wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 03:42 am GMT

PDB ID	:	4V5A
Title	:	Structure of the Ribosome Recycling Factor bound to the Thermus thermophilus 70S ribosome with mRNA, ASL-Phe and tRNA-fMet
Authors	:	Weixlbaumer, A.; Petry, S.; Dunham, C.M.; Selmer, M.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2007-06-28
Resolution	:	3.50 Å(reported)

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

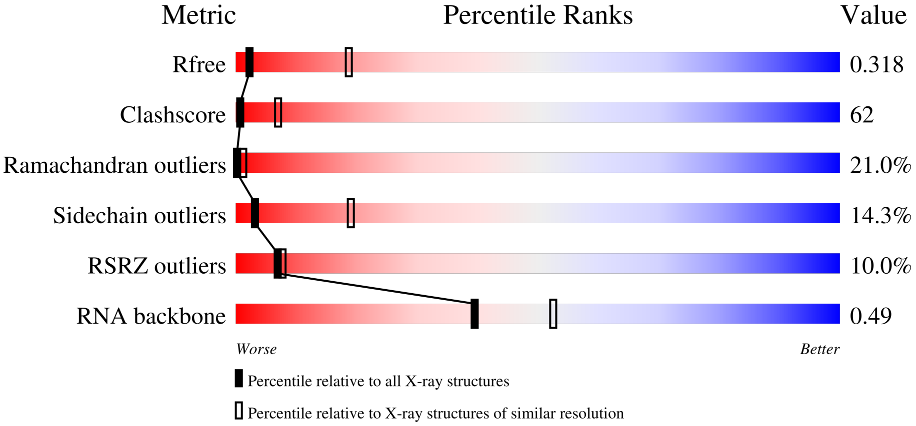
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

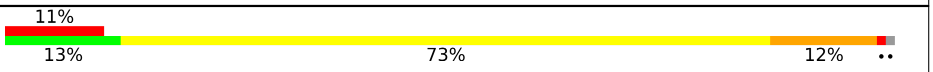
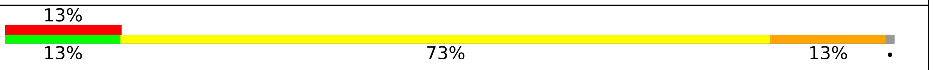
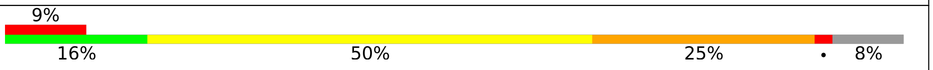
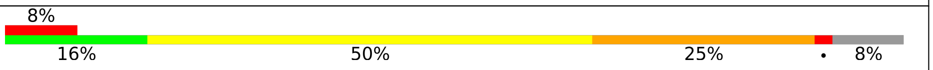
The reported resolution of this entry is 3.50 Å.

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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	 11% 13% 73% 12% ••
1	CA	1522	 13% 13% 73% 13% •
2	AB	256	 9% 16% 50% 25% • 8%
2	CB	256	 8% 16% 50% 25% • 8%

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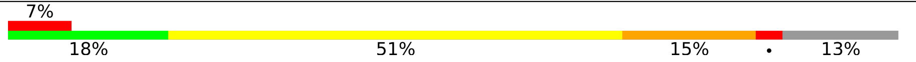
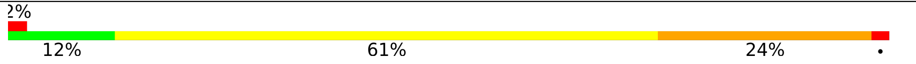
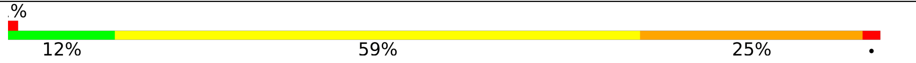
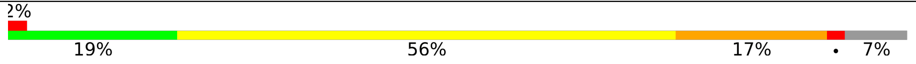
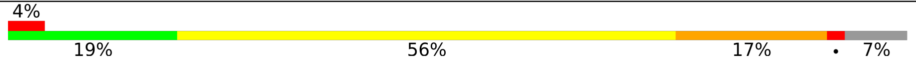
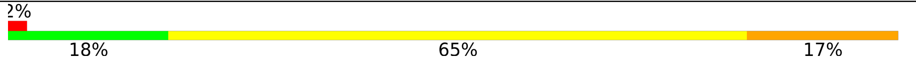
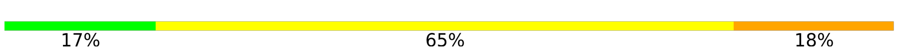
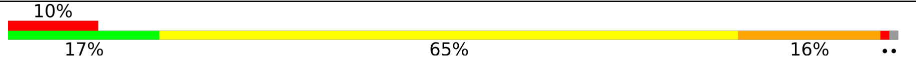
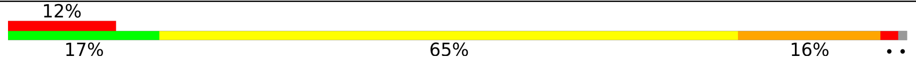
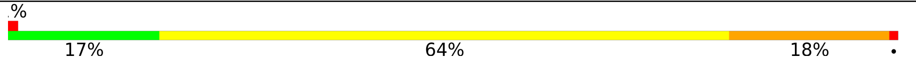
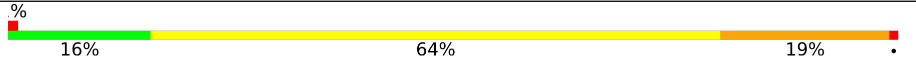
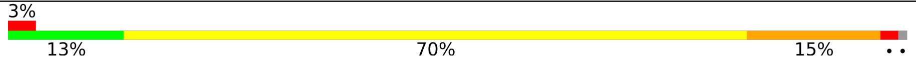
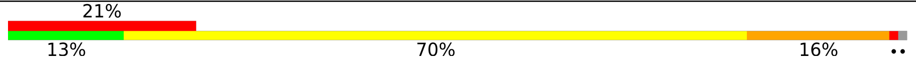
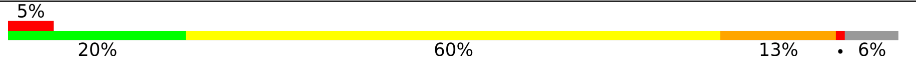
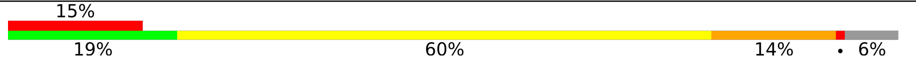
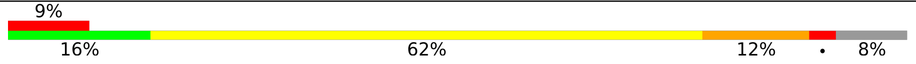
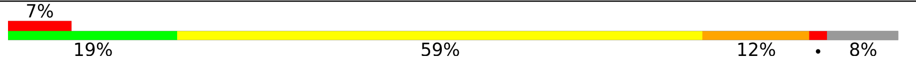
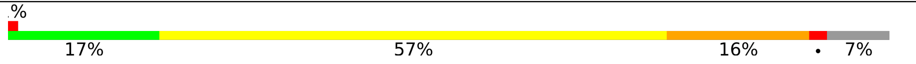
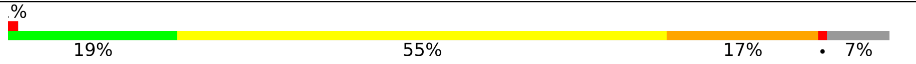
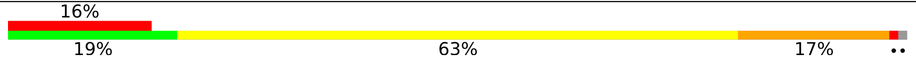
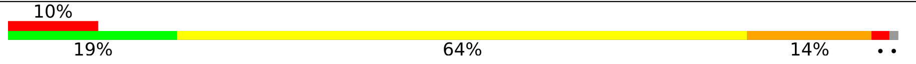
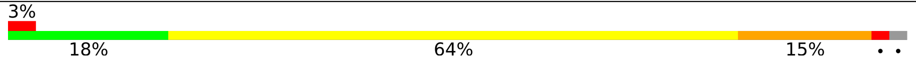
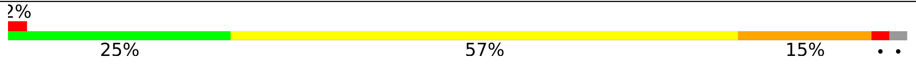
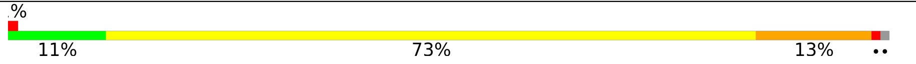
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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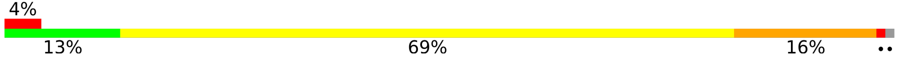
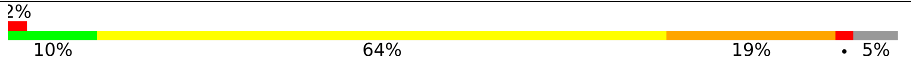
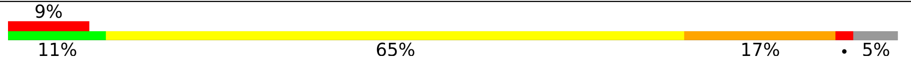
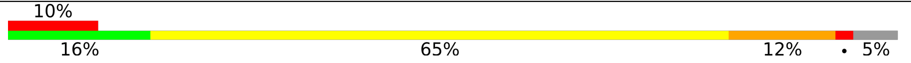
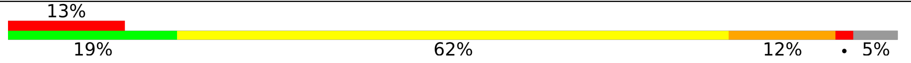
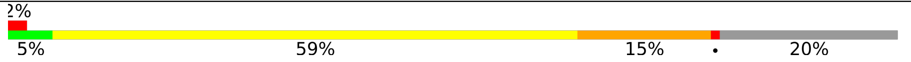
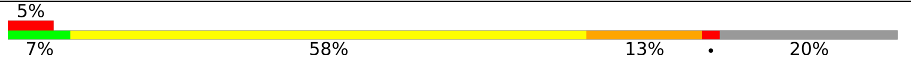
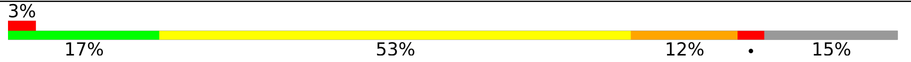
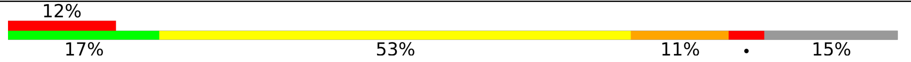
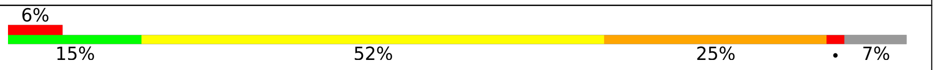
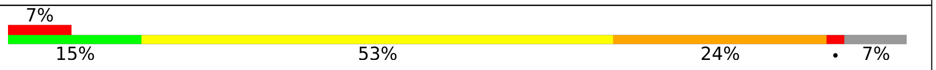
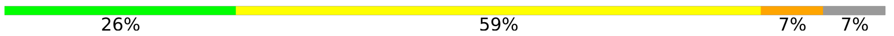
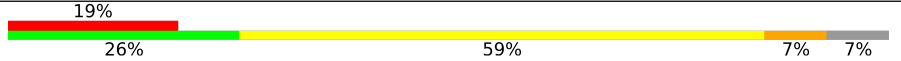
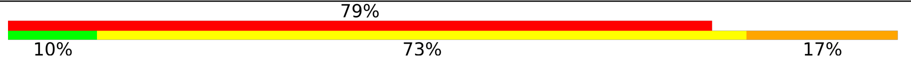
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	CV	76	
23	AW	77	
23	CW	77	
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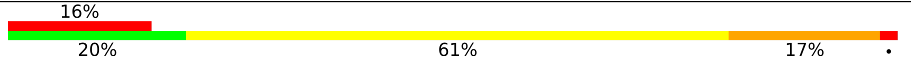
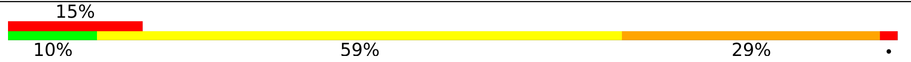
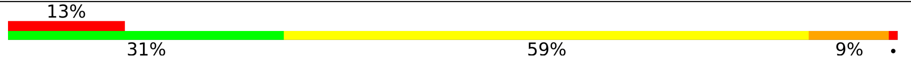
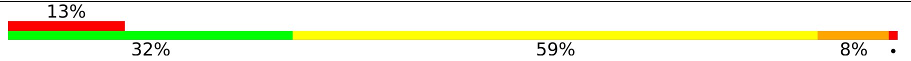
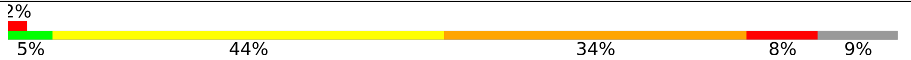
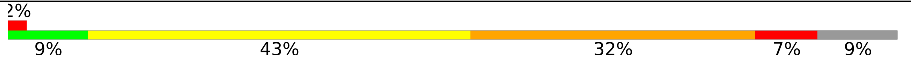
24	CX	31	
25	AY	185	
25	CY	185	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	

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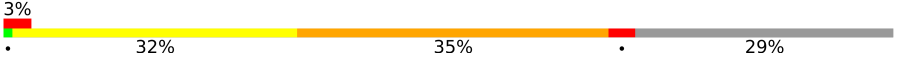
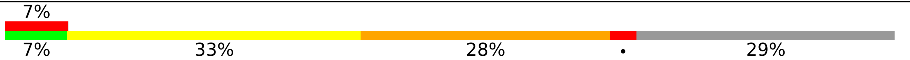
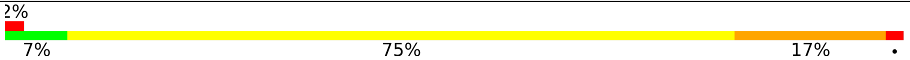
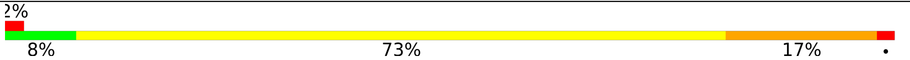
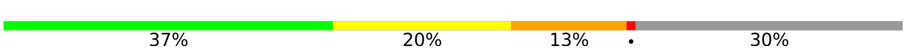
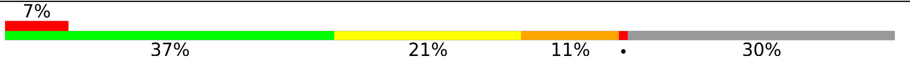
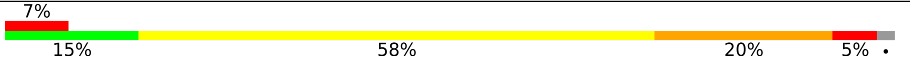
Mol	Chain	Length	Quality of chain
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
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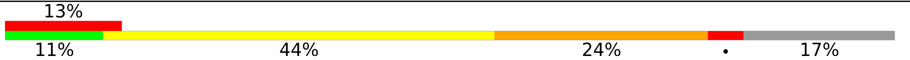
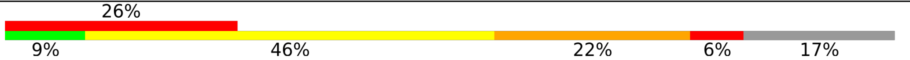
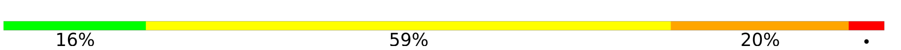
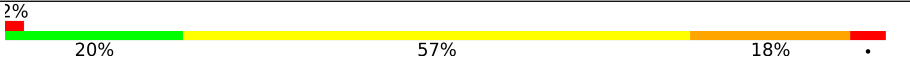
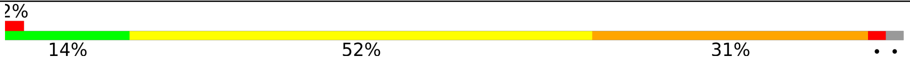
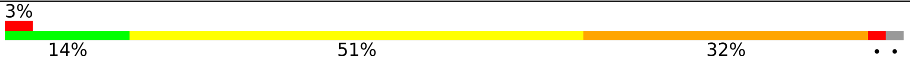
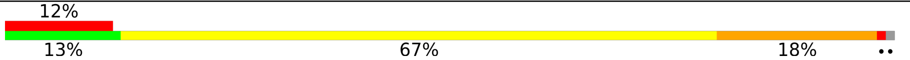
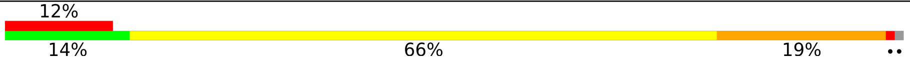
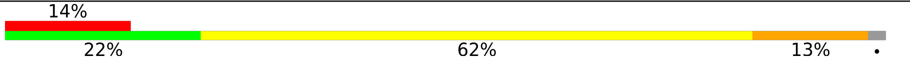
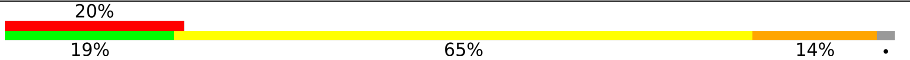
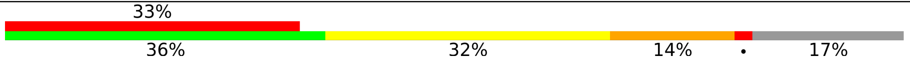
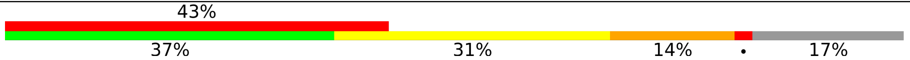
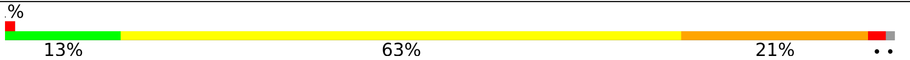
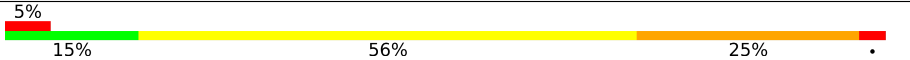
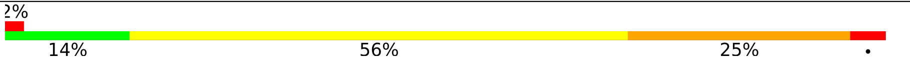
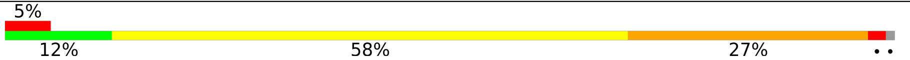
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	BA	2782	
35	DA	2782	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	
40	BF	210	

