A229 U230 C231 G232 A233 C234 U235 C236 C237

C238 A241 G242 U243 A244 G245 C246 G247 G248 C249 C250 A251 G252 C253 G254 A255 A256 A257 G258 C259 C264 A265 G266 C267 C268 U269 A270 A271 A271A C271B C271C C271D U271E C271F C271G C271H C271I C271J U271K U271L C271M U271N C271O C271P C271Q C271R C271S C271T C271U C271V C271W C271X U271Y C271Z G272 C272B C272C C272D

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G337 G338 U339 A340 G348 G349 G352 G353 G354 G355 G356 A357 U358 A359 G360 G361 U362 G363 A363A G363B G363C A363F C364 C365 C366 G372 C375 C376 U380 U384 C385 G386 U387 G388 G389 A394 U395 G396 G397 C404 U405 G406 C409 G410 G411 A412 C413 C414 A415

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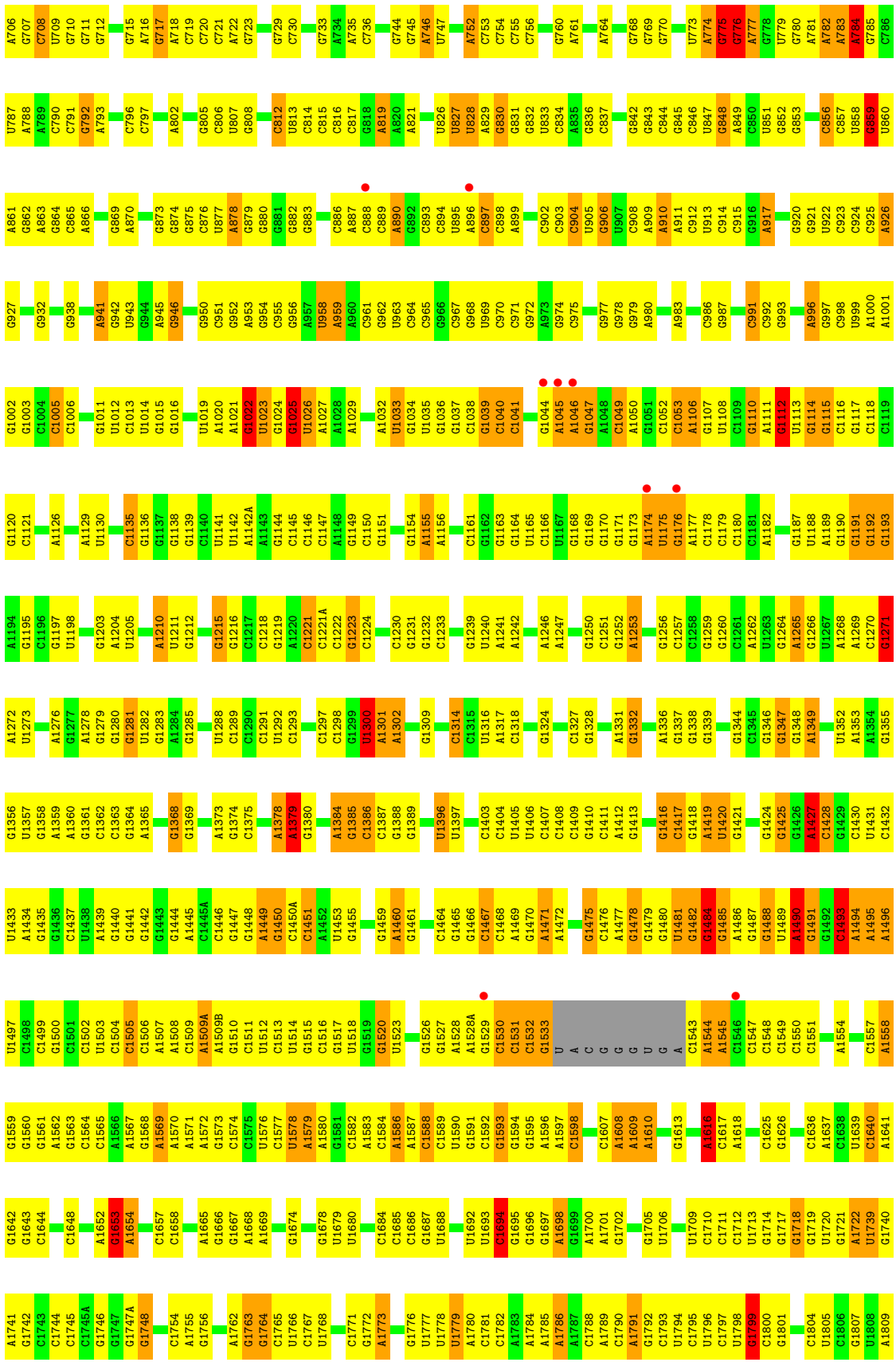
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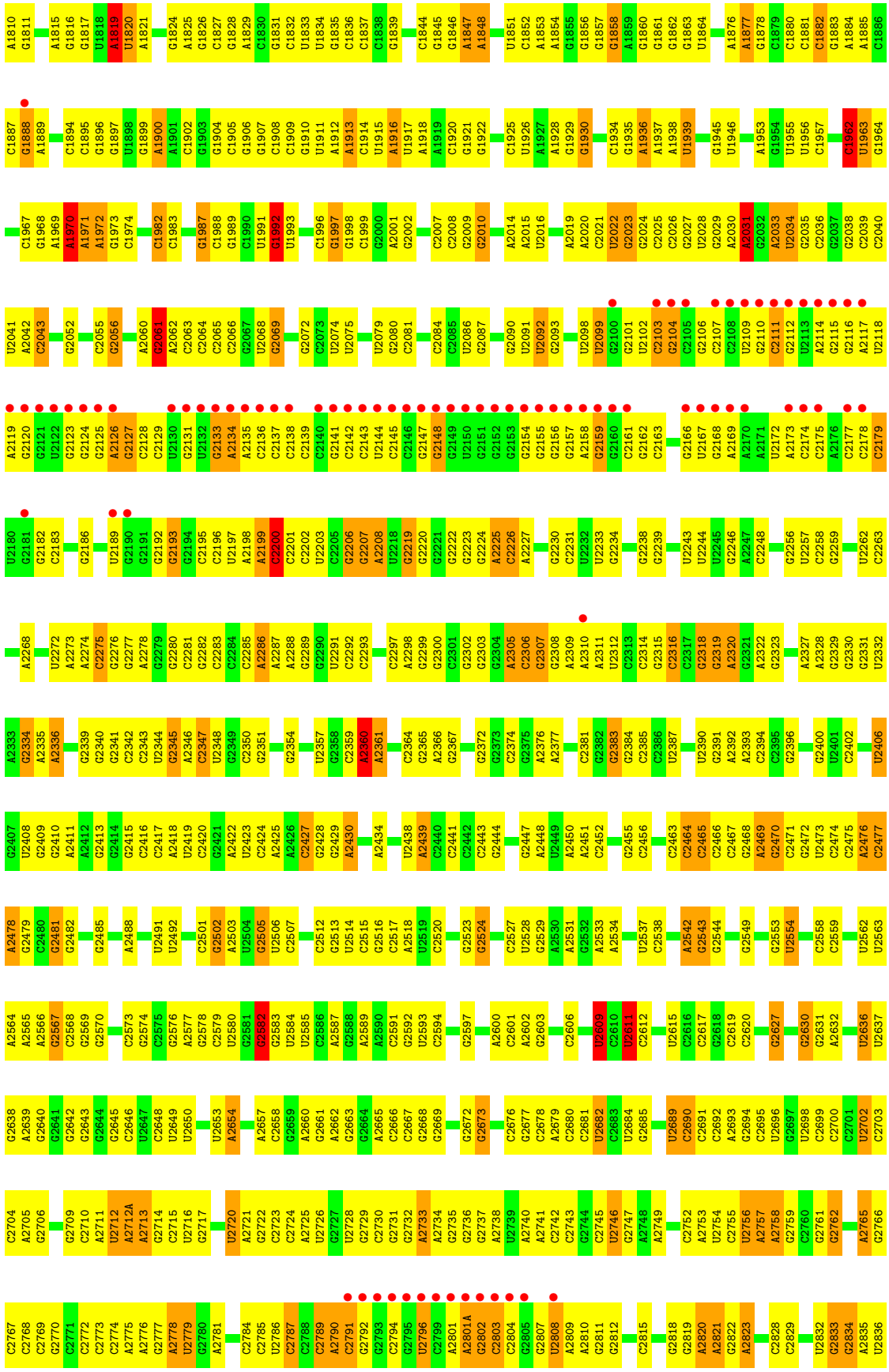
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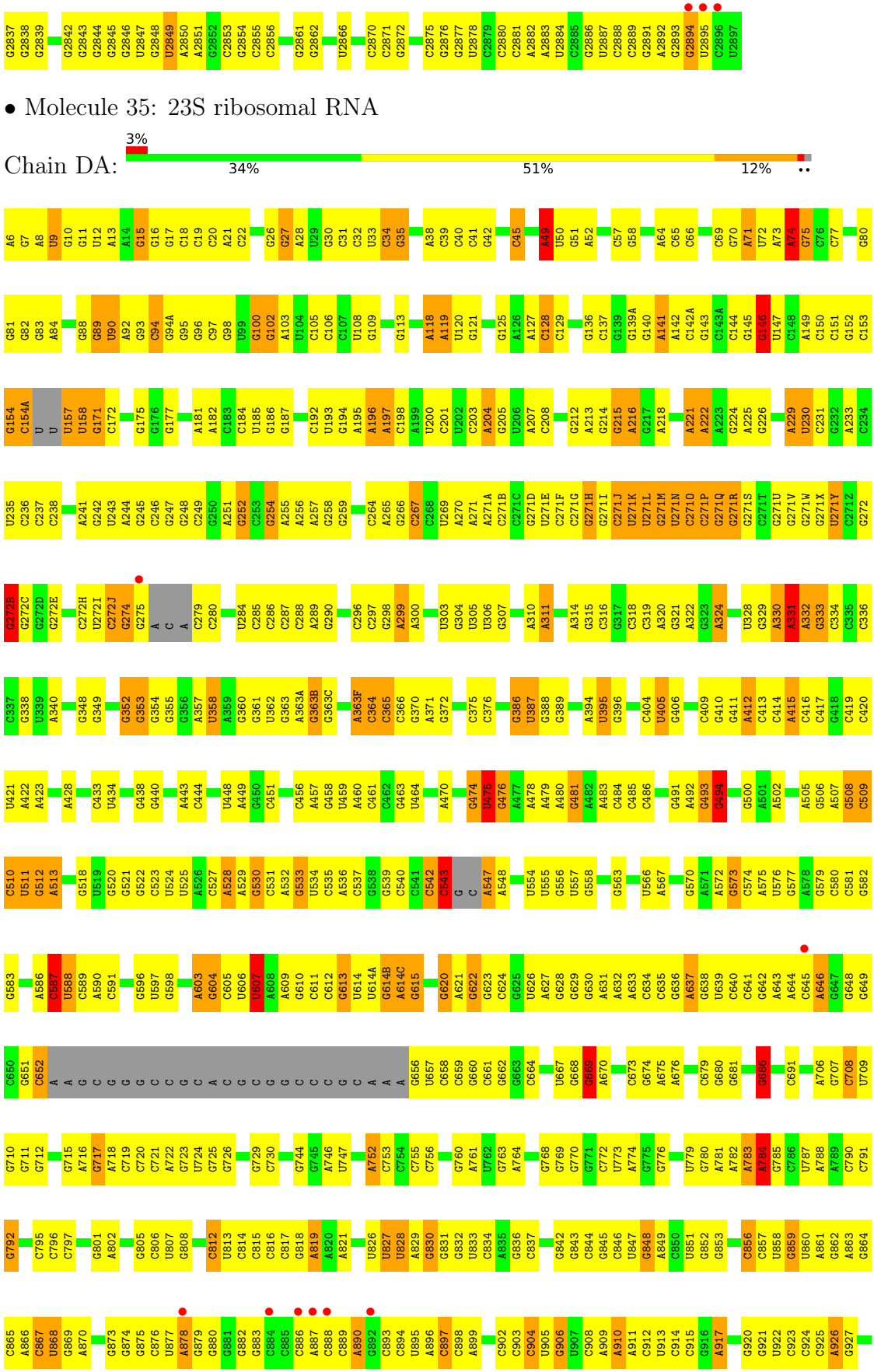
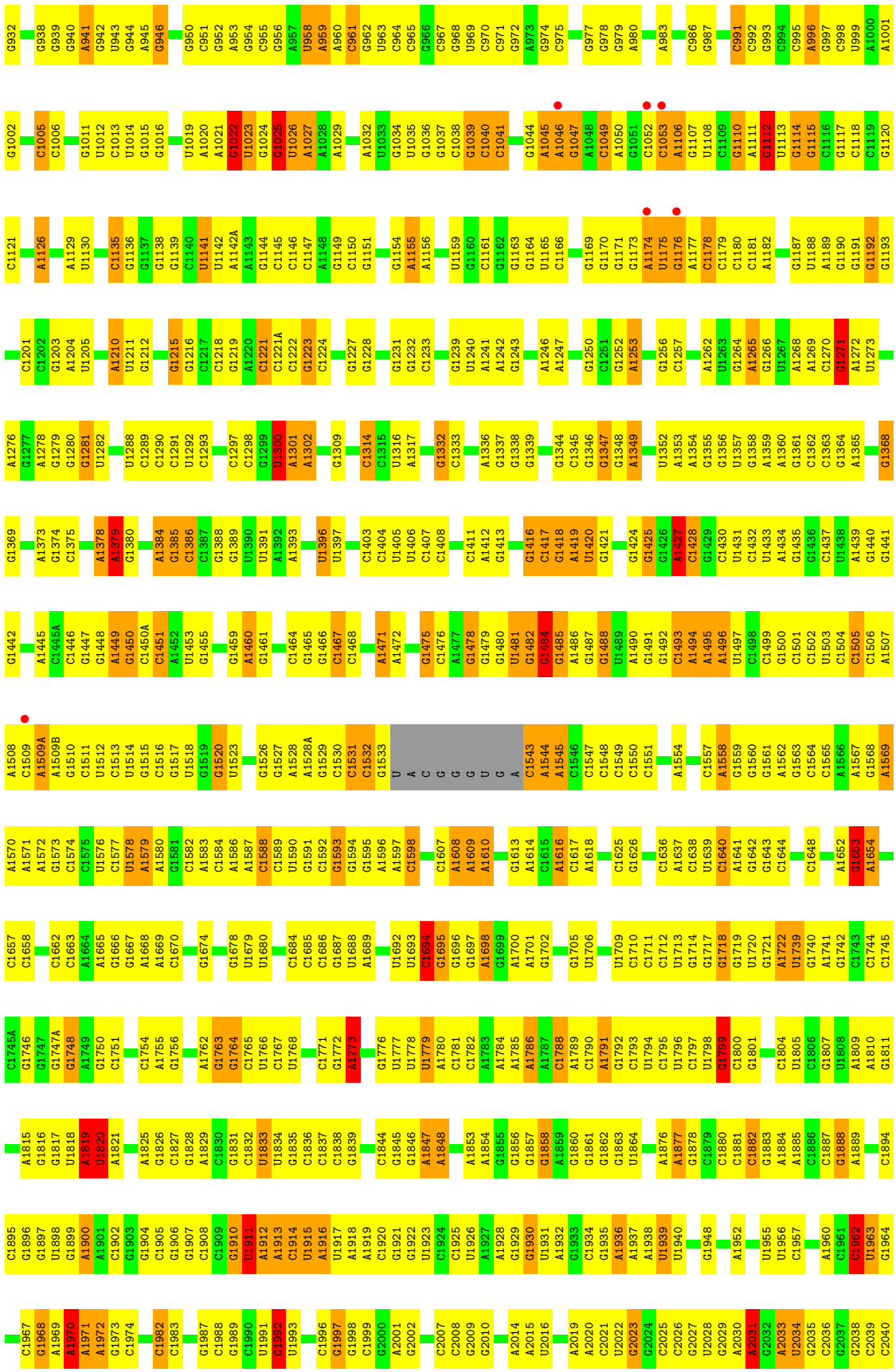

• Molecule 35: 23S ribosomal RNA
Chain DA:
3%
34%
51%
12%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C1201 C1202 G1203 A1204 U1205 A1210 U1211 G1212 G1215 G1216 C1217 C1218 G1219 A1220 C1221 C1221A C1222 G1223 C1224 G1227 G1228 G1231 G1232 C1233 G1239 U1240 A1241 A1242 G1243 A1246 A1247 G1250 C1251 G1252 A1253 G1256 C1257 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273
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G1369 A1373 G1374 C1375 A1378 A1379 G1380 A1384 G1385 C1386 C1387 G1388 G1389 U1390 U1391 A1392 A1393 U1396 U1397 C1403 C1404 U1405 U1406 C1407 C1408 C1411 A1412 G1413 C1416 C1417 G1418 A1419 U1420 G1421 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 G1435 G1436 C1437 U1438 A1439 G1440 G1441
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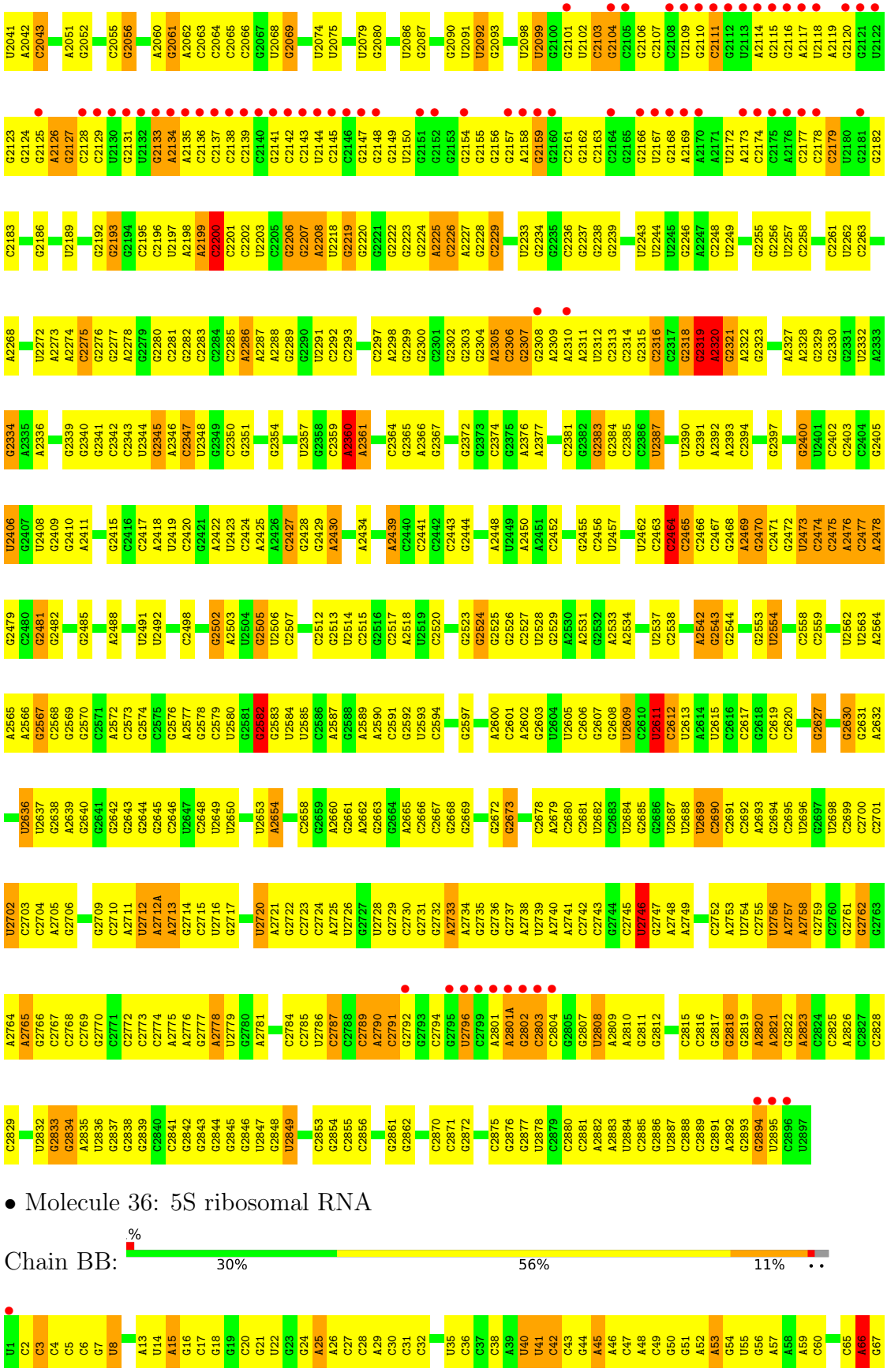
A1815 G1816 G1817 U1818 A1819 U1820 A1821 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833 U1834 G1835 C1836 C1837 C1838 G1839 C1844 G1845 G1846 A1847 A1848 A1853 A1854 G1855 G1856 G1857 G1858 A1859 C1860 G1861 C1862 G1863 U1864 A1876 A1877 G1878 C1879 C1880 C1881 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 C1894
C1895 G1896 G1897 U1898 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 G1948 A1952 U1955 U1956 C1957 A1960 C1961 C1962 U1963 G1964
C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 C1982 C1983 G1987 C1988 G1989 C1990 U1991 G1992 U1993 C1996 G1997 G1998 C1999 G2000 A2001 G2002 C2007 C2008 G2009 G2010 A2014 A2015 U2016 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040

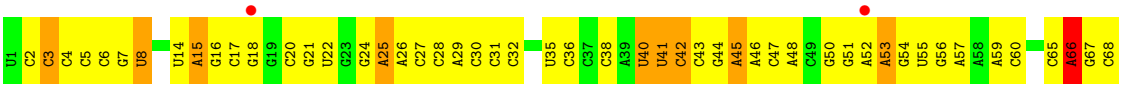


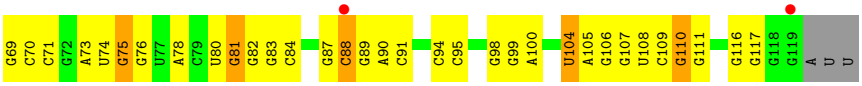
• Molecule 36: 5S ribosomal RNA

Chain BB:

- Molecule 36: 5S ribosomal RNA

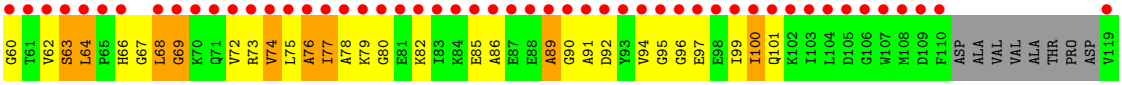
Chain DB:

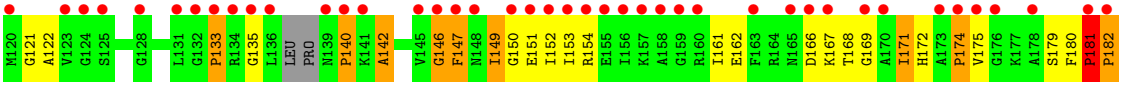


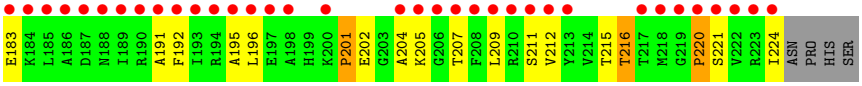


- Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC:

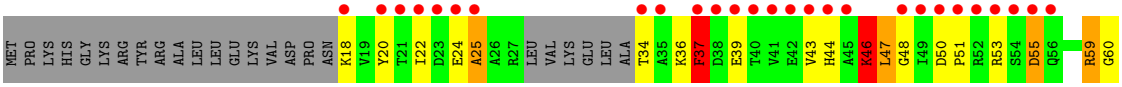


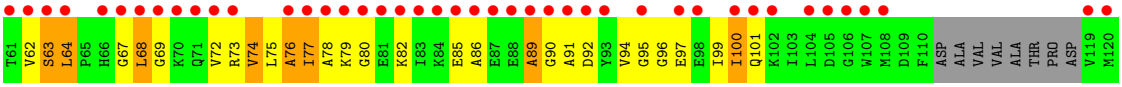


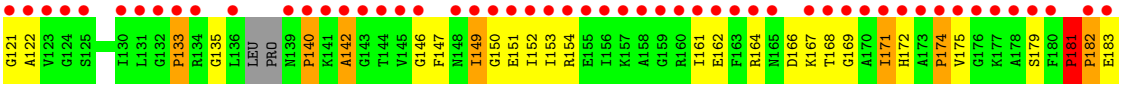


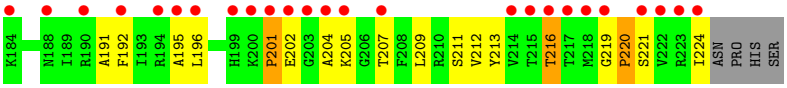
- Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain DC:



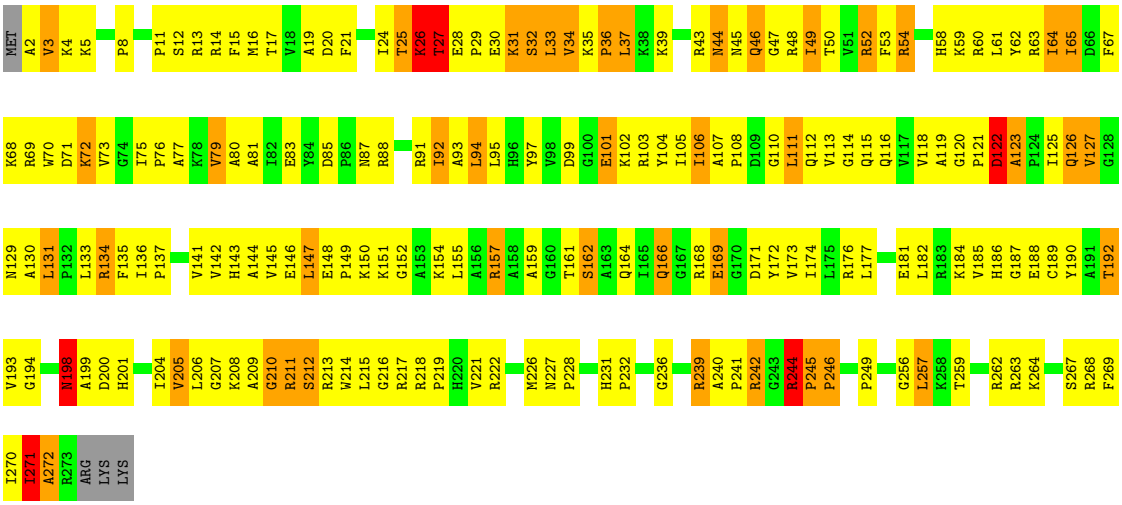






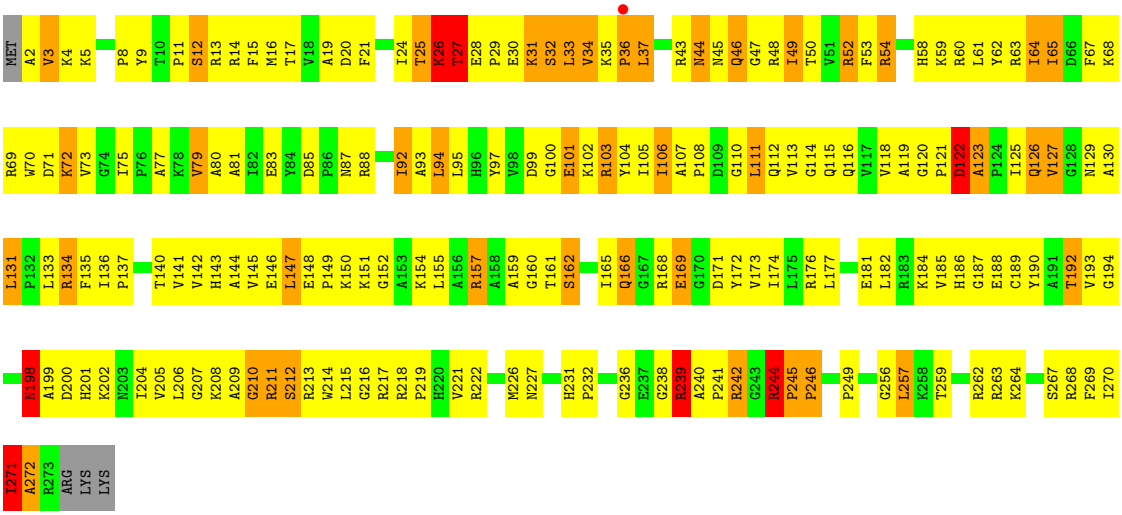
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD: 29% 52% 16%



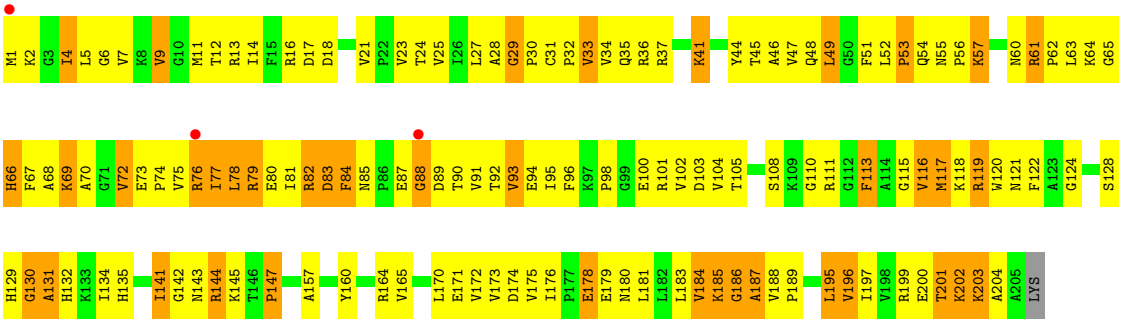
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD: 28% 53% 16%



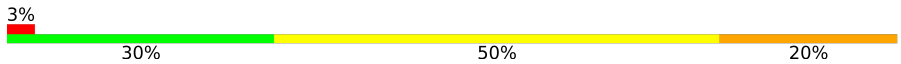
- Molecule 39: 50S RIBOSOMAL PROTEIN L3

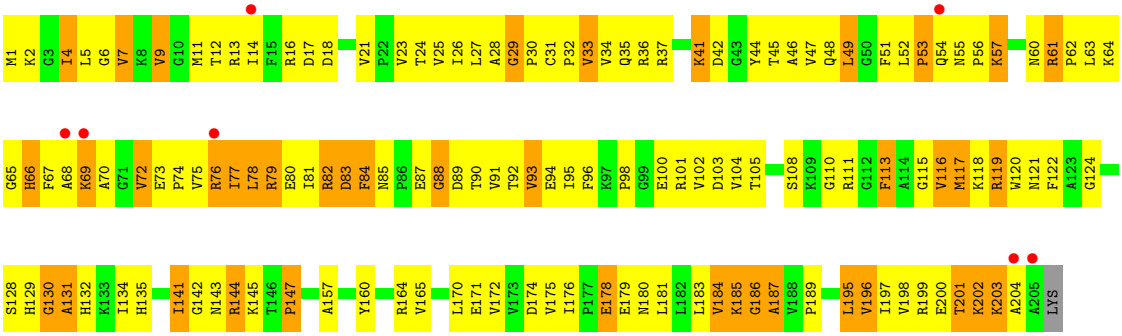
Chain BE: % 31% 50% 19%



• Molecule 39: 50S RIBOSOMAL PROTEIN L3

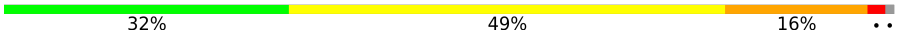
Chain DE:

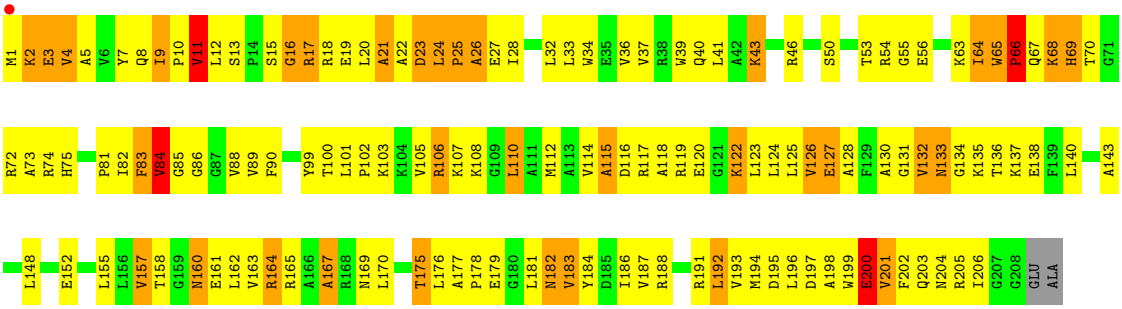




• Molecule 40: 50S RIBOSOMAL PROTEIN L4

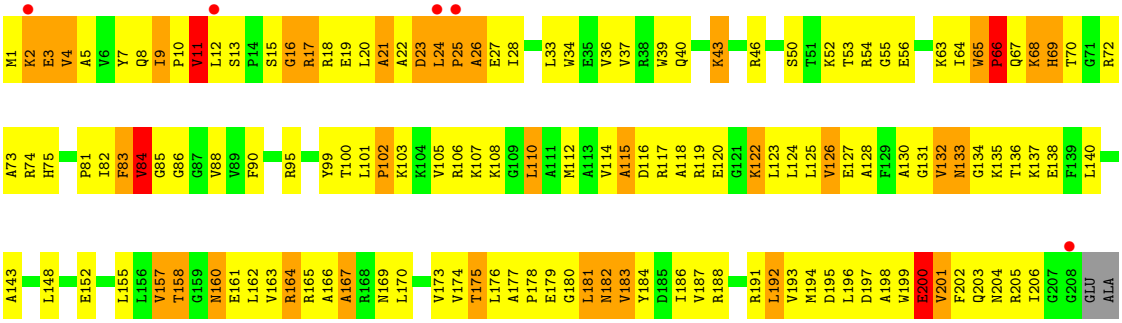
Chain BF:





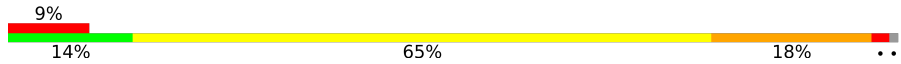
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

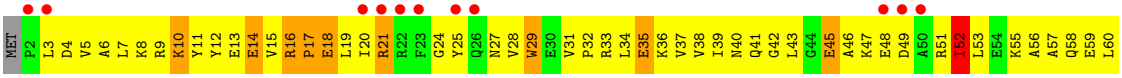
Chain DF:

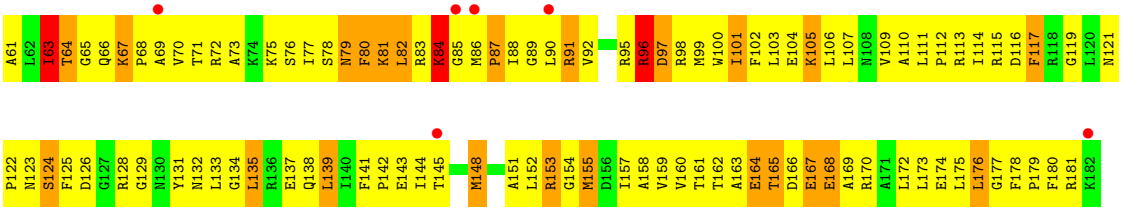


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:

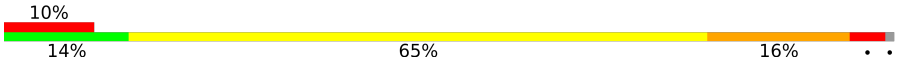


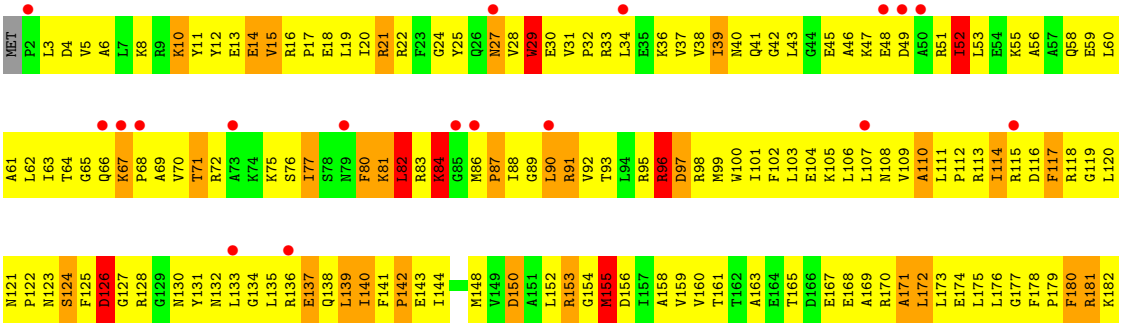




- Molecule 41: 50S RIBOSOMAL PROTEIN L5

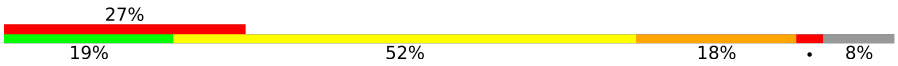
Chain DG:

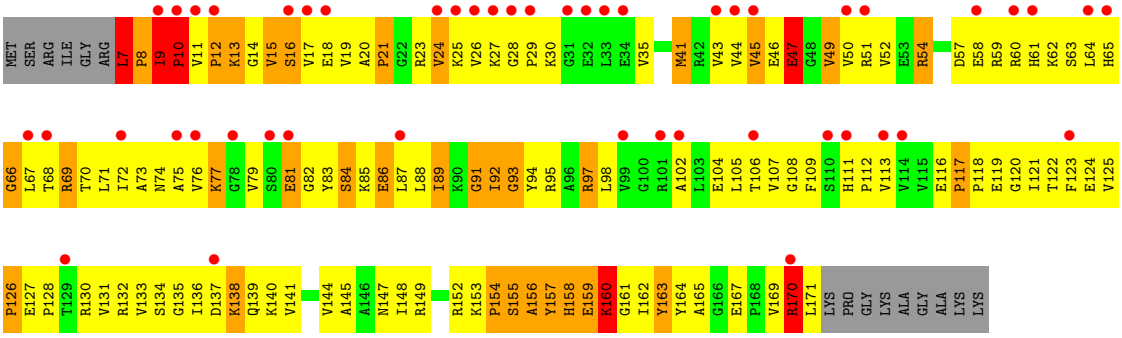




- Molecule 42: 50S RIBOSOMAL PROTEIN L6

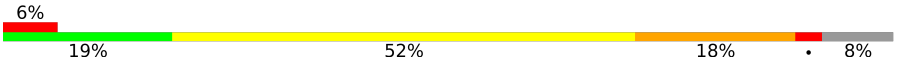
Chain BH:

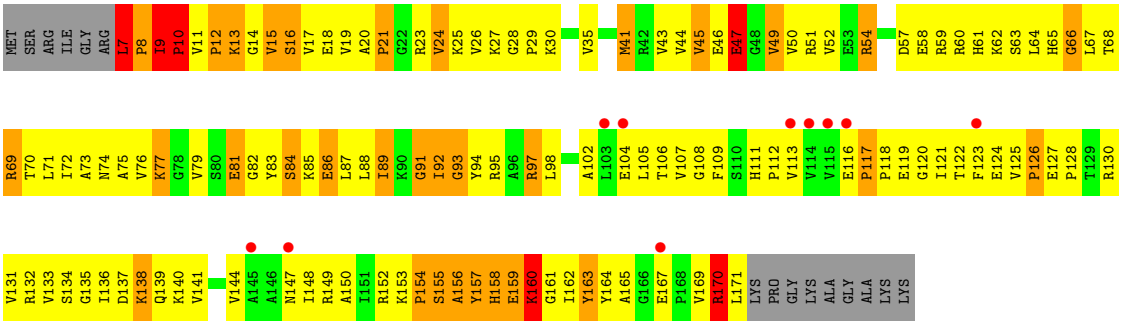




- Molecule 42: 50S RIBOSOMAL PROTEIN L6

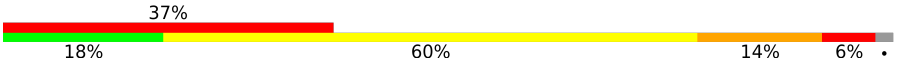
Chain DH:

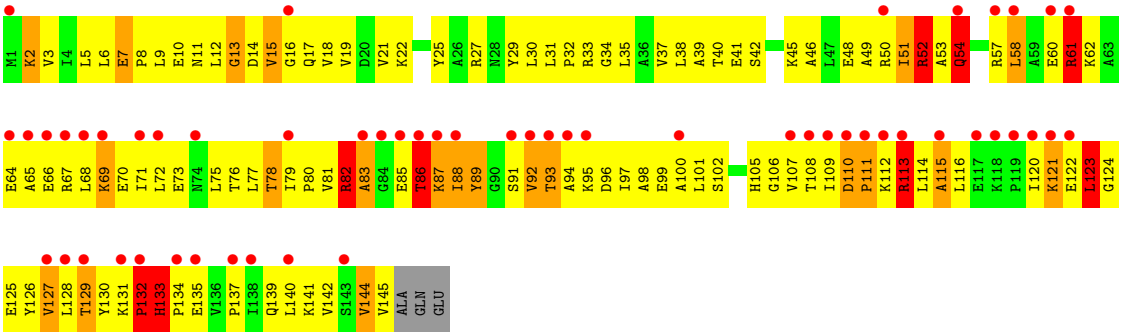




- Molecule 43: 50S RIBOSOMAL PROTEIN L9

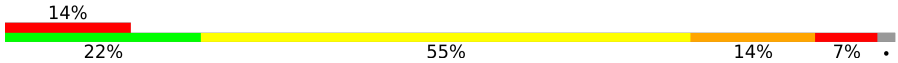
Chain BI:

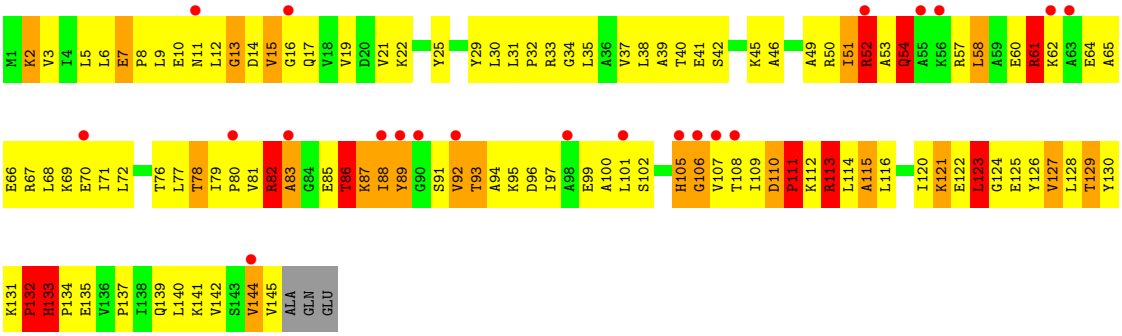




- Molecule 43: 50S RIBOSOMAL PROTEIN L9

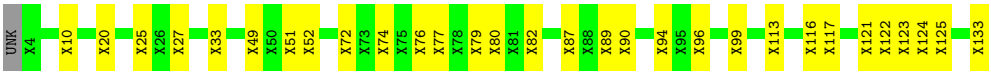
Chain DI:





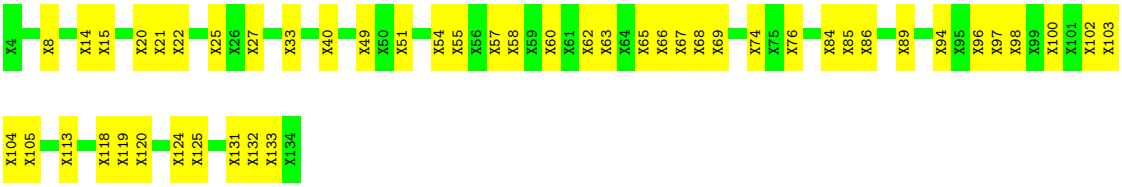
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



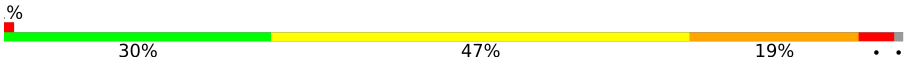
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

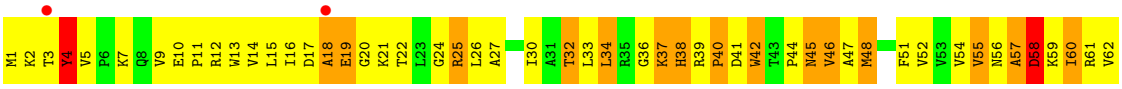
Chain DJ:

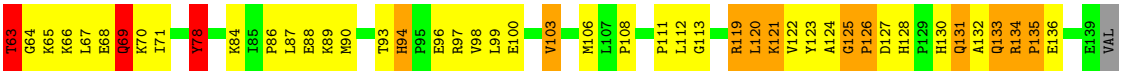


- Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain BN:

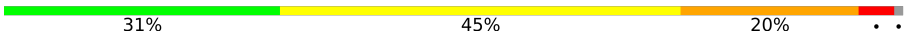






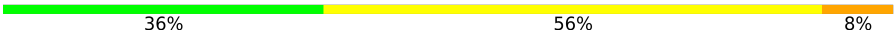
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

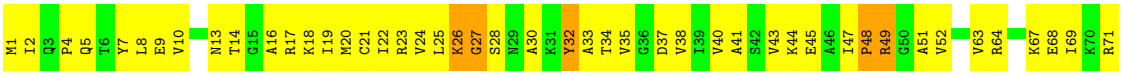
Chain DN:

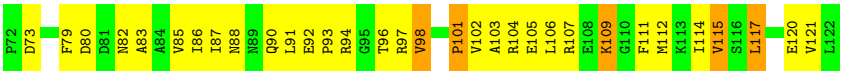


• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO:

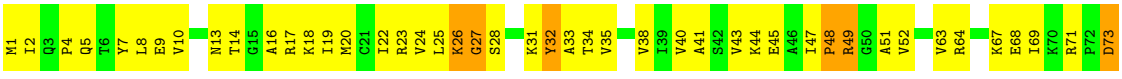


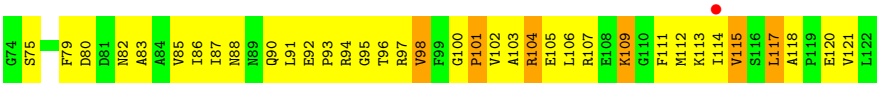




• Molecule 46: 50S RIBOSOMAL PROTEIN L14

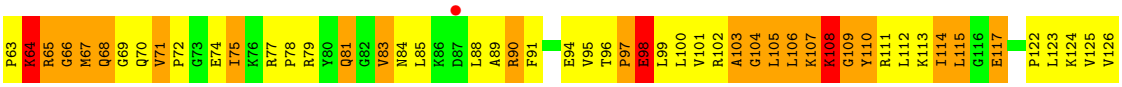
Chain DO:

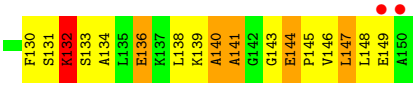




• Molecule 47: 50S RIBOSOMAL PROTEIN L15

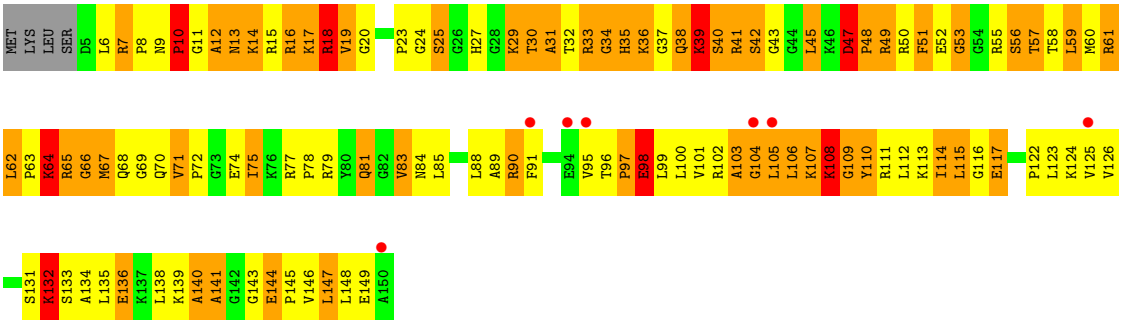
Chain BP:





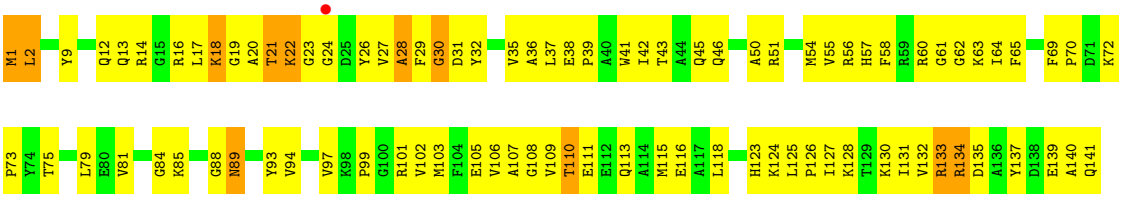
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain DP:



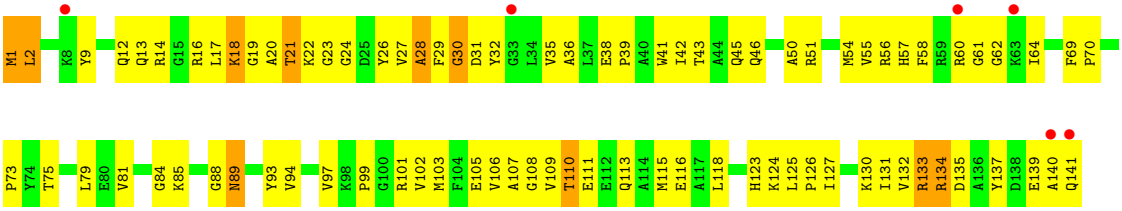
- Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



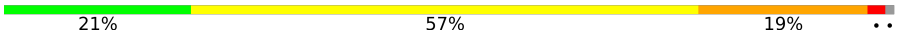
- Molecule 48: 50S RIBOSOMAL PROTEIN L16

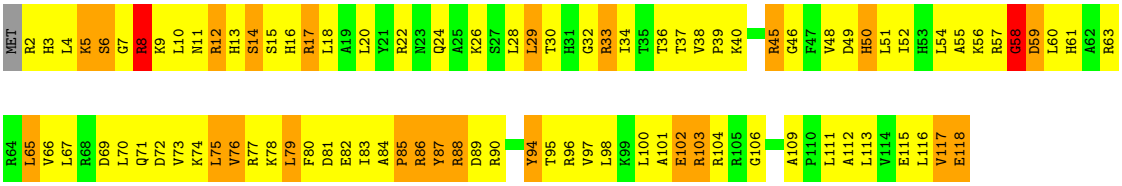
Chain DQ:



- Molecule 49: 50S RIBOSOMAL PROTEIN L17

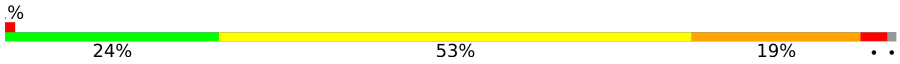
Chain BR:

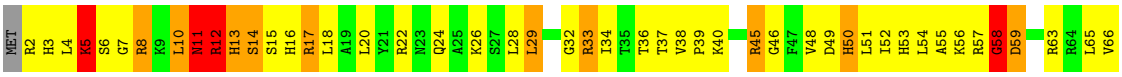


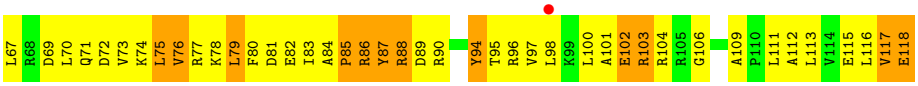


- Molecule 49: 50S RIBOSOMAL PROTEIN L17

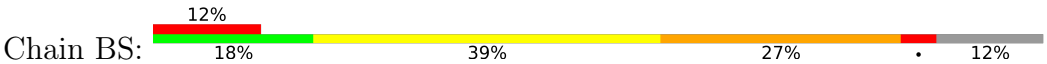
Chain DR:

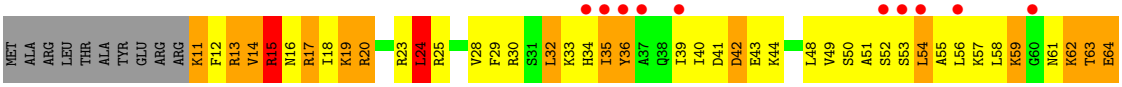


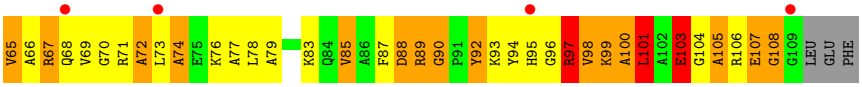




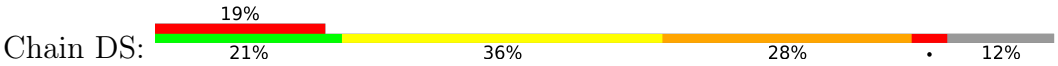
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

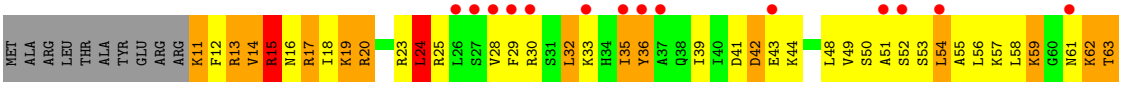


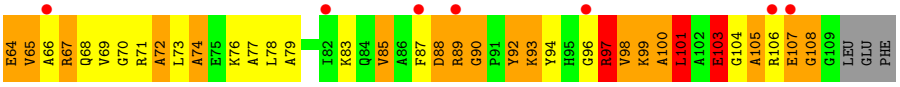




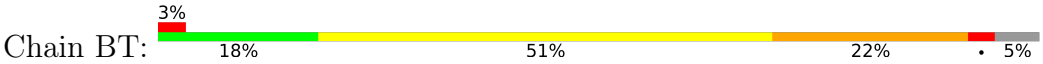
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

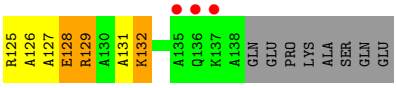




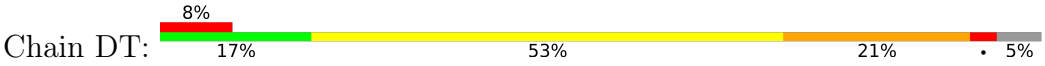


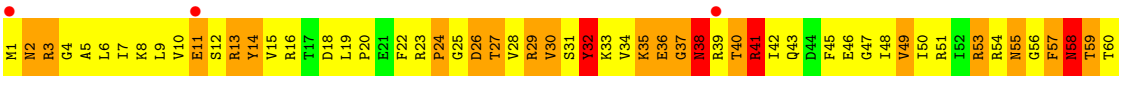
• Molecule 51: 50S RIBOSOMAL PROTEIN L19

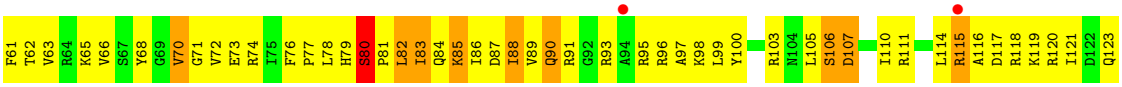


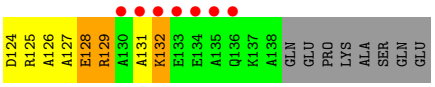


• Molecule 51: 50S RIBOSOMAL PROTEIN L19



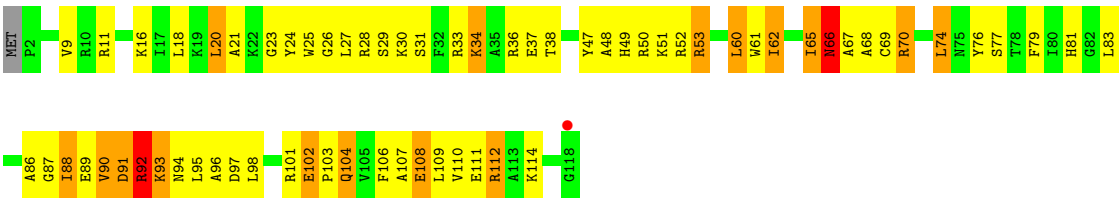






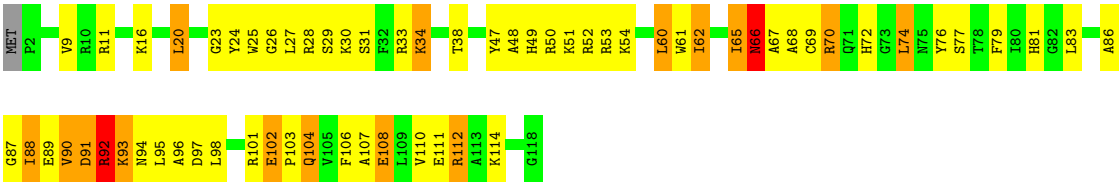
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain BU:



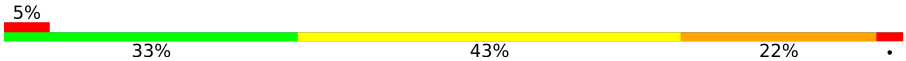
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

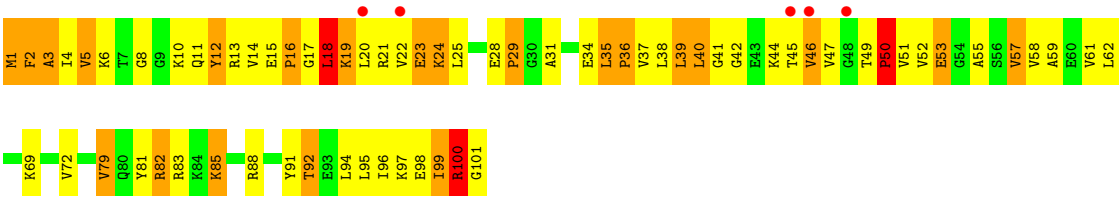
Chain DU:



• Molecule 53: 50S RIBOSOMAL PROTEIN L21

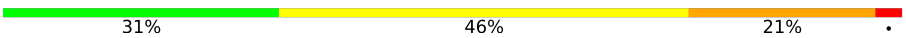
Chain BV:

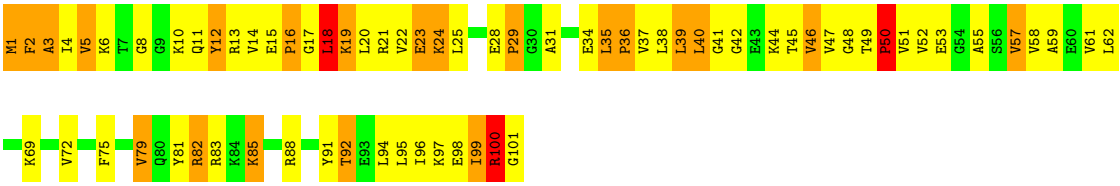




• Molecule 53: 50S RIBOSOMAL PROTEIN L21

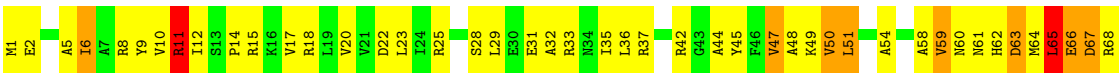
Chain DV:





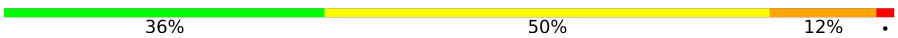
• Molecule 54: 50S RIBOSOMAL PROTEIN L22

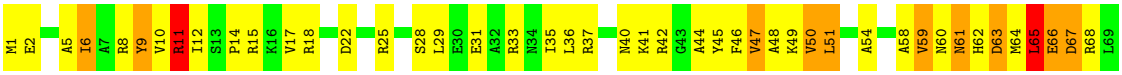
Chain BW:

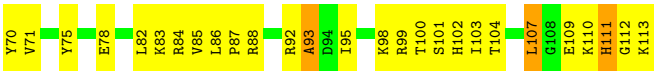


• Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain DW:

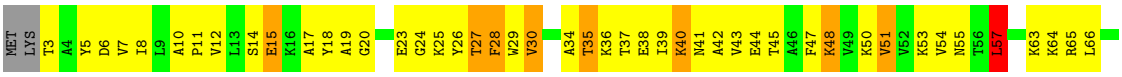


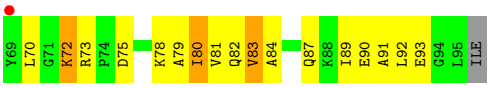




• Molecule 55: 50S RIBOSOMAL PROTEIN L23

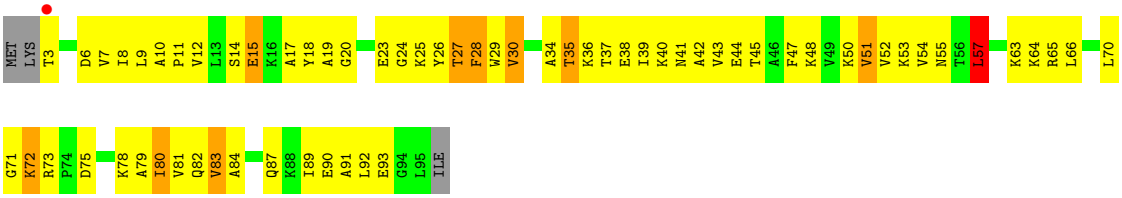
Chain BX:





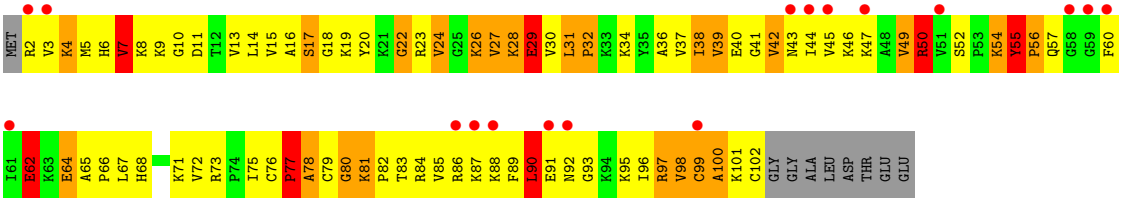
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain DX:



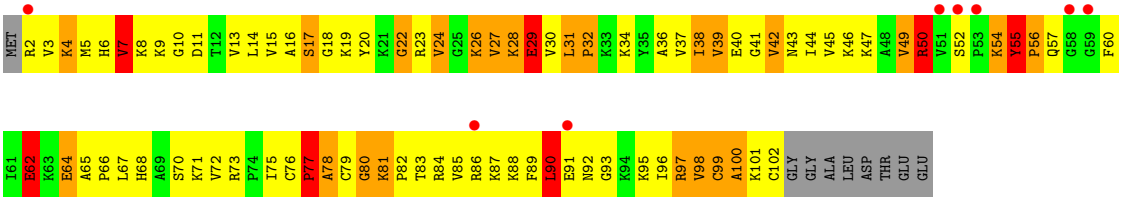
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain BY:



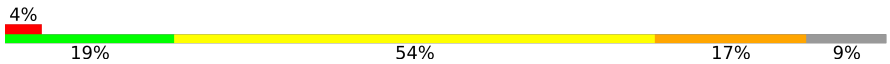
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

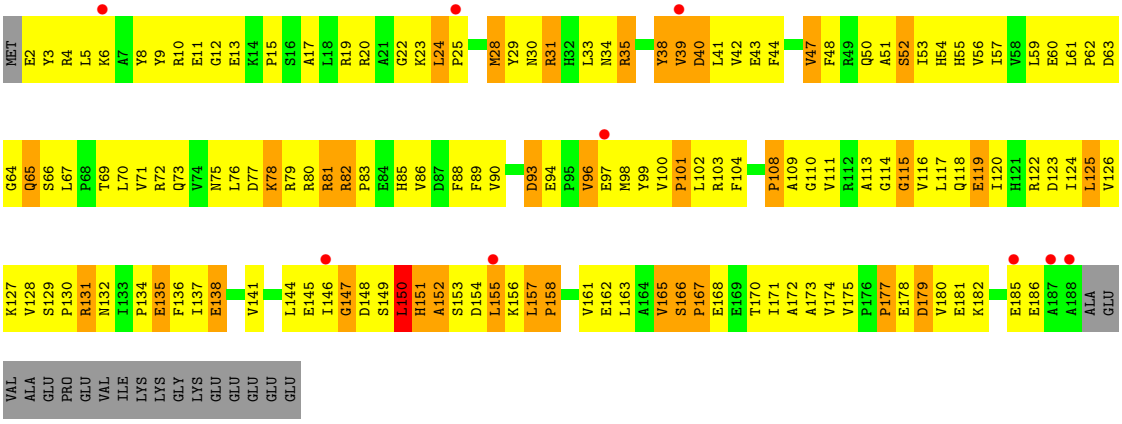
Chain DY:



• Molecule 57: 50S RIBOSOMAL PROTEIN L25

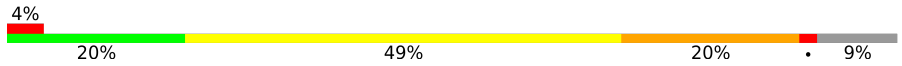
Chain BZ:

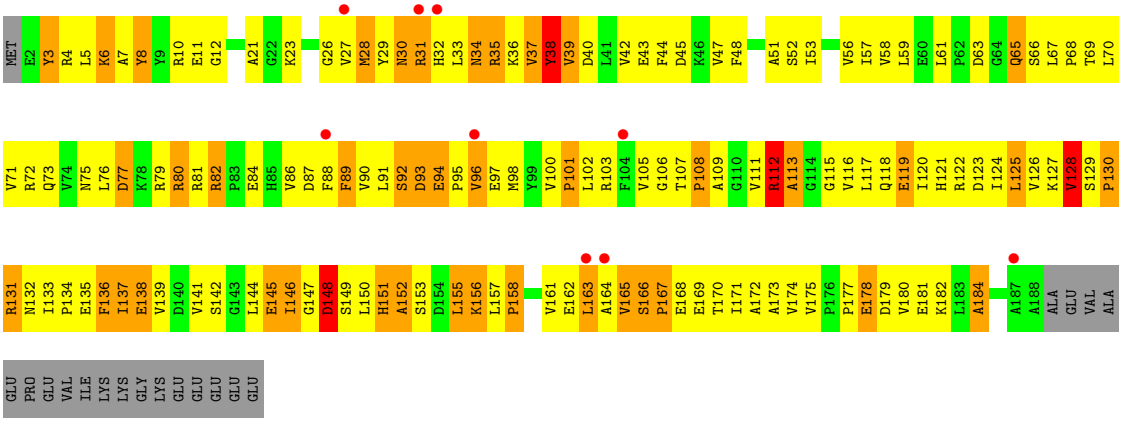




• Molecule 57: 50S RIBOSOMAL PROTEIN L25

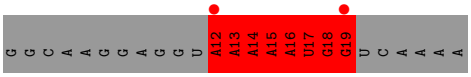
Chain DZ:





• Molecule 58: MRNA

Chain CX:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.04Å 453.51Å 616.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.53 – 3.20 44.53 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.53-3.20) 99.5 (44.53-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.270 0.231 , 0.273	Depositor DCC
R_{free} test set	44837 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	87.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 108.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	296762	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A3P, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.39	0/36252	0.68	9/56580 (0.0%)
1	CA	0.37	1/36253 (0.0%)	0.70	17/56582 (0.0%)
2	AB	0.32	0/1936	0.59	0/2611
2	CB	0.32	0/1936	0.59	0/2611
3	AC	0.30	0/1637	0.55	0/2207
3	CC	0.31	0/1637	0.55	0/2207
4	AD	0.37	0/1722	0.85	6/2306 (0.3%)
4	CD	0.35	0/1722	0.85	6/2306 (0.3%)
5	AE	0.34	0/1163	0.62	0/1566
5	CE	0.34	0/1163	0.61	0/1566
6	AF	0.32	0/856	0.62	0/1154
6	CF	0.34	0/856	0.63	0/1154
7	AG	0.29	0/1276	0.52	0/1709
7	CG	0.29	0/1276	0.51	0/1709
8	AH	0.33	0/1136	0.60	0/1527
8	CH	0.31	0/1136	0.60	0/1527
9	AI	0.32	0/1027	0.57	0/1372
9	CI	0.32	0/1027	0.57	0/1372
10	AJ	0.33	0/808	0.55	0/1087
10	CJ	0.33	0/808	0.55	0/1087
11	AK	0.31	0/900	0.58	0/1213
11	CK	0.33	0/900	0.58	0/1213
12	AL	0.38	0/987	0.87	3/1322 (0.2%)
12	CL	0.37	0/987	0.89	3/1322 (0.2%)
13	AM	0.31	0/941	0.62	0/1258
13	CM	0.32	0/941	0.61	0/1258
14	AN	0.33	0/501	0.54	0/664
14	CN	0.33	0/501	0.54	0/664
15	AO	0.35	0/745	0.60	0/992
15	CO	0.34	0/745	0.60	0/992
16	AP	0.37	0/717	0.61	0/965
16	CP	0.35	0/717	0.59	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.37	0/837	0.62	0/1119
17	CQ	0.34	0/837	0.62	0/1119
18	AR	0.33	0/579	0.60	0/768
18	CR	0.33	0/579	0.59	0/768
19	AS	0.33	0/685	0.54	0/922
19	CS	0.34	0/685	0.54	0/922
20	AT	0.31	0/765	0.57	0/1007
20	CT	0.29	0/765	0.57	0/1007
21	AU	0.45	0/213	0.53	0/279
21	CU	0.45	0/213	0.54	0/279
22	AV	2.00	34/1832 (1.9%)	2.16	50/2855 (1.8%)
22	AW	0.41	0/1832	0.71	0/2855
22	CV	0.44	1/1832 (0.1%)	0.72	0/2855
22	CW	0.40	0/1832	0.71	0/2855
23	AX	2.66	24/383 (6.3%)	4.32	117/595 (19.7%)
24	AY	1.30	4/790 (0.5%)	1.44	14/1055 (1.3%)
24	CY	1.10	0/132	1.27	0/177
25	B0	0.39	0/671	0.64	0/892
25	D0	0.39	0/671	0.63	0/892
26	B1	0.47	0/741	0.75	0/986
26	D1	0.47	0/741	0.78	0/986
27	B2	0.36	0/600	0.63	0/793
27	D2	0.45	0/600	0.71	0/793
28	B3	0.42	0/473	0.68	0/636
28	D3	0.41	0/473	0.67	0/636
29	B4	0.39	0/444	0.65	0/602
29	D4	0.40	0/444	0.65	0/602
30	B5	0.48	0/473	0.76	0/639
30	D5	0.48	0/473	0.76	0/639
31	B6	0.41	0/387	0.64	0/517
31	D6	0.41	0/387	0.64	0/517
32	B7	0.52	0/427	0.68	0/563
32	D7	0.56	0/427	0.71	0/563
33	B8	0.56	0/516	0.94	1/681 (0.1%)
33	D8	0.53	0/516	0.93	1/681 (0.1%)
34	B9	0.33	0/302	0.62	0/397
34	D9	0.34	0/302	0.62	0/397
35	BA	0.60	55/67715 (0.1%)	0.77	106/105714 (0.1%)
35	DA	0.60	28/67714 (0.0%)	0.78	109/105710 (0.1%)
36	BB	0.38	0/2853	0.69	0/4451
36	DB	0.38	0/2853	0.69	0/4451
37	BC	0.33	0/1145	0.60	7/1556 (0.4%)
37	DC	0.33	0/1145	0.60	7/1556 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	BD	0.48	0/2155	0.78	1/2907 (0.0%)
38	DD	0.51	0/2155	0.80	1/2907 (0.0%)
39	BE	0.45	0/1597	0.74	0/2155
39	DE	0.44	0/1597	0.75	0/2155
40	BF	0.47	0/1659	0.75	1/2246 (0.0%)
40	DF	0.50	0/1659	0.75	0/2246
41	BG	0.33	0/1498	0.62	0/2013
41	DG	0.34	0/1498	0.64	0/2013
42	BH	0.61	1/1285 (0.1%)	0.85	3/1741 (0.2%)
42	DH	0.61	1/1285 (0.1%)	0.85	3/1741 (0.2%)
43	BI	0.38	0/1140	1.09	9/1543 (0.6%)
43	DI	0.37	0/1140	1.07	9/1543 (0.6%)
45	BN	0.41	0/1132	0.75	0/1527
45	DN	0.44	0/1132	0.76	0/1527
46	BO	0.44	0/943	0.71	0/1269
46	DO	0.41	0/943	0.69	0/1269
47	BP	0.57	0/1131	1.03	4/1504 (0.3%)
47	DP	0.56	0/1131	1.02	5/1504 (0.3%)
48	BQ	0.40	0/1143	0.63	0/1527
48	DQ	0.37	0/1143	0.63	0/1527
49	BR	0.40	0/974	0.70	1/1302 (0.1%)
49	DR	0.75	3/974 (0.3%)	0.95	6/1302 (0.5%)
50	BS	0.39	0/779	0.67	0/1038
50	DS	0.40	0/779	0.67	0/1038
51	BT	0.42	0/1156	0.74	1/1544 (0.1%)
51	DT	0.40	0/1156	0.72	1/1544 (0.1%)
52	BU	0.43	0/975	0.68	0/1297
52	DU	0.49	0/975	0.71	0/1297
53	BV	0.42	0/790	0.74	0/1057
53	DV	0.46	0/790	0.76	0/1057
54	BW	0.48	0/907	0.75	0/1216
54	DW	0.50	1/907 (0.1%)	0.76	0/1216
55	BX	0.48	0/740	0.71	1/995 (0.1%)
55	DX	0.54	0/740	0.73	1/995 (0.1%)
56	BY	0.48	0/789	0.79	1/1053 (0.1%)
56	DY	0.51	0/789	0.80	1/1053 (0.1%)
57	BZ	0.37	0/1514	0.67	0/2056
57	DZ	0.36	0/1514	0.64	0/2056
58	CX	3.13	24/195 (12.3%)	4.52	67/303 (22.1%)
All	All	0.53	177/318302 (0.1%)	0.78	572/475638 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	10
1	CA	1	9
22	AV	0	1
22	CV	0	1
24	AY	0	1
35	BA	20	57
35	DA	20	70
36	BB	0	1
36	DB	0	2
42	BH	0	1
42	DH	0	1
49	BR	0	1
49	DR	0	2
All	All	42	157