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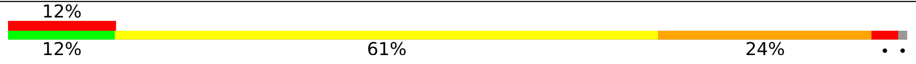
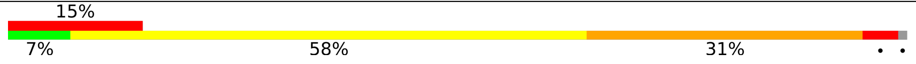
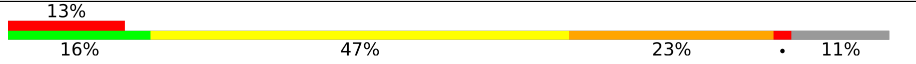
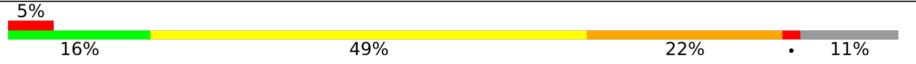
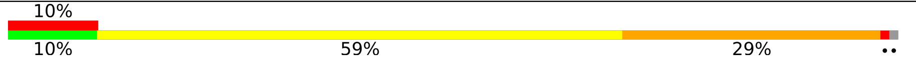
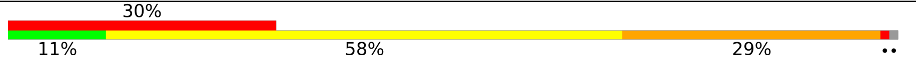
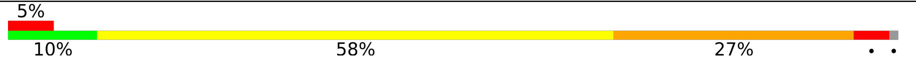
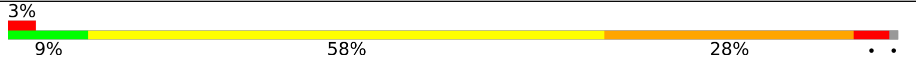
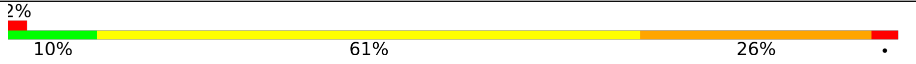
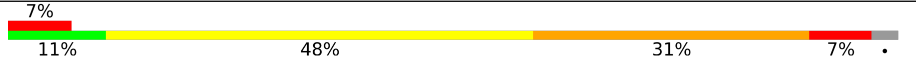
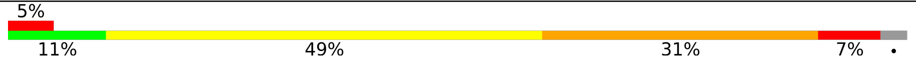
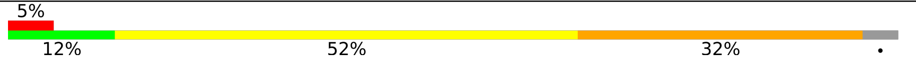
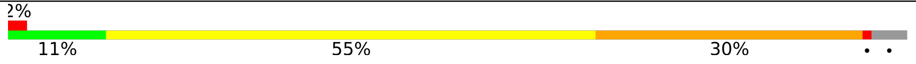
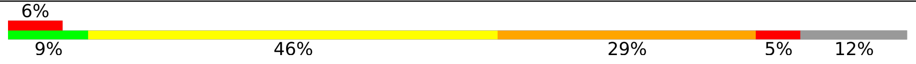
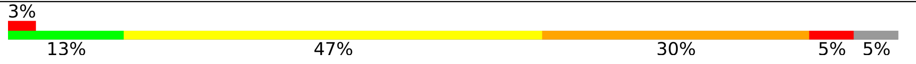
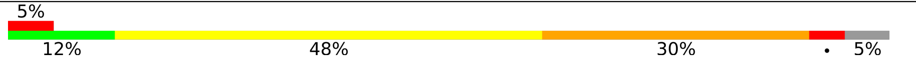
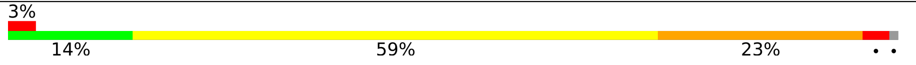
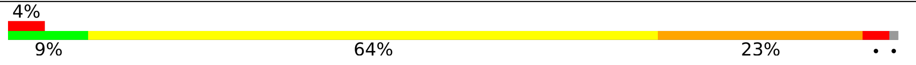
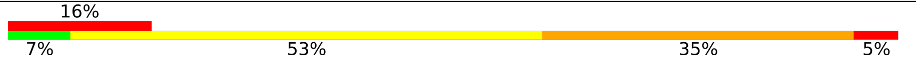
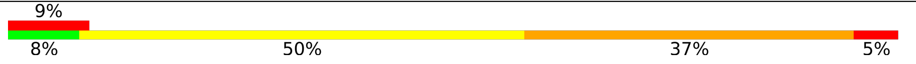
Mol	Chain	Length	Quality of chain
40	DF	210	3% 11% 58% 28% • •
41	BG	182	12% 12% 61% 24% • •
41	DG	182	15% 7% 58% 31% • •
42	BH	180	13% 16% 47% 23% • 11%
42	DH	180	5% 16% 49% 22% • 11%
43	BI	148	10% 10% 59% 29% • •
43	DI	148	30% 11% 58% 29% • •
44	BN	140	5% 10% 58% 27% • •
44	DN	140	3% 9% 58% 28% • •
45	BO	122	2% 10% 61% 26% •
45	DO	122	10% 62% 25% •
46	BP	150	7% 11% 48% 31% 7% •
46	DP	150	5% 11% 49% 31% 7% •
47	BQ	141	5% 12% 52% 32% •
47	DQ	141	2% 11% 55% 30% • •
48	BR	118	10% 48% 36% 5% •
48	DR	118	8% 53% 33% 5% •
49	BS	112	6% 9% 46% 29% 5% 12%
49	DS	112	21% 10% 43% 29% 6% 12%
50	BT	146	3% 13% 47% 30% 5% 5%
50	DT	146	5% 12% 48% 30% • 5%
51	BU	118	3% 14% 59% 23% • •
51	DU	118	4% 9% 64% 23% • •
52	BV	101	16% 7% 53% 35% 5%
52	DV	101	9% 8% 50% 37% 5%

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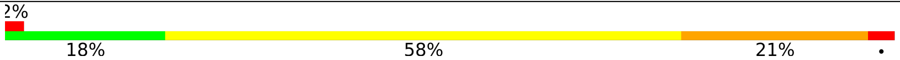
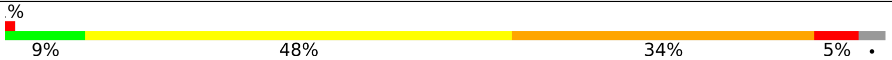
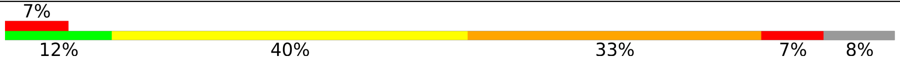
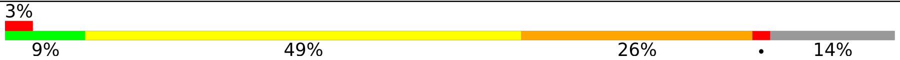
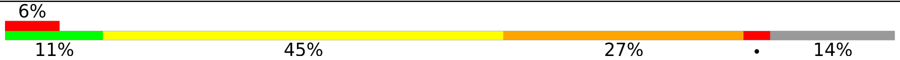
Mol	Chain	Length	Quality of chain
53	BW	113	
53	DW	113	
54	BX	96	
54	DX	96	
55	BY	110	
55	DY	110	
56	BZ	206	
56	DZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	5MU	CW	55	-	-	-	X
57	MG	AA	1615	-	-	-	X
57	MG	AA	1650	-	-	-	X
57	MG	AA	1653	-	-	-	X
57	MG	AA	1706	-	-	-	X
57	MG	AA	1720	-	-	-	X
57	MG	AA	1733	-	-	-	X
57	MG	AA	1734	-	-	-	X
57	MG	AA	1743	-	-	-	X
57	MG	AA	1749	-	-	-	X
57	MG	AA	1762	-	-	-	X
57	MG	AA	1769	-	-	-	X
57	MG	AA	1780	-	-	-	X
57	MG	AA	1789	-	-	-	X
57	MG	AA	1791	-	-	-	X
57	MG	AA	1798	-	-	-	X
57	MG	AK	201	-	-	-	X
57	MG	AV	102	-	-	-	X
57	MG	AW	108	-	-	-	X
57	MG	AW	123	-	-	-	X
57	MG	BA	3006	-	-	-	X
57	MG	BA	3014	-	-	-	X
57	MG	BA	3035	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3101	-	-	-	X
57	MG	BA	3189	-	-	-	X
57	MG	BA	3207	-	-	-	X
57	MG	BA	3227	-	-	-	X
57	MG	BA	3231	-	-	-	X
57	MG	BA	3251	-	-	-	X
57	MG	BA	3281	-	-	-	X
57	MG	BA	3286	-	-	-	X
57	MG	BA	3287	-	-	-	X
57	MG	BA	3292	-	-	-	X
57	MG	BA	3299	-	-	-	X
57	MG	BA	3309	-	-	-	X
57	MG	BA	3316	-	-	-	X
57	MG	BA	3322	-	-	-	X
57	MG	BA	3334	-	-	-	X
57	MG	BA	3379	-	-	-	X
57	MG	BA	3397	-	-	-	X
57	MG	BA	3412	-	-	-	X
57	MG	BA	3423	-	-	-	X
57	MG	BB	204	-	-	-	X
57	MG	BB	209	-	-	-	X
57	MG	BB	210	-	-	-	X
57	MG	BB	213	-	-	-	X
57	MG	BB	220	-	-	-	X
57	MG	CA	1602	-	-	-	X
57	MG	CA	1643	-	-	-	X
57	MG	CA	1646	-	-	-	X
57	MG	CA	1658	-	-	-	X
57	MG	CA	1681	-	-	-	X
57	MG	CA	1686	-	-	-	X
57	MG	CA	1718	-	-	-	X
57	MG	CA	1725	-	-	-	X
57	MG	CA	1731	-	-	-	X
57	MG	CA	1736	-	-	-	X
57	MG	CA	1737	-	-	-	X
57	MG	CA	1738	-	-	-	X
57	MG	CA	1746	-	-	-	X
57	MG	CA	1747	-	-	-	X
57	MG	CA	1759	-	-	-	X
57	MG	CA	1760	-	-	-	X
57	MG	CA	1765	-	-	-	X
57	MG	CA	1767	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	CA	1770	-	-	-	X
57	MG	CA	1785	-	-	-	X
57	MG	CA	1786	-	-	-	X
57	MG	CA	1797	-	-	-	X
57	MG	CE	202	-	-	-	X
57	MG	CN	101	-	-	-	X
57	MG	CV	102	-	-	-	X
57	MG	CW	106	-	-	-	X
57	MG	CW	110	-	-	-	X
57	MG	CW	111	-	-	-	X
57	MG	CW	112	-	-	-	X
57	MG	CW	113	-	-	-	X
57	MG	CW	115	-	-	-	X
57	MG	CW	116	-	-	-	X
57	MG	CW	118	-	-	-	X
57	MG	D1	104	-	-	-	X
57	MG	D2	2601	-	-	-	X
57	MG	DA	3004	-	-	-	X
57	MG	DA	3006	-	-	-	X
57	MG	DA	3049	-	-	-	X
57	MG	DA	3090	-	-	-	X
57	MG	DA	3101	-	-	-	X
57	MG	DA	3127	-	-	-	X
57	MG	DA	3135	-	-	-	X
57	MG	DA	3139	-	-	-	X
57	MG	DA	3140	-	-	-	X
57	MG	DA	3152	-	-	-	X
57	MG	DA	3174	-	-	-	X
57	MG	DA	3176	-	-	-	X
57	MG	DA	3212	-	-	-	X
57	MG	DA	3215	-	-	-	X
57	MG	DA	3220	-	-	-	X
57	MG	DA	3221	-	-	-	X
57	MG	DA	3241	-	-	-	X
57	MG	DA	3258	-	-	-	X
57	MG	DA	3262	-	-	-	X
57	MG	DA	3270	-	-	-	X
57	MG	DA	3271	-	-	-	X
57	MG	DA	3273	-	-	-	X
57	MG	DA	3281	-	-	-	X
57	MG	DA	3282	-	-	-	X
57	MG	DA	3296	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3299	-	-	-	X
57	MG	DA	3301	-	-	-	X
57	MG	DA	3303	-	-	-	X
57	MG	DA	3307	-	-	-	X
57	MG	DA	3326	-	-	-	X
57	MG	DA	3329	-	-	-	X
57	MG	DA	3346	-	-	-	X
57	MG	DA	3358	-	-	-	X
57	MG	DA	3361	-	-	-	X
57	MG	DA	3363	-	-	-	X
57	MG	DA	3367	-	-	-	X
57	MG	DA	3370	-	-	-	X
57	MG	DA	3400	-	-	-	X
57	MG	DA	3409	-	-	-	X
57	MG	DA	3436	-	-	-	X
57	MG	DA	3439	-	-	-	X
57	MG	DA	3441	-	-	-	X
57	MG	DB	202	-	-	-	X
57	MG	DB	219	-	-	-	X
57	MG	DH	201	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 290487 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
1	AA	1504	Total C N O P 32329 14390 5992 10444 1503	0	0	0
1	CA	1504	Total C N O P 32329 14390 5992 10444 1503	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	AB	235	Total C N O S 1901 1213 342 341 5	0	0	1
2	CB	235	Total C N O S 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
3	AC	207	Total C N O S 1613 1016 315 281 1	0	0	1
3	CC	207	Total C N O S 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
4	AD	208	Total C N O S 1703 1066 339 291 7	0	0	0
4	CD	208	Total C N O S 1703 1066 339 291 7	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	CJ	99	Total C N O S 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
11	AK	119	Total C N O S 885 549 168 165 3	0	0	0
11	CK	119	Total C N O S 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
12	AL	125	Total C N O S 971 611 196 163 1	0	0	1
12	CL	125	Total C N O S 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
13	AM	125	Total C N O S 988 611 206 169 2	0	0	1
13	CM	125	Total C N O S 988 611 206 169 2	0	0	1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	AN	60	Total C N O S 492 312 104 72 4	0	0	0
14	CN	60	Total C N O S 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
15	AO	88	Total C N O S 734 459 147 126 2	0	0	0
15	CO	88	Total C N O S 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
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			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 P-SITE RNA ASL-PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	AV	17	362	163	68	115	16	0	0	0
22	CV	17	362	163	68	115	16	0	0	0

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	AW	77	1641	733	297	535	76	0	0	0
23	CW	77	1641	733	297	535	76	0	0	0

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	AX	11	230	104	38	78	10	0	0	0
24	CX	11	230	104	38	78	10	0	0	0

- Molecule 25 is a protein called RIBOSOME RECYCLING FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	AY	185	1478	924	270	282	2	0	0	0
25	CY	185	1478	924	270	282	2	0	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	B0	85	652	403	137	111	1	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	D0	85	Total C N O S 652 403 137 111 1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	6	ALA	GLY	conflict	UNP P60493
B0	8	ALA	GLY	conflict	UNP P60493
D0	6	ALA	GLY	conflict	UNP P60493
D0	8	ALA	GLY	conflict	UNP P60493

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	B1	89	Total C N O 693 435 140 118	0	0	1
27	D1	89	Total C N O 693 435 140 118	0	0	1

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	B2	51	Total C N O S 421 263 85 72 1	0	0	1
28	D2	51	Total C N O S 421 263 85 72 1	0	0	1

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	B4	50	Total C N O 242 143 50 49	0	0	1
30	D4	50	Total C N O 242 143 50 49	0	0	1

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2767	Total	C	N	O	P	0	0	0
			59601	26526	11153	19156	2766			
35	DA	2767	Total	C	N	O	P	0	0	0
			59601	26526	11153	19156	2766			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total 1142	C 691	N 221	O 230	0	0	1
37	DC	191	Total 1143	C 692	N 221	O 230	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	106	ALA	GLY	conflict	UNP Q5SLP7
DC	132	ALA	GLY	conflict	UNP Q5SLP7

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total 1624	C 1035	N 304	O 282	S 3	0	0	1
40	DF	208	Total 1624	C 1035	N 304	O 282	S 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	160	1223	773	229	220	1	0	0	1
42	DH	160	1223	773	229	220	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	146	1132	723	201	207	1	0	0	1
43	DI	146	1132	723	201	207	1	0	0	1

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BQ	136	Total 1080	C 688	N 204	O 183	S 5	0	0	0
47	DQ	136	Total 1080	C 688	N 204	O 183	S 5	0	0	0

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BZ	177	Total 1404	C 897	N 253	O 252	S 2	0	0	1
56	DZ	177	Total 1404	C 897	N 253	O 252	S 2	0	0	1

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	204	Total Mg 204 204	0	0
57	AD	2	Total Mg 2 2	0	0
57	AE	2	Total Mg 2 2	0	0
57	AG	1	Total Mg 1 1	0	0
57	AK	1	Total Mg 1 1	0	0
57	AL	2	Total Mg 2 2	0	0
57	AM	1	Total Mg 1 1	0	0
57	AV	4	Total Mg 4 4	0	0
57	AW	23	Total Mg 23 23	0	0
57	AX	5	Total Mg 5 5	0	0
57	B1	4	Total Mg 4 4	0	0
57	B2	2	Total Mg 2 2	0	0
57	B3	1	Total Mg 1 1	0	0
57	B5	2	Total Mg 2 2	0	0
57	B7	1	Total Mg 1 1	0	0
57	BA	445	Total Mg 445 445	0	0
57	BB	20	Total Mg 20 20	0	0
57	BD	3	Total Mg 3 3	0	0
57	BE	1	Total Mg 1 1	0	0
57	BF	4	Total Mg 4 4	0	0
57	BG	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BN	4	Total Mg 4 4	0	0
57	BO	1	Total Mg 1 1	0	0
57	BP	3	Total Mg 3 3	0	0
57	BU	2	Total Mg 2 2	0	0
57	BX	2	Total Mg 2 2	0	0
57	CA	208	Total Mg 208 208	0	0
57	CE	3	Total Mg 3 3	0	0
57	CG	1	Total Mg 1 1	0	0
57	CL	2	Total Mg 2 2	0	0
57	CN	1	Total Mg 1 1	0	0
57	CV	4	Total Mg 4 4	0	0
57	CW	23	Total Mg 23 23	0	0
57	CX	4	Total Mg 4 4	0	0
57	D1	4	Total Mg 4 4	0	0
57	D2	2	Total Mg 2 2	0	0
57	D3	1	Total Mg 1 1	0	0
57	D5	1	Total Mg 1 1	0	0
57	D7	1	Total Mg 1 1	0	0
57	DA	441	Total Mg 441 441	0	0
57	DB	19	Total Mg 19 19	0	0
57	DD	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	DE	2	Total Mg 2 2	0	0
57	DF	5	Total Mg 5 5	0	0
57	DG	1	Total Mg 1 1	0	0
57	DH	1	Total Mg 1 1	0	0
57	DN	2	Total Mg 2 2	0	0
57	DP	4	Total Mg 4 4	0	0
57	DS	1	Total Mg 1 1	0	0
57	DU	3	Total Mg 3 3	0	0
57	DV	1	Total Mg 1 1	0	0
57	DX	3	Total Mg 3 3	0	0

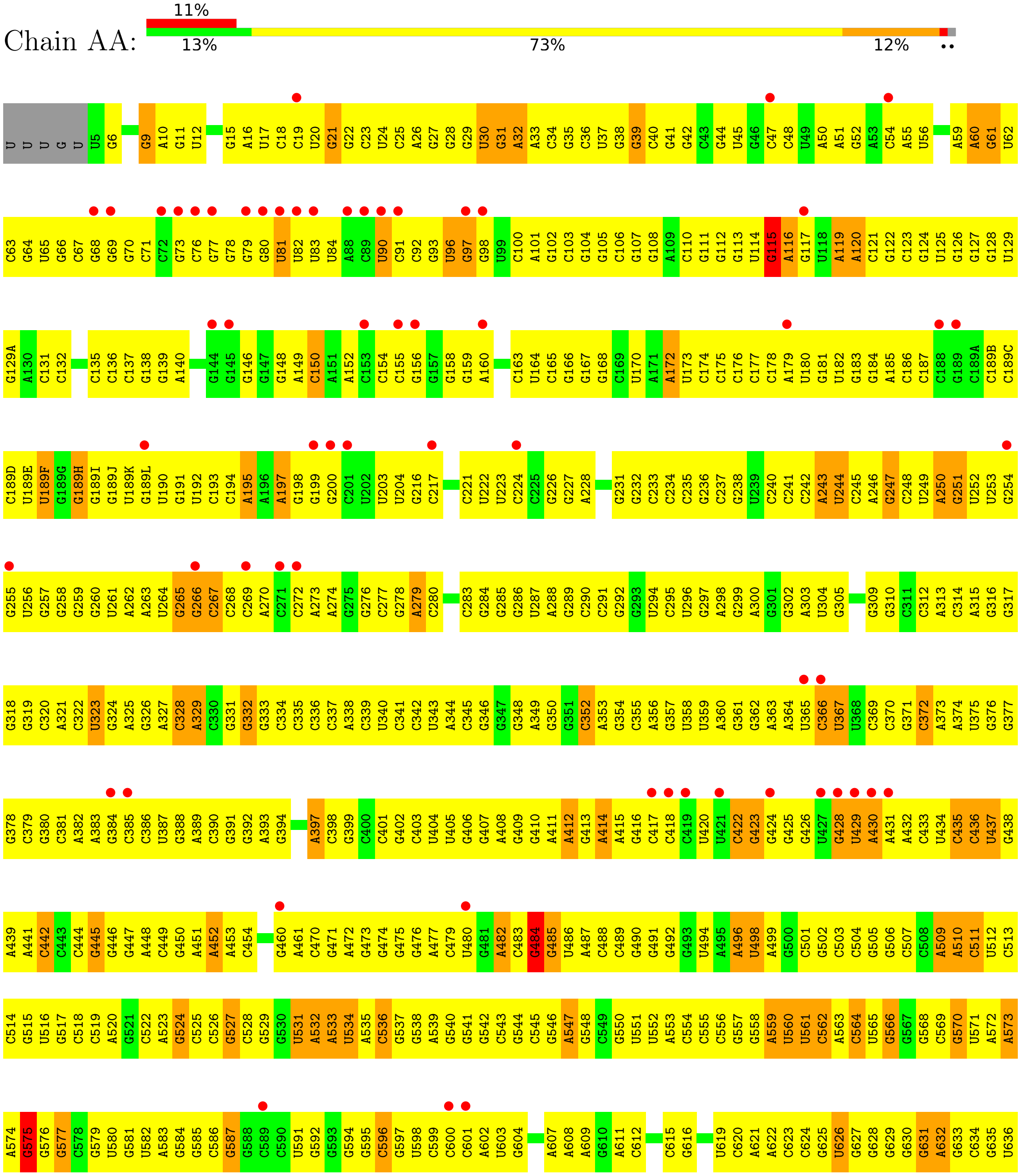
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

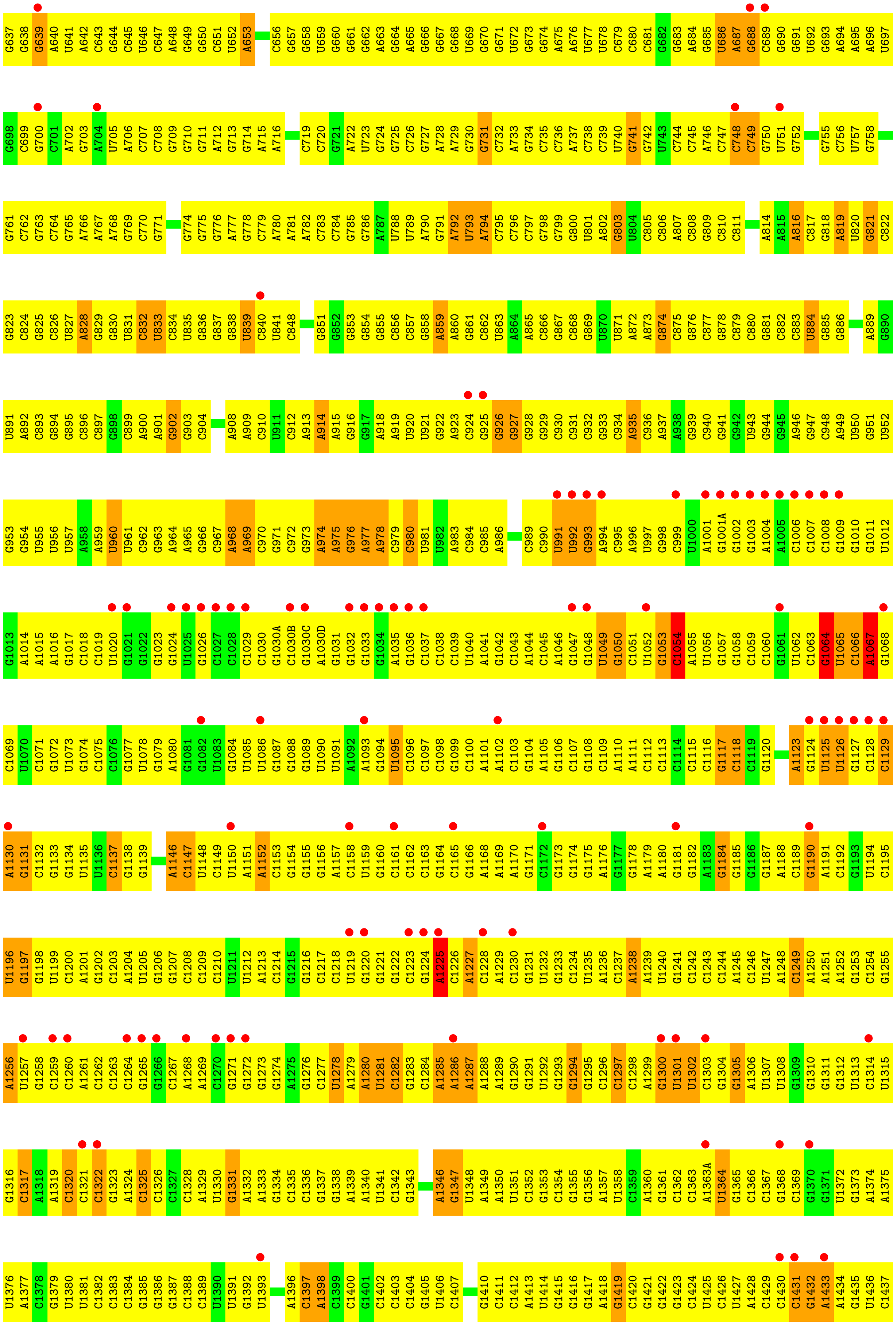
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AD	1	Total Zn 1 1	0	0
58	AN	1	Total Zn 1 1	0	0
58	CD	1	Total Zn 1 1	0	0
58	CN	1	Total Zn 1 1	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: 16S ribosomal RNA





G637 G638 G639 A640 U641 A642 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 C656 G657 G658 U659 G660 C661 G662 A663 G664 A665 G666 G667 G668 U669 G670 C671 U672 G673 G674 A675 A676 U677 U678 C679 C680 C681 G682 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697

G698 C699 G700 C701 A702 G703 A704 U705 A706 C707 C708 G709 G710 G711 A712 G713 G714 A715 A716 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 A733 G734 C735 C736 A737 U738 C739 U740 G741 G742 U743 C744 A745 A746 C747 C748 C749 G750 U751 G752 G755 C756 U757 G758

G761 C762 G763 C764 G765 A766 A767 A768 G769 C770 G771 G774 G775 C776 A777 G778 C779 A780 A781 A782 C783 C784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 G798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 A814 A815 A816 C817 G818 A819 U820 G821 C822

G823 C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 C879 C880 G881 C882 C883 U884 G885 G886 A889 G890

U891 A892 C893 G894 G895 C896 C897 G898 C899 A900 A901 G902 G903 C904 A908 A909 C910 U911 C912 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 G931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 G947 C948 A949 U950 G951 U952

G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 G965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 G985 A986 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012

G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068

C1069 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1077 U1078 G1079 A1080 G1081 G1082 U1083 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 A1123 G1124 U1125 U1126 G1127 C1128 C1129

A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164 C1165 G1166 A1168 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1187 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195

U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1242 G1243 C1244 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 C1254 G1255

A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 G1265 G1266 C1267 A1268 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1296 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 G1311 U1312 U1313 C1314 U1315

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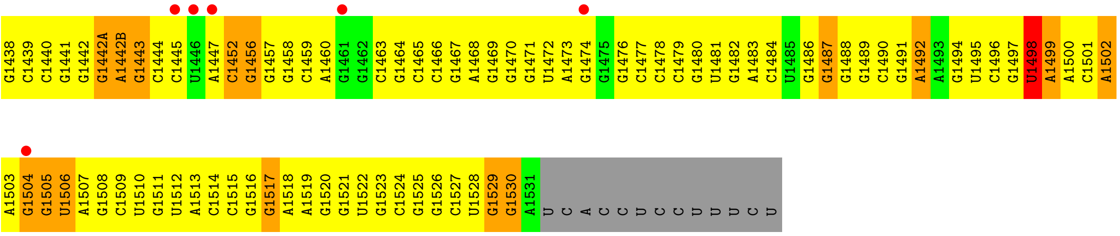
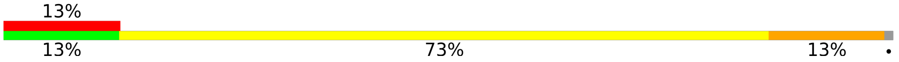
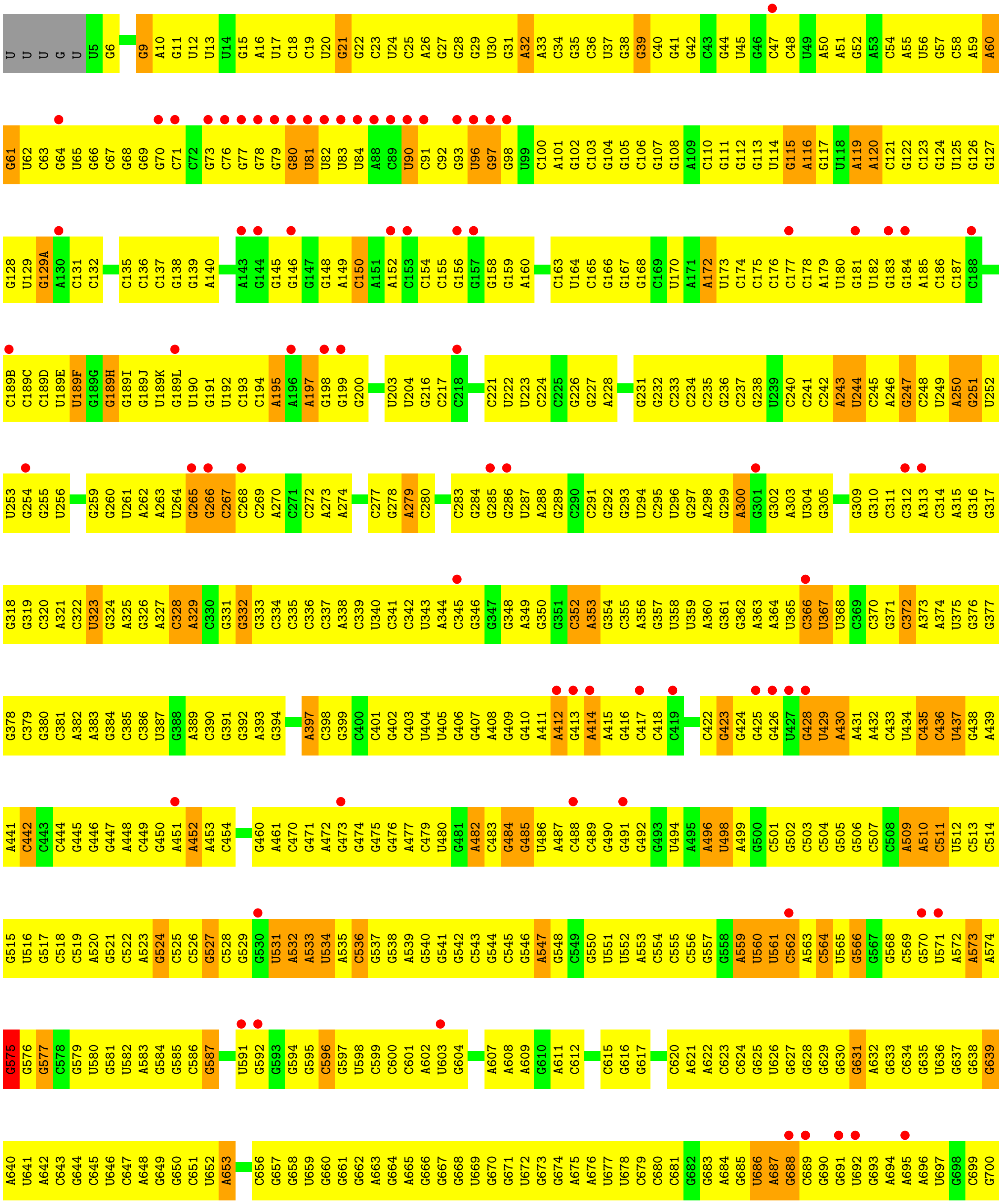
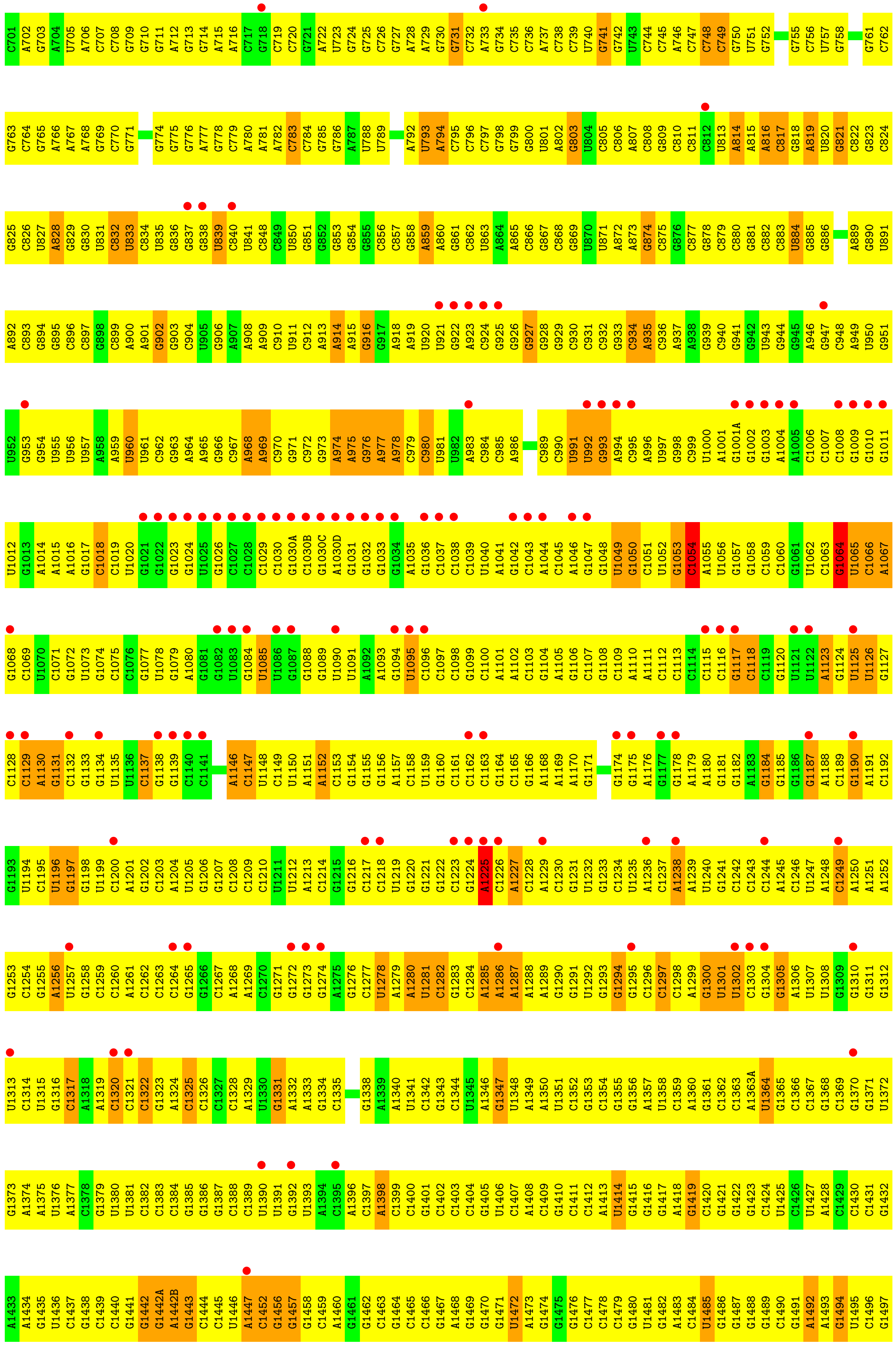