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	53	G	N3-C4	-27.79	1.16	1.35
22	AV	53	G	C2-N3	-27.03	1.11	1.32
22	AV	52	G	N7-C5	-25.47	1.24	1.39
22	AV	52	G	N9-C4	-25.25	1.17	1.38
22	AV	52	G	C5-C6	-22.33	1.20	1.42

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	52	G	C4-C5-N7	30.84	123.13	110.80
22	AV	53	G	N3-C2-N2	-29.82	99.03	119.90
22	AV	52	G	C5-N7-C8	-28.61	89.99	104.30
22	AV	53	G	C5'-C4'-O4'	-26.14	77.74	109.10
22	AV	53	G	N3-C4-N9	-25.89	110.46	126.00

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	575	G	C3'
35	BA	100	G	C1'
35	BA	474	G	C3'
35	BA	587	C	C3'

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Mol	Chain	Res	Type	Atom
35	BA	669	G	C4',C3',C1'

5 of 157 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	115	G	Sidechain
1	AA	120	A	Sidechain
1	AA	575	G	Sidechain
1	AA	587	G	Sidechain
1	AA	731	G	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	AA	32412	0	16354	1303	0
1	CA	32413	0	16353	1701	0
2	AB	1901	0	1951	297	0
2	CB	1901	0	1951	304	0
3	AC	1613	0	1676	245	0
3	CC	1613	0	1677	238	0
4	AD	1692	0	1751	196	0
4	CD	1692	0	1753	218	0
5	AE	1147	0	1206	172	0
5	CE	1147	0	1207	191	0
6	AF	843	0	857	95	0
6	CF	843	0	857	99	0
7	AG	1257	0	1296	134	0
7	CG	1257	0	1296	146	0
8	AH	1116	0	1177	159	0
8	CH	1116	0	1177	167	0
9	AI	1011	0	1041	160	0
9	CI	1011	0	1041	161	0
10	AJ	795	0	840	156	0
10	CJ	795	0	840	157	0
11	AK	885	0	904	99	0
11	CK	885	0	904	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	971	0	1055	118	0
12	CL	971	0	1056	116	0
13	AM	934	0	989	124	0
13	CM	934	0	987	135	0
14	AN	492	0	530	74	0
14	CN	492	0	533	78	0
15	AO	734	0	771	82	0
15	CO	734	0	771	77	0
16	AP	701	0	719	93	0
16	CP	701	0	720	105	0
17	AQ	824	0	890	88	0
17	CQ	824	0	891	91	0
18	AR	574	0	644	90	0
18	CR	574	0	644	88	0
19	AS	671	0	689	118	0
19	CS	671	0	689	112	0
20	AT	763	0	861	74	0
20	CT	763	0	861	75	0
21	AU	209	0	221	42	0
21	CU	209	0	221	39	0
22	AV	1640	0	832	85	0
22	AW	1640	0	837	60	0
22	CV	1640	0	833	134	0
22	CW	1640	0	837	71	0
23	AX	341	0	174	126	0
24	AY	769	0	763	235	0
24	CY	126	0	115	33	0
25	B0	662	0	688	60	0
25	D0	662	0	688	56	0
26	B1	734	0	808	85	0
26	D1	734	0	808	83	0
27	B2	598	0	653	65	0
27	D2	598	0	653	79	0
28	B3	468	0	523	42	0
28	D3	468	0	523	45	0
29	B4	434	0	424	92	0
29	D4	434	0	424	69	0
30	B5	459	0	480	45	0
30	D5	459	0	479	45	0
31	B6	381	0	390	61	0
31	D6	381	0	390	63	0
32	B7	419	0	467	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	D7	419	0	467	34	0
33	B8	508	0	576	123	0
33	D8	508	0	576	122	0
34	B9	299	0	326	28	0
34	D9	299	0	326	30	0
35	BA	60459	0	30475	1944	0
35	DA	60459	0	30466	2109	1
36	BB	2551	0	1295	101	0
36	DB	2551	0	1294	90	1
37	BC	1142	0	865	72	0
37	DC	1142	0	865	71	0
38	BD	2105	0	2182	299	0
38	DD	2105	0	2182	311	0
39	BE	1564	0	1628	223	0
39	DE	1564	0	1628	233	0
40	BF	1624	0	1677	218	0
40	DF	1624	0	1676	225	0
41	BG	1474	0	1534	280	0
41	DG	1474	0	1534	306	0
42	BH	1260	0	1326	250	0
42	DH	1260	0	1326	242	0
43	BI	1125	0	1209	181	0
43	DI	1125	0	1209	169	0
44	BJ	651	0	165	21	0
44	DJ	651	0	166	35	0
45	BN	1105	0	1180	139	0
45	DN	1105	0	1180	133	0
46	BO	933	0	996	101	0
46	DO	933	0	996	114	0
47	BP	1114	0	1187	315	0
47	DP	1114	0	1187	310	0
48	BQ	1122	0	1179	113	0
48	DQ	1122	0	1179	112	0
49	BR	960	0	1021	132	0
49	DR	960	0	1019	127	0
50	BS	771	0	832	143	0
50	DS	771	0	832	132	0
51	BT	1142	0	1202	223	0
51	DT	1142	0	1201	226	0
52	BU	958	0	1015	121	0
52	DU	958	0	1015	116	0
53	BV	779	0	852	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	DV	779	0	852	158	0
54	BW	896	0	953	80	0
54	DW	896	0	952	77	0
55	BX	726	0	778	71	0
55	DX	726	0	778	73	0
56	BY	776	0	870	194	0
56	DY	776	0	870	192	0
57	BZ	1482	0	1503	210	0
57	DZ	1482	0	1503	244	0
58	CX	173	0	89	53	0
59	AA	373	0	0	0	0
59	AC	2	0	0	0	0
59	AD	3	0	0	0	0
59	AH	1	0	0	0	0
59	AI	3	0	0	0	0
59	AL	6	0	0	0	0
59	AN	2	0	0	0	0
59	AO	2	0	0	0	0
59	AP	1	0	0	0	0
59	AQ	3	0	0	0	0
59	AT	1	0	0	0	0
59	AV	7	0	0	0	0
59	AX	4	0	0	0	0
59	AY	3	0	0	0	0
59	B0	2	0	0	0	0
59	B1	1	0	0	0	0
59	B5	3	0	0	0	0
59	B6	1	0	0	0	0
59	B7	1	0	0	0	0
59	BA	709	0	0	0	0
59	BB	6	0	0	0	0
59	BD	5	0	0	0	0
59	BE	4	0	0	0	0
59	BF	1	0	0	0	0
59	BH	4	0	0	0	0
59	BN	1	0	0	0	0
59	BO	1	0	0	0	0
59	BP	4	0	0	5	0
59	BQ	1	0	0	0	0
59	BR	5	0	0	0	0
59	BT	1	0	0	0	0
59	BU	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BY	1	0	0	0	0
59	CA	184	0	0	0	0
59	CC	3	0	0	0	0
59	CD	1	0	0	0	0
59	CH	1	0	0	0	0
59	CJ	2	0	0	0	0
59	CM	3	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	1	0	0	0	0
59	CS	2	0	0	0	0
59	CV	12	0	0	0	0
59	CY	1	0	0	0	0
59	D0	4	0	0	0	0
59	D1	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D5	3	0	0	0	0
59	D6	2	0	0	0	0
59	D7	4	0	0	0	0
59	D8	1	0	0	0	0
59	D9	1	0	0	0	0
59	DA	897	0	0	0	0
59	DB	11	0	0	0	0
59	DD	6	0	0	0	0
59	DE	4	0	0	0	0
59	DF	3	0	0	0	0
59	DN	3	0	0	0	0
59	DO	1	0	0	0	0
59	DP	6	0	0	0	0
59	DR	2	0	0	0	0
59	DT	1	0	0	0	0
59	DU	4	0	0	0	0
59	DW	1	0	0	0	0
59	DY	1	0	0	0	0
60	AD	2	0	0	0	0
60	AN	1	0	0	0	0
60	CD	1	0	0	0	0
61	AA	2	0	0	0	0
All	All	296762	0	199834	19832	1

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 40.

The worst 5 of 19832 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)
3:AC:162:GLN:HB2	23:AX:23:A:C5	1.34	1.59
42:BH:11:VAL:HG22	42:BH:49:VAL:CG1	1.08	1.56
42:DH:11:VAL:HG22	42:DH:49:VAL:CG1	1.08	1.55
1:CA:644:G:C2'	1:CA:645:C:H5"	1.39	1.53
24:AY:57:GLN:HG3	35:BA:1913:A:C2	1.45	1.47

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DA:1411:C:O3'	36:DB:53:A:O2'[1_655]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	233/256 (91%)	133 (57%)	67 (29%)	33 (14%)	0 1
2	CB	233/256 (91%)	133 (57%)	68 (29%)	32 (14%)	0 1
3	AC	205/239 (86%)	130 (63%)	50 (24%)	25 (12%)	0 2
3	CC	205/239 (86%)	128 (62%)	52 (25%)	25 (12%)	0 2
4	AD	206/209 (99%)	139 (68%)	45 (22%)	22 (11%)	0 2
4	CD	206/209 (99%)	138 (67%)	46 (22%)	22 (11%)	0 2
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0 3
5	CE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0 3
6	AF	99/101 (98%)	74 (75%)	13 (13%)	12 (12%)	0 2
6	CF	99/101 (98%)	74 (75%)	13 (13%)	12 (12%)	0 2
7	AG	153/156 (98%)	107 (70%)	35 (23%)	11 (7%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	153/156 (98%)	107 (70%)	35 (23%)	11 (7%)	1	7
8	AH	136/138 (99%)	99 (73%)	31 (23%)	6 (4%)	2	19
8	CH	136/138 (99%)	99 (73%)	30 (22%)	7 (5%)	2	15
9	AI	121/128 (94%)	75 (62%)	31 (26%)	15 (12%)	0	2
9	CI	121/128 (94%)	74 (61%)	33 (27%)	14 (12%)	0	2
10	AJ	97/105 (92%)	64 (66%)	28 (29%)	5 (5%)	2	15
10	CJ	97/105 (92%)	64 (66%)	28 (29%)	5 (5%)	2	15
11	AK	117/129 (91%)	76 (65%)	28 (24%)	13 (11%)	0	2
11	CK	117/129 (91%)	76 (65%)	28 (24%)	13 (11%)	0	2
12	AL	123/135 (91%)	89 (72%)	21 (17%)	13 (11%)	0	2
12	CL	123/135 (91%)	87 (71%)	22 (18%)	14 (11%)	0	2
13	AM	110/126 (87%)	62 (56%)	27 (24%)	21 (19%)	0	0
13	CM	110/126 (87%)	63 (57%)	26 (24%)	21 (19%)	0	0
14	AN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	0	2
14	CN	58/61 (95%)	36 (62%)	16 (28%)	6 (10%)	0	3
15	AO	86/89 (97%)	54 (63%)	25 (29%)	7 (8%)	1	5
15	CO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	5
16	AP	82/88 (93%)	55 (67%)	18 (22%)	9 (11%)	0	2
16	CP	82/88 (93%)	55 (67%)	18 (22%)	9 (11%)	0	2
17	AQ	98/105 (93%)	65 (66%)	21 (21%)	12 (12%)	0	2
17	CQ	98/105 (93%)	66 (67%)	20 (20%)	12 (12%)	0	2
18	AR	68/88 (77%)	36 (53%)	22 (32%)	10 (15%)	0	1
18	CR	68/88 (77%)	35 (52%)	23 (34%)	10 (15%)	0	1
19	AS	83/93 (89%)	48 (58%)	18 (22%)	17 (20%)	0	0
19	CS	83/93 (89%)	48 (58%)	18 (22%)	17 (20%)	0	0
20	AT	97/106 (92%)	62 (64%)	25 (26%)	10 (10%)	0	3
20	CT	97/106 (92%)	62 (64%)	25 (26%)	10 (10%)	0	3
21	AU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	4
21	CU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	4
24	AY	95/97 (98%)	81 (85%)	10 (10%)	4 (4%)	3	20
24	CY	14/97 (14%)	8 (57%)	4 (29%)	2 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	B0	82/85 (96%)	67 (82%)	10 (12%)	5 (6%)	1	12
25	D0	82/85 (96%)	66 (80%)	10 (12%)	6 (7%)	1	7
26	B1	92/98 (94%)	70 (76%)	16 (17%)	6 (6%)	1	10
26	D1	92/98 (94%)	74 (80%)	9 (10%)	9 (10%)	0	3
27	B2	69/72 (96%)	51 (74%)	13 (19%)	5 (7%)	1	7
27	D2	69/72 (96%)	47 (68%)	18 (26%)	4 (6%)	1	13
28	B3	58/60 (97%)	49 (84%)	8 (14%)	1 (2%)	9	42
28	D3	58/60 (97%)	50 (86%)	7 (12%)	1 (2%)	9	42
29	B4	54/71 (76%)	28 (52%)	12 (22%)	14 (26%)	0	0
29	D4	54/71 (76%)	28 (52%)	12 (22%)	14 (26%)	0	0
30	B5	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	0	3
30	D5	57/60 (95%)	41 (72%)	10 (18%)	6 (10%)	0	3
31	B6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	0
31	D6	41/54 (76%)	16 (39%)	16 (39%)	9 (22%)	0	0
32	B7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	37
32	D7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	37
33	B8	62/65 (95%)	35 (56%)	15 (24%)	12 (19%)	0	0
33	D8	62/65 (95%)	34 (55%)	15 (24%)	13 (21%)	0	0
34	B9	34/37 (92%)	24 (71%)	8 (24%)	2 (6%)	1	12
34	D9	34/37 (92%)	24 (71%)	8 (24%)	2 (6%)	1	12
37	BC	183/229 (80%)	75 (41%)	67 (37%)	41 (22%)	0	0
37	DC	183/229 (80%)	76 (42%)	65 (36%)	42 (23%)	0	0
38	BD	270/276 (98%)	199 (74%)	48 (18%)	23 (8%)	1	4
38	DD	270/276 (98%)	198 (73%)	47 (17%)	25 (9%)	0	3
39	BE	203/206 (98%)	142 (70%)	37 (18%)	24 (12%)	0	2
39	DE	203/206 (98%)	143 (70%)	36 (18%)	24 (12%)	0	2
40	BF	206/210 (98%)	137 (66%)	40 (19%)	29 (14%)	0	1
40	DF	206/210 (98%)	137 (66%)	41 (20%)	28 (14%)	0	1
41	BG	177/182 (97%)	109 (62%)	44 (25%)	24 (14%)	0	1
41	DG	177/182 (97%)	107 (60%)	43 (24%)	27 (15%)	0	1
42	BH	163/180 (91%)	90 (55%)	42 (26%)	31 (19%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DH	163/180 (91%)	90 (55%)	42 (26%)	31 (19%)	0	0
43	BI	143/148 (97%)	80 (56%)	36 (25%)	27 (19%)	0	0
43	DI	143/148 (97%)	80 (56%)	36 (25%)	27 (19%)	0	0
45	BN	137/140 (98%)	97 (71%)	20 (15%)	20 (15%)	0	1
45	DN	137/140 (98%)	96 (70%)	21 (15%)	20 (15%)	0	1
46	BO	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	2	16
46	DO	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	2	16
47	BP	144/150 (96%)	70 (49%)	34 (24%)	40 (28%)	0	0
47	DP	144/150 (96%)	70 (49%)	34 (24%)	40 (28%)	0	0
48	BQ	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	0	3
48	DQ	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	0	3
49	BR	115/118 (98%)	80 (70%)	20 (17%)	15 (13%)	0	1
49	DR	115/118 (98%)	82 (71%)	20 (17%)	13 (11%)	0	2
50	BS	97/112 (87%)	46 (47%)	20 (21%)	31 (32%)	0	0
50	DS	97/112 (87%)	46 (47%)	20 (21%)	31 (32%)	0	0
51	BT	136/146 (93%)	79 (58%)	33 (24%)	24 (18%)	0	0
51	DT	136/146 (93%)	80 (59%)	31 (23%)	25 (18%)	0	0
52	BU	115/118 (98%)	87 (76%)	18 (16%)	10 (9%)	1	4
52	DU	115/118 (98%)	88 (76%)	17 (15%)	10 (9%)	1	4
53	BV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	1
53	DV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	1
54	BW	111/113 (98%)	84 (76%)	17 (15%)	10 (9%)	1	4
54	DW	111/113 (98%)	85 (77%)	16 (14%)	10 (9%)	1	4
55	BX	91/96 (95%)	73 (80%)	15 (16%)	3 (3%)	4	25
55	DX	91/96 (95%)	72 (79%)	16 (18%)	3 (3%)	4	25
56	BY	99/110 (90%)	50 (50%)	23 (23%)	26 (26%)	0	0
56	DY	99/110 (90%)	50 (50%)	23 (23%)	26 (26%)	0	0
57	BZ	185/206 (90%)	123 (66%)	38 (20%)	24 (13%)	0	1
57	DZ	185/206 (90%)	101 (55%)	49 (26%)	35 (19%)	0	0
All	All	11855/12786 (93%)	7751 (65%)	2556 (22%)	1548 (13%)	0	1

5 of 1548 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	75	LYS
2	AB	83	MET
2	AB	101	MET
2	AB	150	SER
2	AB	238	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	185 (92%)	17 (8%)	11	39
2	CB	202/220 (92%)	185 (92%)	17 (8%)	11	39
3	AC	160/188 (85%)	151 (94%)	9 (6%)	21	57
3	CC	160/188 (85%)	151 (94%)	9 (6%)	21	57
4	AD	179/181 (99%)	165 (92%)	14 (8%)	12	43
4	CD	179/181 (99%)	164 (92%)	15 (8%)	11	39
5	AE	115/123 (94%)	105 (91%)	10 (9%)	10	37
5	CE	115/123 (94%)	105 (91%)	10 (9%)	10	37
6	AF	90/90 (100%)	87 (97%)	3 (3%)	38	71
6	CF	90/90 (100%)	87 (97%)	3 (3%)	38	71
7	AG	126/127 (99%)	124 (98%)	2 (2%)	62	84
7	CG	126/127 (99%)	124 (98%)	2 (2%)	62	84
8	AH	119/119 (100%)	110 (92%)	9 (8%)	13	45
8	CH	119/119 (100%)	110 (92%)	9 (8%)	13	45
9	AI	98/99 (99%)	88 (90%)	10 (10%)	7	29
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	29
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
11	AK	90/99 (91%)	85 (94%)	5 (6%)	21	57
11	CK	90/99 (91%)	85 (94%)	5 (6%)	21	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/111 (94%)	95 (91%)	9 (9%)	10	37
12	CL	104/111 (94%)	95 (91%)	9 (9%)	10	37
13	AM	94/101 (93%)	86 (92%)	8 (8%)	10	38
13	CM	94/101 (93%)	86 (92%)	8 (8%)	10	38
14	AN	49/50 (98%)	45 (92%)	4 (8%)	11	41
14	CN	49/50 (98%)	45 (92%)	4 (8%)	11	41
15	AO	79/80 (99%)	74 (94%)	5 (6%)	18	52
15	CO	79/80 (99%)	74 (94%)	5 (6%)	18	52
16	AP	72/74 (97%)	67 (93%)	5 (7%)	15	49
16	CP	72/74 (97%)	66 (92%)	6 (8%)	11	40
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	39	71
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	53	79
18	AR	61/77 (79%)	59 (97%)	2 (3%)	38	71
18	CR	61/77 (79%)	59 (97%)	2 (3%)	38	71
19	AS	72/80 (90%)	62 (86%)	10 (14%)	3	16
19	CS	72/80 (90%)	62 (86%)	10 (14%)	3	16
20	AT	76/82 (93%)	67 (88%)	9 (12%)	5	23
20	CT	76/82 (93%)	67 (88%)	9 (12%)	5	23
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	28
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	58
24	AY	78/78 (100%)	42 (54%)	36 (46%)	0	0
24	CY	12/78 (15%)	8 (67%)	4 (33%)	0	0
25	B0	66/67 (98%)	58 (88%)	8 (12%)	5	22
25	D0	66/67 (98%)	58 (88%)	8 (12%)	5	22
26	B1	78/83 (94%)	67 (86%)	11 (14%)	3	16
26	D1	78/83 (94%)	67 (86%)	11 (14%)	3	16
27	B2	66/67 (98%)	59 (89%)	7 (11%)	6	27
27	D2	66/67 (98%)	56 (85%)	10 (15%)	3	13
28	B3	51/52 (98%)	41 (80%)	10 (20%)	1	7
28	D3	51/52 (98%)	41 (80%)	10 (20%)	1	7
29	B4	49/63 (78%)	40 (82%)	9 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	D4	49/63 (78%)	42 (86%)	7 (14%)	3	15
30	B5	51/52 (98%)	47 (92%)	4 (8%)	12	43
30	D5	51/52 (98%)	47 (92%)	4 (8%)	12	43
31	B6	43/52 (83%)	39 (91%)	4 (9%)	9	33
31	D6	43/52 (83%)	38 (88%)	5 (12%)	5	24
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5	22
32	D7	41/42 (98%)	36 (88%)	5 (12%)	5	22
33	B8	53/55 (96%)	45 (85%)	8 (15%)	3	14
33	D8	53/55 (96%)	45 (85%)	8 (15%)	3	14
34	B9	33/34 (97%)	32 (97%)	1 (3%)	41	73
34	D9	33/34 (97%)	32 (97%)	1 (3%)	41	73
37	BC	61/181 (34%)	57 (93%)	4 (7%)	16	51
37	DC	61/181 (34%)	57 (93%)	4 (7%)	16	51
38	BD	213/218 (98%)	176 (83%)	37 (17%)	2	10
38	DD	213/218 (98%)	176 (83%)	37 (17%)	2	10
39	BE	165/166 (99%)	142 (86%)	23 (14%)	3	16
39	DE	165/166 (99%)	142 (86%)	23 (14%)	3	16
40	BF	165/166 (99%)	143 (87%)	22 (13%)	4	18
40	DF	165/166 (99%)	143 (87%)	22 (13%)	4	18
41	BG	155/156 (99%)	133 (86%)	22 (14%)	3	15
41	DG	155/156 (99%)	135 (87%)	20 (13%)	4	19
42	BH	137/148 (93%)	122 (89%)	15 (11%)	6	26
42	DH	137/148 (93%)	122 (89%)	15 (11%)	6	26
43	BI	121/124 (98%)	104 (86%)	17 (14%)	3	16
43	DI	121/124 (98%)	103 (85%)	18 (15%)	3	14
45	BN	117/119 (98%)	97 (83%)	20 (17%)	2	10
45	DN	117/119 (98%)	96 (82%)	21 (18%)	2	9
46	BO	100/100 (100%)	95 (95%)	5 (5%)	24	60
46	DO	100/100 (100%)	94 (94%)	6 (6%)	19	54
47	BP	112/116 (97%)	80 (71%)	32 (29%)	0	1
47	DP	112/116 (97%)	81 (72%)	31 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BQ	111/111 (100%)	104 (94%)	7 (6%)	18	52
48	DQ	111/111 (100%)	104 (94%)	7 (6%)	18	52
49	BR	100/101 (99%)	86 (86%)	14 (14%)	3	16
49	DR	100/101 (99%)	84 (84%)	16 (16%)	2	11
50	BS	77/88 (88%)	64 (83%)	13 (17%)	2	10
50	DS	77/88 (88%)	64 (83%)	13 (17%)	2	10
51	BT	120/127 (94%)	99 (82%)	21 (18%)	2	9
51	DT	120/127 (94%)	100 (83%)	20 (17%)	2	10
52	BU	92/94 (98%)	80 (87%)	12 (13%)	4	19
52	DU	92/94 (98%)	81 (88%)	11 (12%)	5	22
53	BV	82/82 (100%)	68 (83%)	14 (17%)	2	10
53	DV	82/82 (100%)	68 (83%)	14 (17%)	2	10
54	BW	91/92 (99%)	81 (89%)	10 (11%)	6	26
54	DW	91/92 (99%)	81 (89%)	10 (11%)	6	26
55	BX	74/78 (95%)	62 (84%)	12 (16%)	2	11
55	DX	74/78 (95%)	62 (84%)	12 (16%)	2	11
56	BY	84/91 (92%)	70 (83%)	14 (17%)	2	10
56	DY	84/91 (92%)	70 (83%)	14 (17%)	2	10
57	BZ	163/179 (91%)	147 (90%)	16 (10%)	8	31
57	DZ	163/179 (91%)	143 (88%)	20 (12%)	4	21
All	All	9806/10588 (93%)	8674 (88%)	1132 (12%)	5	24

5 of 1132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	DI	86	THR
45	DN	103	VAL
43	DI	82	ARG
51	DT	51	ARG
43	BI	144	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 302 such sidechains are listed below:

Mol	Chain	Res	Type
38	DD	166	GLN
52	DU	71	GLN
39	DE	129	HIS
43	DI	74	ASN
57	DZ	73	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1522 (98%)	206 (13%)	21 (1%)
1	CA	1505/1522 (98%)	235 (15%)	24 (1%)
22	AV	76/77 (98%)	18 (23%)	1 (1%)
22	AW	76/77 (98%)	14 (18%)	1 (1%)
22	CV	76/77 (98%)	20 (26%)	1 (1%)
22	CW	76/77 (98%)	8 (10%)	0
23	AX	15/25 (60%)	14 (93%)	10 (66%)
35	BA	2805/2848 (98%)	485 (17%)	58 (2%)
35	DA	2804/2848 (98%)	487 (17%)	58 (2%)
36	BB	118/122 (96%)	20 (16%)	1 (0%)
36	DB	118/122 (96%)	20 (16%)	1 (0%)
58	CX	8/25 (32%)	7 (87%)	5 (62%)
All	All	9182/9342 (98%)	1534 (16%)	181 (1%)

5 of 1534 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	31	G

5 of 181 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1504	G
35	DA	746	A
58	CX	14	A
35	DA	331	A
35	DA	1301	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	A3P	AA	1493	1	22,28,29	0.82	0	24,42,45	1.57	4 (16%)
1	A3P	CA	1493	1	22,28,29	0.74	0	24,42,45	0.88	2 (8%)

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
1	A3P	AA	1493	1	-	1/8/30/31	0/3/3/3
1	A3P	CA	1493	1	-	2/8/30/31	0/3/3/3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1493	A3P	O2P-P1-O3'	-4.99	83.64	105.99
1	AA	1493	A3P	O3'-P1-O1P	4.11	125.27	109.39
1	CA	1493	A3P	C5-C6-N6	2.23	123.74	120.35
1	CA	1493	A3P	O2P-P1-O1P	2.16	119.13	110.68
1	AA	1493	A3P	C5-C6-N6	2.16	123.63	120.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1493	A3P	C3'-O3'-P1-O3P
1	CA	1493	A3P	C4'-C5'-O5'-P2
1	CA	1493	A3P	C3'-O3'-P1-O2P

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1493	A3P	10	0
1	CA	1493	A3P	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2338 ligands modelled in this entry, 2338 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	AM	3
13	CM	3
9	CI	2
9	AI	2
31	B6	1
31	D6	1
41	BG	1
41	DG	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	7.76
1	D6	46:HIS	C	47:THR	N	7.76
1	BG	112:PRO	C	113:ARG	N	4.73
1	DG	112:PRO	C	113:ARG	N	4.47
1	AM	69:GLU	C	70:LEU	N	4.25

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	AA	1507/1522 (99%)	0.11	40 (2%)	54	39	54, 107, 196, 201	0
1	CA	1507/1522 (99%)	0.83	183 (12%)	4	2	60, 169, 201, 201	0
2	AB	235/256 (91%)	0.41	18 (7%)	13	7	77, 152, 197, 201	0
2	CB	235/256 (91%)	0.99	43 (18%)	1	1	90, 173, 201, 201	0
3	AC	207/239 (86%)	0.52	18 (8%)	10	5	83, 149, 188, 201	0
3	CC	207/239 (86%)	1.38	49 (23%)	0	0	106, 175, 201, 201	0
4	AD	208/209 (99%)	-0.02	1 (0%)	91	86	65, 105, 149, 180	0
4	CD	208/209 (99%)	1.42	56 (26%)	0	0	85, 173, 201, 201	0
5	AE	151/162 (93%)	0.15	3 (1%)	65	51	70, 107, 155, 198	0
5	CE	151/162 (93%)	1.15	39 (25%)	0	0	89, 155, 197, 201	0
6	AF	101/101 (100%)	0.15	3 (2%)	50	34	70, 125, 163, 190	0
6	CF	101/101 (100%)	-0.03	1 (0%)	82	72	65, 110, 155, 184	0
7	AG	155/156 (99%)	0.42	14 (9%)	9	5	85, 141, 184, 201	0
7	CG	155/156 (99%)	0.99	36 (23%)	0	0	86, 164, 200, 201	0
8	AH	138/138 (100%)	0.10	1 (0%)	87	81	66, 108, 151, 171	0
8	CH	138/138 (100%)	0.91	25 (18%)	1	1	79, 157, 189, 201	0
9	AI	127/128 (99%)	1.11	28 (22%)	0	0	94, 164, 200, 201	0
9	CI	127/128 (99%)	2.27	61 (48%)	0	0	115, 177, 201, 201	0
10	AJ	99/105 (94%)	1.64	35 (35%)	0	0	105, 169, 201, 201	0
10	CJ	99/105 (94%)	3.10	58 (58%)	0	0	125, 181, 201, 201	0
11	AK	119/129 (92%)	0.39	8 (6%)	17	10	60, 113, 168, 197	0
11	CK	119/129 (92%)	0.61	11 (9%)	9	5	78, 139, 188, 200	0
12	AL	125/135 (92%)	0.19	2 (1%)	72	59	59, 90, 144, 201	0
12	CL	125/135 (92%)	1.20	28 (22%)	0	0	63, 139, 187, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AM	118/126 (93%)	0.79	18 (15%)	2	1	96, 152, 189, 201	0
13	CM	118/126 (93%)	1.23	27 (22%)	0	0	102, 165, 201, 201	0
14	AN	60/61 (98%)	0.94	10 (16%)	1	1	99, 153, 198, 201	0
14	CN	60/61 (98%)	1.43	14 (23%)	0	0	118, 171, 200, 201	0
15	AO	88/89 (98%)	0.10	1 (1%)	80	69	69, 102, 149, 171	0
15	CO	88/89 (98%)	0.40	4 (4%)	33	21	75, 123, 163, 176	0
16	AP	84/88 (95%)	0.04	1 (1%)	79	67	60, 92, 143, 195	0
16	CP	84/88 (95%)	1.97	38 (45%)	0	0	112, 172, 198, 201	0
17	AQ	100/105 (95%)	-0.07	1 (1%)	82	72	63, 97, 134, 156	0
17	CQ	100/105 (95%)	0.66	11 (11%)	5	3	102, 142, 181, 195	0
18	AR	70/88 (79%)	0.48	5 (7%)	16	9	78, 116, 165, 178	0
18	CR	70/88 (79%)	0.55	5 (7%)	16	9	79, 120, 180, 196	0
19	AS	85/93 (91%)	1.11	17 (20%)	1	1	101, 164, 198, 201	0
19	CS	85/93 (91%)	1.82	31 (36%)	0	0	118, 176, 199, 201	0
20	AT	99/106 (93%)	0.21	3 (3%)	50	34	60, 104, 163, 191	0
20	CT	99/106 (93%)	0.97	16 (16%)	1	1	113, 169, 198, 201	0
21	AU	25/27 (92%)	2.34	11 (44%)	0	0	91, 151, 184, 201	0
21	CU	25/27 (92%)	4.16	20 (80%)	0	0	84, 159, 199, 201	0
22	AV	77/77 (100%)	-0.10	1 (1%)	77	65	55, 106, 161, 194	0
22	AW	77/77 (100%)	2.83	52 (67%)	0	0	125, 201, 201, 201	0
22	CV	77/77 (100%)	0.11	2 (2%)	56	40	50, 131, 174, 182	0
22	CW	77/77 (100%)	3.02	56 (72%)	0	0	146, 201, 201, 201	0
23	AX	16/25 (64%)	2.39	10 (62%)	0	0	84, 199, 201, 201	0
24	AY	97/97 (100%)	1.27	26 (26%)	0	0	99, 149, 192, 201	1 (1%)
24	CY	16/97 (16%)	2.34	9 (56%)	0	0	130, 157, 201, 201	0
25	B0	84/85 (98%)	0.63	7 (8%)	11	6	51, 90, 164, 196	0
25	D0	84/85 (98%)	0.88	12 (14%)	2	1	70, 105, 166, 191	0
26	B1	94/98 (95%)	0.05	3 (3%)	47	31	44, 76, 145, 161	0
26	D1	94/98 (95%)	-0.05	0	100	100	41, 74, 139, 159	0
27	B2	71/72 (98%)	0.13	0	100	100	65, 103, 150, 169	0
27	D2	71/72 (98%)	-0.22	3 (4%)	36	23	42, 71, 129, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	B3	60/60 (100%)	0.38	4 (6%)	17	10	42, 88, 148, 201	0
28	D3	60/60 (100%)	0.35	3 (5%)	28	16	50, 87, 142, 200	0
29	B4	56/71 (78%)	0.20	5 (8%)	9	5	96, 160, 187, 197	0
29	D4	56/71 (78%)	0.88	11 (19%)	1	1	122, 176, 201, 201	0
30	B5	59/60 (98%)	0.26	5 (8%)	10	6	37, 70, 174, 181	0
30	D5	59/60 (98%)	0.46	5 (8%)	10	6	27, 75, 177, 201	0
31	B6	45/54 (83%)	2.83	30 (66%)	0	0	97, 141, 184, 187	0
31	D6	45/54 (83%)	2.19	26 (57%)	0	0	103, 161, 195, 199	0
32	B7	49/49 (100%)	-0.17	0	100	100	38, 55, 112, 194	0
32	D7	49/49 (100%)	-0.15	0	100	100	21, 40, 108, 159	0
33	B8	64/65 (98%)	-0.01	0	100	100	32, 72, 132, 200	0
33	D8	64/65 (98%)	0.24	2 (3%)	49	32	41, 83, 148, 201	0
34	B9	36/37 (97%)	1.94	16 (44%)	0	0	83, 123, 168, 201	0
34	D9	36/37 (97%)	1.91	15 (41%)	0	0	91, 128, 167, 197	0
35	BA	2807/2848 (98%)	0.06	101 (3%)	42	27	32, 74, 188, 201	0
35	DA	2807/2848 (98%)	0.11	87 (3%)	49	32	29, 77, 189, 201	0
36	BB	119/122 (97%)	0.04	1 (0%)	86	78	76, 130, 181, 201	0
36	DB	119/122 (97%)	0.27	4 (3%)	45	29	87, 151, 189, 200	0
37	BC	191/229 (83%)	4.14	156 (81%)	0	0	160, 198, 201, 201	0
37	DC	191/229 (83%)	4.01	148 (77%)	0	0	154, 197, 201, 201	0
38	BD	272/276 (98%)	-0.17	0	100	100	38, 71, 107, 184	0
38	DD	272/276 (98%)	-0.07	1 (0%)	92	89	32, 68, 111, 185	0
39	BE	205/206 (99%)	-0.02	3 (1%)	73	61	36, 83, 157, 201	0
39	DE	205/206 (99%)	0.16	7 (3%)	45	29	25, 91, 157, 201	0
40	BF	208/210 (99%)	-0.22	1 (0%)	91	86	30, 73, 156, 186	0
40	DF	208/210 (99%)	-0.13	5 (2%)	59	44	24, 78, 165, 196	0
41	BG	181/182 (99%)	0.53	17 (9%)	8	4	79, 142, 188, 201	0
41	DG	181/182 (99%)	0.65	18 (9%)	7	4	92, 155, 193, 201	0
42	BH	165/180 (91%)	1.43	48 (29%)	0	0	90, 157, 193, 201	0
42	DH	165/180 (91%)	0.27	10 (6%)	21	12	55, 112, 158, 182	0
43	BI	145/148 (97%)	2.46	55 (37%)	0	0	60, 161, 201, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	DI	145/148 (97%)	0.89	21 (14%) 2 1	70, 130, 200, 201	0
44	BJ	0/131	-	-	-	-
44	DJ	0/131	-	-	-	-
45	BN	139/140 (99%)	-0.05	2 (1%) 75 63	52, 88, 145, 201	0
45	DN	139/140 (99%)	-0.16	0 100 100	44, 79, 140, 189	0
46	BO	122/122 (100%)	-0.35	0 100 100	42, 72, 101, 178	0
46	DO	122/122 (100%)	0.28	1 (0%) 86 78	59, 104, 154, 201	0
47	BP	146/150 (97%)	0.19	3 (2%) 63 49	26, 92, 150, 197	0
47	DP	146/150 (97%)	0.40	7 (4%) 30 18	35, 96, 170, 198	0
48	BQ	141/141 (100%)	0.02	1 (0%) 87 81	48, 89, 132, 201	0
48	DQ	141/141 (100%)	0.34	6 (4%) 35 22	53, 106, 159, 191	0
49	BR	117/118 (99%)	-0.17	0 100 100	39, 76, 125, 150	0
49	DR	117/118 (99%)	0.25	1 (0%) 84 75	53, 90, 147, 162	0
50	BS	99/112 (88%)	0.66	14 (14%) 2 2	75, 133, 182, 189	0
50	DS	99/112 (88%)	1.04	21 (21%) 0 1	95, 145, 196, 201	0
51	BT	138/146 (94%)	0.00	4 (2%) 51 36	51, 87, 182, 201	0
51	DT	138/146 (94%)	0.59	12 (8%) 10 5	68, 131, 194, 201	0
52	BU	117/118 (99%)	-0.11	1 (0%) 84 75	37, 73, 137, 201	0
52	DU	117/118 (99%)	-0.29	0 100 100	25, 62, 114, 174	0
53	BV	101/101 (100%)	0.14	5 (4%) 28 16	35, 103, 143, 201	0
53	DV	101/101 (100%)	-0.17	0 100 100	32, 80, 126, 180	0
54	BW	113/113 (100%)	-0.20	1 (0%) 84 75	43, 70, 133, 201	0
54	DW	113/113 (100%)	-0.27	0 100 100	37, 60, 118, 187	0
55	BX	93/96 (96%)	-0.10	1 (1%) 80 69	43, 89, 125, 140	0
55	DX	93/96 (96%)	-0.22	1 (1%) 80 69	43, 65, 114, 153	0
56	BY	101/110 (91%)	0.93	17 (16%) 1 1	63, 109, 182, 201	0
56	DY	101/110 (91%)	0.45	8 (7%) 12 6	54, 99, 176, 201	0
57	BZ	187/206 (90%)	0.30	9 (4%) 30 18	74, 121, 171, 201	0
57	DZ	187/206 (90%)	0.23	9 (4%) 30 18	76, 133, 187, 201	0
58	CX	8/25 (32%)	1.18	2 (25%) 0 0	106, 165, 200, 201	0
All	All	21297/22390 (95%)	0.48	2106 (9%) 7 4	21, 111, 198, 201	1 (0%)

The worst 5 of 2106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	BI	111	PRO	28.6
3	CC	169	ALA	19.6
10	CJ	72	VAL	17.5
37	DC	176	GLY	17.2
10	CJ	35	SER	16.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	A3P	CA	1493	26/27	0.63	0.44	191,200,203,203	0
1	A3P	AA	1493	26/27	0.90	0.20	151,182,188,189	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DY	201	1/1	-0.35	3.40	168,168,168,168	0
59	MG	CA	1777	1/1	-0.11	0.16	125,125,125,125	0
59	MG	CA	1763	1/1	-0.09	0.59	105,105,105,105	0
59	MG	DA	3345	1/1	0.04	1.22	25,25,25,25	1
59	MG	BT	201	1/1	0.08	0.39	117,117,117,117	0
59	MG	DA	3717	1/1	0.13	0.31	155,155,155,155	0
59	MG	DA	3131	1/1	0.14	0.51	154,154,154,154	0
59	MG	AA	1698	1/1	0.20	0.64	103,103,103,103	0
59	MG	DA	3271	1/1	0.22	0.69	96,96,96,96	0
59	MG	DA	2931	1/1	0.24	0.73	151,151,151,151	1
59	MG	CV	110	1/1	0.24	0.46	105,105,105,105	0
59	MG	DA	3505	1/1	0.26	1.03	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3190	1/1	0.28	1.46	117,117,117,117	0
59	MG	DA	3517	1/1	0.29	0.39	107,107,107,107	0
59	MG	D0	104	1/1	0.30	0.67	98,98,98,98	0
59	MG	DB	204	1/1	0.33	0.21	110,110,110,110	0
59	MG	DA	2944	1/1	0.33	2.47	109,109,109,109	1
59	MG	DA	3042	1/1	0.35	0.42	60,60,60,60	0
59	MG	BA	3335	1/1	0.35	1.65	113,113,113,113	0
59	MG	BA	3132	1/1	0.35	0.42	81,81,81,81	0
59	MG	CA	1754	1/1	0.36	0.31	78,78,78,78	1
59	MG	DA	3590	1/1	0.36	0.47	67,67,67,67	0
59	MG	BA	3529	1/1	0.36	0.70	70,70,70,70	0
59	MG	AV	104	1/1	0.36	0.29	133,133,133,133	0
59	MG	CA	1700	1/1	0.36	0.43	104,104,104,104	0
59	MG	DA	3781	1/1	0.38	0.77	143,143,143,143	0
59	MG	DA	3065	1/1	0.39	0.71	128,128,128,128	0
59	MG	DA	3127	1/1	0.39	0.32	93,93,93,93	0
59	MG	BA	3554	1/1	0.39	0.26	109,109,109,109	0
59	MG	BH	204	1/1	0.40	0.21	57,57,57,57	1
59	MG	CA	1720	1/1	0.41	0.31	106,106,106,106	0
59	MG	CA	1691	1/1	0.41	0.08	103,103,103,103	0
59	MG	DA	3143	1/1	0.41	0.72	113,113,113,113	0
59	MG	AA	1673	1/1	0.42	0.93	90,90,90,90	0
59	MG	AA	1874	1/1	0.42	0.27	111,111,111,111	0
59	MG	CA	1655	1/1	0.42	0.26	84,84,84,84	0
59	MG	DA	2972	1/1	0.43	1.11	97,97,97,97	0
59	MG	CA	1698	1/1	0.44	0.61	73,73,73,73	1
59	MG	DA	3349	1/1	0.44	1.17	141,141,141,141	0
59	MG	CA	1735	1/1	0.44	0.63	127,127,127,127	0
59	MG	DA	3769	1/1	0.45	0.17	142,142,142,142	0
59	MG	BA	3111	1/1	0.45	0.53	79,79,79,79	0
59	MG	BA	3316	1/1	0.45	0.62	98,98,98,98	0
59	MG	BA	3084	1/1	0.45	0.29	88,88,88,88	0
59	MG	DA	3637	1/1	0.46	1.11	88,88,88,88	0
59	MG	DA	3761	1/1	0.46	0.59	96,96,96,96	0
59	MG	DA	2920	1/1	0.47	0.23	15,15,15,15	1
59	MG	AA	1972	1/1	0.47	1.61	98,98,98,98	1
59	MG	DN	202	1/1	0.47	0.60	78,78,78,78	0
59	MG	DA	3017	1/1	0.47	0.41	70,70,70,70	0
59	MG	DA	3485	1/1	0.48	1.83	8,8,8,8	1
59	MG	AA	1757	1/1	0.48	1.55	111,111,111,111	0
59	MG	AA	1605	1/1	0.48	0.33	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1697	1/1	0.48	0.58	83,83,83,83	0
59	MG	BA	2951	1/1	0.48	1.42	142,142,142,142	0
59	MG	BA	3354	1/1	0.48	0.59	76,76,76,76	0
59	MG	BA	3205	1/1	0.49	0.57	78,78,78,78	0
59	MG	DA	3074	1/1	0.49	0.55	129,129,129,129	0
59	MG	CA	1712	1/1	0.49	0.52	88,88,88,88	1
59	MG	DA	3021	1/1	0.49	1.34	87,87,87,87	0
59	MG	BA	3140	1/1	0.49	0.76	113,113,113,113	0
59	MG	BA	2970	1/1	0.50	1.54	101,101,101,101	0
59	MG	AA	1604	1/1	0.50	0.30	118,118,118,118	0
59	MG	DA	3432	1/1	0.50	0.58	86,86,86,86	1
59	MG	AA	1789	1/1	0.50	0.33	108,108,108,108	0
59	MG	AA	1614	1/1	0.50	0.33	113,113,113,113	0
59	MG	CA	1641	1/1	0.51	0.34	84,84,84,84	0
59	MG	BA	3245	1/1	0.51	0.21	116,116,116,116	0
59	MG	BA	3580	1/1	0.51	0.23	135,135,135,135	0
59	MG	AA	1943	1/1	0.52	1.38	60,60,60,60	1
59	MG	D6	102	1/1	0.52	0.92	97,97,97,97	0
59	MG	DA	3449	1/1	0.52	0.47	71,71,71,71	0
59	MG	BA	3006	1/1	0.52	0.95	68,68,68,68	0
59	MG	AA	1666	1/1	0.52	2.59	127,127,127,127	0
59	MG	DA	3489	1/1	0.53	0.55	59,59,59,59	1
59	MG	BA	3585	1/1	0.53	1.84	143,143,143,143	0
59	MG	DF	302	1/1	0.53	1.30	98,98,98,98	0
59	MG	AA	1642	1/1	0.53	0.16	108,108,108,108	0
59	MG	AA	1627	1/1	0.53	1.17	142,142,142,142	0
59	MG	BA	3458	1/1	0.54	1.16	104,104,104,104	0
59	MG	DA	3400	1/1	0.54	0.64	63,63,63,63	1
59	MG	AA	1710	1/1	0.54	0.24	77,77,77,77	0
59	MG	AA	1900	1/1	0.54	0.22	128,128,128,128	0
59	MG	DA	3549	1/1	0.54	0.55	97,97,97,97	0
59	MG	BA	3211	1/1	0.55	0.20	67,67,67,67	0
59	MG	DA	3661	1/1	0.56	0.34	100,100,100,100	0
59	MG	BA	3357	1/1	0.56	0.28	78,78,78,78	1
59	MG	DA	3214	1/1	0.56	0.53	102,102,102,102	0
59	MG	B6	101	1/1	0.56	0.42	111,111,111,111	0
59	MG	BA	2949	1/1	0.56	0.52	102,102,102,102	0
59	MG	BB	204	1/1	0.56	0.15	109,109,109,109	0
59	MG	DA	2976	1/1	0.56	0.65	1,1,1,1	1
59	MG	CA	1756	1/1	0.56	0.66	87,87,87,87	0
59	MG	DA	3439	1/1	0.56	0.28	54,54,54,54	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3563	1/1	0.57	0.52	68,68,68,68	1
59	MG	AA	1828	1/1	0.57	0.25	86,86,86,86	0
59	MG	CA	1676	1/1	0.57	0.29	88,88,88,88	0
59	MG	AA	1635	1/1	0.57	0.70	108,108,108,108	0
59	MG	DA	3666	1/1	0.58	1.14	66,66,66,66	0
59	MG	DA	3298	1/1	0.58	0.34	65,65,65,65	0
59	MG	AA	1883	1/1	0.58	0.85	58,58,58,58	0
59	MG	DA	2984	1/1	0.58	0.42	66,66,66,66	1
59	MG	BA	3234	1/1	0.58	0.59	90,90,90,90	0
59	MG	CA	1726	1/1	0.58	1.02	107,107,107,107	0
59	MG	DE	301	1/1	0.58	0.36	67,67,67,67	0
59	MG	DA	3145	1/1	0.58	1.01	120,120,120,120	0
59	MG	CA	1657	1/1	0.58	0.53	85,85,85,85	0
59	MG	BA	2916	1/1	0.58	0.35	78,78,78,78	0
59	MG	BA	3359	1/1	0.59	0.82	101,101,101,101	0
59	MG	DA	3793	1/1	0.59	0.33	130,130,130,130	0
59	MG	DA	2989	1/1	0.59	0.26	83,83,83,83	0
59	MG	AL	202	1/1	0.59	0.12	73,73,73,73	0
59	MG	DA	3727	1/1	0.59	0.43	70,70,70,70	1
59	MG	CA	1671	1/1	0.59	0.43	99,99,99,99	0
59	MG	DP	202	1/1	0.59	0.60	49,49,49,49	1
59	MG	DA	3640	1/1	0.59	0.46	81,81,81,81	1
59	MG	DA	3786	1/1	0.60	0.38	144,144,144,144	0
59	MG	DA	3240	1/1	0.60	0.07	128,128,128,128	0
59	MG	BA	3301	1/1	0.60	0.63	67,67,67,67	0
59	MG	DD	304	1/1	0.60	0.40	97,97,97,97	0
59	MG	BN	201	1/1	0.60	0.43	64,64,64,64	0
59	MG	BA	3210	1/1	0.60	0.51	106,106,106,106	0
59	MG	DA	3459	1/1	0.60	0.55	92,92,92,92	0
59	MG	AQ	202	1/1	0.60	0.47	97,97,97,97	0
59	MG	DA	3384	1/1	0.60	0.85	120,120,120,120	0
59	MG	AA	1953	1/1	0.61	0.50	120,120,120,120	0
59	MG	DA	3571	1/1	0.61	0.59	96,96,96,96	0
59	MG	BA	3583	1/1	0.61	0.56	81,81,81,81	1
59	MG	AA	1749	1/1	0.61	0.28	74,74,74,74	1
59	MG	BA	3276	1/1	0.61	1.19	125,125,125,125	0
59	MG	BA	2973	1/1	0.61	0.91	85,85,85,85	0
59	MG	DA	2950	1/1	0.61	0.21	80,80,80,80	1
59	MG	AA	1950	1/1	0.62	0.36	81,81,81,81	0
59	MG	AA	1908	1/1	0.62	0.30	65,65,65,65	0
59	MG	DA	3142	1/1	0.62	0.29	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1619	1/1	0.62	0.50	111,111,111,111	0
59	MG	CA	1640	1/1	0.62	0.41	76,76,76,76	0
59	MG	DA	3195	1/1	0.62	0.55	96,96,96,96	0
59	MG	BA	3037	1/1	0.62	0.68	64,64,64,64	0
59	MG	BA	3193	1/1	0.62	0.71	109,109,109,109	0
59	MG	BA	3602	1/1	0.62	1.44	122,122,122,122	1
59	MG	DA	3289	1/1	0.62	0.56	78,78,78,78	0
59	MG	CA	1658	1/1	0.62	0.52	97,97,97,97	0
59	MG	DA	3566	1/1	0.62	0.15	106,106,106,106	0
59	MG	AX	103	1/1	0.62	0.61	112,112,112,112	0
59	MG	CA	1747	1/1	0.62	0.17	79,79,79,79	0
59	MG	DA	3111	1/1	0.62	0.34	83,83,83,83	0
59	MG	DA	3391	1/1	0.62	0.44	73,73,73,73	0
59	MG	BA	3340	1/1	0.63	0.94	99,99,99,99	0
59	MG	BA	3560	1/1	0.63	0.99	83,83,83,83	0
59	MG	BA	3395	1/1	0.63	0.63	84,84,84,84	0
59	MG	DA	3094	1/1	0.63	0.53	87,87,87,87	0
59	MG	DA	3584	1/1	0.63	0.64	80,80,80,80	0
59	MG	BA	3417	1/1	0.63	0.48	68,68,68,68	0
59	MG	DA	3124	1/1	0.63	0.53	81,81,81,81	0
59	MG	DA	2928	1/1	0.63	0.33	61,61,61,61	1
59	MG	BA	2929	1/1	0.63	0.26	90,90,90,90	0
59	MG	DA	3324	1/1	0.63	0.33	66,66,66,66	1
59	MG	DA	3138	1/1	0.63	0.83	139,139,139,139	0
59	MG	BA	2907	1/1	0.63	0.32	108,108,108,108	0
59	MG	DA	3515	1/1	0.64	1.29	108,108,108,108	0
59	MG	AO	101	1/1	0.64	0.39	111,111,111,111	0
59	MG	CA	1615	1/1	0.64	1.19	104,104,104,104	0
59	MG	DA	3552	1/1	0.64	0.42	120,120,120,120	0
59	MG	BA	2923	1/1	0.64	1.07	96,96,96,96	0
59	MG	BA	3248	1/1	0.64	0.35	101,101,101,101	0
59	MG	AA	1648	1/1	0.64	0.78	108,108,108,108	0
59	MG	BA	3284	1/1	0.64	0.55	97,97,97,97	0
59	MG	DA	3417	1/1	0.64	0.57	48,48,48,48	1
59	MG	CA	1766	1/1	0.65	0.30	118,118,118,118	0
59	MG	BA	3097	1/1	0.65	0.45	89,89,89,89	0
59	MG	DA	3072	1/1	0.65	0.44	81,81,81,81	0
59	MG	CA	1681	1/1	0.65	0.42	95,95,95,95	0
59	MG	AA	1935	1/1	0.65	0.25	96,96,96,96	0
59	MG	BA	2953	1/1	0.65	0.58	84,84,84,84	0
59	MG	BA	2967	1/1	0.65	0.28	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3539	1/1	0.65	0.58	70,70,70,70	0
59	MG	DA	3241	1/1	0.65	0.49	34,34,34,34	1
59	MG	BA	3039	1/1	0.65	0.76	81,81,81,81	0
59	MG	AA	1725	1/1	0.65	0.50	70,70,70,70	1
59	MG	DA	3475	1/1	0.66	0.39	115,115,115,115	0
59	MG	AA	1745	1/1	0.66	0.54	50,50,50,50	1
59	MG	DA	3689	1/1	0.66	0.15	123,123,123,123	0
59	MG	BA	3272	1/1	0.66	1.26	126,126,126,126	0
59	MG	CA	1730	1/1	0.66	0.18	106,106,106,106	0
59	MG	AN	102	1/1	0.66	0.12	141,141,141,141	0
59	MG	BA	3199	1/1	0.66	1.88	110,110,110,110	0
59	MG	AA	1851	1/1	0.66	0.48	62,62,62,62	0
59	MG	BA	3113	1/1	0.66	0.13	95,95,95,95	0
59	MG	BA	3121	1/1	0.66	1.00	125,125,125,125	0
59	MG	BA	3336	1/1	0.66	0.24	99,99,99,99	0
59	MG	AA	1891	1/1	0.66	0.37	54,54,54,54	1
59	MG	DA	2988	1/1	0.66	0.54	40,40,40,40	1
59	MG	CA	1779	1/1	0.66	0.51	102,102,102,102	0
59	MG	CJ	201	1/1	0.66	0.41	115,115,115,115	0
59	MG	CS	102	1/1	0.66	0.11	102,102,102,102	0
59	MG	AA	1938	1/1	0.66	1.01	124,124,124,124	0
59	MG	DA	3538	1/1	0.67	0.60	118,118,118,118	0
59	MG	DA	3238	1/1	0.67	0.28	134,134,134,134	0
59	MG	BA	3486	1/1	0.67	0.26	54,54,54,54	0
59	MG	CA	1650	1/1	0.67	0.89	79,79,79,79	0
59	MG	DA	3253	1/1	0.67	0.45	52,52,52,52	0
59	MG	DA	3004	1/1	0.67	0.92	122,122,122,122	0
59	MG	BA	2914	1/1	0.67	1.75	106,106,106,106	0
59	MG	AA	1922	1/1	0.67	0.28	82,82,82,82	0
59	MG	AA	1762	1/1	0.67	0.20	74,74,74,74	0
59	MG	DA	3617	1/1	0.67	0.42	111,111,111,111	0
59	MG	BA	3566	1/1	0.67	0.39	66,66,66,66	1
59	MG	BA	3570	1/1	0.67	0.54	115,115,115,115	0
59	MG	AA	1795	1/1	0.67	0.12	96,96,96,96	0
59	MG	DA	3665	1/1	0.67	0.57	96,96,96,96	0
59	MG	DA	3389	1/1	0.67	1.20	145,145,145,145	0
59	MG	DA	3676	1/1	0.67	0.61	96,96,96,96	0
59	MG	AA	1798	1/1	0.67	0.40	114,114,114,114	0
59	MG	AA	1944	1/1	0.67	0.34	76,76,76,76	0
59	MG	DA	3414	1/1	0.67	0.89	121,121,121,121	0
59	MG	DA	3113	1/1	0.67	1.29	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3123	1/1	0.67	1.02	91,91,91,91	0
59	MG	BA	3213	1/1	0.67	0.63	135,135,135,135	0
59	MG	AA	1766	1/1	0.67	0.71	74,74,74,74	0
59	MG	AY	103	1/1	0.67	0.62	108,108,108,108	0
59	MG	BA	3383	1/1	0.67	0.11	126,126,126,126	0
59	MG	AA	1905	1/1	0.67	0.68	71,71,71,71	1
59	MG	CA	1608	1/1	0.67	0.73	124,124,124,124	0
59	MG	CA	1731	1/1	0.67	0.21	76,76,76,76	0
59	MG	DA	3511	1/1	0.67	1.33	83,83,83,83	0
59	MG	AA	1768	1/1	0.67	0.88	107,107,107,107	0
59	MG	DR	202	1/1	0.67	0.38	65,65,65,65	1
59	MG	BA	3186	1/1	0.67	0.11	81,81,81,81	0
59	MG	AA	1889	1/1	0.68	0.42	115,115,115,115	0
59	MG	BA	3222	1/1	0.68	0.92	108,108,108,108	0
59	MG	AD	303	1/1	0.68	0.47	134,134,134,134	0
59	MG	BA	3112	1/1	0.68	0.41	101,101,101,101	0
59	MG	CA	1739	1/1	0.68	0.53	104,104,104,104	0
59	MG	BA	2901	1/1	0.68	1.43	113,113,113,113	0
59	MG	AA	1829	1/1	0.68	0.55	91,91,91,91	0
59	MG	CA	1649	1/1	0.68	1.08	92,92,92,92	0
59	MG	BA	3514	1/1	0.68	0.39	76,76,76,76	0
59	MG	AA	1708	1/1	0.68	0.38	65,65,65,65	1
59	MG	CA	1773	1/1	0.68	0.42	106,106,106,106	0
59	MG	BA	2984	1/1	0.68	0.32	92,92,92,92	0
59	MG	AA	1857	1/1	0.68	0.18	57,57,57,57	0
59	MG	DA	3404	1/1	0.68	0.43	87,87,87,87	0
59	MG	DA	3096	1/1	0.68	0.44	80,80,80,80	0
59	MG	BA	3019	1/1	0.68	0.95	66,66,66,66	0
59	MG	BA	3317	1/1	0.68	0.88	64,64,64,64	1
59	MG	DA	3747	1/1	0.68	0.54	38,38,38,38	1
59	MG	BA	3327	1/1	0.68	0.55	59,59,59,59	0
59	MG	AA	1735	1/1	0.68	0.77	85,85,85,85	0
59	MG	DA	3780	1/1	0.68	0.46	77,77,77,77	0
59	MG	AA	1722	1/1	0.68	0.76	116,116,116,116	0
59	MG	DA	2914	1/1	0.68	0.59	83,83,83,83	0
59	MG	DA	3137	1/1	0.68	0.27	70,70,70,70	0
59	MG	BA	3082	1/1	0.68	0.29	90,90,90,90	0
59	MG	DA	3495	1/1	0.68	0.62	75,75,75,75	0
59	MG	BA	3604	1/1	0.68	0.66	82,82,82,82	0
59	MG	AA	1959	1/1	0.68	0.83	146,146,146,146	0
59	MG	DA	2936	1/1	0.68	0.67	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3087	1/1	0.68	0.45	87,87,87,87	0
59	MG	CA	1722	1/1	0.68	0.31	73,73,73,73	0
59	MG	DA	2953	1/1	0.68	0.66	99,99,99,99	0
59	MG	CA	1743	1/1	0.69	1.95	81,81,81,81	0
59	MG	DA	3150	1/1	0.69	0.17	98,98,98,98	0
59	MG	DA	2958	1/1	0.69	0.20	59,59,59,59	1
59	MG	CA	1745	1/1	0.69	0.28	112,112,112,112	0
59	MG	DA	3231	1/1	0.69	0.42	98,98,98,98	0
59	MG	BA	3576	1/1	0.69	0.18	97,97,97,97	0
59	MG	DA	2983	1/1	0.69	0.57	79,79,79,79	1
59	MG	BA	3313	1/1	0.69	0.15	70,70,70,70	0
59	MG	BA	3367	1/1	0.69	1.56	96,96,96,96	0
59	MG	CA	1762	1/1	0.69	0.20	95,95,95,95	0
59	MG	CA	1659	1/1	0.69	1.53	100,100,100,100	0
59	MG	DA	3009	1/1	0.69	1.71	83,83,83,83	0
59	MG	DA	3634	1/1	0.69	0.34	83,83,83,83	0
59	MG	DA	3316	1/1	0.69	0.45	59,59,59,59	1
59	MG	BA	3379	1/1	0.69	1.75	114,114,114,114	0
59	MG	DA	3643	1/1	0.69	0.35	113,113,113,113	0
59	MG	DA	3649	1/1	0.69	0.47	66,66,66,66	0
59	MG	BA	3601	1/1	0.69	0.41	79,79,79,79	0
59	MG	DA	3346	1/1	0.69	0.35	59,59,59,59	0
59	MG	CA	1776	1/1	0.69	0.83	83,83,83,83	0
59	MG	AA	1651	1/1	0.69	0.20	76,76,76,76	0
59	MG	BA	3387	1/1	0.69	0.41	87,87,87,87	0
59	MG	BA	3120	1/1	0.69	0.13	101,101,101,101	0
59	MG	BA	3320	1/1	0.69	0.32	92,92,92,92	0
59	MG	BA	2999	1/1	0.69	0.12	86,86,86,86	0
59	MG	CA	1709	1/1	0.69	0.15	85,85,85,85	1
59	MG	AA	1932	1/1	0.69	0.30	82,82,82,82	0
59	MG	DA	3770	1/1	0.69	0.31	85,85,85,85	1
59	MG	AA	1711	1/1	0.69	0.25	90,90,90,90	0
59	MG	BA	3338	1/1	0.69	0.43	97,97,97,97	0
59	MG	DA	3443	1/1	0.69	0.41	133,133,133,133	0
59	MG	DA	2925	1/1	0.69	1.06	108,108,108,108	0
59	MG	CA	1626	1/1	0.69	0.54	112,112,112,112	0
59	MG	DA	3470	1/1	0.69	0.59	75,75,75,75	0
59	MG	DA	3133	1/1	0.69	0.90	120,120,120,120	0
59	MG	DA	3134	1/1	0.69	0.33	74,74,74,74	0
59	MG	AA	1835	1/1	0.69	1.82	102,102,102,102	0
59	MG	BA	3350	1/1	0.69	0.99	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3286	1/1	0.69	0.27	57,57,57,57	0
59	MG	AV	106	1/1	0.69	0.24	87,87,87,87	1
59	MG	BA	3491	1/1	0.70	0.17	70,70,70,70	0
59	MG	DA	3155	1/1	0.70	0.87	78,78,78,78	0
59	MG	DA	3109	1/1	0.70	0.45	90,90,90,90	0
59	MG	BA	3265	1/1	0.70	0.33	66,66,66,66	0
59	MG	AA	1660	1/1	0.70	0.21	82,82,82,82	0
59	MG	DA	3409	1/1	0.70	0.18	53,53,53,53	1
59	MG	BA	3532	1/1	0.70	1.45	88,88,88,88	0
59	MG	BA	3548	1/1	0.70	0.36	92,92,92,92	0
59	MG	AA	1870	1/1	0.70	0.38	73,73,73,73	0
59	MG	B5	101	1/1	0.70	0.57	83,83,83,83	0
59	MG	AA	1956	1/1	0.70	0.56	58,58,58,58	0
59	MG	DA	3022	1/1	0.70	0.47	71,71,71,71	0
59	MG	CA	1601	1/1	0.70	0.27	96,96,96,96	0
59	MG	AA	1728	1/1	0.70	0.30	78,78,78,78	0
59	MG	DA	3321	1/1	0.70	0.32	88,88,88,88	0
59	MG	BA	3016	1/1	0.70	0.36	66,66,66,66	0
59	MG	AA	1640	1/1	0.70	1.72	127,127,127,127	0
59	MG	AA	1667	1/1	0.70	0.25	49,49,49,49	0
59	MG	DA	3146	1/1	0.70	0.59	85,85,85,85	0
59	MG	DA	3374	1/1	0.70	0.36	91,91,91,91	0
59	MG	BA	2971	1/1	0.71	1.10	92,92,92,92	0
59	MG	AA	1818	1/1	0.71	0.13	60,60,60,60	0
59	MG	DA	3168	1/1	0.71	1.16	100,100,100,100	0
59	MG	CA	1609	1/1	0.71	1.04	93,93,93,93	0
59	MG	DA	3203	1/1	0.71	0.75	112,112,112,112	0
59	MG	DA	3210	1/1	0.71	0.29	71,71,71,71	0
59	MG	AA	1820	1/1	0.71	0.32	97,97,97,97	0
59	MG	DA	2908	1/1	0.71	1.43	97,97,97,97	0
59	MG	BA	2991	1/1	0.71	0.98	60,60,60,60	1
59	MG	DA	3680	1/1	0.71	0.76	98,98,98,98	0
59	MG	B0	102	1/1	0.71	0.27	91,91,91,91	0
59	MG	BA	3568	1/1	0.71	0.46	58,58,58,58	0
59	MG	DA	3718	1/1	0.71	0.78	92,92,92,92	0
59	MG	CA	1646	1/1	0.71	0.78	102,102,102,102	0
59	MG	AA	1872	1/1	0.71	0.67	77,77,77,77	0
59	MG	AA	1758	1/1	0.71	0.44	98,98,98,98	0
59	MG	BA	3215	1/1	0.71	0.57	4,4,4,4	1
59	MG	BA	3217	1/1	0.71	0.17	72,72,72,72	0
59	MG	AA	1792	1/1	0.71	0.17	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3525	1/1	0.71	0.99	63,63,63,63	0
59	MG	BA	3331	1/1	0.71	1.51	92,92,92,92	0
59	MG	AA	1702	1/1	0.71	0.28	64,64,64,64	0
59	MG	BA	3487	1/1	0.71	0.29	64,64,64,64	0
59	MG	DD	303	1/1	0.71	0.38	64,64,64,64	0
59	MG	AA	1776	1/1	0.71	0.69	119,119,119,119	0
59	MG	CA	1683	1/1	0.71	0.36	60,60,60,60	0
59	MG	BA	3505	1/1	0.71	0.47	95,95,95,95	0
59	MG	BA	3052	1/1	0.71	0.44	64,64,64,64	0
59	MG	DA	2990	1/1	0.71	0.45	43,43,43,43	1
59	MG	BR	201	1/1	0.71	0.46	47,47,47,47	1
59	MG	BA	3071	1/1	0.71	0.72	110,110,110,110	0
59	MG	CA	1770	1/1	0.72	0.67	54,54,54,54	1
59	MG	BA	3342	1/1	0.72	0.58	127,127,127,127	0
59	MG	CA	1741	1/1	0.72	1.71	106,106,106,106	0
59	MG	AA	1689	1/1	0.72	0.16	82,82,82,82	1
59	MG	DA	3736	1/1	0.72	0.18	77,77,77,77	1
59	MG	DA	3192	1/1	0.72	1.03	70,70,70,70	0
59	MG	AA	1772	1/1	0.72	0.50	85,85,85,85	0
59	MG	BB	203	1/1	0.72	0.36	59,59,59,59	0
59	MG	DA	3582	1/1	0.72	0.58	47,47,47,47	1
59	MG	CM	201	1/1	0.72	0.12	131,131,131,131	0
59	MG	DA	3366	1/1	0.72	0.74	9,9,9,9	1
59	MG	DA	3369	1/1	0.72	0.26	95,95,95,95	0
59	MG	CA	1723	1/1	0.72	0.49	82,82,82,82	0
59	MG	DA	3491	1/1	0.72	1.06	107,107,107,107	0
59	MG	CA	1695	1/1	0.72	0.51	110,110,110,110	0
59	MG	DA	3497	1/1	0.72	0.28	103,103,103,103	0
59	MG	DD	305	1/1	0.72	0.28	1,1,1,1	1
59	MG	BA	3241	1/1	0.72	0.26	44,44,44,44	0
59	MG	D1	101	1/1	0.72	0.23	75,75,75,75	0
59	MG	D6	101	1/1	0.72	0.60	95,95,95,95	0
59	MG	CA	1663	1/1	0.72	0.20	97,97,97,97	0
59	MG	DP	206	1/1	0.72	1.13	82,82,82,82	0
59	MG	DA	3524	1/1	0.72	0.58	61,61,61,61	0
59	MG	BA	3569	1/1	0.72	1.13	113,113,113,113	0
59	MG	BA	3571	1/1	0.73	0.45	77,77,77,77	0
59	MG	BA	3400	1/1	0.73	0.10	87,87,87,87	0
59	MG	AA	1793	1/1	0.73	0.17	75,75,75,75	0
59	MG	BA	3581	1/1	0.73	1.48	95,95,95,95	0
59	MG	BA	3095	1/1	0.73	0.39	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3337	1/1	0.73	0.25	90,90,90,90	0
59	MG	AA	1732	1/1	0.73	0.11	52,52,52,52	0
59	MG	BA	3030	1/1	0.73	0.54	79,79,79,79	0
59	MG	AA	1964	1/1	0.73	1.22	106,106,106,106	0
59	MG	CA	1732	1/1	0.73	0.19	70,70,70,70	0
59	MG	DA	3737	1/1	0.73	0.80	74,74,74,74	0
59	MG	AA	1945	1/1	0.73	1.01	94,94,94,94	1
59	MG	BA	3116	1/1	0.73	0.53	81,81,81,81	0
59	MG	AA	1866	1/1	0.73	0.34	74,74,74,74	0
59	MG	BE	304	1/1	0.73	0.44	46,46,46,46	1
59	MG	DA	3779	1/1	0.73	0.76	122,122,122,122	0
59	MG	DA	3546	1/1	0.73	0.85	11,11,11,11	1
59	MG	DA	3172	1/1	0.73	1.02	102,102,102,102	0
59	MG	BA	2904	1/1	0.73	1.74	104,104,104,104	0
59	MG	BA	3304	1/1	0.73	1.24	90,90,90,90	0
59	MG	CA	1750	1/1	0.73	1.39	102,102,102,102	0
59	MG	DB	209	1/1	0.73	0.24	95,95,95,95	0
59	MG	DA	3075	1/1	0.73	0.15	98,98,98,98	0
59	MG	BA	3122	1/1	0.73	0.92	106,106,106,106	0
59	MG	DA	3419	1/1	0.73	0.89	122,122,122,122	0
59	MG	DA	3423	1/1	0.73	0.45	51,51,51,51	1
59	MG	CA	1755	1/1	0.73	0.29	100,100,100,100	0
59	MG	BA	3374	1/1	0.73	0.73	74,74,74,74	0
59	MG	DN	203	1/1	0.73	0.83	64,64,64,64	1
59	MG	DO	201	1/1	0.73	0.18	117,117,117,117	0
59	MG	BA	3218	1/1	0.73	0.34	111,111,111,111	0
59	MG	AA	1838	1/1	0.73	0.74	80,80,80,80	0
59	MG	BA	3225	1/1	0.73	0.19	62,62,62,62	0
59	MG	BA	2965	1/1	0.73	0.77	84,84,84,84	0
59	MG	BB	206	1/1	0.74	0.63	90,90,90,90	1
59	MG	BA	3493	1/1	0.74	0.47	101,101,101,101	0
59	MG	DA	3326	1/1	0.74	0.54	63,63,63,63	0
59	MG	DA	3329	1/1	0.74	0.41	110,110,110,110	0
59	MG	BA	2986	1/1	0.74	0.36	52,52,52,52	0
59	MG	DA	3693	1/1	0.74	0.41	33,33,33,33	1
59	MG	BA	2987	1/1	0.74	0.24	104,104,104,104	0
59	MG	BA	2908	1/1	0.74	0.16	84,84,84,84	0
59	MG	CV	106	1/1	0.74	0.38	101,101,101,101	0
59	MG	DA	3732	1/1	0.74	0.30	67,67,67,67	0
59	MG	AA	1962	1/1	0.74	0.78	65,65,65,65	0
59	MG	D0	102	1/1	0.74	0.40	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1682	1/1	0.74	1.09	104,104,104,104	0
59	MG	AA	1803	1/1	0.74	0.53	98,98,98,98	0
59	MG	BA	3587	1/1	0.74	0.54	47,47,47,47	0
59	MG	CA	1610	1/1	0.74	2.00	143,143,143,143	0
59	MG	CA	1684	1/1	0.74	0.47	64,64,64,64	0
59	MG	DA	3068	1/1	0.74	0.34	51,51,51,51	0
59	MG	DA	3556	1/1	0.74	0.56	97,97,97,97	0
59	MG	DA	3559	1/1	0.74	0.32	74,74,74,74	0
59	MG	DA	2909	1/1	0.74	0.48	83,83,83,83	0
59	MG	CA	1686	1/1	0.74	0.28	74,74,74,74	0
59	MG	CA	1752	1/1	0.74	0.58	113,113,113,113	0
59	MG	DB	211	1/1	0.74	0.34	80,80,80,80	0
59	MG	DA	3576	1/1	0.74	0.35	87,87,87,87	0
59	MG	DA	3418	1/1	0.74	0.14	88,88,88,88	0
59	MG	CA	1611	1/1	0.74	0.43	86,86,86,86	0
59	MG	BA	3600	1/1	0.74	0.54	63,63,63,63	0
59	MG	DA	3597	1/1	0.74	0.28	66,66,66,66	0
59	MG	AA	1814	1/1	0.74	1.04	77,77,77,77	0
59	MG	CA	1630	1/1	0.74	0.18	68,68,68,68	0
59	MG	BA	3134	1/1	0.74	0.10	65,65,65,65	0
59	MG	BA	3567	1/1	0.74	0.29	76,76,76,76	0
59	MG	AA	1861	1/1	0.74	0.62	77,77,77,77	0
59	MG	CA	1647	1/1	0.74	0.42	77,77,77,77	0
59	MG	AA	1788	1/1	0.74	0.33	80,80,80,80	0
59	MG	AA	1968	1/1	0.75	0.51	95,95,95,95	0
59	MG	DA	2911	1/1	0.75	0.65	91,91,91,91	0
59	MG	CV	101	1/1	0.75	0.31	93,93,93,93	1
59	MG	DA	2919	1/1	0.75	0.23	57,57,57,57	0
59	MG	AA	1738	1/1	0.75	0.83	59,59,59,59	0
59	MG	CV	107	1/1	0.75	0.29	115,115,115,115	0
59	MG	BA	3042	1/1	0.75	0.35	103,103,103,103	0
59	MG	DA	3553	1/1	0.75	0.70	68,68,68,68	0
59	MG	BA	3536	1/1	0.75	0.84	73,73,73,73	0