- Molecule 1: 16S ribosomal RNA

Chain CA:



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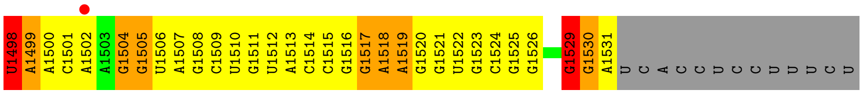
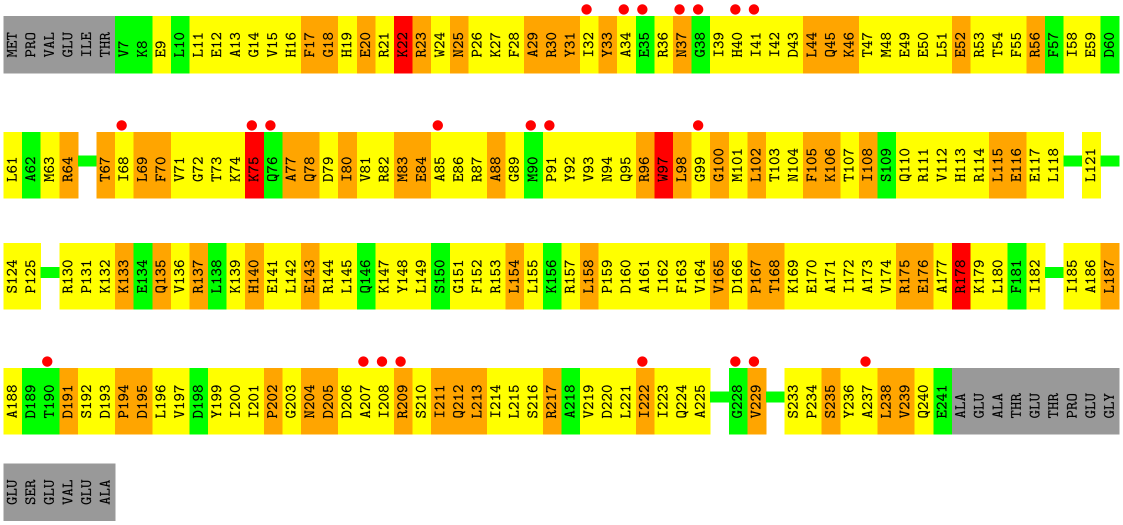
A1433 A1434 G1435 U1436 C1437 G1438 C1439 C1440 G1441 G1442 G1442A A1442B G1443 C1444 C1445 U1446 A1447 C1452 G1456 G1457 G1458 C1459 A1460 G1461 G1462 C1463 G1464 C1465 C1466 G1467 A1468 G1469 G1470 G1471 U1472 A1473 G1474 G1475 G1476 C1477 C1478 C1479 G1480 U1481 G1482 A1483 C1484 U1485 G1486 G1487 G1488 G1489 C1490 G1491 A1492 A1493 G1494 U1495 C1496 G1497



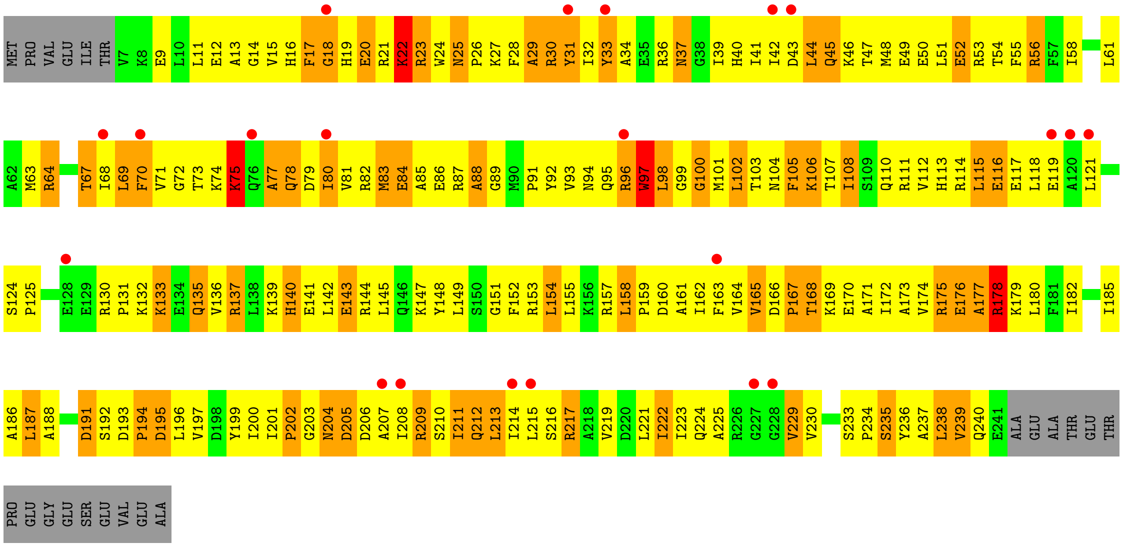
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



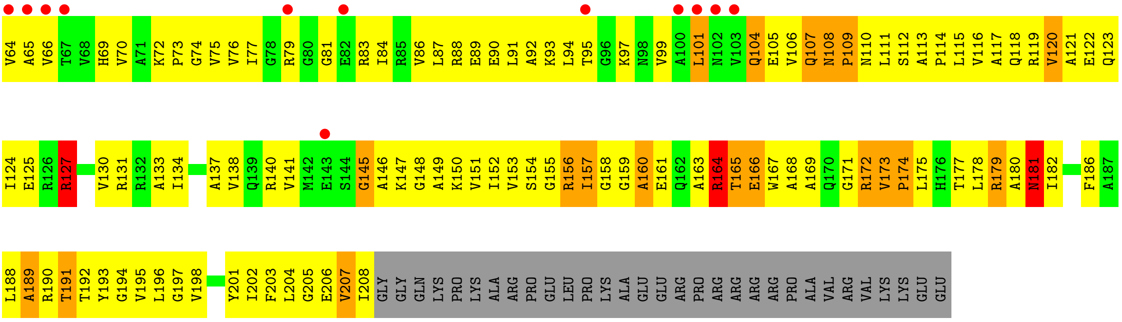
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB:



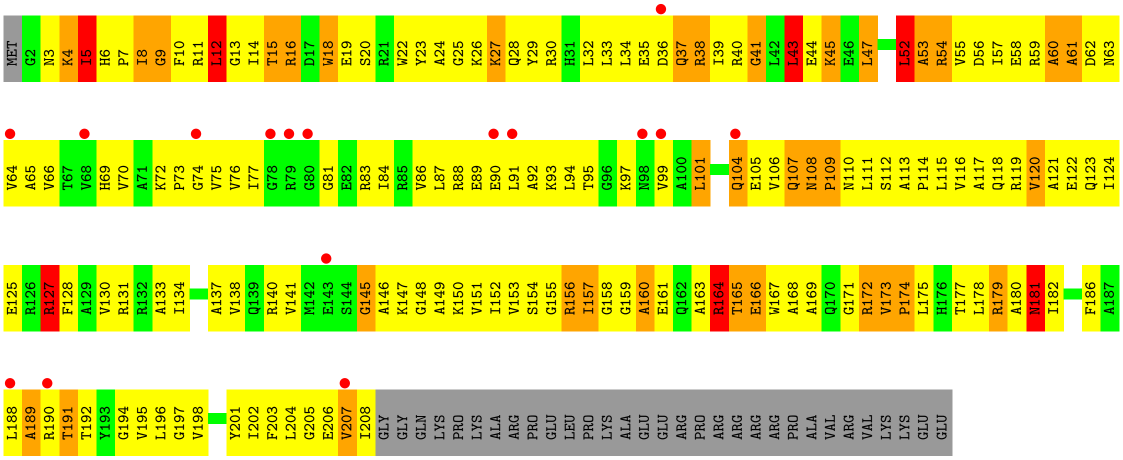
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



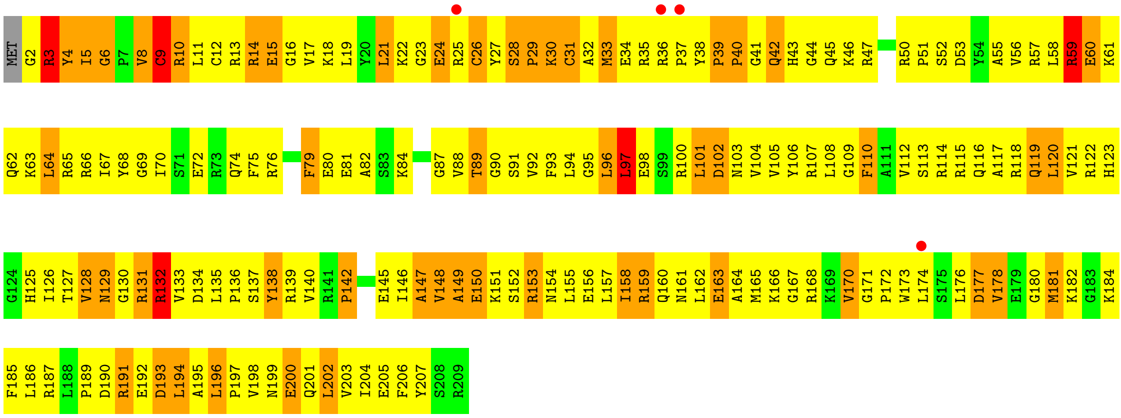
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:



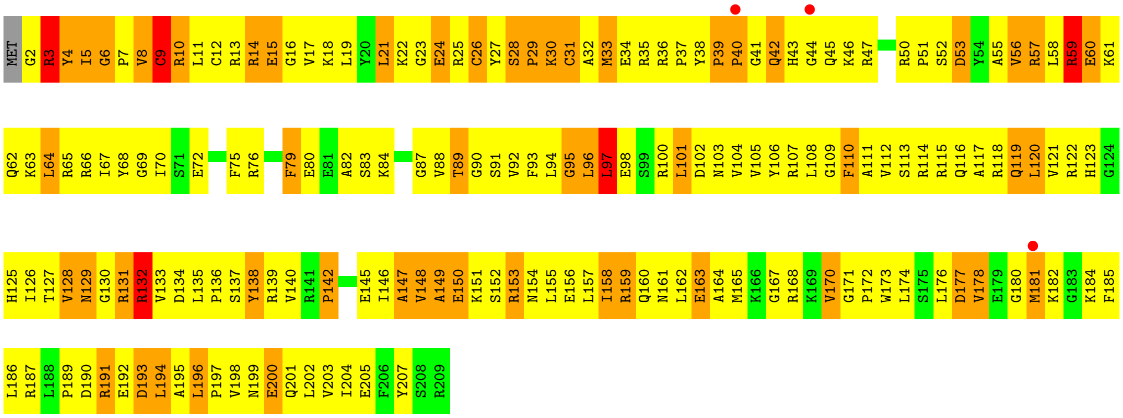
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



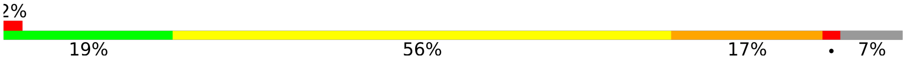
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

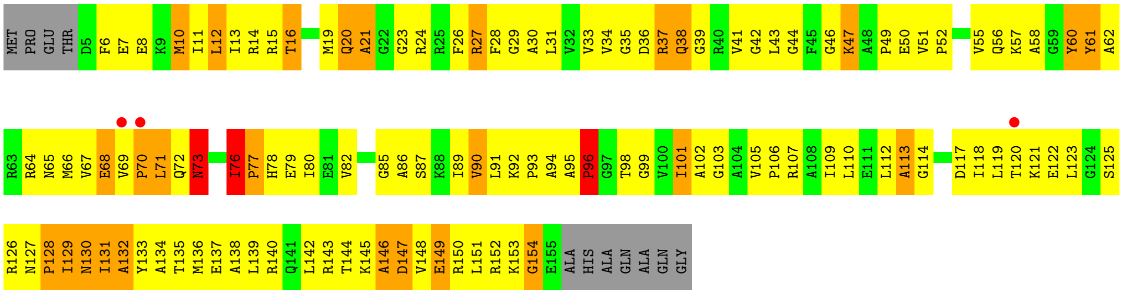
Chain CD:



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

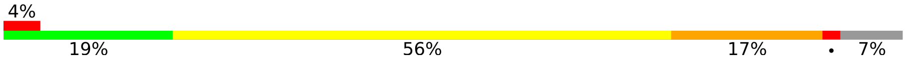
Chain AE:

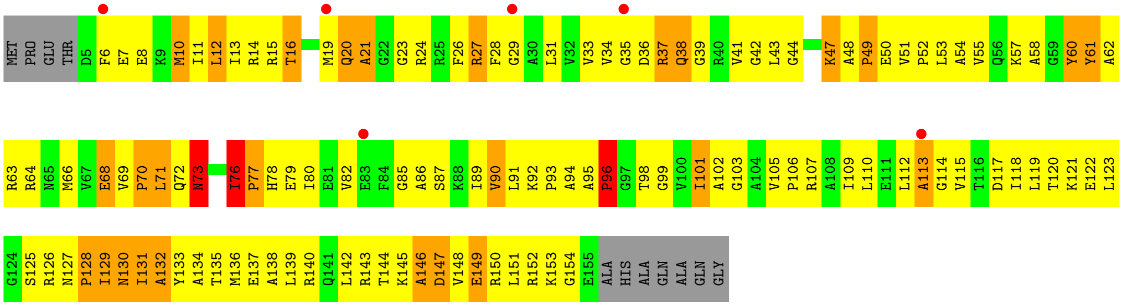




- Molecule 5: 30S RIBOSOMAL PROTEIN S5

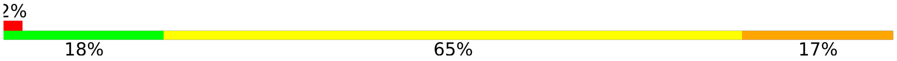
Chain CE:

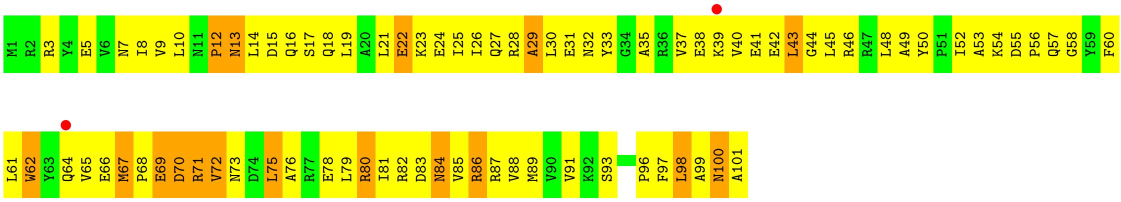




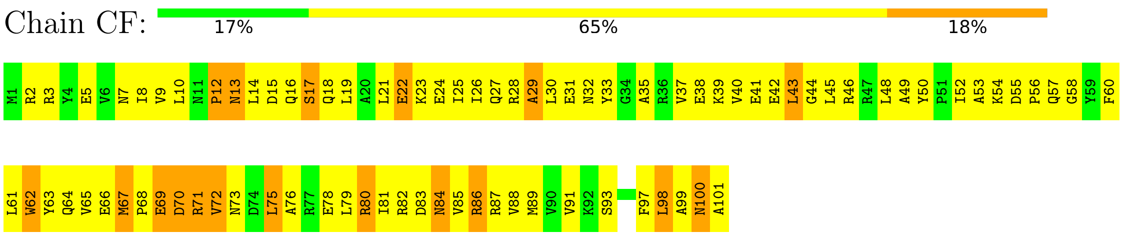
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:

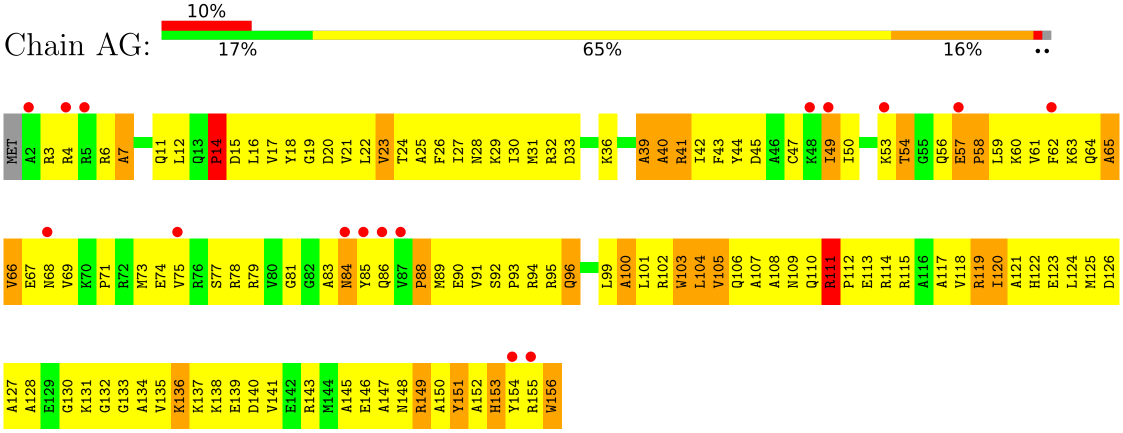




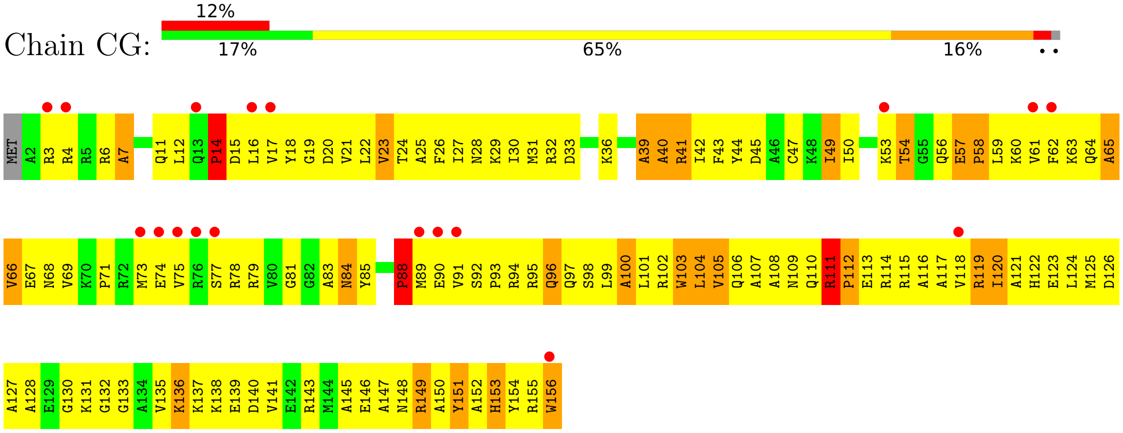
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