59	MG	DA	3496	1/1	0.75	0.26	83,83,83,83	0
59	MG	AA	1652	1/1	0.75	0.18	95,95,95,95	0
59	MG	CC	301	1/1	0.75	0.86	117,117,117,117	0
59	MG	BA	3325	1/1	0.75	0.38	84,84,84,84	0
59	MG	CJ	202	1/1	0.75	0.09	130,130,130,130	0
59	MG	DA	3785	1/1	0.75	1.05	35,35,35,35	1
59	MG	BA	3512	1/1	0.75	0.28	51,51,51,51	0
59	MG	DA	3027	1/1	0.76	0.44	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1775	1/1	0.76	0.26	92,92,92,92	0
59	MG	DA	3357	1/1	0.76	0.34	64,64,64,64	0
59	MG	DA	3710	1/1	0.76	0.61	92,92,92,92	0
59	MG	DA	3165	1/1	0.76	0.52	121,121,121,121	0
59	MG	BA	3384	1/1	0.76	0.82	95,95,95,95	0
59	MG	CA	1662	1/1	0.76	0.12	79,79,79,79	0
59	MG	BA	3196	1/1	0.76	0.48	64,64,64,64	0
59	MG	BA	2992	1/1	0.76	0.28	50,50,50,50	1
59	MG	AA	1620	1/1	0.76	0.63	71,71,71,71	0
59	MG	DA	3208	1/1	0.76	0.44	91,91,91,91	0
59	MG	DA	3403	1/1	0.76	0.23	109,109,109,109	0
59	MG	BA	3102	1/1	0.76	0.67	64,64,64,64	0
59	MG	CA	1619	1/1	0.76	0.21	116,116,116,116	0
59	MG	DA	3777	1/1	0.76	0.27	70,70,70,70	0
59	MG	AO	102	1/1	0.76	1.04	77,77,77,77	0
59	MG	DA	3561	1/1	0.76	0.46	81,81,81,81	1
59	MG	CV	104	1/1	0.76	0.18	86,86,86,86	0
59	MG	DA	2961	1/1	0.76	0.52	126,126,126,126	0
59	MG	CA	1627	1/1	0.76	0.17	71,71,71,71	0
59	MG	CA	1749	1/1	0.76	0.53	16,16,16,16	1
59	MG	CA	1628	1/1	0.76	0.19	88,88,88,88	0
59	MG	DA	3288	1/1	0.76	0.13	60,60,60,60	0
59	MG	BA	3251	1/1	0.76	0.67	100,100,100,100	0
59	MG	AA	1690	1/1	0.76	0.22	81,81,81,81	1
59	MG	DA	3306	1/1	0.76	0.11	56,56,56,56	0
59	MG	DA	3468	1/1	0.76	0.47	76,76,76,76	0
59	MG	BA	3361	1/1	0.76	1.62	105,105,105,105	0
59	MG	BA	3185	1/1	0.76	0.34	75,75,75,75	0
59	MG	BH	201	1/1	0.76	0.29	71,71,71,71	1
59	MG	BA	3501	1/1	0.76	0.25	112,112,112,112	0
59	MG	AA	1624	1/1	0.76	0.73	98,98,98,98	0
59	MG	BA	3375	1/1	0.76	1.10	74,74,74,74	0
59	MG	DA	3341	1/1	0.76	0.57	62,62,62,62	0
59	MG	DA	3670	1/1	0.76	0.47	88,88,88,88	0
59	MG	AA	1948	1/1	0.76	0.59	114,114,114,114	0
59	MG	BA	2993	1/1	0.77	0.87	86,86,86,86	0
59	MG	CA	1607	1/1	0.77	0.11	94,94,94,94	0
59	MG	DA	3307	1/1	0.77	0.32	77,77,77,77	0
59	MG	DA	3730	1/1	0.77	0.49	91,91,91,91	0
59	MG	AA	1777	1/1	0.77	0.37	115,115,115,115	0
59	MG	BA	3588	1/1	0.77	1.38	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3596	1/1	0.77	1.25	107,107,107,107	0
59	MG	AA	1685	1/1	0.77	0.39	30,30,30,30	1
59	MG	DA	3158	1/1	0.77	0.55	130,130,130,130	0
59	MG	CA	1733	1/1	0.77	0.17	76,76,76,76	0
59	MG	DA	3464	1/1	0.77	0.66	62,62,62,62	1
59	MG	BA	3445	1/1	0.77	0.51	111,111,111,111	0
59	MG	AA	1904	1/1	0.77	0.45	81,81,81,81	0
59	MG	BA	3460	1/1	0.77	0.55	40,40,40,40	0
59	MG	DA	3476	1/1	0.77	0.41	120,120,120,120	0
59	MG	AA	1880	1/1	0.77	0.51	102,102,102,102	0
59	MG	BA	2935	1/1	0.77	0.43	102,102,102,102	0
59	MG	DA	3789	1/1	0.77	0.40	68,68,68,68	0
59	MG	DA	3628	1/1	0.77	1.26	93,93,93,93	0
59	MG	CA	1746	1/1	0.77	0.53	85,85,85,85	0
59	MG	DB	207	1/1	0.77	0.41	53,53,53,53	1
59	MG	AA	1630	1/1	0.77	0.31	57,57,57,57	0
59	MG	CA	1634	1/1	0.77	0.12	97,97,97,97	0
59	MG	AA	1912	1/1	0.77	0.32	57,57,57,57	1
59	MG	AA	1915	1/1	0.77	0.48	75,75,75,75	0
59	MG	BA	3043	1/1	0.77	0.38	80,80,80,80	0
59	MG	DA	3392	1/1	0.77	0.36	81,81,81,81	0
59	MG	AA	1625	1/1	0.77	0.48	73,73,73,73	1
59	MG	BA	3311	1/1	0.77	0.37	80,80,80,80	0
59	MG	BA	3391	1/1	0.77	1.34	91,91,91,91	1
59	MG	D9	101	1/1	0.77	0.34	92,92,92,92	1
59	MG	CA	1654	1/1	0.77	0.56	77,77,77,77	0
59	MG	DA	3540	1/1	0.77	0.32	152,152,152,152	0
59	MG	DA	3544	1/1	0.77	0.14	62,62,62,62	0
59	MG	DA	3711	1/1	0.77	0.37	55,55,55,55	1
59	MG	CA	1685	1/1	0.78	0.37	92,92,92,92	0
59	MG	CA	1637	1/1	0.78	0.14	114,114,114,114	0
59	MG	BA	3173	1/1	0.78	0.30	102,102,102,102	1
59	MG	CA	1692	1/1	0.78	0.23	140,140,140,140	0
59	MG	BA	3115	1/1	0.78	0.41	93,93,93,93	0
59	MG	AA	1869	1/1	0.78	0.59	75,75,75,75	0
59	MG	DA	3420	1/1	0.78	0.62	100,100,100,100	0
59	MG	DA	3421	1/1	0.78	0.18	71,71,71,71	0
59	MG	CA	1751	1/1	0.78	0.26	69,69,69,69	1
59	MG	AA	1770	1/1	0.78	0.37	76,76,76,76	0
59	MG	BA	3414	1/1	0.78	0.36	67,67,67,67	0
59	MG	BA	3017	1/1	0.78	0.94	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3594	1/1	0.78	0.23	83,83,83,83	0
59	MG	DA	3577	1/1	0.78	0.16	92,92,92,92	0
59	MG	CA	1758	1/1	0.78	0.56	126,126,126,126	0
59	MG	DA	3014	1/1	0.78	0.46	108,108,108,108	0
59	MG	BA	3421	1/1	0.78	0.33	68,68,68,68	0
59	MG	BA	3430	1/1	0.78	0.36	68,68,68,68	0
59	MG	DA	3607	1/1	0.78	0.29	104,104,104,104	0
59	MG	BA	2927	1/1	0.78	0.33	83,83,83,83	1
59	MG	BA	3281	1/1	0.78	0.47	94,94,94,94	0
59	MG	BA	3326	1/1	0.78	0.62	77,77,77,77	0
59	MG	CA	1622	1/1	0.78	0.75	99,99,99,99	0
59	MG	BA	3025	1/1	0.78	0.22	83,83,83,83	0
59	MG	DA	3354	1/1	0.78	0.27	52,52,52,52	0
59	MG	AA	1794	1/1	0.78	0.47	106,106,106,106	0
59	MG	BA	3290	1/1	0.78	0.38	86,86,86,86	0
59	MG	DA	3200	1/1	0.78	0.57	62,62,62,62	0
59	MG	CA	1737	1/1	0.78	0.12	120,120,120,120	0
59	MG	DN	201	1/1	0.78	0.23	19,19,19,19	1
59	MG	BA	3004	1/1	0.78	1.52	84,84,84,84	0
59	MG	DA	3673	1/1	0.78	0.81	116,116,116,116	0
59	MG	BA	3303	1/1	0.78	0.14	88,88,88,88	0
59	MG	DA	3107	1/1	0.78	0.61	103,103,103,103	0
59	MG	DA	3222	1/1	0.78	0.30	79,79,79,79	0
59	MG	DA	2951	1/1	0.78	0.46	102,102,102,102	0
59	MG	DA	3235	1/1	0.78	0.48	110,110,110,110	0
59	MG	BA	3492	1/1	0.79	0.15	31,31,31,31	1
59	MG	BA	3085	1/1	0.79	0.45	68,68,68,68	0
59	MG	AA	1736	1/1	0.79	1.18	101,101,101,101	0
59	MG	AA	1910	1/1	0.79	0.17	120,120,120,120	0
59	MG	DA	3340	1/1	0.79	0.28	96,96,96,96	0
59	MG	CV	112	1/1	0.79	0.20	69,69,69,69	0
59	MG	CA	1680	1/1	0.79	0.98	102,102,102,102	0
59	MG	DA	3105	1/1	0.79	0.89	92,92,92,92	0
59	MG	AA	1754	1/1	0.79	0.12	124,124,124,124	0
59	MG	DA	3763	1/1	0.79	0.52	62,62,62,62	1
59	MG	AA	1644	1/1	0.79	0.32	84,84,84,84	0
59	MG	CA	1765	1/1	0.79	1.09	94,94,94,94	0
59	MG	DA	3363	1/1	0.79	0.39	69,69,69,69	0
59	MG	DA	3112	1/1	0.79	0.10	87,87,87,87	0
59	MG	DA	3220	1/1	0.79	0.93	117,117,117,117	0
59	MG	DA	3493	1/1	0.79	0.39	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3528	1/1	0.79	0.46	73,73,73,73	0
59	MG	BA	3104	1/1	0.79	0.51	78,78,78,78	0
59	MG	AA	1703	1/1	0.79	0.15	44,44,44,44	1
59	MG	DA	3390	1/1	0.79	0.56	60,60,60,60	1
59	MG	BA	3032	1/1	0.79	0.36	88,88,88,88	0
59	MG	BA	3547	1/1	0.79	0.26	78,78,78,78	0
59	MG	DA	3005	1/1	0.79	0.11	69,69,69,69	0
59	MG	BA	3141	1/1	0.79	0.59	104,104,104,104	0
59	MG	BA	3380	1/1	0.79	1.22	133,133,133,133	0
59	MG	DA	3537	1/1	0.79	0.49	56,56,56,56	0
59	MG	DA	3671	1/1	0.79	0.89	103,103,103,103	0
59	MG	DA	3015	1/1	0.79	0.37	81,81,81,81	0
59	MG	BA	3479	1/1	0.79	0.52	133,133,133,133	0
59	MG	BA	3146	1/1	0.79	1.09	113,113,113,113	0
59	MG	DA	3686	1/1	0.79	0.34	107,107,107,107	0
59	MG	AA	1787	1/1	0.79	0.20	109,109,109,109	0
59	MG	BA	3346	1/1	0.79	0.52	71,71,71,71	0
59	MG	DA	3695	1/1	0.79	0.42	81,81,81,81	0
59	MG	DA	3702	1/1	0.79	0.43	80,80,80,80	0
59	MG	CA	1716	1/1	0.79	0.53	110,110,110,110	0
59	MG	DA	2942	1/1	0.79	0.80	27,27,27,27	1
59	MG	AA	1781	1/1	0.80	0.32	111,111,111,111	0
59	MG	BA	3142	1/1	0.80	0.17	67,67,67,67	0
59	MG	DA	3688	1/1	0.80	0.35	107,107,107,107	1
59	MG	AA	1617	1/1	0.80	0.16	109,109,109,109	0
59	MG	DA	3514	1/1	0.80	0.40	82,82,82,82	0
59	MG	BA	3378	1/1	0.80	0.40	79,79,79,79	0
59	MG	DA	3007	1/1	0.80	0.28	57,57,57,57	0
59	MG	DA	3161	1/1	0.80	0.64	61,61,61,61	0
59	MG	BA	3157	1/1	0.80	0.56	60,60,60,60	0
59	MG	DA	3368	1/1	0.80	0.52	104,104,104,104	0
59	MG	BA	3590	1/1	0.80	0.17	90,90,90,90	0
59	MG	BA	3324	1/1	0.80	0.41	63,63,63,63	0
59	MG	DA	3191	1/1	0.80	0.21	83,83,83,83	0
59	MG	BA	3027	1/1	0.80	0.33	74,74,74,74	0
59	MG	DA	2905	1/1	0.80	0.08	80,80,80,80	0
59	MG	DA	3547	1/1	0.80	0.72	89,89,89,89	0
59	MG	CA	1696	1/1	0.80	1.10	79,79,79,79	0
59	MG	DA	3751	1/1	0.80	0.59	82,82,82,82	0
59	MG	DA	3756	1/1	0.80	0.44	106,106,106,106	0
59	MG	DA	3758	1/1	0.80	0.89	95,95,95,95	0
59	MG	BA	3176	1/1	0.80	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3385	1/1	0.80	0.35	63,63,63,63	1
59	MG	DA	3060	1/1	0.80	0.59	77,77,77,77	0
59	MG	BA	2979	1/1	0.80	0.42	66,66,66,66	0
59	MG	DA	2918	1/1	0.80	0.49	91,91,91,91	0
59	MG	CA	1703	1/1	0.80	1.03	82,82,82,82	0
59	MG	DA	3227	1/1	0.80	0.44	73,73,73,73	0
59	MG	AA	1800	1/1	0.80	0.94	114,114,114,114	0
59	MG	DA	2921	1/1	0.80	1.66	114,114,114,114	0
59	MG	AA	1802	1/1	0.80	0.28	119,119,119,119	0
59	MG	CA	1767	1/1	0.80	0.44	73,73,73,73	0
59	MG	AA	1671	1/1	0.80	1.36	107,107,107,107	0
59	MG	DB	202	1/1	0.80	0.46	55,55,55,55	0
59	MG	AA	1890	1/1	0.80	0.49	78,78,78,78	0
59	MG	DA	2938	1/1	0.80	0.16	17,17,17,17	1
59	MG	AA	1759	1/1	0.80	0.38	51,51,51,51	0
59	MG	AA	1970	1/1	0.80	0.33	107,107,107,107	0
59	MG	BA	3563	1/1	0.80	0.49	80,80,80,80	0
59	MG	BA	3209	1/1	0.80	0.31	61,61,61,61	0
59	MG	DA	3467	1/1	0.80	0.36	109,109,109,109	0
59	MG	BA	3443	1/1	0.80	0.14	76,76,76,76	0
59	MG	AA	1971	1/1	0.80	0.66	125,125,125,125	0
59	MG	DA	2959	1/1	0.80	0.38	61,61,61,61	0
59	MG	AA	1865	1/1	0.80	0.37	96,96,96,96	0
59	MG	AA	1607	1/1	0.80	0.26	73,73,73,73	0
59	MG	AA	1764	1/1	0.80	1.02	65,65,65,65	0
59	MG	BA	3480	1/1	0.80	0.35	55,55,55,55	0
59	MG	DA	3338	1/1	0.80	0.22	68,68,68,68	0
59	MG	CA	1677	1/1	0.80	0.95	88,88,88,88	1
59	MG	AA	1675	1/1	0.80	0.35	52,52,52,52	1
59	MG	AA	1752	1/1	0.81	0.38	51,51,51,51	1
59	MG	DA	3629	1/1	0.81	0.32	45,45,45,45	0
59	MG	DA	3035	1/1	0.81	0.27	84,84,84,84	0
59	MG	BA	3101	1/1	0.81	0.42	79,79,79,79	0
59	MG	DA	3043	1/1	0.81	0.37	80,80,80,80	0
59	MG	DA	3642	1/1	0.81	0.57	88,88,88,88	0
59	MG	CA	1631	1/1	0.81	0.35	59,59,59,59	0
59	MG	AA	1734	1/1	0.81	0.21	9,9,9,9	1
59	MG	BA	3170	1/1	0.81	0.15	56,56,56,56	0
59	MG	DA	3435	1/1	0.81	0.29	47,47,47,47	0
59	MG	DA	3228	1/1	0.81	0.31	79,79,79,79	0
59	MG	DA	3230	1/1	0.81	0.31	94,94,94,94	0
59	MG	BA	3556	1/1	0.81	1.11	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1761	1/1	0.81	0.26	87,87,87,87	0
59	MG	DA	3236	1/1	0.81	0.37	63,63,63,63	0
59	MG	BA	3363	1/1	0.81	0.50	92,92,92,92	0
59	MG	DA	3078	1/1	0.81	0.66	73,73,73,73	0
59	MG	DA	3083	1/1	0.81	0.45	104,104,104,104	0
59	MG	DA	3085	1/1	0.81	0.14	68,68,68,68	0
59	MG	DA	3086	1/1	0.81	0.26	60,60,60,60	0
59	MG	CA	1642	1/1	0.81	0.24	85,85,85,85	0
59	MG	CA	1644	1/1	0.81	0.36	92,92,92,92	0
59	MG	DA	3704	1/1	0.81	0.22	74,74,74,74	0
59	MG	AA	1867	1/1	0.81	0.36	65,65,65,65	0
59	MG	DA	3302	1/1	0.81	0.64	57,57,57,57	0
59	MG	DA	3712	1/1	0.81	0.96	108,108,108,108	0
59	MG	DA	3714	1/1	0.81	1.07	109,109,109,109	0
59	MG	BE	301	1/1	0.81	0.46	88,88,88,88	0
59	MG	CA	1715	1/1	0.81	0.16	80,80,80,80	0
59	MG	CA	1771	1/1	0.81	0.82	96,96,96,96	0
59	MG	BA	3471	1/1	0.81	0.61	96,96,96,96	0
59	MG	DA	3506	1/1	0.81	1.06	73,73,73,73	1
59	MG	DA	3733	1/1	0.81	0.13	43,43,43,43	0
59	MG	AA	1646	1/1	0.81	0.61	106,106,106,106	0
59	MG	DA	3116	1/1	0.81	0.16	78,78,78,78	0
59	MG	CA	1721	1/1	0.81	0.72	111,111,111,111	0
59	MG	DA	3330	1/1	0.81	0.34	1,1,1,1	1
59	MG	DA	3518	1/1	0.81	0.36	62,62,62,62	1
59	MG	DA	3519	1/1	0.81	0.33	77,77,77,77	0
59	MG	AA	1678	1/1	0.81	0.37	76,76,76,76	0
59	MG	AA	1618	1/1	0.81	0.54	78,78,78,78	0
59	MG	BA	3044	1/1	0.81	0.65	64,64,64,64	0
59	MG	BA	3488	1/1	0.81	0.53	66,66,66,66	1
59	MG	AH	201	1/1	0.81	0.89	102,102,102,102	0
59	MG	DA	3136	1/1	0.81	0.48	97,97,97,97	0
59	MG	CS	101	1/1	0.81	0.15	97,97,97,97	1
59	MG	AA	1743	1/1	0.81	0.21	87,87,87,87	0
59	MG	BA	3333	1/1	0.81	0.36	72,72,72,72	0
59	MG	DA	3548	1/1	0.81	0.38	50,50,50,50	1
59	MG	DA	3358	1/1	0.81	0.27	93,93,93,93	0
59	MG	CA	1664	1/1	0.81	0.24	91,91,91,91	0
59	MG	BA	3582	1/1	0.81	0.46	63,63,63,63	0
59	MG	CA	1738	1/1	0.81	0.18	80,80,80,80	0
59	MG	AA	1879	1/1	0.81	0.48	74,74,74,74	0
59	MG	DA	2993	1/1	0.81	0.79	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3376	1/1	0.81	0.80	93,93,93,93	0
59	MG	AA	1730	1/1	0.81	0.27	77,77,77,77	1
59	MG	CY	101	1/1	0.81	0.41	143,143,143,143	0
59	MG	DA	3575	1/1	0.81	0.72	89,89,89,89	0
59	MG	CA	1679	1/1	0.81	0.15	65,65,65,65	1
59	MG	BA	3127	1/1	0.81	0.41	71,71,71,71	0
59	MG	DA	3578	1/1	0.81	0.65	105,105,105,105	0
59	MG	AA	1957	1/1	0.81	0.81	75,75,75,75	0
59	MG	D3	101	1/1	0.81	1.94	1,1,1,1	1
59	MG	AA	1747	1/1	0.81	0.77	119,119,119,119	0
59	MG	DA	3593	1/1	0.81	0.32	61,61,61,61	0
59	MG	AA	1621	1/1	0.81	1.22	98,98,98,98	0
59	MG	DR	201	1/1	0.81	0.22	108,108,108,108	0
59	MG	DA	3197	1/1	0.81	0.21	67,67,67,67	0
59	MG	BA	3096	1/1	0.81	0.91	102,102,102,102	0
59	MG	AA	1806	1/1	0.82	0.17	81,81,81,81	0
59	MG	DA	3679	1/1	0.82	0.29	51,51,51,51	0
59	MG	DA	3164	1/1	0.82	0.26	55,55,55,55	0
59	MG	DA	3040	1/1	0.82	0.58	81,81,81,81	0
59	MG	BA	3083	1/1	0.82	0.27	80,80,80,80	0
59	MG	AA	1739	1/1	0.82	0.90	73,73,73,73	1
59	MG	BA	3249	1/1	0.82	0.92	79,79,79,79	0
59	MG	BA	2976	1/1	0.82	0.13	97,97,97,97	0
59	MG	DA	3066	1/1	0.82	0.18	113,113,113,113	0
59	MG	CA	1775	1/1	0.82	0.12	70,70,70,70	1
59	MG	CA	1725	1/1	0.82	0.47	76,76,76,76	1
59	MG	BA	3259	1/1	0.82	0.23	59,59,59,59	0
59	MG	BA	3578	1/1	0.82	0.18	76,76,76,76	0
59	MG	DA	3383	1/1	0.82	0.62	135,135,135,135	0
59	MG	CA	1670	1/1	0.82	0.28	66,66,66,66	0
59	MG	DA	2940	1/1	0.82	0.45	106,106,106,106	0
59	MG	CH	201	1/1	0.82	0.64	37,37,37,37	1
59	MG	BA	3382	1/1	0.82	0.12	77,77,77,77	0
59	MG	AA	1663	1/1	0.82	0.50	95,95,95,95	0
59	MG	BA	3497	1/1	0.82	1.26	85,85,85,85	0
59	MG	BA	3092	1/1	0.82	0.22	101,101,101,101	0
59	MG	BA	3274	1/1	0.82	0.46	83,83,83,83	0
59	MG	AA	1631	1/1	0.82	1.12	85,85,85,85	0
59	MG	DA	3750	1/1	0.82	0.85	84,84,84,84	0
59	MG	DA	3412	1/1	0.82	0.48	42,42,42,42	0
59	MG	AA	1723	1/1	0.82	0.16	91,91,91,91	0
59	MG	BA	3522	1/1	0.82	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1609	1/1	0.82	0.56	59,59,59,59	0
59	MG	CV	109	1/1	0.82	0.13	95,95,95,95	0
59	MG	DA	3574	1/1	0.82	0.68	70,70,70,70	1
59	MG	BA	3339	1/1	0.82	0.81	63,63,63,63	1
59	MG	AA	1907	1/1	0.82	0.52	96,96,96,96	0
59	MG	DA	3286	1/1	0.82	0.42	112,112,112,112	0
59	MG	AA	1780	1/1	0.82	0.44	154,154,154,154	0
59	MG	DA	3130	1/1	0.82	1.24	108,108,108,108	0
59	MG	DA	3583	1/1	0.82	0.48	64,64,64,64	0
59	MG	DA	3293	1/1	0.82	0.70	70,70,70,70	0
59	MG	DA	3587	1/1	0.82	0.75	74,74,74,74	0
59	MG	DA	3296	1/1	0.82	0.27	46,46,46,46	1
59	MG	CA	1693	1/1	0.82	0.70	73,73,73,73	0
59	MG	BA	3539	1/1	0.82	0.30	97,97,97,97	1
59	MG	DA	3462	1/1	0.82	0.87	78,78,78,78	0
59	MG	DA	3612	1/1	0.82	0.50	77,77,77,77	0
59	MG	BA	3546	1/1	0.82	0.75	83,83,83,83	0
59	MG	AA	1837	1/1	0.82	0.26	75,75,75,75	0
59	MG	AA	1726	1/1	0.82	0.32	70,70,70,70	1
59	MG	BA	3003	1/1	0.82	0.33	75,75,75,75	0
59	MG	DA	3474	1/1	0.82	2.41	99,99,99,99	0
59	MG	D7	104	1/1	0.82	0.22	82,82,82,82	1
59	MG	BA	3309	1/1	0.82	0.25	58,58,58,58	0
59	MG	DA	3144	1/1	0.82	0.50	131,131,131,131	0
59	MG	AA	1700	1/1	0.82	0.62	90,90,90,90	0
59	MG	CA	1711	1/1	0.82	0.11	65,65,65,65	1
59	MG	BA	3312	1/1	0.82	0.28	53,53,53,53	0
59	MG	DA	3023	1/1	0.82	0.38	41,41,41,41	0
59	MG	AA	1769	1/1	0.82	0.48	101,101,101,101	0
59	MG	DA	3343	1/1	0.82	0.43	69,69,69,69	0
59	MG	DA	3503	1/1	0.82	0.30	59,59,59,59	0
59	MG	DA	3500	1/1	0.83	0.47	84,84,84,84	0
59	MG	AA	1839	1/1	0.83	0.37	74,74,74,74	0
59	MG	DA	3159	1/1	0.83	0.41	85,85,85,85	0
59	MG	DA	3028	1/1	0.83	0.40	79,79,79,79	0
59	MG	CA	1760	1/1	0.83	0.24	52,52,52,52	1
59	MG	AA	1842	1/1	0.83	0.12	58,58,58,58	0
59	MG	BA	3502	1/1	0.83	1.80	132,132,132,132	0
59	MG	BA	2977	1/1	0.83	1.03	93,93,93,93	0
59	MG	DA	3177	1/1	0.83	0.22	71,71,71,71	0
59	MG	DA	3046	1/1	0.83	0.36	95,95,95,95	0
59	MG	DA	3522	1/1	0.83	0.53	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3056	1/1	0.83	0.71	65,65,65,65	0
59	MG	DA	3193	1/1	0.83	0.17	68,68,68,68	0
59	MG	DA	2917	1/1	0.83	0.99	89,89,89,89	0
59	MG	CA	1764	1/1	0.83	0.19	82,82,82,82	0
59	MG	BA	3509	1/1	0.83	0.52	58,58,58,58	0
59	MG	BA	3029	1/1	0.83	0.31	92,92,92,92	0
59	MG	DA	3388	1/1	0.83	0.65	78,78,78,78	0
59	MG	BA	3260	1/1	0.83	0.40	77,77,77,77	0
59	MG	AA	1825	1/1	0.83	0.72	71,71,71,71	0
59	MG	BA	3524	1/1	0.83	0.42	103,103,103,103	0
59	MG	CA	1643	1/1	0.83	0.12	80,80,80,80	0
59	MG	BA	3598	1/1	0.83	0.49	110,110,110,110	0
59	MG	BA	3526	1/1	0.83	1.19	76,76,76,76	0
59	MG	BA	3390	1/1	0.83	0.14	65,65,65,65	0
59	MG	DA	3407	1/1	0.83	0.51	77,77,77,77	1
59	MG	DA	3092	1/1	0.83	0.69	106,106,106,106	0
59	MG	BA	3268	1/1	0.83	0.18	88,88,88,88	1
59	MG	CA	1780	1/1	0.83	0.68	47,47,47,47	1
59	MG	DA	3102	1/1	0.83	0.40	86,86,86,86	0
59	MG	BA	2983	1/1	0.83	0.20	63,63,63,63	0
59	MG	AA	1856	1/1	0.83	0.48	80,80,80,80	0
59	MG	DA	3773	1/1	0.83	0.28	90,90,90,90	0
59	MG	AA	1942	1/1	0.83	0.22	98,98,98,98	0
59	MG	BA	3541	1/1	0.83	0.93	82,82,82,82	0
59	MG	DA	3269	1/1	0.83	0.47	44,44,44,44	0
59	MG	DA	3429	1/1	0.83	0.65	23,23,23,23	1
59	MG	DA	3270	1/1	0.83	0.17	55,55,55,55	0
59	MG	AA	1966	1/1	0.83	0.27	99,99,99,99	0
59	MG	AA	1665	1/1	0.83	0.67	60,60,60,60	0
59	MG	DA	3791	1/1	0.83	0.62	76,76,76,76	0
59	MG	AX	101	1/1	0.83	0.44	113,113,113,113	0
59	MG	BH	202	1/1	0.83	0.13	95,95,95,95	0
59	MG	DA	3595	1/1	0.83	0.79	75,75,75,75	0
59	MG	DA	3457	1/1	0.83	0.74	68,68,68,68	0
59	MG	BA	3553	1/1	0.83	0.32	106,106,106,106	0
59	MG	AA	1969	1/1	0.83	0.71	83,83,83,83	0
59	MG	BO	201	1/1	0.83	0.25	88,88,88,88	0
59	MG	BA	3352	1/1	0.83	0.24	72,72,72,72	0
59	MG	BA	3353	1/1	0.83	0.66	107,107,107,107	0
59	MG	BA	3070	1/1	0.83	0.47	108,108,108,108	0
59	MG	BA	2994	1/1	0.83	0.48	80,80,80,80	0
59	MG	AA	1715	1/1	0.83	0.99	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3002	1/1	0.83	1.67	83,83,83,83	0
59	MG	AA	1704	1/1	0.83	0.29	84,84,84,84	0
59	MG	AA	1610	1/1	0.83	0.50	77,77,77,77	0
59	MG	AA	1683	1/1	0.83	0.57	47,47,47,47	1
59	MG	AA	1919	1/1	0.83	0.16	78,78,78,78	0
59	MG	D7	103	1/1	0.83	1.99	69,69,69,69	0
59	MG	BA	3154	1/1	0.83	0.34	54,54,54,54	0
59	MG	AI	203	1/1	0.83	0.27	138,138,138,138	0
59	MG	DA	3650	1/1	0.84	0.36	106,106,106,106	0
59	MG	DA	3148	1/1	0.84	1.15	120,120,120,120	0
59	MG	CA	1719	1/1	0.84	0.28	95,95,95,95	0
59	MG	DA	3154	1/1	0.84	0.34	58,58,58,58	0
59	MG	AA	1947	1/1	0.84	0.66	79,79,79,79	0
59	MG	BA	3200	1/1	0.84	0.12	31,31,31,31	0
59	MG	BA	3425	1/1	0.84	0.44	48,48,48,48	0
59	MG	DA	3048	1/1	0.84	0.71	63,63,63,63	0
59	MG	DA	3344	1/1	0.84	0.27	75,75,75,75	0
59	MG	BA	3544	1/1	0.84	0.33	62,62,62,62	0
59	MG	DA	2927	1/1	0.84	0.35	1,1,1,1	1
59	MG	DA	3508	1/1	0.84	0.30	88,88,88,88	0
59	MG	AA	1661	1/1	0.84	0.44	34,34,34,34	1
59	MG	DA	3512	1/1	0.84	0.37	104,104,104,104	0
59	MG	AA	1849	1/1	0.84	0.20	80,80,80,80	0
59	MG	BA	3444	1/1	0.84	0.76	69,69,69,69	0
59	MG	DA	3070	1/1	0.84	0.12	59,59,59,59	0
59	MG	DA	3706	1/1	0.84	0.74	66,66,66,66	0
59	MG	DA	2937	1/1	0.84	0.33	63,63,63,63	1
59	MG	BA	3130	1/1	0.84	0.17	62,62,62,62	0
59	MG	BA	3020	1/1	0.84	0.50	103,103,103,103	0
59	MG	BA	3300	1/1	0.84	0.48	71,71,71,71	0
59	MG	DA	3372	1/1	0.84	0.25	82,82,82,82	0
59	MG	DA	3081	1/1	0.84	0.26	75,75,75,75	0
59	MG	BA	2943	1/1	0.84	0.17	92,92,92,92	1
59	MG	DA	3205	1/1	0.84	0.47	130,130,130,130	0
59	MG	BA	3477	1/1	0.84	1.31	128,128,128,128	0
59	MG	BA	3358	1/1	0.84	0.11	100,100,100,100	0
59	MG	AA	1850	1/1	0.84	0.81	89,89,89,89	0
59	MG	BA	3216	1/1	0.84	0.38	73,73,73,73	0
59	MG	DA	3739	1/1	0.84	0.27	95,95,95,95	0
59	MG	CV	105	1/1	0.84	0.17	82,82,82,82	0
59	MG	DA	3224	1/1	0.84	0.39	85,85,85,85	0
59	MG	DA	3098	1/1	0.84	0.87	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3101	1/1	0.84	1.26	97,97,97,97	0
59	MG	AA	1955	1/1	0.84	0.30	64,64,64,64	1
59	MG	DA	3406	1/1	0.84	1.62	38,38,38,38	1
59	MG	AA	1790	1/1	0.84	0.42	96,96,96,96	0
59	MG	AA	1854	1/1	0.84	0.20	71,71,71,71	0
59	MG	DA	2979	1/1	0.84	0.37	42,42,42,42	0
59	MG	DA	3567	1/1	0.84	1.21	98,98,98,98	0
59	MG	BA	3150	1/1	0.84	0.40	145,145,145,145	0
59	MG	DA	3573	1/1	0.84	0.34	86,86,86,86	0
59	MG	DA	3239	1/1	0.84	0.14	96,96,96,96	0
59	MG	BA	3232	1/1	0.84	0.31	64,64,64,64	0
59	MG	AA	1936	1/1	0.84	0.20	135,135,135,135	0
59	MG	CA	1621	1/1	0.84	0.38	89,89,89,89	0
59	MG	DA	3263	1/1	0.84	0.33	125,125,125,125	0
59	MG	DA	3581	1/1	0.84	0.26	88,88,88,88	1
59	MG	DA	3792	1/1	0.84	0.44	77,77,77,77	0
59	MG	DA	3266	1/1	0.84	0.38	57,57,57,57	0
59	MG	DA	3121	1/1	0.84	0.35	69,69,69,69	0
59	MG	DB	203	1/1	0.84	0.17	30,30,30,30	1
59	MG	AA	1645	1/1	0.84	1.01	56,56,56,56	1
59	MG	BA	3165	1/1	0.84	0.71	77,77,77,77	0
59	MG	DA	3274	1/1	0.84	0.08	73,73,73,73	0
59	MG	DA	3591	1/1	0.84	0.65	19,19,19,19	1
59	MG	AA	1643	1/1	0.84	0.17	92,92,92,92	0
59	MG	BA	3105	1/1	0.84	1.08	79,79,79,79	0
59	MG	AA	1779	1/1	0.84	0.22	114,114,114,114	0
59	MG	AA	1881	1/1	0.84	0.52	98,98,98,98	0
59	MG	BA	3005	1/1	0.84	1.23	105,105,105,105	0
59	MG	BA	3592	1/1	0.84	0.25	100,100,100,100	0
59	MG	BA	3523	1/1	0.84	1.10	122,122,122,122	0
59	MG	AA	1827	1/1	0.84	0.20	85,85,85,85	0
59	MG	BA	3013	1/1	0.84	0.44	60,60,60,60	0
59	MG	DA	2910	1/1	0.84	0.80	68,68,68,68	0
59	MG	DP	205	1/1	0.84	0.42	63,63,63,63	0
59	MG	BA	3270	1/1	0.84	0.27	60,60,60,60	0
59	MG	BA	3412	1/1	0.84	0.36	95,95,95,95	0
59	MG	DA	3481	1/1	0.84	0.52	73,73,73,73	0
59	MG	DT	201	1/1	0.84	0.77	5,5,5,5	1
59	MG	BA	3074	1/1	0.84	0.49	36,36,36,36	0
59	MG	DA	2969	1/1	0.85	1.03	98,98,98,98	0
59	MG	BA	3365	1/1	0.85	1.28	112,112,112,112	0
59	MG	DA	3093	1/1	0.85	0.36	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	D2	101	1/1	0.85	0.36	62,62,62,62	0
59	MG	BA	2917	1/1	0.85	0.26	84,84,84,84	0
59	MG	DA	2982	1/1	0.85	0.33	97,97,97,97	0
59	MG	BA	2963	1/1	0.85	1.13	113,113,113,113	0
59	MG	CA	1718	1/1	0.85	0.25	87,87,87,87	0
59	MG	CA	1605	1/1	0.85	0.85	49,49,49,49	1
59	MG	DA	3212	1/1	0.85	0.43	105,105,105,105	0
59	MG	AA	1719	1/1	0.85	0.84	76,76,76,76	1
59	MG	DA	3219	1/1	0.85	0.47	62,62,62,62	0
59	MG	BA	3328	1/1	0.85	0.66	76,76,76,76	0
59	MG	DA	3379	1/1	0.85	0.46	72,72,72,72	0
59	MG	DA	2901	1/1	0.85	0.33	51,51,51,51	0
59	MG	DA	3526	1/1	0.85	0.10	11,11,11,11	1
59	MG	CA	1768	1/1	0.85	0.15	71,71,71,71	0
59	MG	BA	3034	1/1	0.85	0.23	51,51,51,51	0
59	MG	AA	1674	1/1	0.85	0.26	48,48,48,48	0
59	MG	BA	3011	1/1	0.85	0.91	107,107,107,107	0
59	MG	CA	1614	1/1	0.85	0.42	72,72,72,72	0
59	MG	BA	3179	1/1	0.85	0.26	66,66,66,66	0
59	MG	DA	3126	1/1	0.85	0.28	60,60,60,60	0
59	MG	BA	3287	1/1	0.85	0.14	104,104,104,104	0
59	MG	DA	3735	1/1	0.85	0.16	90,90,90,90	0
59	MG	BA	3229	1/1	0.85	1.18	88,88,88,88	0
59	MG	BA	2989	1/1	0.85	0.27	82,82,82,82	0
59	MG	BA	3597	1/1	0.85	0.72	53,53,53,53	1
59	MG	DA	3244	1/1	0.85	0.30	29,29,29,29	0
59	MG	DA	3748	1/1	0.85	0.67	125,125,125,125	0
59	MG	DA	3248	1/1	0.85	0.26	62,62,62,62	0
59	MG	BA	3551	1/1	0.85	0.95	82,82,82,82	0
59	MG	BA	2928	1/1	0.85	0.80	116,116,116,116	0
59	MG	DA	3265	1/1	0.85	0.79	82,82,82,82	0
59	MG	DA	2926	1/1	0.85	0.44	45,45,45,45	1
59	MG	BA	3239	1/1	0.85	0.29	77,77,77,77	0
59	MG	BA	3555	1/1	0.85	0.68	60,60,60,60	0
59	MG	AA	1602	1/1	0.85	0.18	71,71,71,71	0
59	MG	BA	3133	1/1	0.85	0.21	57,57,57,57	0
59	MG	BA	3045	1/1	0.85	0.16	75,75,75,75	0
59	MG	BA	3565	1/1	0.85	0.38	79,79,79,79	0
59	MG	DA	3438	1/1	0.85	0.23	76,76,76,76	0
59	MG	DA	3147	1/1	0.85	0.17	90,90,90,90	0
59	MG	BA	3503	1/1	0.85	0.37	65,65,65,65	1
59	MG	BA	3138	1/1	0.85	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3451	1/1	0.85	0.15	80,80,80,80	1
59	MG	DA	3151	1/1	0.85	0.92	73,73,73,73	0
59	MG	AA	1712	1/1	0.85	0.77	188,188,188,188	0
59	MG	DA	2949	1/1	0.85	0.33	98,98,98,98	1
59	MG	AA	1713	1/1	0.85	0.12	70,70,70,70	0
59	MG	DA	3594	1/1	0.85	0.23	63,63,63,63	1
59	MG	DA	3314	1/1	0.85	0.15	71,71,71,71	0
59	MG	CA	1701	1/1	0.85	0.27	83,83,83,83	0
59	MG	AA	1949	1/1	0.85	0.49	42,42,42,42	1
59	MG	CA	1705	1/1	0.85	0.45	62,62,62,62	0
59	MG	DA	3076	1/1	0.85	0.27	75,75,75,75	0
59	MG	DA	3619	1/1	0.85	0.27	69,69,69,69	0
59	MG	DA	3627	1/1	0.85	0.31	70,70,70,70	0
59	MG	AA	1692	1/1	0.85	0.32	89,89,89,89	0
59	MG	DA	3169	1/1	0.85	1.38	67,67,67,67	0
59	MG	DA	3630	1/1	0.85	0.41	99,99,99,99	0
59	MG	DA	3482	1/1	0.85	0.34	37,37,37,37	1
59	MG	DA	3335	1/1	0.85	0.50	48,48,48,48	0
59	MG	DA	3170	1/1	0.85	0.47	98,98,98,98	0
59	MG	BA	3075	1/1	0.85	0.44	87,87,87,87	0
59	MG	DA	3492	1/1	0.85	0.88	62,62,62,62	0
59	MG	DA	2962	1/1	0.85	0.70	84,84,84,84	0
59	MG	DA	3181	1/1	0.85	0.36	49,49,49,49	0
59	MG	DA	3190	1/1	0.85	0.35	97,97,97,97	0
59	MG	DA	2967	1/1	0.85	0.32	35,35,35,35	1
59	MG	DA	3498	1/1	0.85	0.42	82,82,82,82	0
59	MG	BA	3194	1/1	0.86	0.12	67,67,67,67	0
59	MG	AA	1939	1/1	0.86	0.29	74,74,74,74	1
59	MG	DA	3654	1/1	0.86	0.36	78,78,78,78	0
59	MG	AA	1717	1/1	0.86	0.32	120,120,120,120	0
59	MG	BA	3278	1/1	0.86	0.43	71,71,71,71	0
59	MG	BA	3124	1/1	0.86	0.45	62,62,62,62	0
59	MG	DA	3667	1/1	0.86	0.43	46,46,46,46	1
59	MG	DA	3047	1/1	0.86	0.75	88,88,88,88	0
59	MG	BA	3564	1/1	0.86	0.66	113,113,113,113	0
59	MG	CA	1689	1/1	0.86	0.13	96,96,96,96	1
59	MG	BA	3355	1/1	0.86	0.24	26,26,26,26	0
59	MG	DA	3678	1/1	0.86	0.46	100,100,100,100	0
59	MG	DA	3063	1/1	0.86	0.23	50,50,50,50	0
59	MG	BA	3201	1/1	0.86	0.23	50,50,50,50	0
59	MG	DA	2922	1/1	0.86	0.33	65,65,65,65	0
59	MG	AA	1641	1/1	0.86	0.15	68,68,68,68	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1613	1/1	0.86	0.93	74,74,74,74	0
59	MG	CA	1613	1/1	0.86	0.37	73,73,73,73	0
59	MG	AA	1855	1/1	0.86	0.31	69,69,69,69	0
59	MG	DA	3698	1/1	0.86	0.19	25,25,25,25	0
59	MG	BA	2939	1/1	0.86	0.32	80,80,80,80	0
59	MG	BA	2940	1/1	0.86	0.42	63,63,63,63	0
59	MG	CA	1774	1/1	0.86	1.63	111,111,111,111	1
59	MG	AA	1833	1/1	0.86	0.28	87,87,87,87	0
59	MG	DA	3367	1/1	0.86	0.57	28,28,28,28	1
59	MG	DA	3202	1/1	0.86	0.17	70,70,70,70	0
59	MG	BA	3370	1/1	0.86	0.52	105,105,105,105	0
59	MG	CA	1625	1/1	0.86	0.16	62,62,62,62	0
59	MG	BA	2948	1/1	0.86	0.21	64,64,64,64	0
59	MG	DA	3529	1/1	0.86	0.10	42,42,42,42	0
59	MG	DA	3091	1/1	0.86	0.39	119,119,119,119	0
59	MG	DA	3211	1/1	0.86	0.23	65,65,65,65	0
59	MG	BA	3498	1/1	0.86	1.07	85,85,85,85	1
59	MG	AA	1611	1/1	0.86	0.39	66,66,66,66	0
59	MG	DA	3386	1/1	0.86	0.41	99,99,99,99	0
59	MG	AA	1740	1/1	0.86	0.39	94,94,94,94	0
59	MG	DA	2952	1/1	0.86	0.49	44,44,44,44	0
59	MG	BA	3145	1/1	0.86	0.35	89,89,89,89	0
59	MG	DA	3223	1/1	0.86	0.38	37,37,37,37	0
59	MG	DA	2955	1/1	0.86	0.33	34,34,34,34	1
59	MG	CA	1632	1/1	0.86	0.48	94,94,94,94	0
59	MG	DA	3401	1/1	0.86	0.80	65,65,65,65	0
59	MG	BA	3036	1/1	0.86	0.34	98,98,98,98	0
59	MG	CA	1636	1/1	0.86	0.53	77,77,77,77	0
59	MG	BA	3507	1/1	0.86	0.42	55,55,55,55	0
59	MG	DA	2963	1/1	0.86	0.32	39,39,39,39	1
59	MG	BA	3149	1/1	0.86	0.33	86,86,86,86	0
59	MG	BA	3098	1/1	0.86	0.41	62,62,62,62	0
59	MG	BA	3233	1/1	0.86	0.15	73,73,73,73	0
59	MG	DA	3778	1/1	0.86	0.21	115,115,115,115	0
59	MG	BA	3595	1/1	0.86	0.63	65,65,65,65	0
59	MG	AA	1742	1/1	0.86	0.27	63,63,63,63	1
59	MG	BA	2961	1/1	0.86	0.13	79,79,79,79	0
59	MG	DA	3125	1/1	0.86	0.46	118,118,118,118	0
59	MG	DA	3252	1/1	0.86	0.19	87,87,87,87	0
59	MG	AA	1659	1/1	0.86	0.20	107,107,107,107	0
59	MG	AA	1782	1/1	0.86	0.36	103,103,103,103	0
59	MG	BA	3107	1/1	0.86	0.62	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1894	1/1	0.86	0.21	90,90,90,90	0
59	MG	DA	3436	1/1	0.86	0.33	104,104,104,104	0
59	MG	DA	3268	1/1	0.86	0.30	35,35,35,35	0
59	MG	AA	1797	1/1	0.86	0.28	76,76,76,76	0
59	MG	BA	3049	1/1	0.86	0.19	66,66,66,66	0
59	MG	BA	3415	1/1	0.86	0.43	69,69,69,69	1
59	MG	AA	1937	1/1	0.86	0.18	58,58,58,58	0
59	MG	DA	3453	1/1	0.86	0.22	84,84,84,84	0
59	MG	BD	302	1/1	0.86	0.32	52,52,52,52	0
59	MG	DA	3139	1/1	0.86	0.27	89,89,89,89	0
59	MG	DA	3615	1/1	0.86	0.80	86,86,86,86	0
59	MG	BA	3189	1/1	0.86	0.36	62,62,62,62	0
59	MG	BA	3423	1/1	0.86	0.40	67,67,67,67	1
59	MG	BA	3266	1/1	0.86	0.17	65,65,65,65	0
59	MG	D8	101	1/1	0.86	0.19	74,74,74,74	0
59	MG	DA	3301	1/1	0.86	0.20	32,32,32,32	0
59	MG	BA	3064	1/1	0.86	0.41	45,45,45,45	0
59	MG	DA	3632	1/1	0.86	0.49	56,56,56,56	0
59	MG	BH	203	1/1	0.86	0.46	75,75,75,75	0
59	MG	BA	3432	1/1	0.86	0.46	59,59,59,59	0
59	MG	DA	3480	1/1	0.86	0.27	87,87,87,87	0
59	MG	DA	2906	1/1	0.86	0.34	93,93,93,93	1
59	MG	AA	1903	1/1	0.86	0.39	79,79,79,79	0
60	ZN	CD	301	1/1	0.86	0.24	151,151,151,151	0
59	MG	BA	2954	1/1	0.87	0.28	59,59,59,59	0
59	MG	DA	2945	1/1	0.87	0.73	102,102,102,102	0
59	MG	BA	3603	1/1	0.87	0.25	74,74,74,74	0
59	MG	BA	2958	1/1	0.87	0.28	46,46,46,46	0
59	MG	BA	3060	1/1	0.87	1.10	98,98,98,98	0
59	MG	BA	3144	1/1	0.87	0.32	73,73,73,73	0
59	MG	BA	3267	1/1	0.87	1.16	94,94,94,94	0
59	MG	BA	2990	1/1	0.87	0.21	77,77,77,77	0
59	MG	AA	1731	1/1	0.87	0.35	81,81,81,81	0
59	MG	AA	1686	1/1	0.87	0.17	81,81,81,81	0
59	MG	DA	3359	1/1	0.87	0.33	64,64,64,64	0
59	MG	AD	302	1/1	0.87	0.07	96,96,96,96	0
59	MG	AA	1940	1/1	0.87	0.25	86,86,86,86	0
59	MG	BA	3080	1/1	0.87	0.59	83,83,83,83	0
59	MG	AA	1902	1/1	0.87	0.10	90,90,90,90	0
59	MG	BA	3408	1/1	0.87	0.39	73,73,73,73	0
59	MG	DA	3250	1/1	0.87	0.29	69,69,69,69	0
59	MG	DA	3079	1/1	0.87	0.68	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3118	1/1	0.87	0.07	59,59,59,59	0
59	MG	BA	3348	1/1	0.87	0.26	61,61,61,61	0
59	MG	DA	3753	1/1	0.87	0.79	83,83,83,83	0
59	MG	BA	3575	1/1	0.87	0.37	92,92,92,92	0
59	MG	DA	2907	1/1	0.87	0.41	83,83,83,83	0
59	MG	BA	3171	1/1	0.87	0.30	29,29,29,29	0
59	MG	DA	3387	1/1	0.87	0.42	77,77,77,77	0
59	MG	DA	3167	1/1	0.87	0.32	40,40,40,40	0
59	MG	AA	1917	1/1	0.87	0.31	78,78,78,78	0
59	MG	AA	1699	1/1	0.87	0.19	71,71,71,71	0
59	MG	BA	3230	1/1	0.87	0.52	85,85,85,85	0
59	MG	AA	1756	1/1	0.87	0.19	91,91,91,91	0
59	MG	DA	3396	1/1	0.87	0.30	62,62,62,62	0
59	MG	CA	1668	1/1	0.87	0.32	94,94,94,94	0
59	MG	DA	3001	1/1	0.87	0.07	79,79,79,79	0
59	MG	DA	3783	1/1	0.87	1.06	90,90,90,90	0
59	MG	DA	3291	1/1	0.87	0.37	88,88,88,88	0
59	MG	BA	3181	1/1	0.87	0.51	42,42,42,42	0
59	MG	DA	3295	1/1	0.87	0.78	99,99,99,99	0
59	MG	BA	3086	1/1	0.87	0.18	123,123,123,123	0
59	MG	DA	3648	1/1	0.87	0.63	100,100,100,100	0
59	MG	DA	3521	1/1	0.87	0.22	99,99,99,99	0
59	MG	CD	302	1/1	0.87	0.25	68,68,68,68	0
59	MG	DA	3651	1/1	0.87	0.35	93,93,93,93	0
59	MG	DA	3411	1/1	0.87	0.18	67,67,67,67	1
59	MG	DA	3299	1/1	0.87	0.47	75,75,75,75	0
59	MG	AA	1608	1/1	0.87	0.41	58,58,58,58	0
59	MG	BA	3040	1/1	0.87	0.65	79,79,79,79	0
59	MG	DA	3532	1/1	0.87	0.27	79,79,79,79	0
59	MG	DA	3304	1/1	0.87	0.48	84,84,84,84	0
59	MG	AA	1906	1/1	0.87	0.36	65,65,65,65	1
59	MG	CA	1618	1/1	0.87	0.31	79,79,79,79	0
59	MG	BA	3246	1/1	0.87	0.24	68,68,68,68	0
59	MG	BA	3540	1/1	0.87	0.87	66,66,66,66	1
59	MG	DA	3427	1/1	0.87	0.39	78,78,78,78	0
59	MG	DA	2930	1/1	0.87	1.30	1,1,1,1	1
59	MG	DA	3682	1/1	0.87	0.19	103,103,103,103	0
59	MG	AA	1639	1/1	0.87	1.31	79,79,79,79	0
59	MG	BA	3542	1/1	0.87	0.35	102,102,102,102	0
59	MG	AV	103	1/1	0.87	0.12	72,72,72,72	0
59	MG	DA	3691	1/1	0.87	0.10	59,59,59,59	0
59	MG	DA	3036	1/1	0.87	0.47	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3473	1/1	0.87	0.91	87,87,87,87	0
59	MG	AA	1656	1/1	0.87	0.30	98,98,98,98	1
59	MG	BA	3258	1/1	0.87	0.52	69,69,69,69	0
59	MG	BA	3308	1/1	0.88	0.28	53,53,53,53	1
59	MG	CA	1623	1/1	0.88	0.08	81,81,81,81	0
59	MG	CC	303	1/1	0.88	0.12	113,113,113,113	0
59	MG	CA	1624	1/1	0.88	0.35	86,86,86,86	0
59	MG	DA	3502	1/1	0.88	0.28	74,74,74,74	0
59	MG	AA	1694	1/1	0.88	0.24	56,56,56,56	1
59	MG	DA	3201	1/1	0.88	0.35	62,62,62,62	0
59	MG	DA	3080	1/1	0.88	0.19	56,56,56,56	0
59	MG	BA	3110	1/1	0.88	0.23	55,55,55,55	0
59	MG	AA	1774	1/1	0.88	0.51	120,120,120,120	0
59	MG	BA	3046	1/1	0.88	0.12	90,90,90,90	0
59	MG	BA	3584	1/1	0.88	0.26	65,65,65,65	0
59	MG	BA	3047	1/1	0.88	0.68	89,89,89,89	0
59	MG	DA	3373	1/1	0.88	0.69	75,75,75,75	0
59	MG	BA	3244	1/1	0.88	0.49	88,88,88,88	0
59	MG	DA	3690	1/1	0.88	0.31	62,62,62,62	0
59	MG	AA	1748	1/1	0.88	0.46	23,23,23,23	1
59	MG	DA	2960	1/1	0.88	0.91	57,57,57,57	1
59	MG	DA	3382	1/1	0.88	0.11	101,101,101,101	0
59	MG	AA	1807	1/1	0.88	0.42	61,61,61,61	0
59	MG	AA	1809	1/1	0.88	1.31	92,92,92,92	0
59	MG	DA	3703	1/1	0.88	0.19	41,41,41,41	0
59	MG	DA	3385	1/1	0.88	0.24	43,43,43,43	0
59	MG	AA	1813	1/1	0.88	0.41	134,134,134,134	0
59	MG	DA	3708	1/1	0.88	1.26	100,100,100,100	0
59	MG	BA	3521	1/1	0.88	0.33	119,119,119,119	0
59	MG	BA	3393	1/1	0.88	0.20	104,104,104,104	0
59	MG	DA	3106	1/1	0.88	0.24	77,77,77,77	0
59	MG	BA	3394	1/1	0.88	0.32	85,85,85,85	0
59	MG	DA	2974	1/1	0.88	0.69	47,47,47,47	1
59	MG	AA	1791	1/1	0.88	0.30	93,93,93,93	0
59	MG	BA	3253	1/1	0.88	0.37	52,52,52,52	1
59	MG	DA	3728	1/1	0.88	0.42	46,46,46,46	1
59	MG	DA	2981	1/1	0.88	0.36	127,127,127,127	0
59	MG	BA	3329	1/1	0.88	0.46	1,1,1,1	1
59	MG	BA	3256	1/1	0.88	0.32	122,122,122,122	0
59	MG	BA	3192	1/1	0.88	0.71	90,90,90,90	0
59	MG	BA	3534	1/1	0.88	0.56	56,56,56,56	0
59	MG	BA	2902	1/1	0.88	0.32	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1681	1/1	0.88	0.24	106,106,106,106	0
59	MG	DA	2991	1/1	0.88	0.35	44,44,44,44	1
59	MG	DA	3128	1/1	0.88	0.30	86,86,86,86	0
59	MG	BA	3263	1/1	0.88	0.99	76,76,76,76	0
59	MG	BA	3015	1/1	0.88	0.07	105,105,105,105	0
59	MG	DA	3132	1/1	0.88	0.59	49,49,49,49	0
59	MG	DA	3755	1/1	0.88	0.15	128,128,128,128	0
59	MG	DA	3572	1/1	0.88	0.53	56,56,56,56	1
59	MG	CA	1660	1/1	0.88	0.35	99,99,99,99	0
59	MG	BA	3198	1/1	0.88	0.35	102,102,102,102	0
59	MG	DA	3135	1/1	0.88	0.29	51,51,51,51	0
59	MG	AA	1819	1/1	0.88	0.08	75,75,75,75	0
59	MG	DA	2904	1/1	0.88	1.06	66,66,66,66	0
59	MG	AA	1633	1/1	0.88	1.30	72,72,72,72	1
59	MG	DA	3776	1/1	0.88	0.45	58,58,58,58	0
59	MG	AA	1676	1/1	0.88	0.29	68,68,68,68	0
59	MG	BA	2915	1/1	0.88	0.37	70,70,70,70	0
59	MG	AA	1920	1/1	0.88	0.14	73,73,73,73	0
59	MG	AA	1755	1/1	0.88	0.25	34,34,34,34	1
59	MG	DA	3585	1/1	0.88	0.35	78,78,78,78	0
59	MG	BA	2921	1/1	0.88	0.12	51,51,51,51	0
59	MG	DA	3442	1/1	0.88	0.45	71,71,71,71	0
59	MG	BP	201	1/1	0.88	0.31	24,24,24,24	0
59	MG	DA	3788	1/1	0.88	0.25	124,124,124,124	0
59	MG	DA	3446	1/1	0.88	0.37	52,52,52,52	0
59	MG	BA	3465	1/1	0.88	0.55	37,37,37,37	0
59	MG	DA	3034	1/1	0.88	0.45	98,98,98,98	0
59	MG	BA	2922	1/1	0.88	1.25	95,95,95,95	0
59	MG	DA	3797	1/1	0.88	0.36	56,56,56,56	0
59	MG	DA	3598	1/1	0.88	0.62	83,83,83,83	0
59	MG	BY	201	1/1	0.88	0.23	50,50,50,50	0
59	MG	DA	3037	1/1	0.88	0.54	58,58,58,58	0
59	MG	DB	205	1/1	0.88	0.50	82,82,82,82	0
59	MG	BA	3472	1/1	0.88	0.98	100,100,100,100	0
59	MG	AA	1929	1/1	0.88	0.26	69,69,69,69	0
59	MG	BA	3285	1/1	0.88	0.18	96,96,96,96	0
59	MG	AA	1931	1/1	0.88	0.25	87,87,87,87	0
59	MG	DA	3163	1/1	0.88	0.33	49,49,49,49	0
59	MG	DA	2923	1/1	0.88	0.17	94,94,94,94	0
59	MG	AA	1615	1/1	0.88	1.12	67,67,67,67	0
59	MG	DA	3631	1/1	0.88	0.41	41,41,41,41	0
59	MG	BA	3483	1/1	0.88	0.53	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3479	1/1	0.88	0.59	127,127,127,127	0
59	MG	BA	3485	1/1	0.88	0.64	103,103,103,103	0
59	MG	AQ	203	1/1	0.88	1.01	130,130,130,130	0
59	MG	AA	1958	1/1	0.88	0.11	106,106,106,106	0
59	MG	AA	1729	1/1	0.88	0.23	50,50,50,50	0
59	MG	DA	3067	1/1	0.88	0.29	106,106,106,106	0
59	MG	BA	3572	1/1	0.88	0.90	68,68,68,68	0
59	MG	DA	3185	1/1	0.88	0.23	79,79,79,79	0
59	MG	AV	105	1/1	0.88	0.15	80,80,80,80	0
59	MG	AA	1771	1/1	0.88	0.59	95,95,95,95	0
59	MG	DA	3659	1/1	0.88	0.45	88,88,88,88	0
59	MG	AA	1668	1/1	0.89	0.66	78,78,78,78	0
59	MG	CA	1638	1/1	0.89	0.29	61,61,61,61	0
59	MG	DA	3380	1/1	0.89	0.31	43,43,43,43	0
59	MG	AA	1805	1/1	0.89	0.19	102,102,102,102	0
59	MG	BA	3180	1/1	0.89	0.29	42,42,42,42	0
59	MG	DA	2996	1/1	0.89	0.51	71,71,71,71	1
59	MG	AA	1691	1/1	0.89	0.59	90,90,90,90	0
59	MG	BA	3183	1/1	0.89	0.17	54,54,54,54	0
59	MG	AA	1784	1/1	0.89	0.30	92,92,92,92	0
59	MG	BA	3050	1/1	0.89	0.12	73,73,73,73	0
59	MG	BA	3187	1/1	0.89	0.57	37,37,37,37	0
59	MG	AA	1923	1/1	0.89	0.43	55,55,55,55	0
59	MG	BA	3409	1/1	0.89	0.55	104,104,104,104	0
59	MG	DA	3245	1/1	0.89	0.31	78,78,78,78	0
59	MG	DA	3395	1/1	0.89	0.41	83,83,83,83	0
59	MG	BA	3007	1/1	0.89	0.33	93,93,93,93	0
59	MG	BA	3008	1/1	0.89	0.34	123,123,123,123	0
59	MG	CA	1656	1/1	0.89	0.51	73,73,73,73	0
59	MG	BB	202	1/1	0.89	0.50	62,62,62,62	0
59	MG	DA	3260	1/1	0.89	0.70	33,33,33,33	0
59	MG	BA	3067	1/1	0.89	0.21	34,34,34,34	0
59	MG	AA	1831	1/1	0.89	0.84	89,89,89,89	0
59	MG	BA	3195	1/1	0.89	0.35	85,85,85,85	0
59	MG	DA	3555	1/1	0.89	1.19	105,105,105,105	0
59	MG	DA	3267	1/1	0.89	0.36	62,62,62,62	0
59	MG	AA	1832	1/1	0.89	0.52	140,140,140,140	0
59	MG	DA	3413	1/1	0.89	1.26	84,84,84,84	0
59	MG	BD	304	1/1	0.89	0.32	49,49,49,49	0
59	MG	BA	3014	1/1	0.89	0.35	79,79,79,79	0
59	MG	BA	3428	1/1	0.89	1.06	72,72,72,72	0
59	MG	BA	3429	1/1	0.89	1.00	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	2972	1/1	0.89	0.49	63,63,63,63	1
59	MG	BA	3077	1/1	0.89	0.47	71,71,71,71	0
59	MG	BA	3435	1/1	0.89	0.61	70,70,70,70	0
59	MG	DA	3153	1/1	0.89	0.56	68,68,68,68	0
59	MG	BA	3436	1/1	0.89	0.16	62,62,62,62	0
59	MG	DA	3754	1/1	0.89	0.79	34,34,34,34	1
59	MG	DA	3049	1/1	0.89	1.46	96,96,96,96	0
59	MG	DA	3433	1/1	0.89	0.65	1,1,1,1	1
59	MG	DA	3757	1/1	0.89	0.65	86,86,86,86	0
59	MG	DA	3156	1/1	0.89	0.56	73,73,73,73	0
59	MG	BA	3437	1/1	0.89	0.31	60,60,60,60	0
59	MG	BA	3440	1/1	0.89	0.42	72,72,72,72	0
59	MG	DA	3768	1/1	0.89	0.06	58,58,58,58	1
59	MG	BQ	201	1/1	0.89	0.27	72,72,72,72	0
59	MG	AA	1679	1/1	0.89	0.32	53,53,53,53	1
59	MG	AA	1864	1/1	0.89	0.20	67,67,67,67	0
59	MG	BA	3208	1/1	0.89	0.37	27,27,27,27	0
59	MG	BA	3558	1/1	0.89	0.40	78,78,78,78	0
59	MG	BA	3275	1/1	0.89	0.19	38,38,38,38	0
59	MG	BA	3562	1/1	0.89	0.52	71,71,71,71	0
59	MG	AA	1810	1/1	0.89	0.24	71,71,71,71	0
59	MG	AA	1963	1/1	0.89	0.76	74,74,74,74	0
59	MG	DA	3782	1/1	0.89	0.27	51,51,51,51	0
59	MG	AA	1601	1/1	0.89	0.17	74,74,74,74	0
59	MG	DA	3463	1/1	0.89	0.56	83,83,83,83	0
59	MG	BA	3282	1/1	0.89	0.38	47,47,47,47	0
59	MG	DA	3614	1/1	0.89	0.26	100,100,100,100	0
59	MG	BA	3212	1/1	0.89	0.57	52,52,52,52	0
59	MG	AA	1695	1/1	0.89	0.19	65,65,65,65	0
59	MG	AA	1868	1/1	0.89	0.25	100,100,100,100	0
59	MG	BA	3364	1/1	0.89	0.92	66,66,66,66	1
59	MG	DA	3794	1/1	0.89	0.17	79,79,79,79	0
59	MG	DA	3796	1/1	0.89	0.28	95,95,95,95	1
59	MG	AA	1705	1/1	0.89	1.06	105,105,105,105	0
59	MG	AA	1801	1/1	0.89	0.22	130,130,130,130	0
59	MG	BA	3574	1/1	0.89	0.30	53,53,53,53	0
59	MG	AA	1843	1/1	0.89	0.71	99,99,99,99	0
59	MG	BA	3371	1/1	0.89	0.15	63,63,63,63	0
59	MG	AA	1848	1/1	0.89	0.29	117,117,117,117	0
59	MG	BA	2950	1/1	0.89	0.29	55,55,55,55	1
59	MG	DA	3353	1/1	0.89	0.12	84,84,84,84	0
59	MG	DD	301	1/1	0.89	0.38	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3376	1/1	0.89	0.24	68,68,68,68	1
59	MG	DA	3206	1/1	0.89	0.32	66,66,66,66	0
59	MG	CV	108	1/1	0.89	0.25	101,101,101,101	0
59	MG	BA	3228	1/1	0.89	0.62	99,99,99,99	0
59	MG	DF	301	1/1	0.89	0.35	17,17,17,17	1
59	MG	DA	3360	1/1	0.89	0.22	99,99,99,99	0
59	MG	CA	1629	1/1	0.89	0.29	98,98,98,98	0
59	MG	DA	3365	1/1	0.89	0.47	92,92,92,92	0
59	MG	AC	302	1/1	0.89	0.12	163,163,163,163	0
59	MG	DA	3213	1/1	0.89	0.65	67,67,67,67	0
59	MG	AA	1875	1/1	0.89	0.23	62,62,62,62	0
59	MG	D0	101	1/1	0.89	0.16	16,16,16,16	1
59	MG	DA	3371	1/1	0.89	0.14	59,59,59,59	1
59	MG	BA	2996	1/1	0.89	0.28	68,68,68,68	0
59	MG	DA	3509	1/1	0.89	0.47	39,39,39,39	0
59	MG	DA	3510	1/1	0.89	0.10	59,59,59,59	0
59	MG	AA	1677	1/1	0.89	0.28	76,76,76,76	1
59	MG	BA	3001	1/1	0.89	0.28	117,117,117,117	0
59	MG	BA	3422	1/1	0.90	0.16	68,68,68,68	0
59	MG	DA	3186	1/1	0.90	0.18	42,42,42,42	0
59	MG	DA	3189	1/1	0.90	0.27	80,80,80,80	0
59	MG	BA	3048	1/1	0.90	0.19	90,90,90,90	0
59	MG	DA	3696	1/1	0.90	0.53	80,80,80,80	0
59	MG	DA	3415	1/1	0.90	0.53	41,41,41,41	0
59	MG	DA	3100	1/1	0.90	0.55	67,67,67,67	0
59	MG	BA	3123	1/1	0.90	0.41	105,105,105,105	0
59	MG	BA	3172	1/1	0.90	0.43	80,80,80,80	0
59	MG	BA	3321	1/1	0.90	0.34	58,58,58,58	0
59	MG	DA	3312	1/1	0.90	0.29	48,48,48,48	0
59	MG	DA	3709	1/1	0.90	0.22	61,61,61,61	0
59	MG	CA	1708	1/1	0.90	0.20	64,64,64,64	1
59	MG	BA	2930	1/1	0.90	0.20	85,85,85,85	0
59	MG	DA	3320	1/1	0.90	0.13	78,78,78,78	0
59	MG	BA	3511	1/1	0.90	0.33	73,73,73,73	0
59	MG	DA	2916	1/1	0.90	0.15	57,57,57,57	0
59	MG	DA	3006	1/1	0.90	0.38	107,107,107,107	0
59	MG	BA	3174	1/1	0.90	0.25	83,83,83,83	0
59	MG	BA	3372	1/1	0.90	0.37	70,70,70,70	0
59	MG	BA	3573	1/1	0.90	0.70	75,75,75,75	0
59	MG	DA	3568	1/1	0.90	0.64	73,73,73,73	0
59	MG	BA	3125	1/1	0.90	0.23	70,70,70,70	0
59	MG	AQ	201	1/1	0.90	0.09	97,97,97,97	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1651	1/1	0.90	0.17	84,84,84,84	0
59	MG	BA	3128	1/1	0.90	0.53	92,92,92,92	0
59	MG	BU	201	1/1	0.90	0.51	46,46,46,46	0
59	MG	DA	3745	1/1	0.90	0.51	56,56,56,56	0
59	MG	DA	3218	1/1	0.90	0.38	130,130,130,130	0
59	MG	DA	3455	1/1	0.90	0.47	71,71,71,71	0
59	MG	AA	1716	1/1	0.90	0.23	82,82,82,82	0
59	MG	DA	3580	1/1	0.90	0.26	34,34,34,34	0
59	MG	DA	3752	1/1	0.90	0.38	96,96,96,96	0
59	MG	BA	3330	1/1	0.90	0.39	88,88,88,88	0
59	MG	DA	3221	1/1	0.90	0.73	77,77,77,77	0
59	MG	BA	3000	1/1	0.90	0.10	80,80,80,80	0
59	MG	BA	3446	1/1	0.90	0.30	99,99,99,99	0
59	MG	DA	3466	1/1	0.90	0.56	40,40,40,40	0
59	MG	CQ	201	1/1	0.90	0.08	98,98,98,98	1
59	MG	DA	2935	1/1	0.90	1.26	12,12,12,12	1
59	MG	AA	1941	1/1	0.90	0.56	63,63,63,63	0
59	MG	DA	3767	1/1	0.90	0.64	67,67,67,67	0
59	MG	DA	3472	1/1	0.90	0.35	79,79,79,79	1
59	MG	CA	1661	1/1	0.90	0.19	65,65,65,65	0
59	MG	BA	2941	1/1	0.90	0.27	62,62,62,62	0
59	MG	CV	103	1/1	0.90	0.15	67,67,67,67	0
59	MG	DA	3477	1/1	0.90	0.62	76,76,76,76	0
59	MG	DA	3601	1/1	0.90	0.24	39,39,39,39	0
59	MG	DA	3602	1/1	0.90	0.29	76,76,76,76	0
59	MG	AA	1817	1/1	0.90	0.14	71,71,71,71	0
59	MG	DA	3237	1/1	0.90	0.33	37,37,37,37	0
59	MG	BA	3188	1/1	0.90	0.09	58,58,58,58	0
59	MG	AA	1930	1/1	0.90	0.16	64,64,64,64	0
59	MG	AA	1834	1/1	0.90	0.34	94,94,94,94	0
59	MG	DA	3059	1/1	0.90	0.59	77,77,77,77	0
59	MG	DA	3621	1/1	0.90	0.35	76,76,76,76	1
59	MG	AA	1960	1/1	0.90	0.18	72,72,72,72	0
59	MG	BA	3543	1/1	0.90	0.69	71,71,71,71	0
59	MG	CA	1744	1/1	0.90	0.22	57,57,57,57	0
59	MG	DA	3378	1/1	0.90	0.45	96,96,96,96	0
59	MG	AA	1847	1/1	0.90	0.37	76,76,76,76	0
59	MG	AI	201	1/1	0.90	0.29	163,163,163,163	0
59	MG	AA	1761	1/1	0.90	1.23	83,83,83,83	0
59	MG	DA	3499	1/1	0.90	0.35	90,90,90,90	0
59	MG	BA	3148	1/1	0.90	0.76	106,106,106,106	0
59	MG	DA	3501	1/1	0.90	0.49	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3401	1/1	0.90	0.09	75,75,75,75	0
59	MG	BA	2957	1/1	0.90	0.46	81,81,81,81	0
59	MG	AA	1918	1/1	0.90	0.29	64,64,64,64	0
59	MG	BA	3151	1/1	0.90	0.20	65,65,65,65	0
59	MG	DB	210	1/1	0.90	0.36	56,56,56,56	0
59	MG	DA	3507	1/1	0.90	0.31	5,5,5,5	1
59	MG	DA	3652	1/1	0.90	0.13	74,74,74,74	0
59	MG	AA	1603	1/1	0.90	0.20	74,74,74,74	0
59	MG	BA	3557	1/1	0.90	0.99	37,37,37,37	1