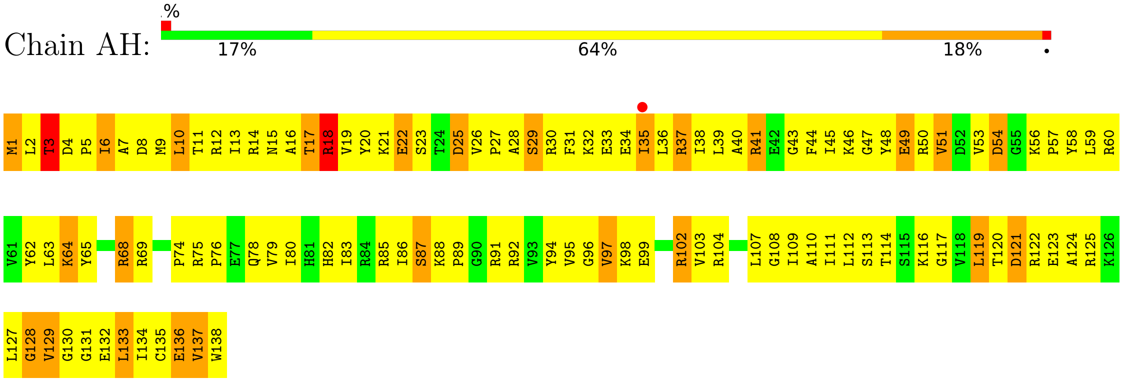
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



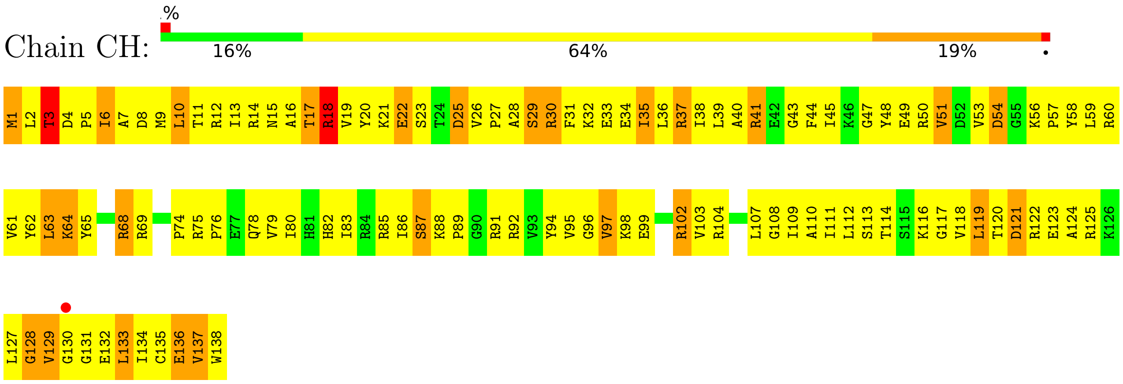
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



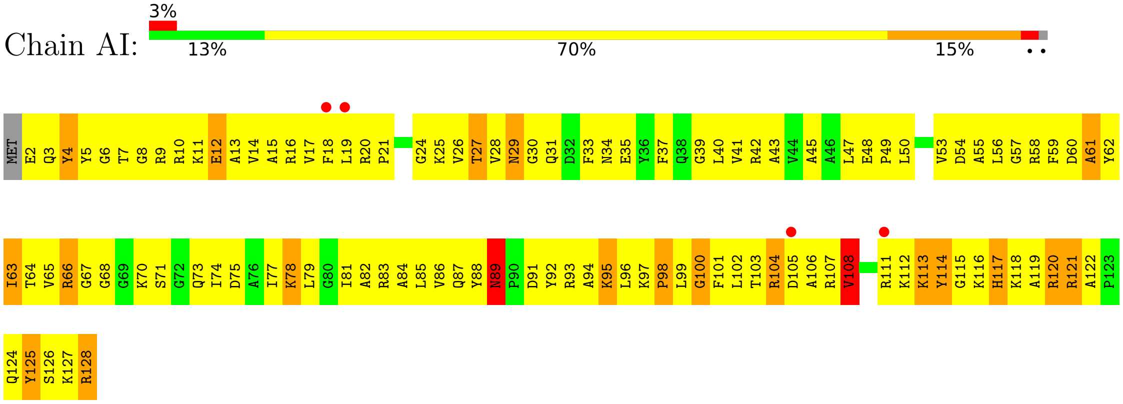
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



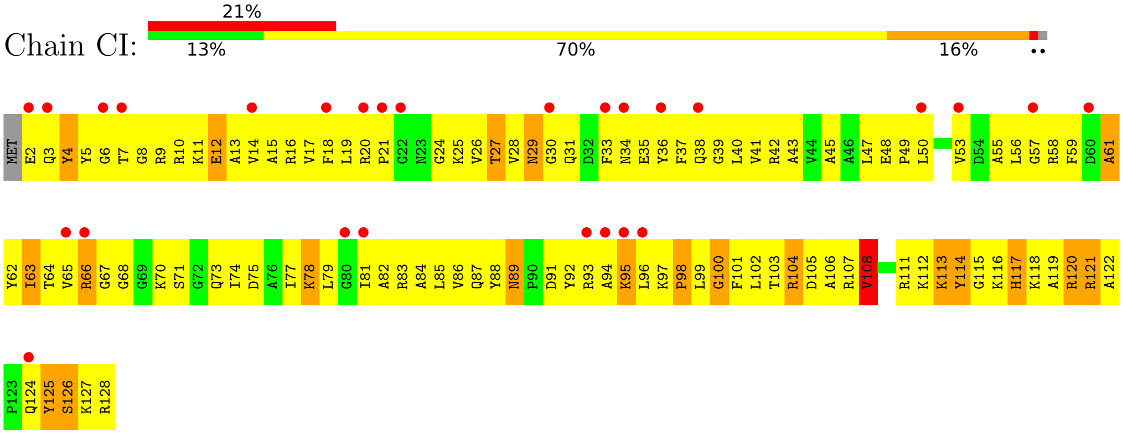
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



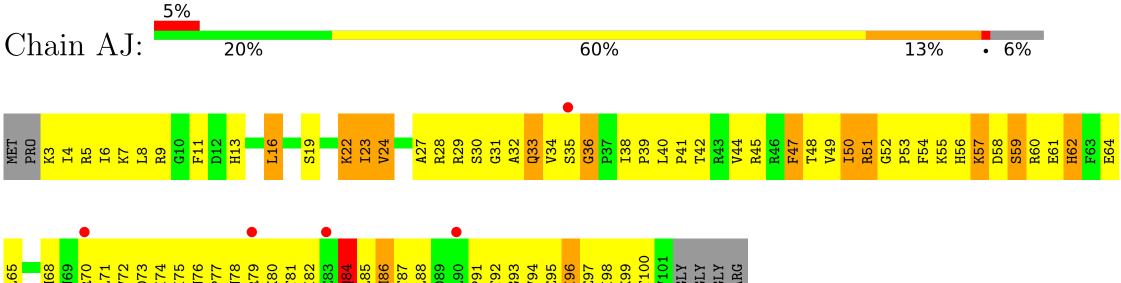
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



- Molecule 9: 30S RIBOSOMAL PROTEIN S9

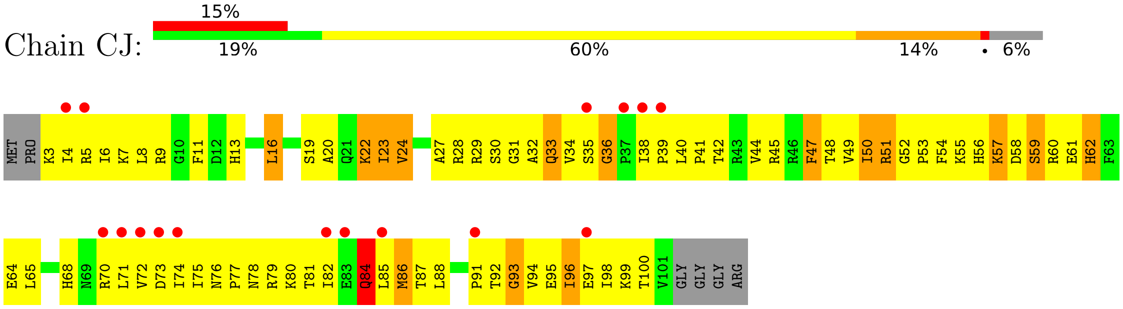


- Molecule 10: 30S RIBOSOMAL PROTEIN S10



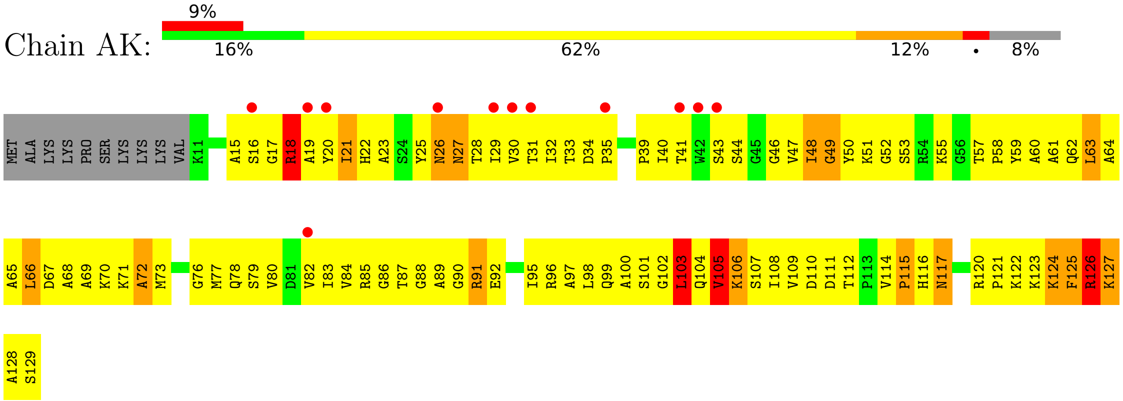
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



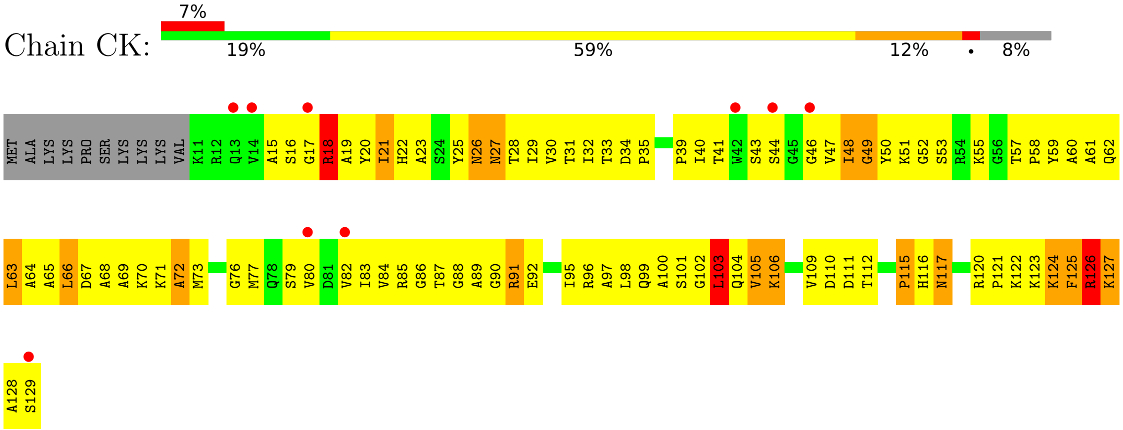
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



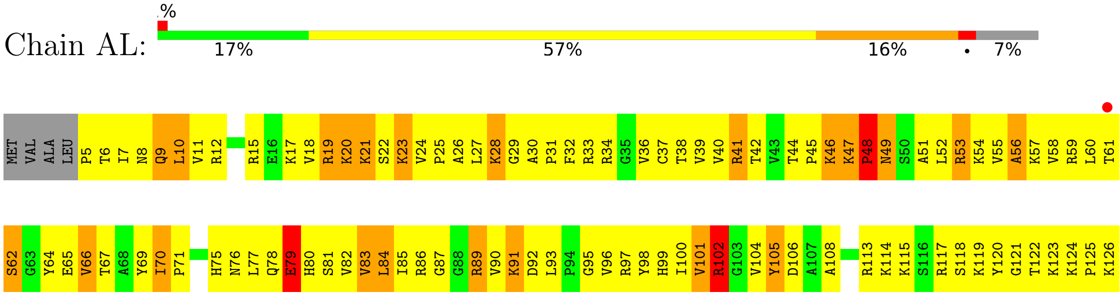
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

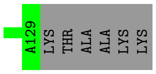
Chain CK:



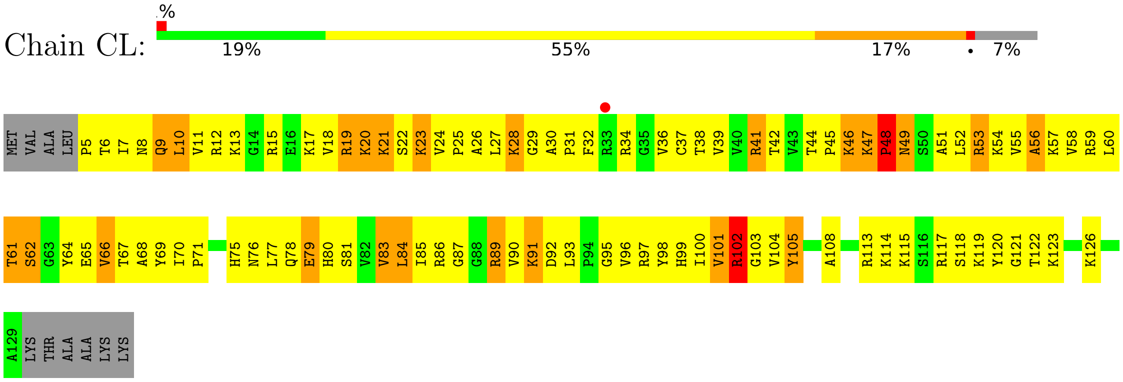
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:

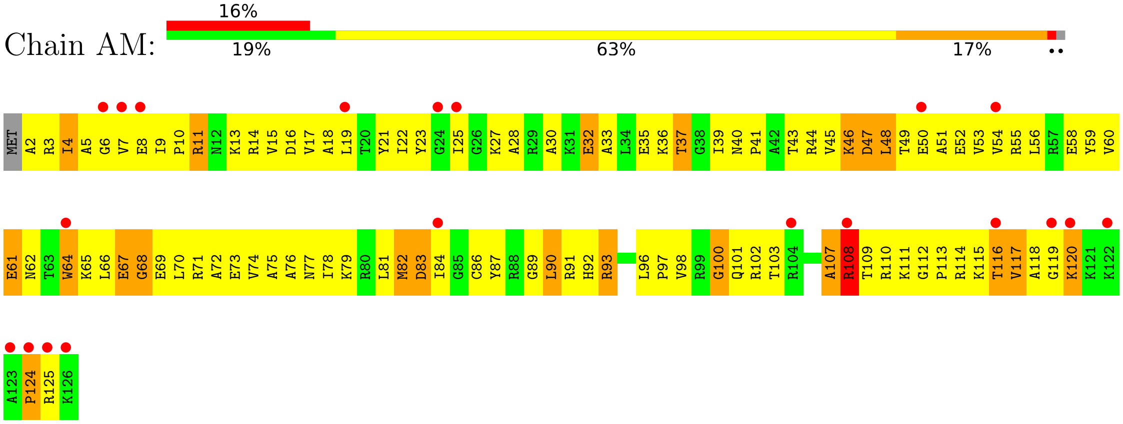




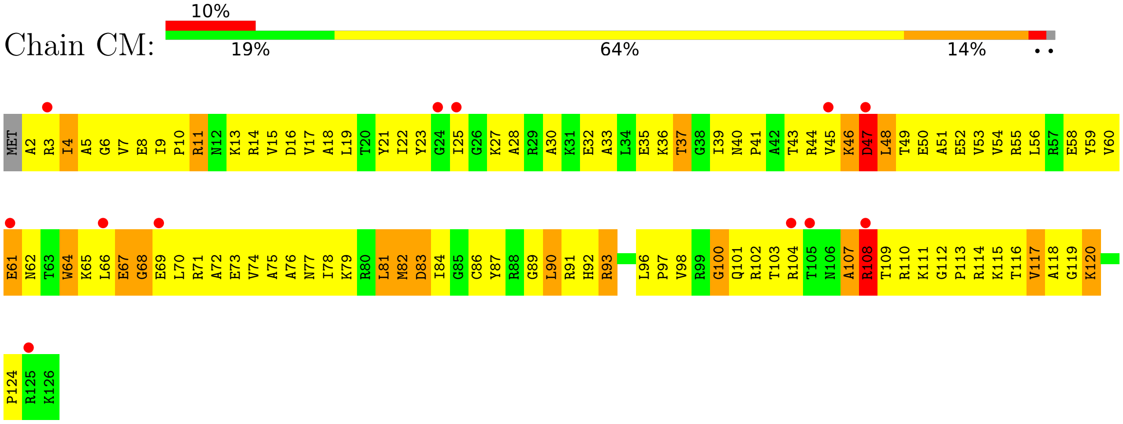
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



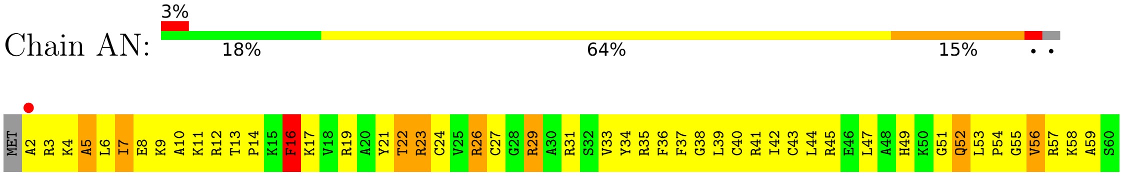
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