59	MG	D7	102	1/1	0.90	0.30	75,75,75,75	0
59	MG	AA	1862	1/1	0.90	0.37	65,65,65,65	0
59	MG	DA	3272	1/1	0.90	0.22	79,79,79,79	1
59	MG	DA	3273	1/1	0.90	0.59	54,54,54,54	0
59	MG	DF	303	1/1	0.90	0.21	22,22,22,22	1
59	MG	BA	3495	1/1	0.90	0.20	69,69,69,69	0
59	MG	DA	3397	1/1	0.90	0.56	72,72,72,72	0
59	MG	DA	3280	1/1	0.90	0.21	58,58,58,58	0
59	MG	CA	1694	1/1	0.90	0.20	93,93,93,93	0
59	MG	BA	3158	1/1	0.90	0.22	33,33,33,33	0
59	MG	AA	1733	1/1	0.90	0.14	71,71,71,71	0
59	MG	DA	2902	1/1	0.90	0.41	42,42,42,42	0
59	MG	CA	1635	1/1	0.90	0.22	93,93,93,93	0
59	MG	DA	3684	1/1	0.90	0.29	82,82,82,82	0
59	MG	DA	3408	1/1	0.90	0.30	41,41,41,41	0
59	MG	DA	3528	1/1	0.90	0.28	80,80,80,80	0
59	MG	DA	2987	1/1	0.90	0.28	68,68,68,68	0
59	MG	DA	3516	1/1	0.91	0.85	97,97,97,97	0
59	MG	DA	2915	1/1	0.91	0.35	48,48,48,48	0
59	MG	DA	3620	1/1	0.91	0.13	70,70,70,70	0
59	MG	BA	3051	1/1	0.91	0.17	68,68,68,68	0
59	MG	DA	3624	1/1	0.91	0.43	71,71,71,71	0
59	MG	AC	301	1/1	0.91	0.14	173,173,173,173	0
59	MG	BA	3250	1/1	0.91	0.25	51,51,51,51	0
59	MG	BA	3058	1/1	0.91	0.27	74,74,74,74	0
59	MG	BA	3059	1/1	0.91	0.23	98,98,98,98	0
59	MG	AY	102	1/1	0.91	0.76	104,104,104,104	1
59	MG	BA	3061	1/1	0.91	0.32	63,63,63,63	0
59	MG	DA	3002	1/1	0.91	0.07	78,78,78,78	0
59	MG	CV	102	1/1	0.91	0.08	92,92,92,92	0
59	MG	DA	3759	1/1	0.91	0.58	49,49,49,49	0
59	MG	BA	3135	1/1	0.91	0.24	86,86,86,86	0
59	MG	BA	3063	1/1	0.91	0.34	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3261	1/1	0.91	0.77	34,34,34,34	1
59	MG	BA	3033	1/1	0.91	0.32	69,69,69,69	0
59	MG	BA	3579	1/1	0.91	0.71	71,71,71,71	0
59	MG	DA	3541	1/1	0.91	0.21	96,96,96,96	0
59	MG	DA	3013	1/1	0.91	0.45	68,68,68,68	0
59	MG	DA	3545	1/1	0.91	0.11	58,58,58,58	0
59	MG	BA	3537	1/1	0.91	0.30	28,28,28,28	0
59	MG	DA	3180	1/1	0.91	0.34	115,115,115,115	0
59	MG	AA	1821	1/1	0.91	0.40	65,65,65,65	0
59	MG	DA	3184	1/1	0.91	0.27	63,63,63,63	0
59	MG	CA	1753	1/1	0.91	0.09	103,103,103,103	0
59	MG	DA	3108	1/1	0.91	0.24	81,81,81,81	0
59	MG	BA	3410	1/1	0.91	0.47	42,42,42,42	0
59	MG	DA	3784	1/1	0.91	0.34	123,123,123,123	0
59	MG	BA	3319	1/1	0.91	0.52	33,33,33,33	0
59	MG	BA	3010	1/1	0.91	0.65	95,95,95,95	0
59	MG	AV	102	1/1	0.91	0.79	106,106,106,106	0
59	MG	CA	1759	1/1	0.91	0.79	98,98,98,98	0
59	MG	DA	3117	1/1	0.91	0.42	88,88,88,88	0
59	MG	CA	1603	1/1	0.91	0.32	112,112,112,112	0
59	MG	DA	3198	1/1	0.91	0.54	31,31,31,31	0
59	MG	CA	1706	1/1	0.91	0.09	47,47,47,47	0
59	MG	D1	102	1/1	0.91	0.27	80,80,80,80	0
59	MG	AL	205	1/1	0.91	0.29	47,47,47,47	1
59	MG	DB	201	1/1	0.91	0.15	59,59,59,59	0
59	MG	B5	102	1/1	0.91	0.21	32,32,32,32	1
59	MG	DA	3488	1/1	0.91	0.28	28,28,28,28	0
59	MG	AA	1680	1/1	0.91	0.27	75,75,75,75	0
59	MG	AA	1707	1/1	0.91	0.27	97,97,97,97	0
59	MG	DA	2954	1/1	0.91	0.51	47,47,47,47	1
59	MG	DA	3579	1/1	0.91	0.34	110,110,110,110	0
59	MG	CA	1713	1/1	0.91	0.26	65,65,65,65	1
59	MG	AA	1693	1/1	0.91	0.10	56,56,56,56	1
59	MG	DA	3311	1/1	0.91	0.91	96,96,96,96	0
59	MG	BA	3427	1/1	0.91	0.61	63,63,63,63	0
59	MG	BA	3018	1/1	0.91	0.15	38,38,38,38	0
59	MG	AV	107	1/1	0.91	0.25	58,58,58,58	0
59	MG	AA	1878	1/1	0.91	0.16	76,76,76,76	0
59	MG	DE	303	1/1	0.91	0.23	42,42,42,42	0
59	MG	DA	3062	1/1	0.91	0.41	88,88,88,88	0
59	MG	BA	3377	1/1	0.91	0.27	59,59,59,59	0
59	MG	BA	3240	1/1	0.91	0.60	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AX	102	1/1	0.91	0.12	87,87,87,87	0
59	MG	DA	3716	1/1	0.91	0.50	103,103,103,103	0
59	MG	BA	3242	1/1	0.91	0.38	60,60,60,60	0
59	MG	BA	3162	1/1	0.91	0.68	41,41,41,41	0
59	MG	BA	2938	1/1	0.91	0.20	64,64,64,64	1
59	MG	BA	3513	1/1	0.91	0.38	77,77,77,77	0
59	MG	BA	2962	1/1	0.91	0.63	70,70,70,70	0
59	MG	BB	205	1/1	0.91	0.12	69,69,69,69	1
59	MG	DA	3609	1/1	0.91	0.53	63,63,63,63	0
59	MG	DA	2913	1/1	0.91	0.37	15,15,15,15	1
59	MG	BA	3520	1/1	0.91	0.23	80,80,80,80	0
59	MG	DA	3424	1/1	0.91	1.01	84,84,84,84	0
59	MG	AA	1927	1/1	0.92	0.13	113,113,113,113	0
59	MG	BA	2980	1/1	0.92	0.32	47,47,47,47	0
59	MG	BA	3023	1/1	0.92	0.28	64,64,64,64	0
59	MG	DA	3534	1/1	0.92	0.47	73,73,73,73	1
59	MG	DA	3536	1/1	0.92	0.26	37,37,37,37	1
59	MG	BA	3431	1/1	0.92	0.57	79,79,79,79	0
59	MG	BA	3203	1/1	0.92	0.40	75,75,75,75	0
59	MG	BA	3204	1/1	0.92	0.90	71,71,71,71	0
59	MG	CA	1665	1/1	0.92	0.13	79,79,79,79	0
59	MG	BA	2981	1/1	0.92	0.20	80,80,80,80	0
59	MG	BA	2982	1/1	0.92	0.14	58,58,58,58	1
59	MG	AA	1873	1/1	0.92	0.44	117,117,117,117	0
59	MG	CA	1675	1/1	0.92	0.59	93,93,93,93	0
59	MG	AA	1840	1/1	0.92	0.34	76,76,76,76	0
59	MG	DA	3044	1/1	0.92	0.23	78,78,78,78	0
59	MG	BA	2985	1/1	0.92	0.74	84,84,84,84	0
59	MG	DA	3550	1/1	0.92	0.46	86,86,86,86	0
59	MG	BA	3552	1/1	0.92	0.17	54,54,54,54	1
59	MG	DA	3713	1/1	0.92	0.19	67,67,67,67	0
59	MG	BA	3283	1/1	0.92	0.29	58,58,58,58	0
59	MG	DA	3554	1/1	0.92	0.08	95,95,95,95	0
59	MG	AA	1951	1/1	0.92	0.33	82,82,82,82	0
59	MG	CA	1682	1/1	0.92	0.33	53,53,53,53	0
59	MG	DA	3721	1/1	0.92	0.19	171,171,171,171	0
59	MG	DA	3300	1/1	0.92	0.32	67,67,67,67	0
59	MG	DA	3428	1/1	0.92	0.32	65,65,65,65	0
59	MG	BA	3457	1/1	0.92	0.53	72,72,72,72	0
59	MG	AA	1952	1/1	0.92	0.88	97,97,97,97	0
59	MG	BA	3093	1/1	0.92	0.20	52,52,52,52	0
59	MG	AA	1701	1/1	0.92	0.33	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3569	1/1	0.92	0.61	102,102,102,102	0
59	MG	DA	3175	1/1	0.92	0.20	28,28,28,28	0
59	MG	DA	3308	1/1	0.92	0.23	103,103,103,103	0
59	MG	DA	3744	1/1	0.92	0.27	93,93,93,93	1
59	MG	DA	3309	1/1	0.92	0.59	76,76,76,76	0
59	MG	CA	1687	1/1	0.92	0.08	63,63,63,63	0
59	MG	AA	1876	1/1	0.92	0.27	92,92,92,92	1
59	MG	CA	1690	1/1	0.92	0.42	60,60,60,60	0
59	MG	BA	3561	1/1	0.92	1.32	122,122,122,122	0
59	MG	BA	3293	1/1	0.92	0.17	82,82,82,82	0
59	MG	AI	202	1/1	0.92	0.17	117,117,117,117	0
59	MG	BA	3474	1/1	0.92	0.56	53,53,53,53	0
59	MG	AA	1746	1/1	0.92	0.31	66,66,66,66	0
59	MG	DA	3458	1/1	0.92	0.51	59,59,59,59	0
59	MG	DA	3327	1/1	0.92	0.12	39,39,39,39	1
59	MG	BA	3223	1/1	0.92	0.22	80,80,80,80	0
59	MG	AA	1844	1/1	0.92	0.22	107,107,107,107	0
59	MG	BA	3306	1/1	0.92	0.26	57,57,57,57	0
59	MG	CA	1699	1/1	0.92	0.21	64,64,64,64	0
59	MG	AA	1863	1/1	0.92	0.30	80,80,80,80	0
59	MG	AL	206	1/1	0.92	0.19	53,53,53,53	1
59	MG	AA	1662	1/1	0.92	0.43	68,68,68,68	0
59	MG	DA	3471	1/1	0.92	0.55	63,63,63,63	0
59	MG	DA	2957	1/1	0.92	0.42	47,47,47,47	0
59	MG	CA	1704	1/1	0.92	0.10	71,71,71,71	0
59	MG	BA	2952	1/1	0.92	0.47	96,96,96,96	0
59	MG	DA	3204	1/1	0.92	0.22	70,70,70,70	0
59	MG	BA	3109	1/1	0.92	0.31	35,35,35,35	0
59	MG	AA	1765	1/1	0.92	0.09	107,107,107,107	1
59	MG	BA	3386	1/1	0.92	0.34	72,72,72,72	0
59	MG	BA	2906	1/1	0.92	0.36	92,92,92,92	0
59	MG	DA	2966	1/1	0.92	0.96	51,51,51,51	1
59	MG	DA	3484	1/1	0.92	0.86	58,58,58,58	0
59	MG	AA	1629	1/1	0.92	0.31	80,80,80,80	0
59	MG	AA	1709	1/1	0.92	0.26	85,85,85,85	1
59	MG	BA	3500	1/1	0.92	0.35	79,79,79,79	0
59	MG	BA	2910	1/1	0.92	0.24	83,83,83,83	1
59	MG	AA	1634	1/1	0.92	0.47	70,70,70,70	1
59	MG	BA	3117	1/1	0.92	0.78	98,98,98,98	0
59	MG	BA	3504	1/1	0.92	0.23	59,59,59,59	0
59	MG	BA	3398	1/1	0.92	0.69	53,53,53,53	0
59	MG	AA	1852	1/1	0.92	0.37	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AT	201	1/1	0.92	0.23	76,76,76,76	1
59	MG	BA	3407	1/1	0.92	0.29	64,64,64,64	0
59	MG	DA	3636	1/1	0.92	0.15	50,50,50,50	0
59	MG	BA	3591	1/1	0.92	0.83	93,93,93,93	0
59	MG	DA	3375	1/1	0.92	0.44	57,57,57,57	0
59	MG	AV	101	1/1	0.92	0.75	52,52,52,52	1
59	MG	BA	2919	1/1	0.92	0.43	44,44,44,44	1
59	MG	BA	2920	1/1	0.92	0.28	42,42,42,42	0
59	MG	BA	3518	1/1	0.92	0.30	64,64,64,64	0
59	MG	D7	101	1/1	0.92	0.56	89,89,89,89	0
59	MG	DA	3000	1/1	0.92	0.06	105,105,105,105	0
59	MG	AA	1811	1/1	0.92	0.26	49,49,49,49	0
59	MG	BA	3413	1/1	0.92	0.70	73,73,73,73	0
59	MG	DA	3657	1/1	0.92	0.32	59,59,59,59	0
59	MG	BA	3191	1/1	0.92	0.75	78,78,78,78	0
59	MG	DE	302	1/1	0.92	0.24	39,39,39,39	1
59	MG	AA	1760	1/1	0.92	0.37	45,45,45,45	0
59	MG	BA	3068	1/1	0.92	0.63	59,59,59,59	0
59	MG	BA	2975	1/1	0.92	0.58	57,57,57,57	0
59	MG	BA	3262	1/1	0.92	0.27	50,50,50,50	0
59	MG	DA	3668	1/1	0.92	0.28	93,93,93,93	0
59	MG	DA	3669	1/1	0.92	0.40	39,39,39,39	0
59	MG	DA	3011	1/1	0.92	0.27	40,40,40,40	0
59	MG	AA	1946	1/1	0.92	0.40	77,77,77,77	0
59	MG	DA	3394	1/1	0.92	0.30	63,63,63,63	0
59	MG	DA	3520	1/1	0.92	0.41	103,103,103,103	0
59	MG	BA	3072	1/1	0.92	0.33	101,101,101,101	0
59	MG	BA	3426	1/1	0.92	0.76	77,77,77,77	0
59	MG	DA	3140	1/1	0.92	0.66	77,77,77,77	0
59	MG	DA	3016	1/1	0.92	0.28	51,51,51,51	0
59	MG	DU	201	1/1	0.92	0.21	68,68,68,68	0
59	MG	AA	1926	1/1	0.92	0.16	59,59,59,59	0
59	MG	DA	3685	1/1	0.92	0.15	69,69,69,69	0
59	MG	BA	3499	1/1	0.93	0.36	43,43,43,43	0
59	MG	DA	3297	1/1	0.93	0.65	53,53,53,53	0
59	MG	BA	3310	1/1	0.93	0.64	68,68,68,68	0
59	MG	BA	3362	1/1	0.93	0.51	43,43,43,43	0
59	MG	AA	1786	1/1	0.93	0.14	123,123,123,123	0
59	MG	DA	3073	1/1	0.93	0.42	64,64,64,64	0
59	MG	AA	1737	1/1	0.93	0.54	69,69,69,69	0
59	MG	AA	1916	1/1	0.93	0.09	70,70,70,70	0
59	MG	DA	3305	1/1	0.93	0.56	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3182	1/1	0.93	0.21	73,73,73,73	0
59	MG	DA	3183	1/1	0.93	0.28	94,94,94,94	0
59	MG	BA	3366	1/1	0.93	0.55	71,71,71,71	0
59	MG	BA	3315	1/1	0.93	0.68	74,74,74,74	0
59	MG	AA	1727	1/1	0.93	0.14	84,84,84,84	1
59	MG	BA	3510	1/1	0.93	0.71	41,41,41,41	0
59	MG	DA	3570	1/1	0.93	0.38	62,62,62,62	0
59	MG	CA	1602	1/1	0.93	0.15	76,76,76,76	0
59	MG	DA	3723	1/1	0.93	0.48	101,101,101,101	0
59	MG	DA	3724	1/1	0.93	0.28	73,73,73,73	0
59	MG	D0	103	1/1	0.93	0.35	74,74,74,74	0
59	MG	DA	3319	1/1	0.93	0.13	47,47,47,47	0
59	MG	BA	2988	1/1	0.93	0.14	35,35,35,35	0
59	MG	DA	3731	1/1	0.93	0.26	45,45,45,45	1
59	MG	BA	3214	1/1	0.93	0.55	85,85,85,85	0
59	MG	DA	3322	1/1	0.93	0.56	89,89,89,89	0
59	MG	BA	3373	1/1	0.93	0.21	56,56,56,56	0
59	MG	DA	2970	1/1	0.93	0.35	41,41,41,41	1
59	MG	BA	3089	1/1	0.93	0.32	33,33,33,33	0
59	MG	AA	1898	1/1	0.93	0.27	65,65,65,65	0
59	MG	DA	3740	1/1	0.93	0.22	50,50,50,50	0
59	MG	DA	3743	1/1	0.93	0.26	50,50,50,50	1
59	MG	DA	3095	1/1	0.93	0.56	42,42,42,42	0
59	MG	DA	3334	1/1	0.93	0.19	56,56,56,56	0
59	MG	BA	3519	1/1	0.93	0.82	88,88,88,88	0
59	MG	DA	2978	1/1	0.93	0.34	33,33,33,33	0
59	MG	AA	1687	1/1	0.93	0.10	101,101,101,101	0
59	MG	AA	1799	1/1	0.93	0.13	80,80,80,80	0
59	MG	DA	3588	1/1	0.93	0.39	83,83,83,83	0
59	MG	BA	3219	1/1	0.93	0.43	57,57,57,57	0
59	MG	DA	3207	1/1	0.93	0.19	84,84,84,84	0
59	MG	BA	3184	1/1	0.93	0.34	38,38,38,38	0
59	MG	DA	3209	1/1	0.93	0.49	50,50,50,50	0
59	MG	CA	1616	1/1	0.93	0.15	62,62,62,62	0
59	MG	BA	2966	1/1	0.93	0.55	64,64,64,64	0
59	MG	DA	3478	1/1	0.93	1.02	112,112,112,112	0
59	MG	DA	3352	1/1	0.93	0.32	58,58,58,58	0
59	MG	DA	3762	1/1	0.93	0.13	99,99,99,99	0
59	MG	BA	3054	1/1	0.93	0.27	100,100,100,100	0
59	MG	DA	3765	1/1	0.93	0.56	69,69,69,69	0
59	MG	DA	3766	1/1	0.93	0.79	100,100,100,100	0
59	MG	CA	1757	1/1	0.93	0.14	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3355	1/1	0.93	0.15	80,80,80,80	0
59	MG	BA	3021	1/1	0.93	0.57	78,78,78,78	0
59	MG	DA	3215	1/1	0.93	0.48	69,69,69,69	0
59	MG	DA	2903	1/1	0.93	0.48	43,43,43,43	0
59	MG	DA	3774	1/1	0.93	0.64	84,84,84,84	0
59	MG	DA	3616	1/1	0.93	0.36	51,51,51,51	0
59	MG	BA	3455	1/1	0.93	0.79	65,65,65,65	0
59	MG	BA	3531	1/1	0.93	0.54	53,53,53,53	0
59	MG	DA	3364	1/1	0.93	0.34	59,59,59,59	0
59	MG	BA	3456	1/1	0.93	0.58	33,33,33,33	0
59	MG	AA	1714	1/1	0.93	0.21	66,66,66,66	0
59	MG	BA	3279	1/1	0.93	0.35	59,59,59,59	0
59	MG	BA	2968	1/1	0.93	0.59	72,72,72,72	0
59	MG	BA	3463	1/1	0.93	0.68	66,66,66,66	0
59	MG	BA	3026	1/1	0.93	0.43	105,105,105,105	0
59	MG	BA	3388	1/1	0.93	0.59	100,100,100,100	0
59	MG	AA	1670	1/1	0.93	0.21	28,28,28,28	1
59	MG	DA	3633	1/1	0.93	0.65	75,75,75,75	0
59	MG	CA	1769	1/1	0.93	0.23	68,68,68,68	0
59	MG	AA	1720	1/1	0.93	0.55	37,37,37,37	1
59	MG	CA	1633	1/1	0.93	0.09	70,70,70,70	0
59	MG	AA	1767	1/1	0.93	0.35	77,77,77,77	0
59	MG	CA	1702	1/1	0.93	0.17	104,104,104,104	0
59	MG	BA	2911	1/1	0.93	0.30	94,94,94,94	0
59	MG	BA	3069	1/1	0.93	0.57	100,100,100,100	0
59	MG	BA	2912	1/1	0.93	0.48	57,57,57,57	0
59	MG	CA	1778	1/1	0.93	0.35	88,88,88,88	0
59	MG	DA	3025	1/1	0.93	0.24	108,108,108,108	0
59	MG	DA	2924	1/1	0.93	0.30	65,65,65,65	0
59	MG	BA	3349	1/1	0.93	0.33	68,68,68,68	0
59	MG	DA	3655	1/1	0.93	0.79	91,91,91,91	0
59	MG	BA	2945	1/1	0.93	0.34	113,113,113,113	0
59	MG	DA	3255	1/1	0.93	0.41	51,51,51,51	0
59	MG	BA	3403	1/1	0.93	0.17	69,69,69,69	0
59	MG	AA	1928	1/1	0.93	0.34	42,42,42,42	0
59	MG	AA	1885	1/1	0.93	0.37	57,57,57,57	0
59	MG	AA	1887	1/1	0.93	0.24	72,72,72,72	0
59	MG	DA	2932	1/1	0.93	0.21	1,1,1,1	1
59	MG	DA	2933	1/1	0.93	0.25	51,51,51,51	0
59	MG	DA	2934	1/1	0.93	0.19	48,48,48,48	1
59	MG	CA	1714	1/1	0.93	0.61	83,83,83,83	0
59	MG	BD	305	1/1	0.93	0.14	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AY	101	1/1	0.93	1.19	6,6,6,6	1
59	MG	DA	3530	1/1	0.93	0.29	122,122,122,122	0
59	MG	CP	101	1/1	0.93	0.06	81,81,81,81	0
59	MG	DA	3157	1/1	0.93	0.23	52,52,52,52	0
59	MG	DA	3050	1/1	0.93	0.54	40,40,40,40	0
59	MG	DP	201	1/1	0.93	0.11	36,36,36,36	1
59	MG	DA	3276	1/1	0.93	0.30	58,58,58,58	0
59	MG	DA	2939	1/1	0.93	0.82	1,1,1,1	1
59	MG	CA	1648	1/1	0.93	0.81	90,90,90,90	0
59	MG	DA	3287	1/1	0.93	0.14	66,66,66,66	0
59	MG	BA	3164	1/1	0.93	0.83	44,44,44,44	0
59	MG	BF	301	1/1	0.93	0.37	60,60,60,60	0
59	MG	AA	1909	1/1	0.93	0.11	87,87,87,87	1
59	MG	AA	1804	1/1	0.93	0.47	90,90,90,90	0
59	MG	BA	3360	1/1	0.93	0.39	80,80,80,80	0
59	MG	BA	3549	1/1	0.94	0.63	84,84,84,84	0
59	MG	BA	3550	1/1	0.94	0.42	103,103,103,103	0
59	MG	AA	1616	1/1	0.94	0.54	61,61,61,61	0
59	MG	DA	3672	1/1	0.94	0.23	74,74,74,74	0
59	MG	BA	2995	1/1	0.94	0.35	84,84,84,84	0
59	MG	DA	3674	1/1	0.94	0.70	55,55,55,55	0
59	MG	BA	3227	1/1	0.94	0.23	78,78,78,78	0
59	MG	DA	3677	1/1	0.94	0.31	45,45,45,45	0
59	MG	CA	1604	1/1	0.94	0.19	63,63,63,63	0
59	MG	DA	3087	1/1	0.94	0.33	33,33,33,33	0
59	MG	DA	3089	1/1	0.94	0.19	81,81,81,81	0
59	MG	AA	1961	1/1	0.94	0.24	87,87,87,87	0
59	MG	DA	3683	1/1	0.94	0.69	46,46,46,46	0
59	MG	CA	1606	1/1	0.94	0.10	60,60,60,60	0
59	MG	DA	3513	1/1	0.94	0.13	95,95,95,95	0
59	MG	BA	2997	1/1	0.94	0.37	82,82,82,82	0
59	MG	BA	2909	1/1	0.94	0.20	50,50,50,50	0
59	MG	BA	2956	1/1	0.94	0.27	37,37,37,37	1
59	MG	AA	1796	1/1	0.94	0.14	61,61,61,61	0
59	MG	AA	1836	1/1	0.94	0.34	114,114,114,114	0
59	MG	DA	2965	1/1	0.94	0.65	52,52,52,52	0
59	MG	CA	1612	1/1	0.94	0.24	58,58,58,58	0
59	MG	BA	3475	1/1	0.94	0.19	59,59,59,59	0
59	MG	BA	3476	1/1	0.94	0.27	58,58,58,58	0
59	MG	BA	3236	1/1	0.94	0.88	86,86,86,86	0
59	MG	BA	2959	1/1	0.94	0.26	65,65,65,65	0
59	MG	BA	3178	1/1	0.94	0.96	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1710	1/1	0.94	0.21	51,51,51,51	0
59	MG	DA	3233	1/1	0.94	0.20	152,152,152,152	0
59	MG	AA	1606	1/1	0.94	0.24	77,77,77,77	0
59	MG	DA	3531	1/1	0.94	0.32	82,82,82,82	0
59	MG	AA	1654	1/1	0.94	0.13	58,58,58,58	1
59	MG	BA	3053	1/1	0.94	1.01	62,62,62,62	0
59	MG	DA	3115	1/1	0.94	0.47	39,39,39,39	0
59	MG	AA	1871	1/1	0.94	0.22	144,144,144,144	0
59	MG	AA	1892	1/1	0.94	0.19	75,75,75,75	0
59	MG	BA	3489	1/1	0.94	0.10	22,22,22,22	0
59	MG	DA	3242	1/1	0.94	0.34	31,31,31,31	0
59	MG	BA	3392	1/1	0.94	0.85	87,87,87,87	0
59	MG	DA	3722	1/1	0.94	0.56	86,86,86,86	0
59	MG	DA	3542	1/1	0.94	0.18	74,74,74,74	0
59	MG	AA	1826	1/1	0.94	0.15	83,83,83,83	0
59	MG	DA	3393	1/1	0.94	0.28	6,6,6,6	1
59	MG	BA	3009	1/1	0.94	0.42	80,80,80,80	0
59	MG	DA	3249	1/1	0.94	0.26	68,68,68,68	0
59	MG	AA	1895	1/1	0.94	0.22	72,72,72,72	0
59	MG	BA	3496	1/1	0.94	0.32	44,44,44,44	0
59	MG	BA	3396	1/1	0.94	0.66	86,86,86,86	0
59	MG	CA	1724	1/1	0.94	0.52	102,102,102,102	0
59	MG	DA	2997	1/1	0.94	0.53	43,43,43,43	0
59	MG	AA	1896	1/1	0.94	0.20	78,78,78,78	0
59	MG	DA	3738	1/1	0.94	0.21	89,89,89,89	0
59	MG	AA	1973	1/1	0.94	0.22	69,69,69,69	0
59	MG	BA	3066	1/1	0.94	0.67	57,57,57,57	0
59	MG	AA	1921	1/1	0.94	0.47	86,86,86,86	0
59	MG	AA	1750	1/1	0.94	0.20	54,54,54,54	1
59	MG	BA	2924	1/1	0.94	0.52	73,73,73,73	0
59	MG	DA	3746	1/1	0.94	0.69	71,71,71,71	0
59	MG	AA	1899	1/1	0.94	0.37	63,63,63,63	0
59	MG	BA	3129	1/1	0.94	0.41	42,42,42,42	0
59	MG	BA	3411	1/1	0.94	0.49	76,76,76,76	0
59	MG	BA	3508	1/1	0.94	0.51	39,39,39,39	0
59	MG	AX	104	1/1	0.94	0.45	43,43,43,43	0
59	MG	BA	3341	1/1	0.94	0.41	33,33,33,33	0
59	MG	AA	1925	1/1	0.94	0.13	72,72,72,72	0
59	MG	DA	3277	1/1	0.94	0.40	42,42,42,42	0
59	MG	BA	3345	1/1	0.94	0.59	37,37,37,37	0
59	MG	DA	3281	1/1	0.94	0.45	31,31,31,31	0
59	MG	BA	3416	1/1	0.94	0.72	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3073	1/1	0.94	0.50	52,52,52,52	0
59	MG	DA	3149	1/1	0.94	0.31	26,26,26,26	0
59	MG	BA	3515	1/1	0.94	0.15	47,47,47,47	1
59	MG	BA	3517	1/1	0.94	0.25	98,98,98,98	0
59	MG	DA	3292	1/1	0.94	0.46	106,106,106,106	0
59	MG	AD	304	1/1	0.94	0.19	135,135,135,135	0
59	MG	BA	3269	1/1	0.94	0.15	63,63,63,63	0
59	MG	DA	3030	1/1	0.94	0.74	59,59,59,59	0
59	MG	AA	1841	1/1	0.94	0.39	42,42,42,42	0
59	MG	DA	3586	1/1	0.94	0.54	34,34,34,34	0
59	MG	DA	3772	1/1	0.94	0.17	69,69,69,69	0
59	MG	AA	1901	1/1	0.94	0.69	65,65,65,65	0
59	MG	BA	3606	1/1	0.94	0.55	65,65,65,65	0
59	MG	DA	3444	1/1	0.94	0.42	31,31,31,31	0
59	MG	DA	3445	1/1	0.94	0.25	55,55,55,55	0
59	MG	DA	3592	1/1	0.94	0.50	58,58,58,58	0
59	MG	BB	201	1/1	0.94	0.38	46,46,46,46	0
59	MG	DA	3447	1/1	0.94	0.77	70,70,70,70	0
59	MG	BA	3079	1/1	0.94	0.16	37,37,37,37	0
59	MG	DA	3162	1/1	0.94	0.37	122,122,122,122	0
59	MG	DA	3041	1/1	0.94	0.22	78,78,78,78	0
59	MG	AA	1859	1/1	0.94	0.20	44,44,44,44	0
59	MG	BA	3207	1/1	0.94	0.43	43,43,43,43	0
59	MG	AA	1669	1/1	0.94	0.28	50,50,50,50	0
59	MG	DA	3787	1/1	0.94	0.53	95,95,95,95	0
59	MG	AA	1647	1/1	0.94	0.15	35,35,35,35	0
59	MG	DA	3460	1/1	0.94	0.17	73,73,73,73	0
59	MG	DA	3461	1/1	0.94	0.54	77,77,77,77	0
59	MG	BA	2942	1/1	0.94	0.64	110,110,110,110	0
59	MG	B7	101	1/1	0.94	0.89	93,93,93,93	0
59	MG	BA	3147	1/1	0.94	0.50	72,72,72,72	0
59	MG	DA	3173	1/1	0.94	0.46	48,48,48,48	0
59	MG	DA	3315	1/1	0.94	0.46	77,77,77,77	0
59	MG	BA	2944	1/1	0.94	0.29	43,43,43,43	0
59	MG	DA	3622	1/1	0.94	0.06	58,58,58,58	0
59	MG	DA	3623	1/1	0.94	0.16	28,28,28,28	0
59	MG	DA	3317	1/1	0.94	0.51	62,62,62,62	0
59	MG	DA	3318	1/1	0.94	0.12	59,59,59,59	0
59	MG	DB	206	1/1	0.94	0.09	65,65,65,65	1
59	MG	DA	3053	1/1	0.94	0.38	33,33,33,33	0
59	MG	DA	3054	1/1	0.94	0.08	69,69,69,69	0
59	MG	AA	1664	1/1	0.94	0.15	17,17,17,17	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3057	1/1	0.94	0.22	32,32,32,32	0
59	MG	DA	3323	1/1	0.94	0.75	58,58,58,58	0
59	MG	BA	2946	1/1	0.94	0.42	49,49,49,49	0
59	MG	DA	3325	1/1	0.94	0.33	109,109,109,109	0
59	MG	AA	1783	1/1	0.94	0.55	73,73,73,73	0
59	MG	CA	1678	1/1	0.94	0.14	45,45,45,45	1
59	MG	AA	1934	1/1	0.94	0.22	68,68,68,68	0
59	MG	DA	3064	1/1	0.94	0.22	51,51,51,51	0
59	MG	BA	2905	1/1	0.94	0.34	52,52,52,52	0
59	MG	DA	3486	1/1	0.94	0.62	38,38,38,38	0
59	MG	BA	3297	1/1	0.94	0.22	34,34,34,34	0
59	MG	BA	3450	1/1	0.94	0.62	60,60,60,60	0
59	MG	BA	3451	1/1	0.94	0.18	55,55,55,55	0
59	MG	DA	3194	1/1	0.94	0.23	92,92,92,92	0
59	MG	BA	3545	1/1	0.94	0.42	79,79,79,79	0
59	MG	DA	3494	1/1	0.94	0.38	41,41,41,41	0
59	MG	BA	3453	1/1	0.94	0.07	120,120,120,120	0
59	MG	AA	1622	1/1	0.94	0.31	70,70,70,70	0
59	MG	DA	3660	1/1	0.94	0.67	78,78,78,78	0
59	MG	BR	203	1/1	0.94	0.45	83,83,83,83	0
59	MG	DA	3662	1/1	0.94	0.28	59,59,59,59	0
59	MG	BA	3159	1/1	0.94	0.45	72,72,72,72	0
59	MG	DA	3347	1/1	0.94	0.21	71,71,71,71	0
59	MG	DU	202	1/1	0.94	0.31	8,8,8,8	1
59	MG	DW	201	1/1	0.94	0.30	36,36,36,36	1
59	MG	DA	2946	1/1	0.94	0.35	96,96,96,96	0
59	MG	CA	1781	1/1	0.94	0.17	74,74,74,74	0
59	MG	AA	1877	1/1	0.95	0.41	61,61,61,61	0
59	MG	DA	3692	1/1	0.95	0.87	61,61,61,61	0
59	MG	CA	1672	1/1	0.95	0.16	92,92,92,92	0
59	MG	CA	1673	1/1	0.95	0.28	62,62,62,62	0
59	MG	DA	3430	1/1	0.95	0.23	25,25,25,25	0
59	MG	DA	3551	1/1	0.95	0.55	53,53,53,53	0
59	MG	DA	3700	1/1	0.95	0.32	59,59,59,59	0
59	MG	DA	3431	1/1	0.95	0.33	38,38,38,38	0
59	MG	CA	1674	1/1	0.95	0.18	90,90,90,90	0
59	MG	BA	3221	1/1	0.95	0.59	42,42,42,42	0
59	MG	DA	3434	1/1	0.95	0.55	44,44,44,44	0
59	MG	DA	3707	1/1	0.95	0.39	55,55,55,55	1
59	MG	B1	101	1/1	0.95	0.14	50,50,50,50	1
59	MG	DA	3557	1/1	0.95	0.14	64,64,64,64	0
59	MG	DA	3558	1/1	0.95	0.42	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3449	1/1	0.95	0.14	69,69,69,69	0
59	MG	BA	3022	1/1	0.95	0.08	43,43,43,43	0
59	MG	DA	3097	1/1	0.95	0.32	69,69,69,69	0
59	MG	DA	3565	1/1	0.95	0.16	54,54,54,54	0
59	MG	BA	2998	1/1	0.95	0.23	54,54,54,54	0
59	MG	BA	3226	1/1	0.95	0.48	78,78,78,78	0
59	MG	BA	3277	1/1	0.95	0.48	44,44,44,44	0
59	MG	DA	3719	1/1	0.95	0.45	73,73,73,73	0
59	MG	BA	3337	1/1	0.95	0.75	37,37,37,37	0
59	MG	DA	2995	1/1	0.95	0.13	44,44,44,44	0
59	MG	BA	3094	1/1	0.95	0.41	32,32,32,32	0
59	MG	BA	3056	1/1	0.95	0.24	156,156,156,156	0
59	MG	DA	3726	1/1	0.95	0.22	65,65,65,65	0
59	MG	AA	1816	1/1	0.95	0.28	64,64,64,64	0
59	MG	BA	3586	1/1	0.95	0.91	86,86,86,86	0
59	MG	DA	3729	1/1	0.95	0.23	96,96,96,96	0
59	MG	BA	3461	1/1	0.95	0.51	41,41,41,41	0
59	MG	DA	3328	1/1	0.95	0.28	34,34,34,34	0
59	MG	DA	3003	1/1	0.95	0.30	36,36,36,36	0
59	MG	CA	1688	1/1	0.95	0.11	79,79,79,79	0
59	MG	DA	3734	1/1	0.95	0.17	74,74,74,74	0
59	MG	DA	2912	1/1	0.95	0.30	68,68,68,68	0
59	MG	BA	3462	1/1	0.95	0.46	28,28,28,28	0
59	MG	AA	1897	1/1	0.95	0.23	68,68,68,68	0
59	MG	DA	3119	1/1	0.95	0.14	66,66,66,66	0
59	MG	DA	3008	1/1	0.95	0.28	70,70,70,70	0
59	MG	BA	3231	1/1	0.95	0.39	28,28,28,28	0
59	MG	BA	3466	1/1	0.95	0.26	38,38,38,38	0
59	MG	BA	3533	1/1	0.95	0.44	83,83,83,83	0
59	MG	DA	3469	1/1	0.95	0.47	65,65,65,65	0
59	MG	AA	1724	1/1	0.95	0.16	86,86,86,86	1
59	MG	DA	3226	1/1	0.95	0.70	54,54,54,54	0
59	MG	BA	3535	1/1	0.95	0.18	81,81,81,81	0
59	MG	BA	3100	1/1	0.95	0.23	47,47,47,47	0
59	MG	BA	3028	1/1	0.95	0.33	58,58,58,58	0
59	MG	AA	1853	1/1	0.95	0.29	74,74,74,74	0
59	MG	BA	3237	1/1	0.95	0.20	58,58,58,58	0
59	MG	DA	3596	1/1	0.95	0.43	54,54,54,54	1
59	MG	BA	3292	1/1	0.95	0.26	29,29,29,29	0
59	MG	BA	3103	1/1	0.95	0.30	69,69,69,69	0
59	MG	BA	3478	1/1	0.95	0.44	28,28,28,28	0
59	MG	BA	3605	1/1	0.95	0.83	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3605	1/1	0.95	0.32	63,63,63,63	0
59	MG	BA	3295	1/1	0.95	0.59	51,51,51,51	0
59	MG	AA	1632	1/1	0.95	0.23	97,97,97,97	0
59	MG	DA	3611	1/1	0.95	0.46	31,31,31,31	0
59	MG	DA	3764	1/1	0.95	0.24	75,75,75,75	0
59	MG	BA	3481	1/1	0.95	0.44	59,59,59,59	0
59	MG	CA	1784	1/1	0.95	0.65	76,76,76,76	0
59	MG	DA	3487	1/1	0.95	0.67	42,42,42,42	1
59	MG	BA	3299	1/1	0.95	0.40	66,66,66,66	0
59	MG	CC	302	1/1	0.95	0.68	114,114,114,114	0
59	MG	DA	3490	1/1	0.95	0.13	29,29,29,29	1
59	MG	BA	3065	1/1	0.95	0.38	50,50,50,50	0
59	MG	BA	3031	1/1	0.95	0.44	58,58,58,58	0
59	MG	DA	3370	1/1	0.95	0.54	68,68,68,68	0
59	MG	DA	3775	1/1	0.95	0.66	86,86,86,86	0
59	MG	AA	1882	1/1	0.95	0.20	57,57,57,57	0
59	MG	BA	2955	1/1	0.95	0.69	84,84,84,84	0
59	MG	AA	1773	1/1	0.95	0.14	50,50,50,50	0
59	MG	BA	3035	1/1	0.95	0.68	42,42,42,42	0
59	MG	DA	3256	1/1	0.95	0.58	42,42,42,42	0
59	MG	DA	3257	1/1	0.95	0.70	29,29,29,29	0
59	MG	DA	3258	1/1	0.95	0.18	48,48,48,48	0
59	MG	DA	2941	1/1	0.95	0.08	27,27,27,27	1
59	MG	AA	1884	1/1	0.95	0.08	89,89,89,89	0
59	MG	DA	3381	1/1	0.95	0.67	43,43,43,43	0
59	MG	DA	3152	1/1	0.95	0.43	108,108,108,108	0
59	MG	BA	3114	1/1	0.95	0.10	80,80,80,80	0
59	MG	DA	3639	1/1	0.95	0.32	37,37,37,37	0
59	MG	DA	3052	1/1	0.95	0.30	68,68,68,68	0
59	MG	DA	3790	1/1	0.95	1.41	29,29,29,29	1
59	MG	CA	1717	1/1	0.95	0.14	78,78,78,78	0
59	MG	AA	1697	1/1	0.95	0.83	76,76,76,76	0
59	MG	DA	3645	1/1	0.95	0.24	78,78,78,78	0
59	MG	DA	3647	1/1	0.95	0.50	36,36,36,36	0
59	MG	DA	3795	1/1	0.95	0.44	25,25,25,25	0
59	MG	BA	3424	1/1	0.95	0.36	64,64,64,64	0
59	MG	BA	2931	1/1	0.95	0.19	44,44,44,44	0
59	MG	BA	3368	1/1	0.95	0.38	62,62,62,62	0
59	MG	DA	3160	1/1	0.95	0.32	68,68,68,68	0
59	MG	CA	1652	1/1	0.95	0.48	78,78,78,78	0
59	MG	DA	3653	1/1	0.95	0.55	82,82,82,82	0
59	MG	AA	1637	1/1	0.95	0.15	78,78,78,78	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1846	1/1	0.95	0.46	45,45,45,45	0
59	MG	BA	3012	1/1	0.95	0.46	34,34,34,34	0
59	MG	DB	208	1/1	0.95	0.17	86,86,86,86	0
59	MG	DA	3278	1/1	0.95	0.25	57,57,57,57	0
59	MG	DA	3279	1/1	0.95	0.60	70,70,70,70	0
59	MG	DA	2956	1/1	0.95	0.26	38,38,38,38	0
59	MG	AA	1824	1/1	0.95	0.15	83,83,83,83	0
59	MG	DD	302	1/1	0.95	0.20	53,53,53,53	0
59	MG	DA	3664	1/1	0.95	0.14	85,85,85,85	0
59	MG	DA	3283	1/1	0.95	0.12	65,65,65,65	0
59	MG	DA	3402	1/1	0.95	0.29	16,16,16,16	0
59	MG	CA	1727	1/1	0.95	0.14	74,74,74,74	0
59	MG	CA	1729	1/1	0.95	0.24	88,88,88,88	0
59	MG	DA	3527	1/1	0.95	0.06	46,46,46,46	0
59	MG	CV	111	1/1	0.95	0.14	71,71,71,71	0
59	MG	DA	3171	1/1	0.95	0.27	71,71,71,71	0
59	MG	DA	3071	1/1	0.95	0.25	71,71,71,71	0
59	MG	AA	1721	1/1	0.95	0.14	111,111,111,111	0
59	MG	DA	3174	1/1	0.95	0.38	93,93,93,93	0
59	MG	AL	203	1/1	0.95	0.25	81,81,81,81	0
59	MG	DA	3535	1/1	0.95	0.52	52,52,52,52	0
59	MG	BA	3433	1/1	0.95	0.22	61,61,61,61	0
59	MG	DA	2964	1/1	0.95	0.44	54,54,54,54	0
59	MG	DP	203	1/1	0.95	0.37	53,53,53,53	0
59	MG	BR	205	1/1	0.95	0.16	76,76,76,76	0
59	MG	DA	3681	1/1	0.95	0.10	28,28,28,28	0
59	MG	BA	3264	1/1	0.95	0.37	42,42,42,42	0
59	MG	AA	1965	1/1	0.95	1.21	97,97,97,97	0
59	MG	BU	202	1/1	0.95	0.37	39,39,39,39	0
59	MG	AA	1684	1/1	0.95	0.19	87,87,87,87	0
59	MG	DA	3543	1/1	0.95	0.32	71,71,71,71	0
59	MG	CA	1740	1/1	0.95	0.88	85,85,85,85	0
59	MG	AA	1638	1/1	0.95	0.35	119,119,119,119	0
59	MG	AA	1911	1/1	0.95	0.14	55,55,55,55	0
59	MG	CA	1783	1/1	0.96	0.10	83,83,83,83	0
59	MG	DA	3450	1/1	0.96	0.17	100,100,100,100	0
59	MG	BA	3318	1/1	0.96	0.48	63,63,63,63	0
59	MG	CA	1639	1/1	0.96	0.18	95,95,95,95	0
59	MG	DA	3454	1/1	0.96	0.48	35,35,35,35	0
59	MG	DA	3118	1/1	0.96	0.15	63,63,63,63	0
59	MG	DA	2929	1/1	0.96	0.21	10,10,10,10	1
59	MG	DA	3019	1/1	0.96	0.67	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3020	1/1	0.96	0.28	52,52,52,52	0
59	MG	BA	3369	1/1	0.96	0.25	65,65,65,65	0
59	MG	DA	3336	1/1	0.96	0.56	31,31,31,31	0
59	MG	AA	1612	1/1	0.96	0.09	55,55,55,55	0
59	MG	AA	1815	1/1	0.96	0.20	76,76,76,76	0
59	MG	DA	3225	1/1	0.96	0.43	32,32,32,32	0
59	MG	DA	3465	1/1	0.96	0.43	26,26,26,26	0
59	MG	BD	303	1/1	0.96	0.22	35,35,35,35	0
59	MG	DA	3026	1/1	0.96	0.34	60,60,60,60	0
59	MG	AA	1741	1/1	0.96	0.17	54,54,54,54	0
59	MG	BA	3494	1/1	0.96	0.56	77,77,77,77	0
59	MG	BA	2903	1/1	0.96	0.42	37,37,37,37	0
59	MG	CM	202	1/1	0.96	0.21	151,151,151,151	0
59	MG	DA	3589	1/1	0.96	0.70	47,47,47,47	0
59	MG	DA	3348	1/1	0.96	0.58	43,43,43,43	0
59	MG	DA	3234	1/1	0.96	0.42	118,118,118,118	0
59	MG	BE	302	1/1	0.96	0.14	30,30,30,30	0
59	MG	BA	2925	1/1	0.96	0.45	33,33,33,33	0
59	MG	BA	3038	1/1	0.96	0.18	17,17,17,17	0
59	MG	DA	3038	1/1	0.96	0.35	32,32,32,32	0
59	MG	DA	3039	1/1	0.96	0.35	88,88,88,88	0
59	MG	AA	1628	1/1	0.96	0.10	84,84,84,84	0
59	MG	BA	3559	1/1	0.96	0.22	45,45,45,45	0
59	MG	DA	2943	1/1	0.96	0.07	71,71,71,71	1
59	MG	DA	3741	1/1	0.96	0.26	43,43,43,43	0
59	MG	DA	3483	1/1	0.96	0.57	55,55,55,55	0
59	MG	DA	3603	1/1	0.96	0.18	60,60,60,60	0
59	MG	DA	3604	1/1	0.96	0.50	39,39,39,39	0
59	MG	BA	3106	1/1	0.96	0.11	35,35,35,35	0
59	MG	AA	1830	1/1	0.96	0.36	86,86,86,86	0
59	MG	DA	3608	1/1	0.96	0.34	61,61,61,61	0
59	MG	DA	3247	1/1	0.96	0.58	41,41,41,41	0
59	MG	DA	3610	1/1	0.96	0.20	112,112,112,112	0
59	MG	BA	3108	1/1	0.96	0.67	56,56,56,56	0
59	MG	BA	3434	1/1	0.96	0.38	68,68,68,68	0
59	MG	CA	1728	1/1	0.96	0.18	88,88,88,88	0
59	MG	DA	3251	1/1	0.96	0.23	53,53,53,53	0
59	MG	BA	3041	1/1	0.96	0.42	37,37,37,37	0
59	MG	BP	204	1/1	0.96	0.27	24,24,24,24	1
59	MG	DA	3618	1/1	0.96	0.66	72,72,72,72	0
59	MG	DA	3254	1/1	0.96	0.09	59,59,59,59	0
59	MG	DA	3051	1/1	0.96	0.34	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AL	204	1/1	0.96	0.05	90,90,90,90	0
59	MG	BA	3334	1/1	0.96	0.17	60,60,60,60	0
59	MG	BR	202	1/1	0.96	0.18	24,24,24,24	0
59	MG	DA	3055	1/1	0.96	0.49	51,51,51,51	0
59	MG	DA	3626	1/1	0.96	0.33	34,34,34,34	0
59	MG	AA	1623	1/1	0.96	1.02	66,66,66,66	0
59	MG	DA	3262	1/1	0.96	0.29	59,59,59,59	1
59	MG	BA	3197	1/1	0.96	0.31	54,54,54,54	0
59	MG	DA	3058	1/1	0.96	0.28	32,32,32,32	0
59	MG	DA	3771	1/1	0.96	0.68	71,71,71,71	0
59	MG	AA	1751	1/1	0.96	0.07	104,104,104,104	0
59	MG	BA	3153	1/1	0.96	0.12	93,93,93,93	0
59	MG	BA	3076	1/1	0.96	0.23	30,30,30,30	0
59	MG	BA	3389	1/1	0.96	0.45	56,56,56,56	0
59	MG	BA	2932	1/1	0.96	0.49	63,63,63,63	0
59	MG	BA	3291	1/1	0.96	0.54	41,41,41,41	0
59	MG	DA	3638	1/1	0.96	0.33	21,21,21,21	0
59	MG	BA	3452	1/1	0.96	0.45	45,45,45,45	0
59	MG	BA	2933	1/1	0.96	0.25	36,36,36,36	0
59	MG	DA	3166	1/1	0.96	0.29	30,30,30,30	0
59	MG	DA	3275	1/1	0.96	0.27	63,63,63,63	0
59	MG	DA	3644	1/1	0.96	0.66	54,54,54,54	0
59	MG	D5	103	1/1	0.96	0.11	88,88,88,88	0
59	MG	AA	1886	1/1	0.96	0.64	84,84,84,84	0
59	MG	BA	3081	1/1	0.96	0.59	64,64,64,64	0
59	MG	BA	2936	1/1	0.96	0.30	43,43,43,43	0
59	MG	BA	3298	1/1	0.96	0.25	67,67,67,67	0
59	MG	DA	3399	1/1	0.96	0.22	62,62,62,62	0
59	MG	BA	3459	1/1	0.96	0.33	44,44,44,44	0
59	MG	DA	3282	1/1	0.96	0.38	31,31,31,31	0
59	MG	BA	2937	1/1	0.96	0.34	40,40,40,40	0
59	MG	DA	3285	1/1	0.96	0.31	37,37,37,37	0
59	MG	BA	3168	1/1	0.96	0.32	24,24,24,24	0
59	MG	DA	3658	1/1	0.96	0.27	53,53,53,53	0
59	MG	DA	3405	1/1	0.96	0.11	63,63,63,63	0
59	MG	DA	3077	1/1	0.96	0.77	68,68,68,68	0
59	MG	AA	1858	1/1	0.96	0.28	60,60,60,60	0
59	MG	DA	3179	1/1	0.96	0.53	66,66,66,66	0
59	MG	BA	3527	1/1	0.96	0.63	86,86,86,86	0
59	MG	BA	3402	1/1	0.96	0.46	37,37,37,37	0
59	MG	AA	1744	1/1	0.96	0.08	80,80,80,80	0
59	MG	DA	3533	1/1	0.96	0.19	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3404	1/1	0.96	0.31	34,34,34,34	0
59	MG	DA	2985	1/1	0.96	0.46	39,39,39,39	0
59	MG	CA	1617	1/1	0.96	0.06	66,66,66,66	0
59	MG	BA	3405	1/1	0.96	0.46	44,44,44,44	0
59	MG	DA	3188	1/1	0.96	0.32	31,31,31,31	0
59	MG	BA	3406	1/1	0.96	0.47	52,52,52,52	0
59	MG	CA	1620	1/1	0.96	0.70	87,87,87,87	0
59	MG	DA	3675	1/1	0.96	0.42	39,39,39,39	0
59	MG	BA	3593	1/1	0.96	0.09	41,41,41,41	0
59	MG	DA	3422	1/1	0.96	0.73	63,63,63,63	0
59	MG	DD	306	1/1	0.96	0.09	60,60,60,60	0
59	MG	DA	2992	1/1	0.96	0.77	103,103,103,103	0
59	MG	BA	3255	1/1	0.96	0.24	55,55,55,55	0
59	MG	DA	3426	1/1	0.96	0.38	28,28,28,28	0
59	MG	AA	1860	1/1	0.96	0.39	61,61,61,61	0
59	MG	BA	2913	1/1	0.96	0.72	51,51,51,51	0
59	MG	B0	101	1/1	0.96	0.89	73,73,73,73	0
59	MG	BA	3538	1/1	0.96	0.09	37,37,37,37	0
59	MG	DA	3310	1/1	0.96	0.39	90,90,90,90	1
59	MG	DA	3099	1/1	0.96	0.31	67,67,67,67	0
59	MG	AA	1924	1/1	0.96	1.03	84,84,84,84	0
59	MG	AA	1696	1/1	0.96	0.21	90,90,90,90	0
59	MG	AA	1822	1/1	0.96	0.33	60,60,60,60	0
59	MG	AA	1763	1/1	0.96	0.24	88,88,88,88	0
59	MG	DP	204	1/1	0.96	0.28	15,15,15,15	0
59	MG	BA	3314	1/1	0.96	0.52	29,29,29,29	0
59	MG	BA	2947	1/1	0.96	0.31	45,45,45,45	0
59	MG	DA	3694	1/1	0.96	0.25	107,107,107,107	0
59	MG	DA	3440	1/1	0.96	0.16	50,50,50,50	1
59	MG	BA	3484	1/1	0.96	0.31	94,94,94,94	0
59	MG	BA	3607	1/1	0.96	0.71	95,95,95,95	0
59	MG	BA	3220	1/1	0.96	0.64	54,54,54,54	0
59	MG	BA	3418	1/1	0.96	1.28	69,69,69,69	0
59	MG	AA	1650	1/1	0.96	0.33	73,73,73,73	0
60	ZN	AN	101	1/1	0.96	0.14	153,153,153,153	0
59	MG	DA	3114	1/1	0.96	0.52	55,55,55,55	0
59	MG	CA	1748	1/1	0.97	0.08	102,102,102,102	0
59	MG	DA	3715	1/1	0.97	0.20	64,64,64,64	0
59	MG	BA	3062	1/1	0.97	0.21	61,61,61,61	0
59	MG	DA	2968	1/1	0.97	0.13	1,1,1,1	1
59	MG	BA	3294	1/1	0.97	0.30	73,73,73,73	0
59	MG	DA	3061	1/1	0.97	0.29	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3720	1/1	0.97	0.14	66,66,66,66	0
59	MG	DA	3361	1/1	0.97	0.37	42,42,42,42	0
59	MG	DA	3362	1/1	0.97	0.42	39,39,39,39	0
59	MG	BA	3589	1/1	0.97	0.10	41,41,41,41	0
59	MG	AA	1672	1/1	0.97	0.16	77,77,77,77	0
59	MG	DA	3725	1/1	0.97	0.36	71,71,71,71	0
59	MG	BA	3351	1/1	0.97	0.29	26,26,26,26	0
59	MG	BA	3167	1/1	0.97	0.28	36,36,36,36	0
59	MG	DA	2977	1/1	0.97	0.41	60,60,60,60	0
59	MG	BA	3247	1/1	0.97	0.21	62,62,62,62	1
59	MG	DA	3600	1/1	0.97	0.30	30,30,30,30	0
59	MG	DA	3259	1/1	0.97	0.52	32,32,32,32	0
59	MG	BA	3206	1/1	0.97	0.51	59,59,59,59	0
59	MG	DA	3069	1/1	0.97	0.19	50,50,50,50	0
59	MG	DA	2980	1/1	0.97	0.20	69,69,69,69	0
59	MG	AA	1823	1/1	0.97	0.29	68,68,68,68	0
59	MG	DA	3606	1/1	0.97	0.12	88,88,88,88	1
59	MG	BA	3356	1/1	0.97	0.25	45,45,45,45	0
59	MG	BA	2926	1/1	0.97	0.22	20,20,20,20	0
59	MG	BA	3302	1/1	0.97	1.20	69,69,69,69	0
59	MG	DA	3377	1/1	0.97	0.26	16,16,16,16	0
59	MG	BA	3599	1/1	0.97	0.07	83,83,83,83	0
59	MG	BA	2969	1/1	0.97	0.26	41,41,41,41	0
59	MG	DA	3613	1/1	0.97	0.13	56,56,56,56	1
59	MG	AA	1913	1/1	0.97	0.10	72,72,72,72	0
59	MG	AA	1914	1/1	0.97	0.25	56,56,56,56	0
59	MG	BA	3307	1/1	0.97	0.43	75,75,75,75	0
59	MG	BA	3099	1/1	0.97	0.37	30,30,30,30	0
59	MG	DA	3749	1/1	0.97	0.22	80,80,80,80	1
59	MG	BA	3257	1/1	0.97	0.74	42,42,42,42	0
59	MG	DA	3082	1/1	0.97	0.17	82,82,82,82	0
59	MG	BA	3175	1/1	0.97	0.36	25,25,25,25	0
59	MG	DA	3178	1/1	0.97	0.35	29,29,29,29	0
59	MG	DA	3084	1/1	0.97	0.39	57,57,57,57	0
59	MG	DA	3504	1/1	0.97	0.26	60,60,60,60	0
59	MG	DA	2994	1/1	0.97	0.63	60,60,60,60	0
59	MG	BA	3419	1/1	0.97	0.23	49,49,49,49	0
59	MG	BA	3609	1/1	0.97	0.20	56,56,56,56	0
59	MG	DA	3088	1/1	0.97	0.10	65,65,65,65	0
59	MG	DA	3760	1/1	0.97	0.32	52,52,52,52	0
59	MG	AA	1706	1/1	0.97	0.07	44,44,44,44	1
59	MG	DA	3284	1/1	0.97	0.39	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3090	1/1	0.97	0.24	35,35,35,35	0
59	MG	DA	2998	1/1	0.97	0.28	49,49,49,49	0
59	MG	CA	1772	1/1	0.97	0.21	79,79,79,79	0
59	MG	DA	3398	1/1	0.97	0.47	31,31,31,31	1
59	MG	BA	3177	1/1	0.97	0.36	45,45,45,45	0
59	MG	AA	1845	1/1	0.97	0.28	53,53,53,53	0
59	MG	DA	3290	1/1	0.97	0.35	32,32,32,32	0
59	MG	BA	2974	1/1	0.97	0.54	38,38,38,38	0
59	MG	AA	1753	1/1	0.97	0.06	110,110,110,110	0
59	MG	DA	3641	1/1	0.97	0.70	68,68,68,68	0
59	MG	AA	1778	1/1	0.97	0.12	84,84,84,84	0
59	MG	DA	3294	1/1	0.97	0.09	80,80,80,80	1
59	MG	AA	1933	1/1	0.97	0.21	67,67,67,67	0
59	MG	BA	2934	1/1	0.97	0.36	57,57,57,57	0
59	MG	DA	3646	1/1	0.97	0.81	57,57,57,57	0
59	MG	DA	3196	1/1	0.97	0.19	100,100,100,100	0
59	MG	CA	1707	1/1	0.97	0.10	79,79,79,79	0
59	MG	B5	103	1/1	0.97	0.33	36,36,36,36	0
59	MG	DA	3199	1/1	0.97	0.41	30,30,30,30	0
59	MG	CA	1782	1/1	0.97	0.24	52,52,52,52	0
59	MG	AA	1893	1/1	0.97	0.27	56,56,56,56	0
59	MG	DA	3303	1/1	0.97	0.28	54,54,54,54	0
59	MG	BA	3224	1/1	0.97	0.37	79,79,79,79	0
59	MG	BA	3323	1/1	0.97	0.53	36,36,36,36	0
59	MG	BE	303	1/1	0.97	0.34	22,22,22,22	0
59	MG	AA	1808	1/1	0.97	0.48	57,57,57,57	0
59	MG	CA	1645	1/1	0.97	0.12	50,50,50,50	0
59	MG	BA	3273	1/1	0.97	0.55	31,31,31,31	0
59	MG	BA	2918	1/1	0.97	0.56	76,76,76,76	1
59	MG	BA	3381	1/1	0.97	0.29	42,42,42,42	0
59	MG	DA	3425	1/1	0.97	0.21	56,56,56,56	0
59	MG	AA	1626	1/1	0.97	0.64	89,89,89,89	0
59	MG	DA	3024	1/1	0.97	0.23	92,92,92,92	0
59	MG	BA	3055	1/1	0.97	0.73	92,92,92,92	0
59	MG	CM	203	1/1	0.97	0.12	123,123,123,123	0
59	MG	BA	3506	1/1	0.97	0.16	42,42,42,42	0
59	MG	DA	3120	1/1	0.97	0.24	106,106,106,106	0
59	MG	DA	3217	1/1	0.97	0.63	69,69,69,69	0
59	MG	AA	1636	1/1	0.97	0.22	53,53,53,53	0
59	MG	BA	3057	1/1	0.97	0.44	68,68,68,68	0
59	MG	DA	3032	1/1	0.97	0.37	34,34,34,34	0
59	MG	DA	3033	1/1	0.97	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1649	1/1	0.97	0.17	63,63,63,63	0
59	MG	AA	1954	1/1	0.97	1.03	67,67,67,67	0
59	MG	BA	3447	1/1	0.97	0.10	90,90,90,90	0
59	MG	DA	3441	1/1	0.97	0.64	55,55,55,55	0
59	MG	BA	3448	1/1	0.97	0.40	40,40,40,40	0
59	MG	BA	2964	1/1	0.97	0.17	96,96,96,96	0
59	MG	BR	204	1/1	0.97	0.21	26,26,26,26	0
59	MG	BA	3155	1/1	0.97	0.48	29,29,29,29	0
59	MG	DA	3560	1/1	0.97	0.19	58,58,58,58	0
59	MG	DA	3331	1/1	0.97	0.16	45,45,45,45	1
59	MG	DA	3332	1/1	0.97	0.31	26,26,26,26	0
59	MG	DA	3687	1/1	0.97	0.16	43,43,43,43	0
59	MG	DA	3564	1/1	0.97	0.32	42,42,42,42	0
59	MG	DA	3448	1/1	0.97	0.20	55,55,55,55	0
59	MG	BA	3088	1/1	0.97	0.86	62,62,62,62	0
59	MG	BA	3516	1/1	0.97	0.80	64,64,64,64	0
59	MG	DA	3232	1/1	0.97	0.32	59,59,59,59	0
59	MG	BA	3119	1/1	0.97	0.34	30,30,30,30	0
59	MG	AA	1812	1/1	0.97	1.00	70,70,70,70	0
59	MG	CA	1666	1/1	0.97	0.08	63,63,63,63	0
59	MG	DA	3456	1/1	0.97	0.73	56,56,56,56	0
59	MG	CA	1667	1/1	0.97	0.07	66,66,66,66	0
59	MG	DA	3342	1/1	0.97	0.29	58,58,58,58	0
59	MG	BA	3161	1/1	0.97	0.27	39,39,39,39	0
59	MG	CA	1669	1/1	0.97	0.15	57,57,57,57	0
59	MG	BA	3288	1/1	0.97	0.45	38,38,38,38	0
59	MG	DA	3705	1/1	0.97	0.55	58,58,58,58	0
59	MG	BA	3289	1/1	0.97	0.33	39,39,39,39	0
59	MG	BA	3091	1/1	0.97	0.30	62,62,62,62	0
59	MG	BA	3202	1/1	0.97	0.28	24,24,24,24	0
59	MG	DA	3243	1/1	0.97	0.81	64,64,64,64	0
59	MG	DA	3351	1/1	0.97	0.17	77,77,77,77	0
59	MG	BA	3399	1/1	0.97	0.58	146,146,146,146	0
59	MG	BA	3525	1/1	0.97	0.26	44,44,44,44	0
59	MG	BA	3243	1/1	0.97	0.46	25,25,25,25	0
59	MG	BA	3442	1/1	0.98	0.25	65,65,65,65	0
59	MG	BA	3482	1/1	0.98	0.49	144,144,144,144	0
59	MG	DA	3473	1/1	0.98	0.53	38,38,38,38	0
59	MG	DA	3216	1/1	0.98	0.36	36,36,36,36	0
59	MG	BA	3143	1/1	0.98	0.37	149,149,149,149	0
59	MG	DA	2986	1/1	0.98	0.21	142,142,142,142	0
59	MG	BA	3347	1/1	0.98	0.50	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3045	1/1	0.98	0.16	47,47,47,47	0
59	MG	AA	1657	1/1	0.98	0.14	77,77,77,77	0
59	MG	D5	101	1/1	0.98	0.30	48,48,48,48	0
59	MG	BA	3166	1/1	0.98	0.47	89,89,89,89	0
59	MG	DA	3103	1/1	0.98	0.35	60,60,60,60	0
59	MG	DA	3350	1/1	0.98	0.49	34,34,34,34	0
59	MG	DA	3699	1/1	0.98	0.19	62,62,62,62	0
59	MG	DA	3416	1/1	0.98	0.35	35,35,35,35	0
59	MG	DA	3701	1/1	0.98	0.11	55,55,55,55	0
59	MG	DA	3625	1/1	0.98	0.43	29,29,29,29	0
59	MG	BA	3126	1/1	0.98	0.12	36,36,36,36	0
59	MG	BA	3261	1/1	0.98	0.28	41,41,41,41	0
59	MG	BA	3608	1/1	0.98	0.42	31,31,31,31	0
59	MG	CA	1734	1/1	0.98	0.15	56,56,56,56	0
59	MG	DA	3229	1/1	0.98	0.08	51,51,51,51	0
59	MG	DA	3356	1/1	0.98	0.55	32,32,32,32	0
59	MG	BA	3235	1/1	0.98	0.20	40,40,40,40	0
59	MG	DA	3110	1/1	0.98	0.72	200,200,200,200	0
59	MG	DA	3562	1/1	0.98	0.13	25,25,25,25	1
59	MG	DA	3635	1/1	0.98	0.44	31,31,31,31	0
59	MG	CA	1736	1/1	0.98	0.14	60,60,60,60	0
59	MG	BA	3490	1/1	0.98	0.60	19,19,19,19	0
59	MG	BA	2960	1/1	0.98	0.58	84,84,84,84	0
59	MG	DA	2999	1/1	0.98	0.05	91,91,91,91	0
59	MG	DA	2947	1/1	0.98	0.15	86,86,86,86	0
59	MG	DA	2948	1/1	0.98	0.34	75,75,75,75	0
59	MG	AA	1888	1/1	0.98	0.22	58,58,58,58	0
59	MG	BA	3238	1/1	0.98	0.52	110,110,110,110	0
59	MG	AA	1967	1/1	0.98	0.28	67,67,67,67	0
59	MG	CA	1742	1/1	0.98	0.09	81,81,81,81	0
59	MG	BA	3454	1/1	0.98	0.56	64,64,64,64	0
59	MG	BD	301	1/1	0.98	0.37	25,25,25,25	0
59	MG	DA	3437	1/1	0.98	0.18	12,12,12,12	1
59	MG	BA	3090	1/1	0.98	0.14	27,27,27,27	0
59	MG	AN	103	1/1	0.98	0.25	147,147,147,147	0
59	MG	AA	1655	1/1	0.98	0.05	101,101,101,101	0
59	MG	AL	201	1/1	0.98	0.11	87,87,87,87	0
59	MG	AA	1653	1/1	0.98	0.07	68,68,68,68	1
59	MG	DA	3129	1/1	0.98	0.41	72,72,72,72	0
59	MG	BA	3136	1/1	0.98	0.19	34,34,34,34	0
59	MG	DA	3656	1/1	0.98	0.17	75,75,75,75	0
59	MG	DA	3313	1/1	0.98	0.28	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3156	1/1	0.98	0.34	27,27,27,27	0
59	MG	BA	3137	1/1	0.98	0.22	43,43,43,43	0
59	MG	AA	1785	1/1	0.98	0.03	108,108,108,108	0
59	MG	BA	3305	1/1	0.98	0.41	28,28,28,28	0
59	MG	BA	3397	1/1	0.98	0.34	75,75,75,75	0
59	MG	DA	3663	1/1	0.98	0.60	55,55,55,55	0
59	MG	DE	304	1/1	0.98	0.35	22,22,22,22	0
59	MG	BA	3467	1/1	0.98	0.15	93,93,93,93	0
59	MG	DA	3742	1/1	0.98	0.58	51,51,51,51	0
59	MG	DA	3452	1/1	0.98	0.45	30,30,30,30	0
59	MG	BA	3468	1/1	0.98	0.44	36,36,36,36	0
59	MG	BA	3470	1/1	0.98	0.42	35,35,35,35	0
59	MG	DA	3523	1/1	0.98	0.18	34,34,34,34	0
59	MG	BA	2978	1/1	0.98	0.48	75,75,75,75	0
59	MG	BA	3182	1/1	0.98	0.25	60,60,60,60	0
59	MG	DA	3141	1/1	0.98	0.36	99,99,99,99	0
59	MG	DA	2971	1/1	0.98	0.20	20,20,20,20	0
59	MG	BP	203	1/1	0.98	0.24	88,88,88,88	0
59	MG	DA	3029	1/1	0.98	0.19	30,30,30,30	0
59	MG	BA	3160	1/1	0.98	0.33	49,49,49,49	0
59	MG	DA	2975	1/1	0.98	0.32	56,56,56,56	0
59	MG	BA	3280	1/1	0.98	0.43	38,38,38,38	0
59	MG	AA	1688	1/1	0.98	0.07	22,22,22,22	1
59	MG	BA	3254	1/1	0.98	0.28	93,93,93,93	0
59	MG	DA	3333	1/1	0.98	0.35	55,55,55,55	0
59	MG	DU	203	1/1	0.98	0.47	36,36,36,36	0
59	MG	DU	204	1/1	0.98	0.29	19,19,19,19	0
59	MG	BA	3024	1/1	0.98	0.35	79,79,79,79	0
59	MG	BA	3344	1/1	0.98	0.51	45,45,45,45	0
59	MG	BA	3439	1/1	0.98	0.25	37,37,37,37	0
59	MG	BA	3163	1/1	0.98	0.42	35,35,35,35	0
59	MG	DA	3122	1/1	0.99	0.69	38,38,38,38	0
59	MG	BA	3420	1/1	0.99	0.35	71,71,71,71	0
59	MG	DA	3187	1/1	0.99	0.56	44,44,44,44	0
59	MG	CA	1653	1/1	0.99	0.34	39,39,39,39	0
59	MG	AP	101	1/1	0.99	0.16	93,93,93,93	0
59	MG	BP	202	1/1	0.99	0.14	69,69,69,69	1
59	MG	DA	3697	1/1	0.99	0.30	32,32,32,32	0
59	MG	BA	3530	1/1	0.99	0.22	33,33,33,33	0
59	MG	DA	3010	1/1	0.99	0.24	49,49,49,49	0
59	MG	BA	3252	1/1	0.99	0.15	75,75,75,75	0
59	MG	DA	3012	1/1	0.99	0.60	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3438	1/1	0.99	0.23	29,29,29,29	0
59	MG	BA	3271	1/1	0.99	0.46	29,29,29,29	0
59	MG	DA	3264	1/1	0.99	0.30	47,47,47,47	1
59	MG	D5	102	1/1	0.99	0.07	63,63,63,63	0
59	MG	AA	1658	1/1	0.99	0.17	106,106,106,106	0
59	MG	DA	3104	1/1	0.99	0.11	63,63,63,63	0
59	MG	DA	3410	1/1	0.99	0.41	25,25,25,25	0
59	MG	BA	3441	1/1	0.99	0.15	40,40,40,40	0
59	MG	DA	3339	1/1	0.99	0.47	37,37,37,37	0
59	MG	DA	3018	1/1	0.99	0.13	76,76,76,76	0
59	MG	BA	3139	1/1	0.99	0.33	27,27,27,27	0
59	MG	BA	3577	1/1	0.99	0.44	38,38,38,38	0
59	MG	BA	3152	1/1	0.99	0.33	34,34,34,34	0
59	MG	AA	1718	1/1	0.99	0.17	98,98,98,98	0
59	MG	BA	3343	1/1	0.99	0.50	32,32,32,32	0
59	MG	BA	3296	1/1	0.99	0.55	27,27,27,27	0
59	MG	BA	3464	1/1	0.99	0.54	43,43,43,43	0
59	MG	DA	3176	1/1	0.99	0.47	37,37,37,37	0
59	MG	DA	2973	1/1	0.99	0.41	21,21,21,21	0
59	MG	BA	3078	1/1	0.99	0.20	18,18,18,18	0
59	MG	BA	3332	1/1	0.99	0.47	19,19,19,19	0
59	MG	DA	3246	1/1	0.99	0.30	32,32,32,32	0
59	MG	BA	3169	1/1	0.99	0.36	24,24,24,24	0
59	MG	BA	3131	1/1	0.99	0.35	43,43,43,43	0
59	MG	DA	3031	1/1	0.99	0.38	51,51,51,51	0
59	MG	BA	3469	1/1	0.99	0.17	102,102,102,102	0
59	MG	BA	3322	1/1	0.99	0.68	24,24,24,24	0
60	ZN	AD	305	1/1	1.00	0.22	88,88,88,88	0
59	MG	DA	3599	1/1	1.00	0.22	39,39,39,39	0
60	ZN	AD	301	1/1	1.00	0.23	106,106,106,106	0

6.5 Other polymers (i)

There are no such residues in this entry.