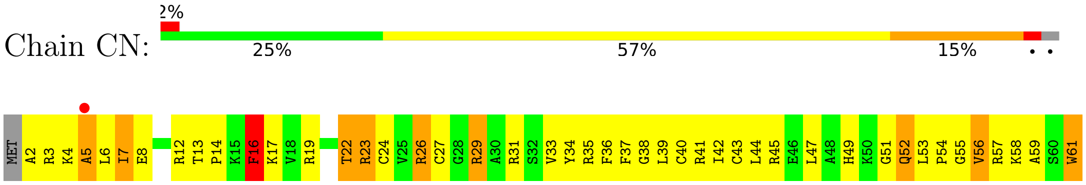


- Molecule 14: 30S RIBOSOMAL PROTEIN S14



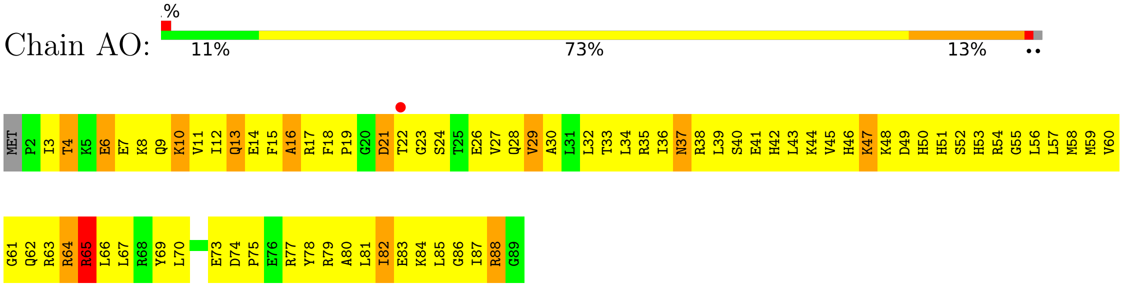
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CN:



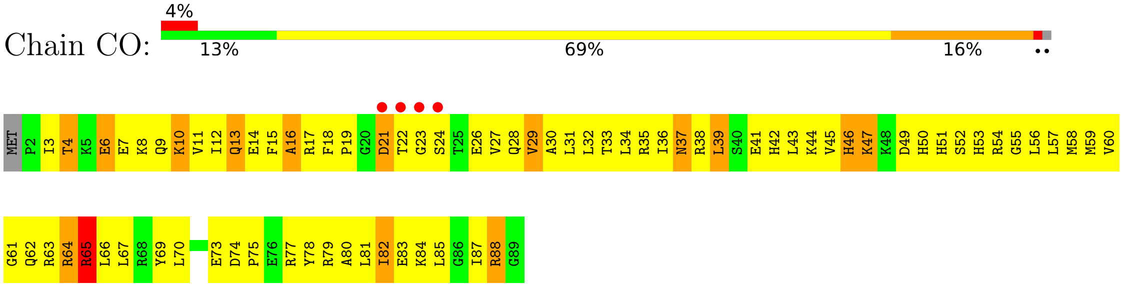
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



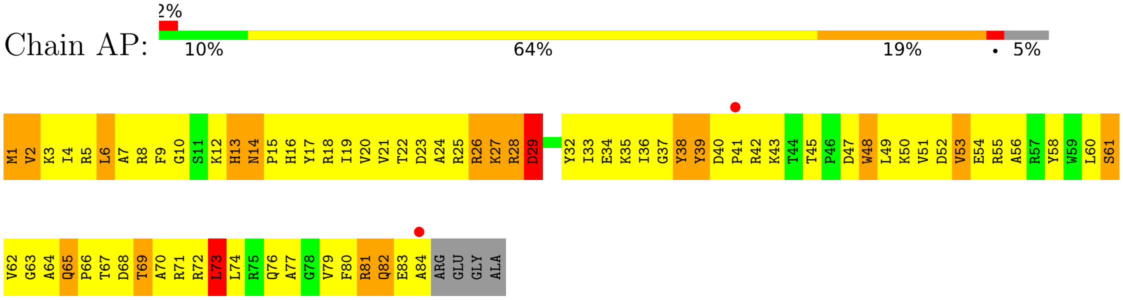
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



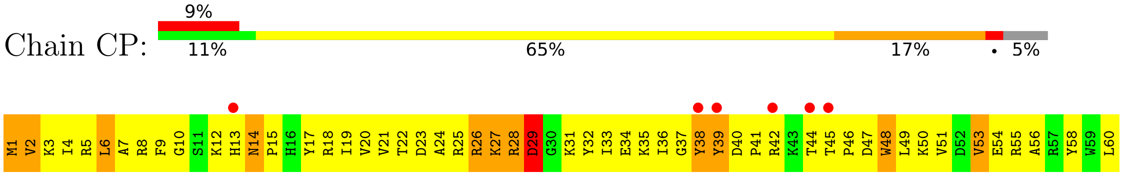
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

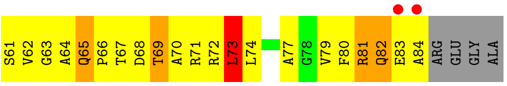
Chain AP:



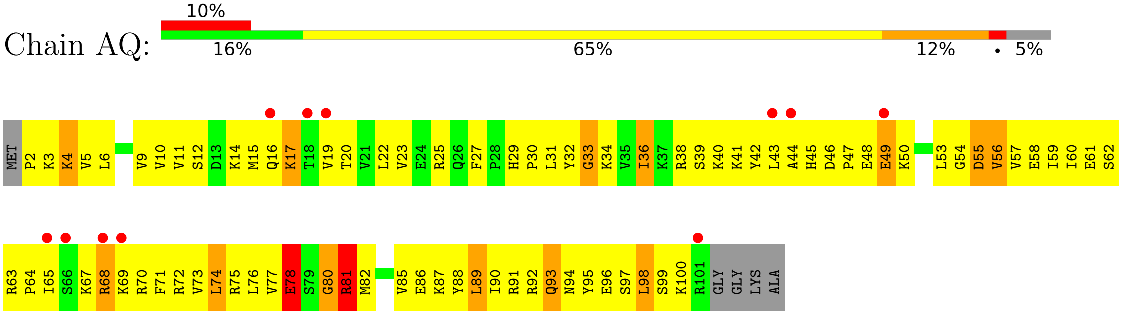
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:

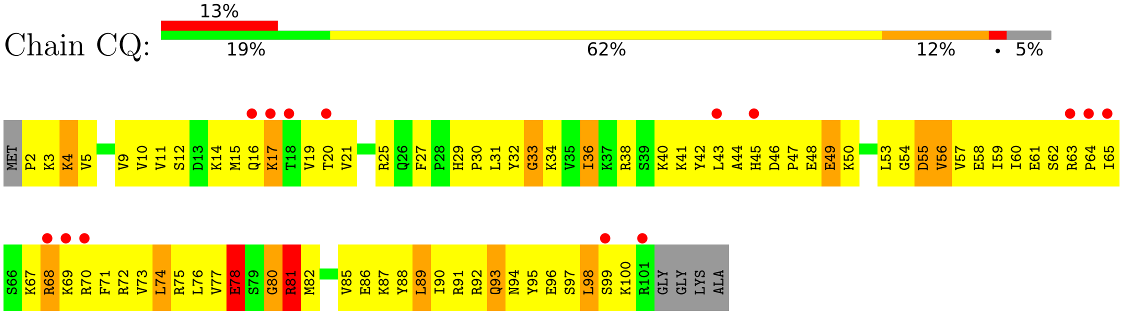




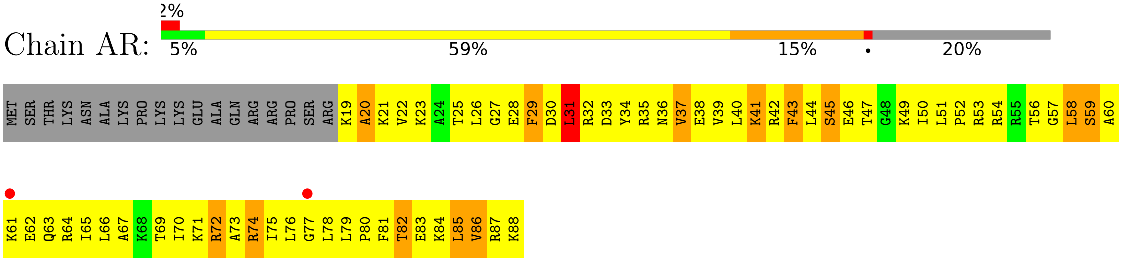
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



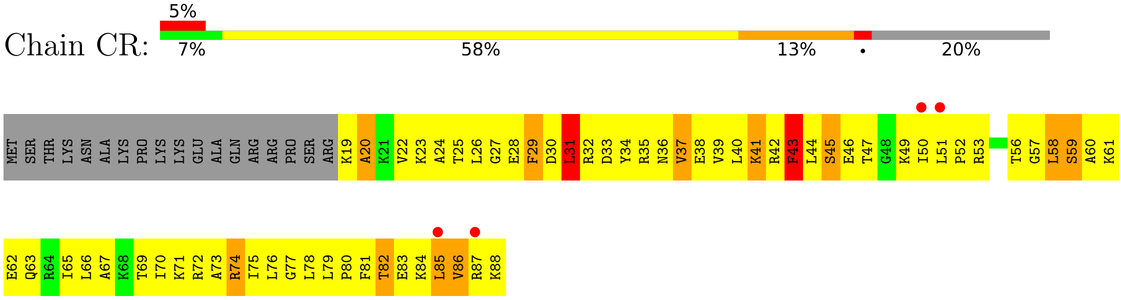
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



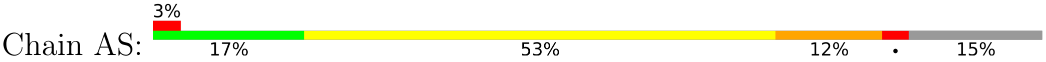
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

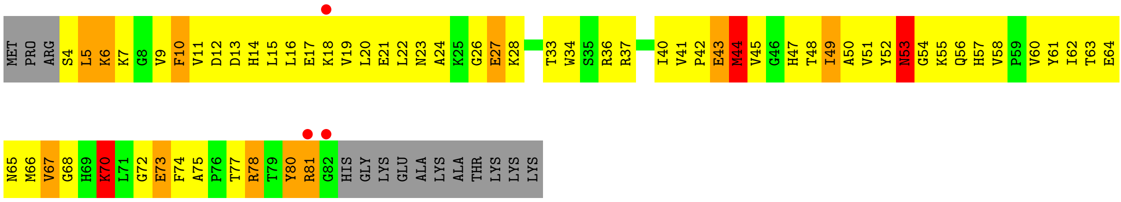


- Molecule 18: 30S RIBOSOMAL PROTEIN S18



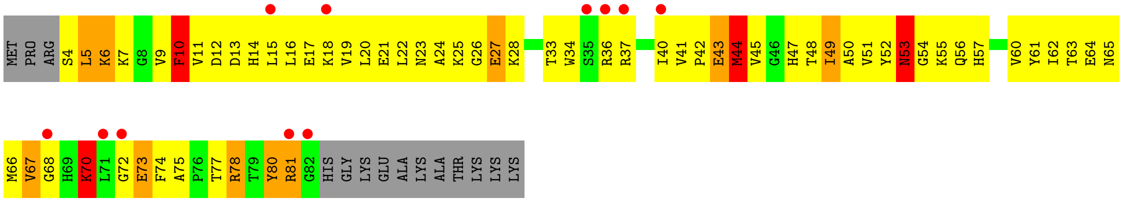
- Molecule 19: 30S RIBOSOMAL PROTEIN S19





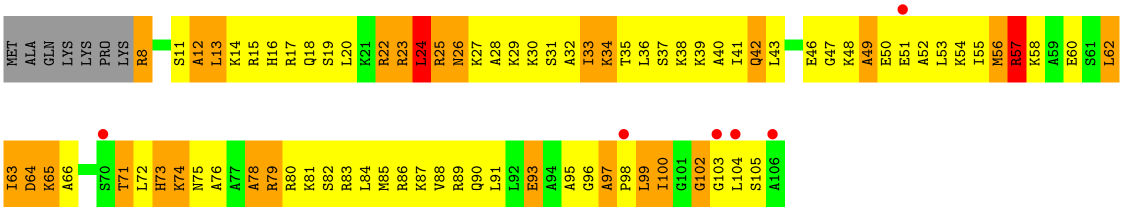
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



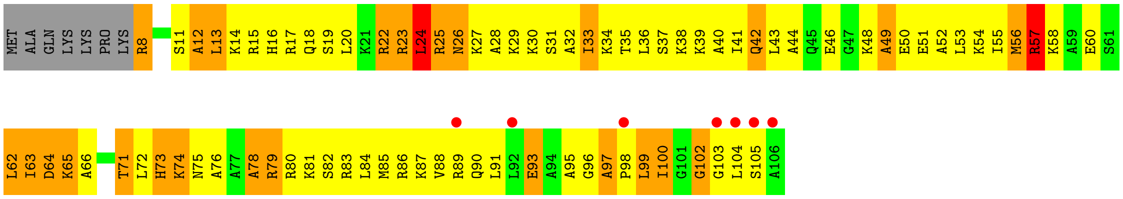
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



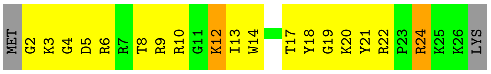
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



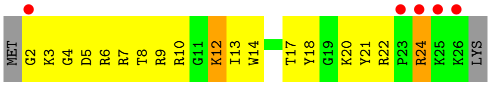
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



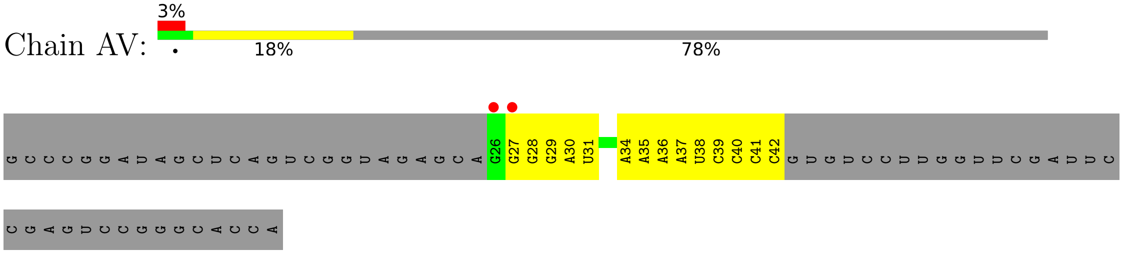
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



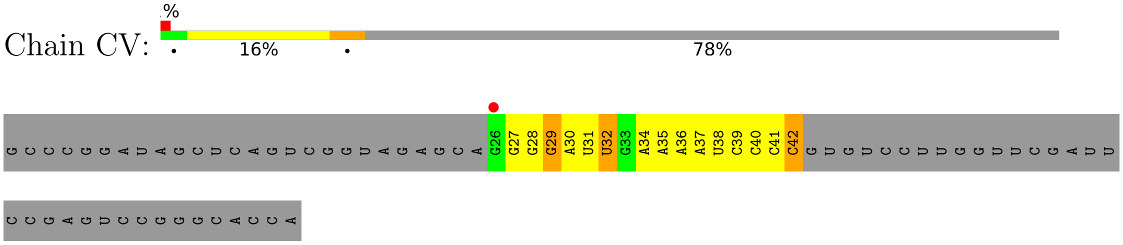
- Molecule 22: P-SITE RNA ASL-PHE

Chain AV:



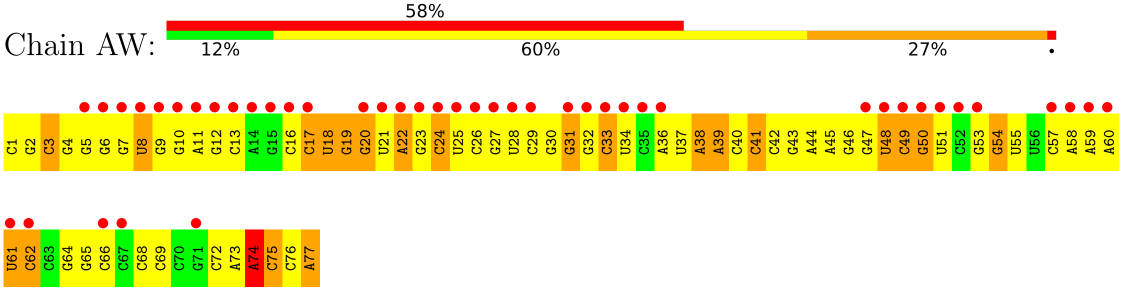
- Molecule 22: P-SITE RNA ASL-PHE

Chain CV:



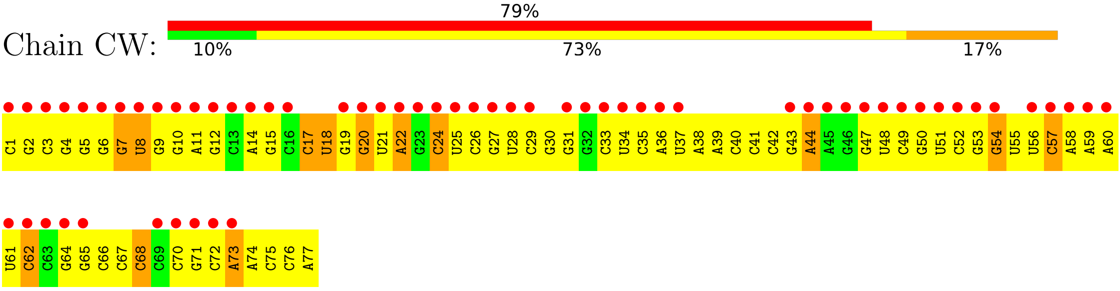
- Molecule 23: TRNA-FMET

Chain AW:



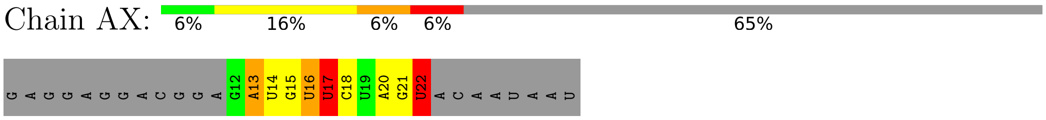
- Molecule 23: TRNA-FMET

Chain CW:

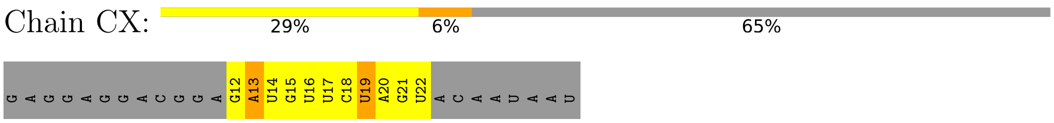


- Molecule 24: MRNA

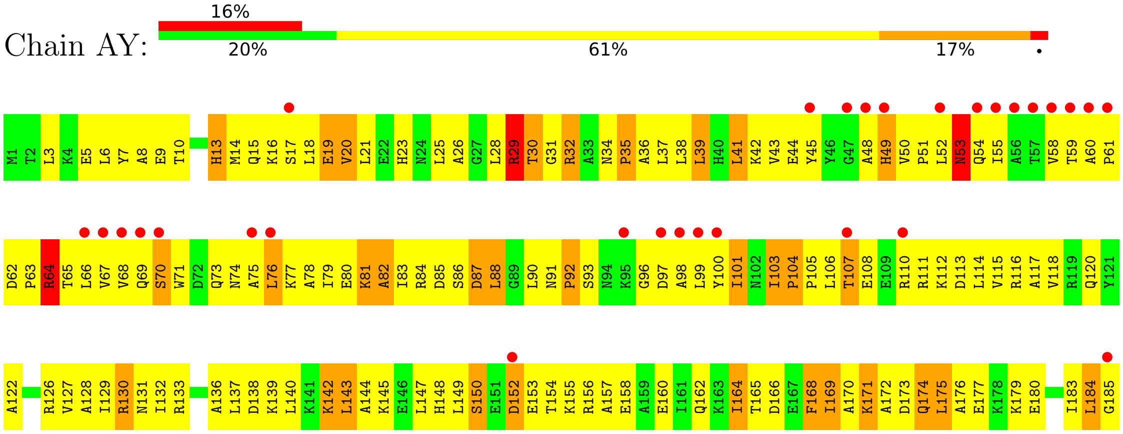
Chain AX:



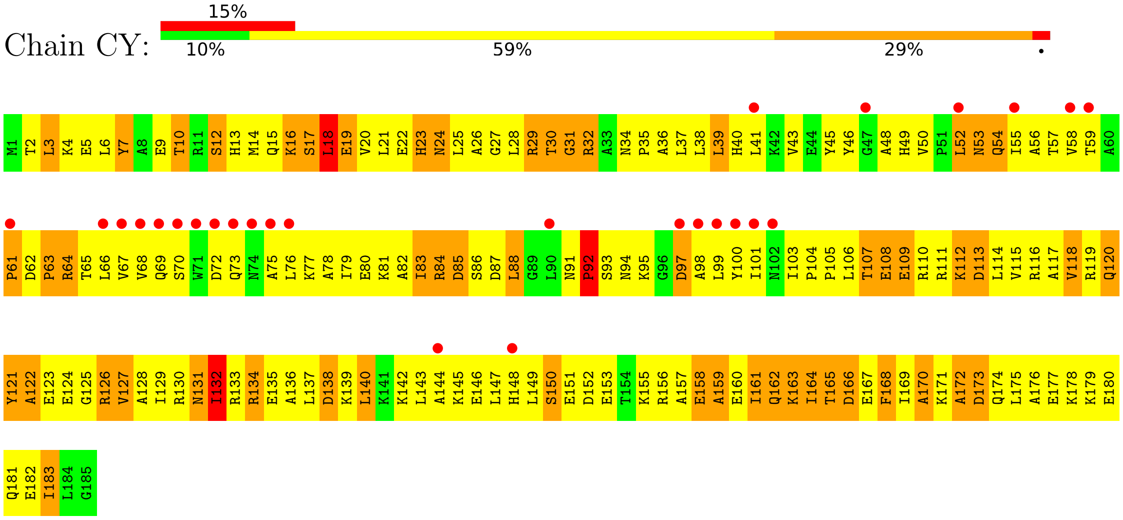
- Molecule 24: MRNA



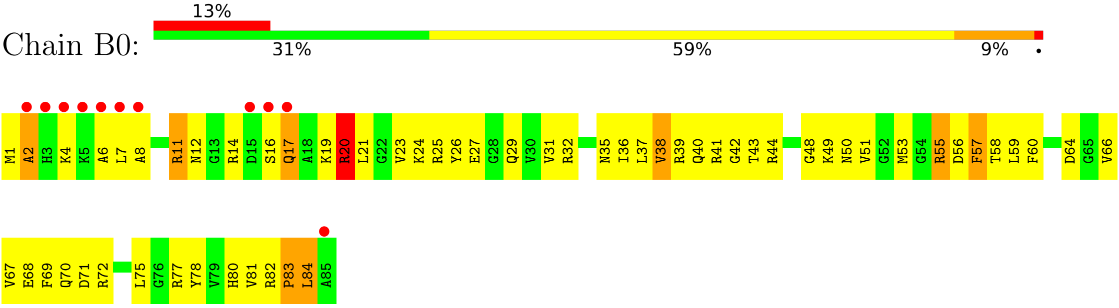
- Molecule 25: RIBOSOME RECYCLING FACTOR



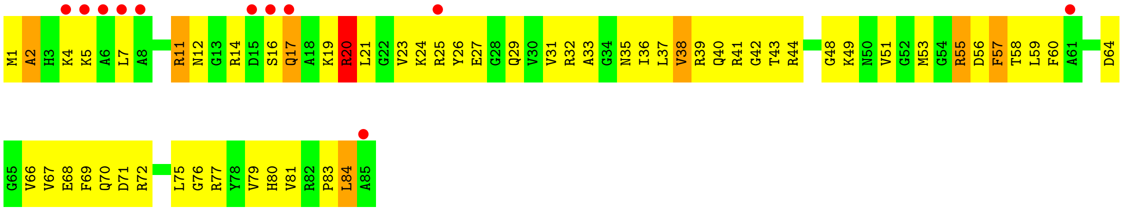
- Molecule 25: RIBOSOME RECYCLING FACTOR



- Molecule 26: 50S RIBOSOMAL PROTEIN L27

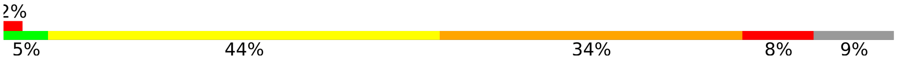


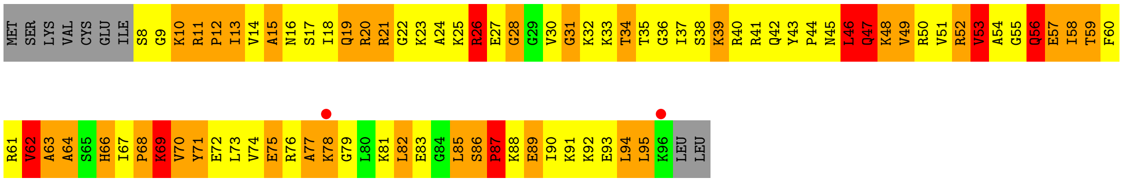
- Molecule 26: 50S RIBOSOMAL PROTEIN L27



- Molecule 27: 50S RIBOSOMAL PROTEIN L28

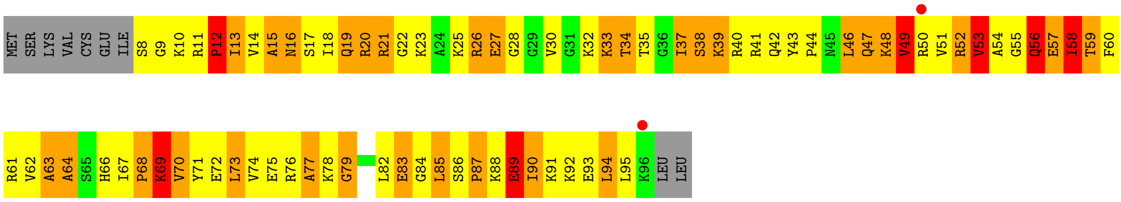
Chain B1:





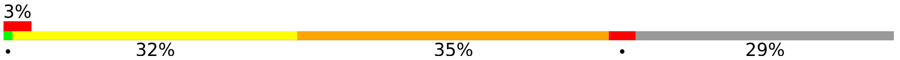
- Molecule 27: 50S RIBOSOMAL PROTEIN L28

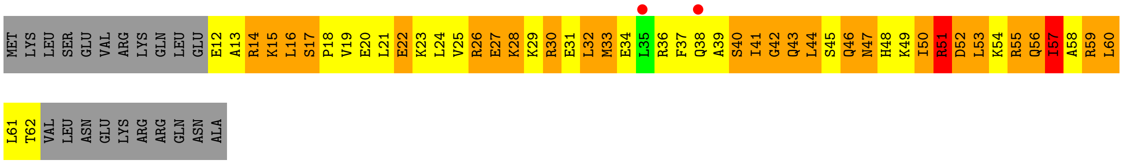
Chain D1:



- Molecule 28: 50S RIBOSOMAL PROTEIN L29

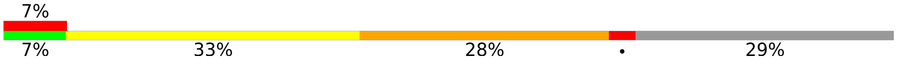
Chain B2:

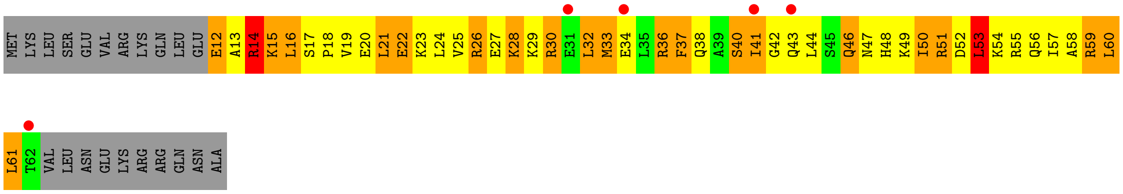




- Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:





- Molecule 29: 50S RIBOSOMAL PROTEIN L30

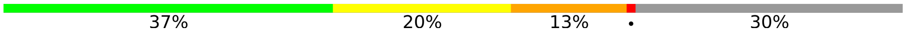
Chain B3:

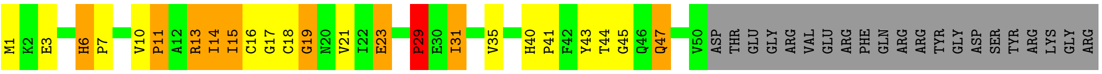
- Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:

- Molecule 30: 50S RIBOSOMAL PROTEIN L31

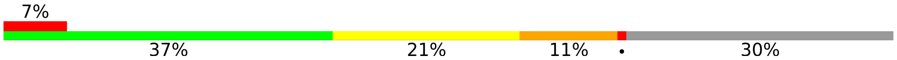
Chain B4:

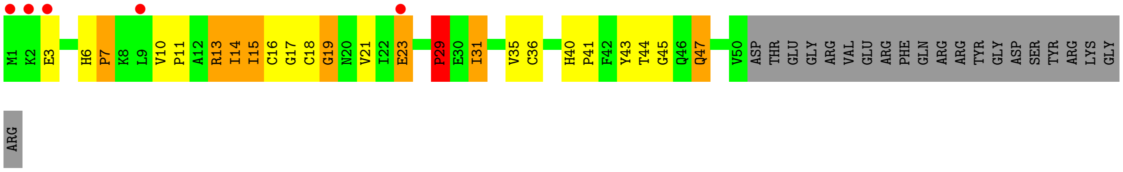




- Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain D4:





- Molecule 31: 50S RIBOSOMAL PROTEIN L32

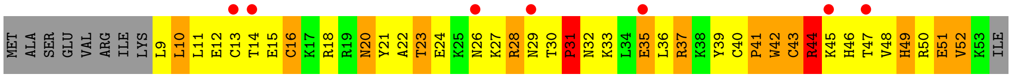
Chain B5:

- Molecule 31: 50S RIBOSOMAL PROTEIN L32

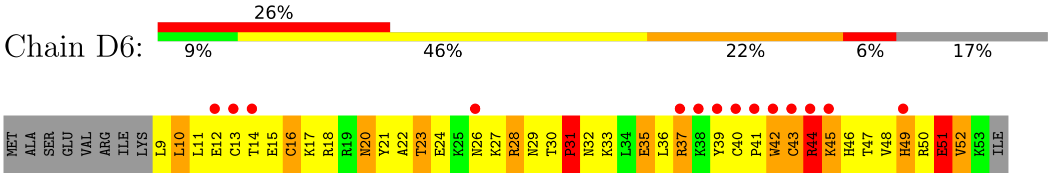
Chain D5:

- Molecule 32: 50S RIBOSOMAL PROTEIN L33

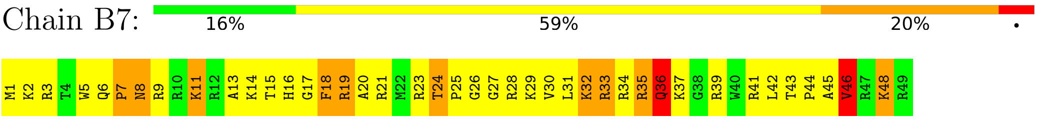
Chain B6:



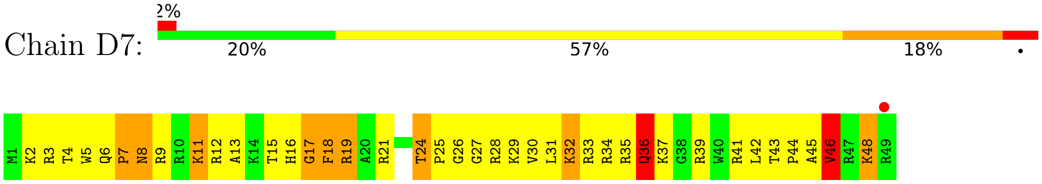
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



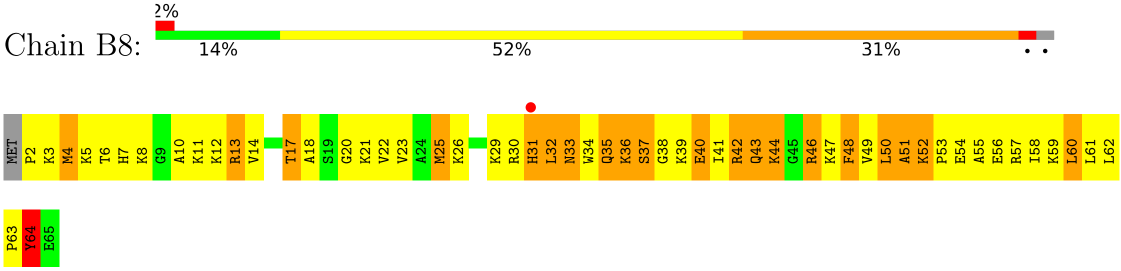
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



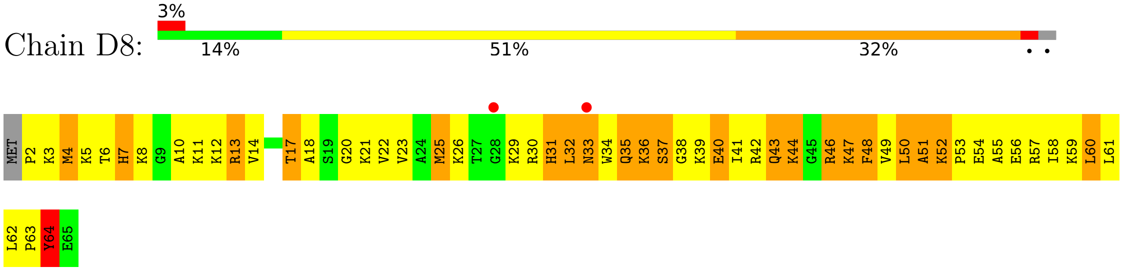
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



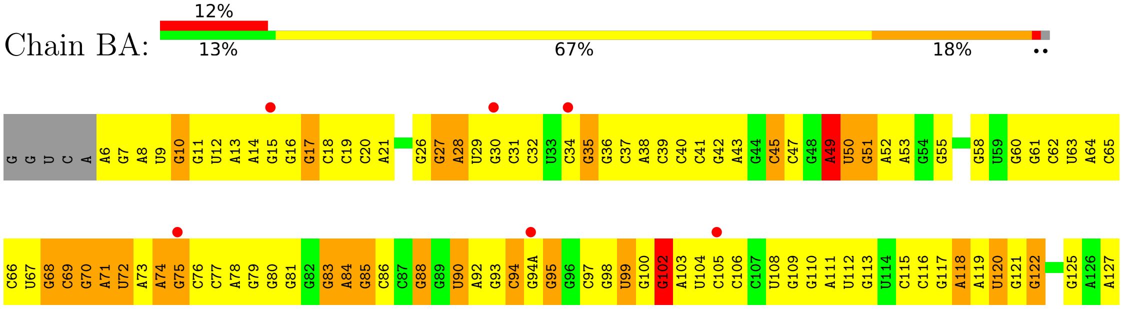
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

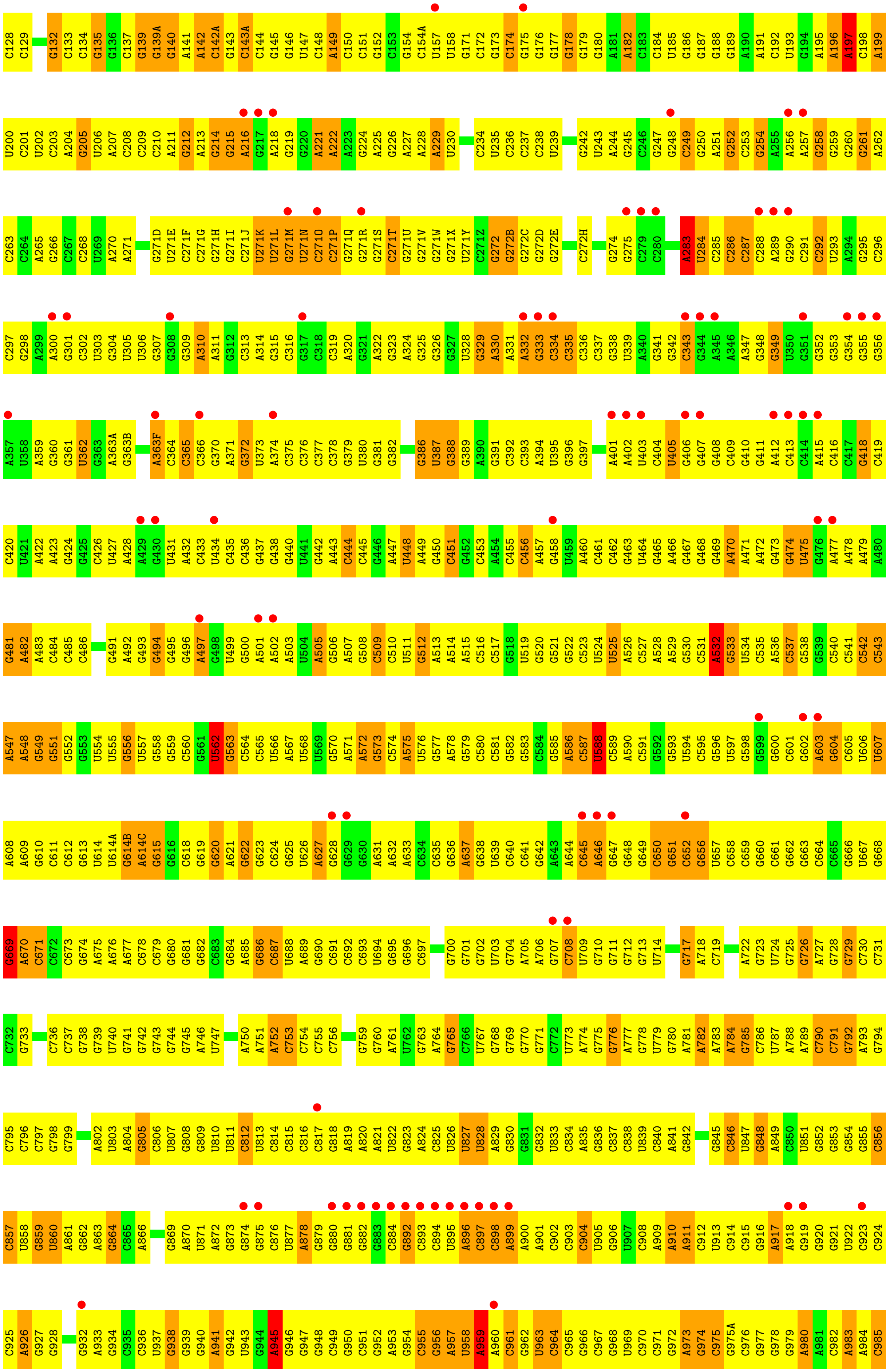


- Molecule 34: 50S RIBOSOMAL PROTEIN L35



- Molecule 35: 23S ribosomal RNA

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U200 C201 U202 C203 A204 G205 U206 A207 G208 C209 C210 A211 G212 A213 G214 G215 A216 G217 A218 G219 G220 A221 A222 A223 G224 A225 G226 A227 A228 A229 U230 C234 U235 C236 C237 G238 U239 G242 U243 A244 G245 C246 G247 G248 C249 G250 A251 G252 C253 G254 A255 A256 A257 G258 G259 G260 G261 A262
C263 C264 A265 G266 C267 C268 U269 A270 A271 G271D U271E C271F C271G G271H G271I C271J U271K U271L G271M U271N C271O C271P G271Q G271R G271S C271T G271U G271V G271W G271X U271Y C271Z G272 G272B C272C G272D G272E C272H G274 G275 C279 C280 A283 U284 C285 C286 C287 C288 A289 G290 C291 C292 U293 A294 G295 C296
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C732 G733 C736 C737 G738 G739 U740 G741 G742 G743 G744 G745 A746 U747 A750 A751 A752 C753 C754 C755 C756 G759 G760 A761 U762 G763 A764 G765 C766 U767 G768 G769 G770 G771 C772 U773 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794
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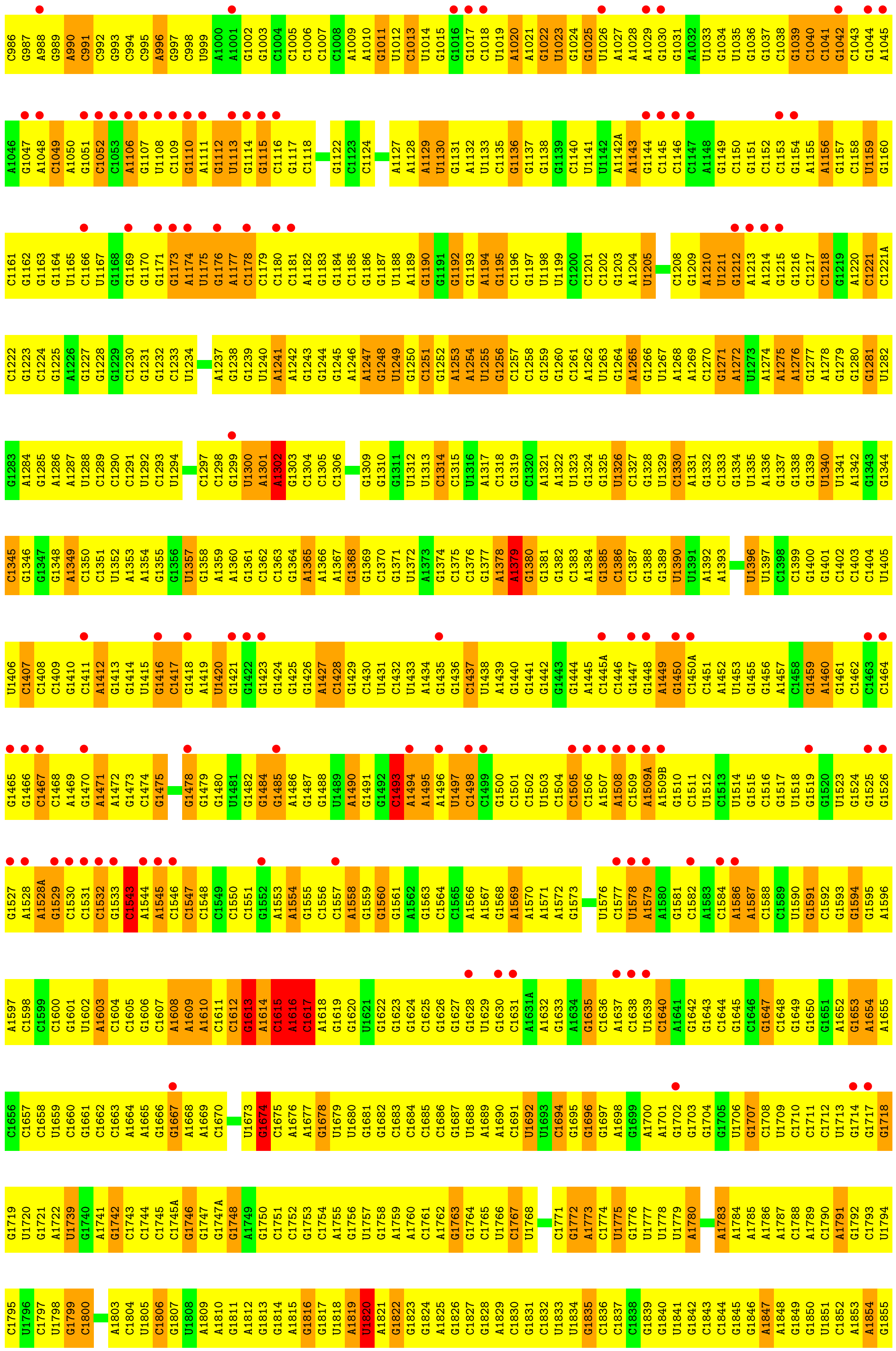
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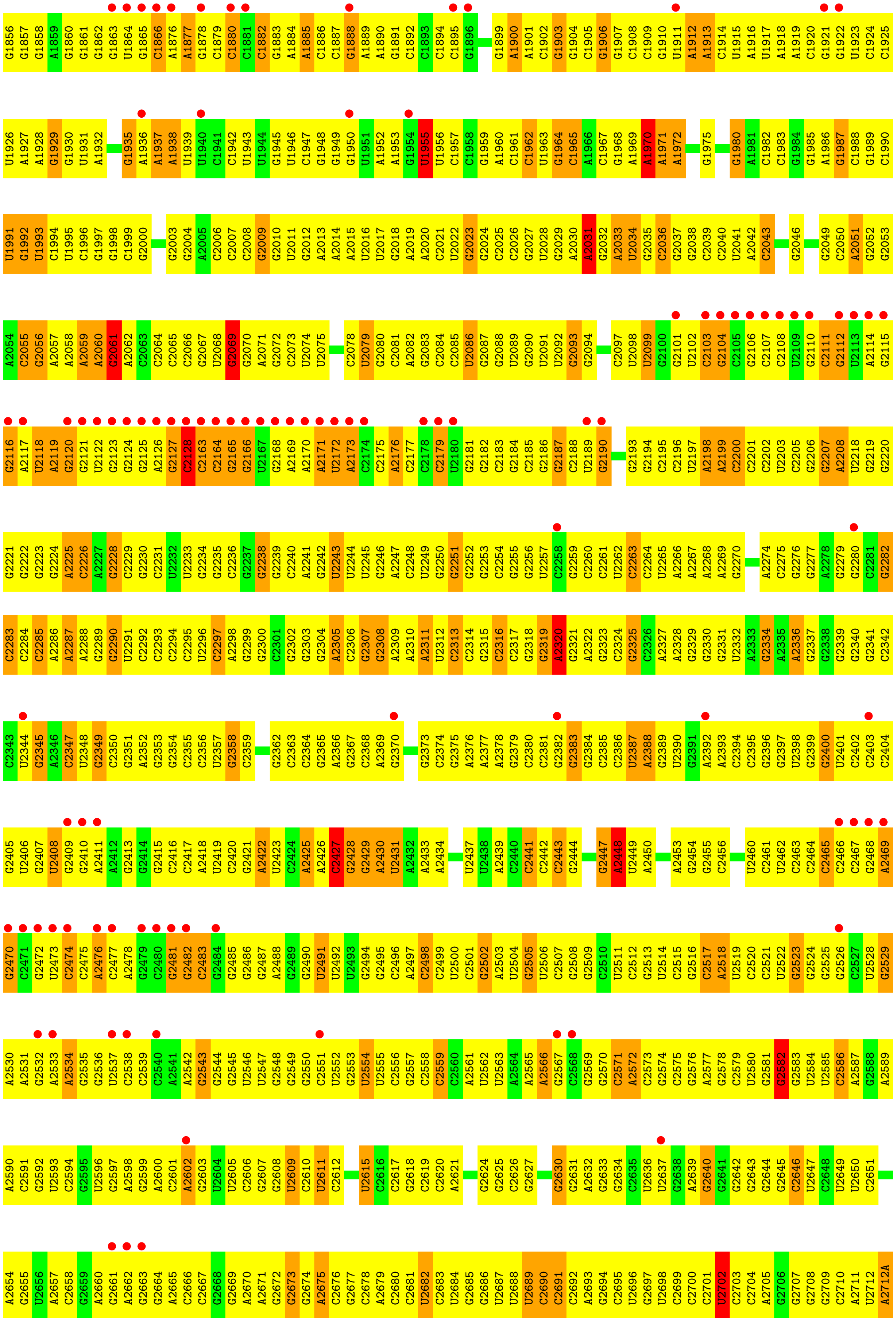
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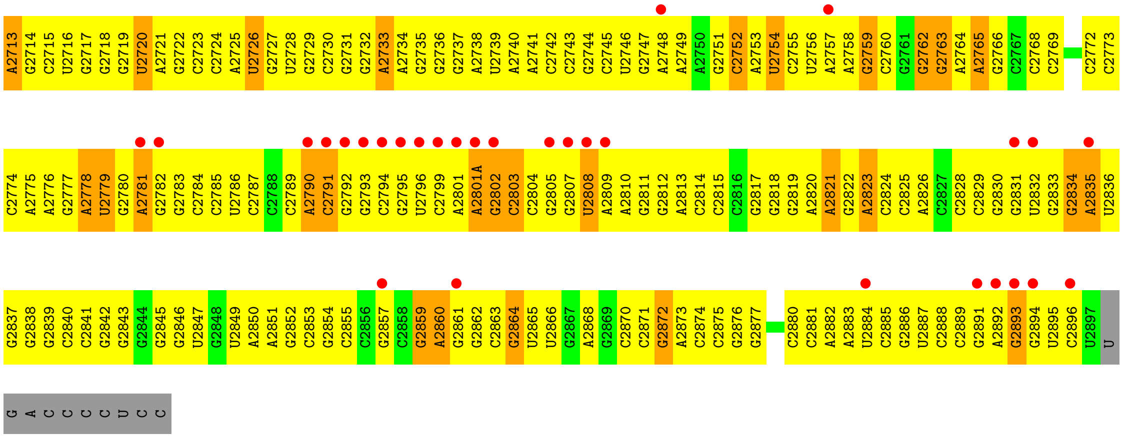

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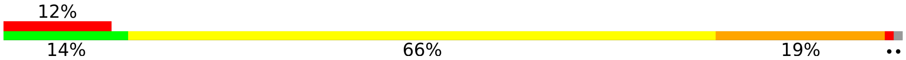

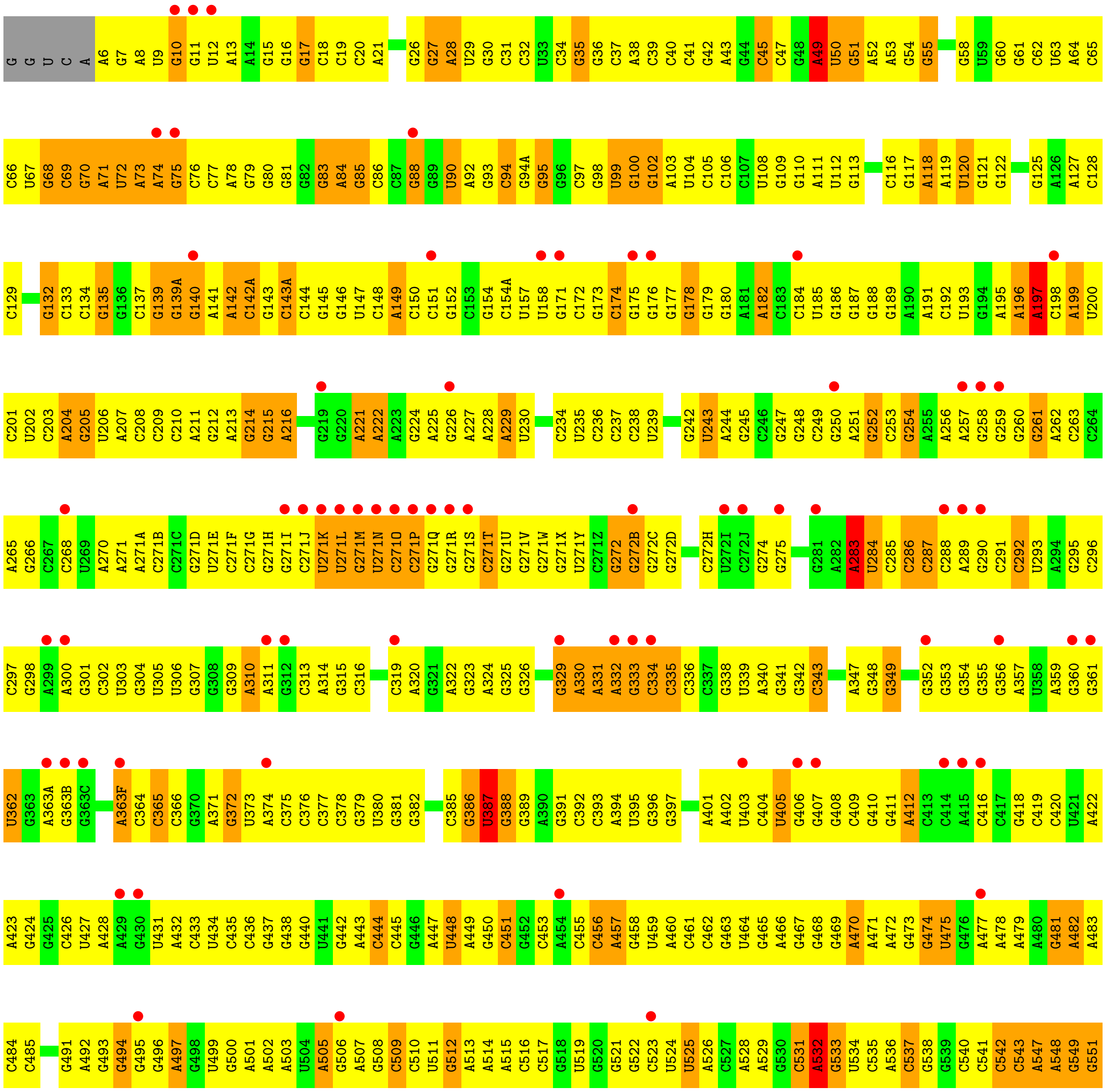

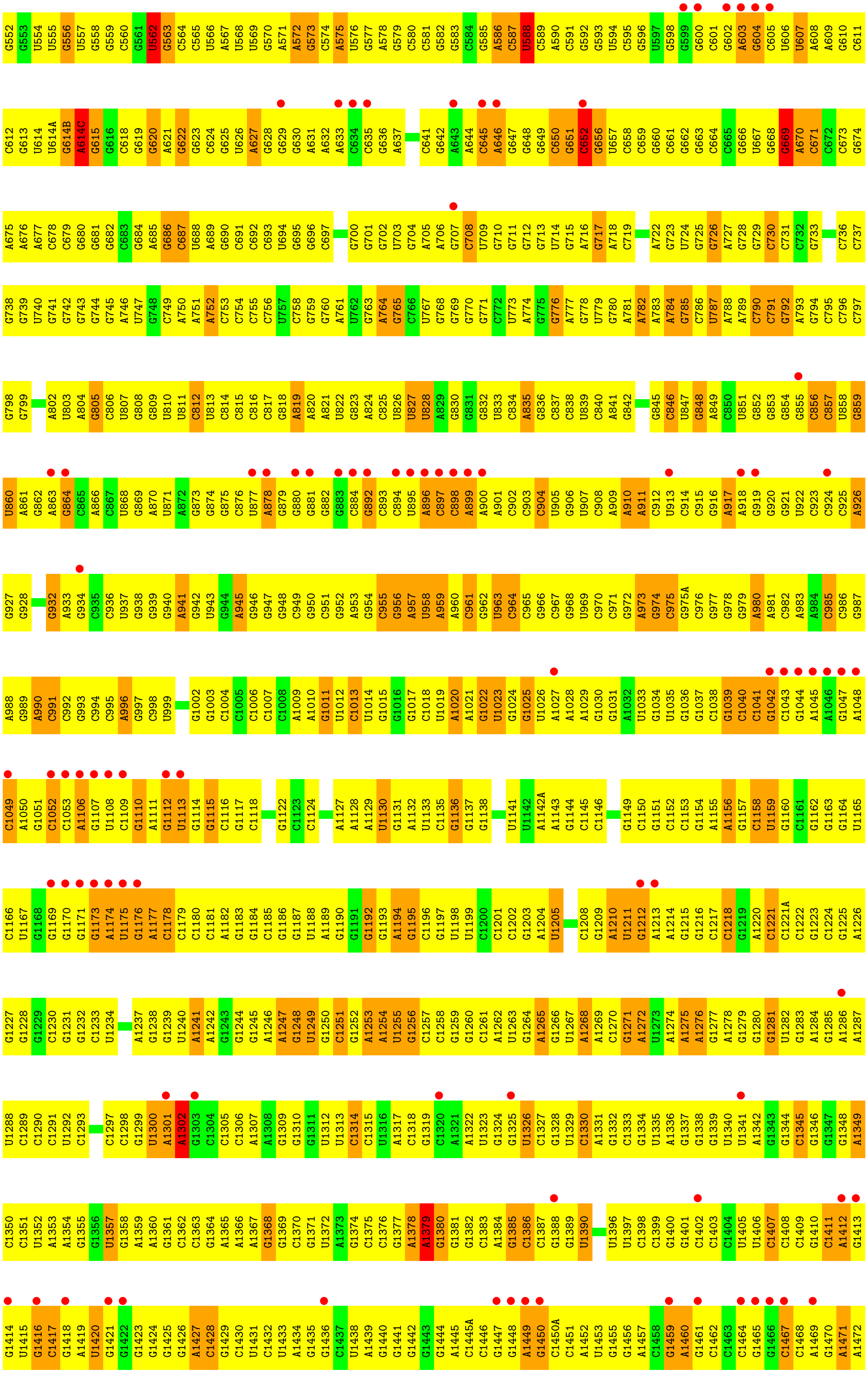
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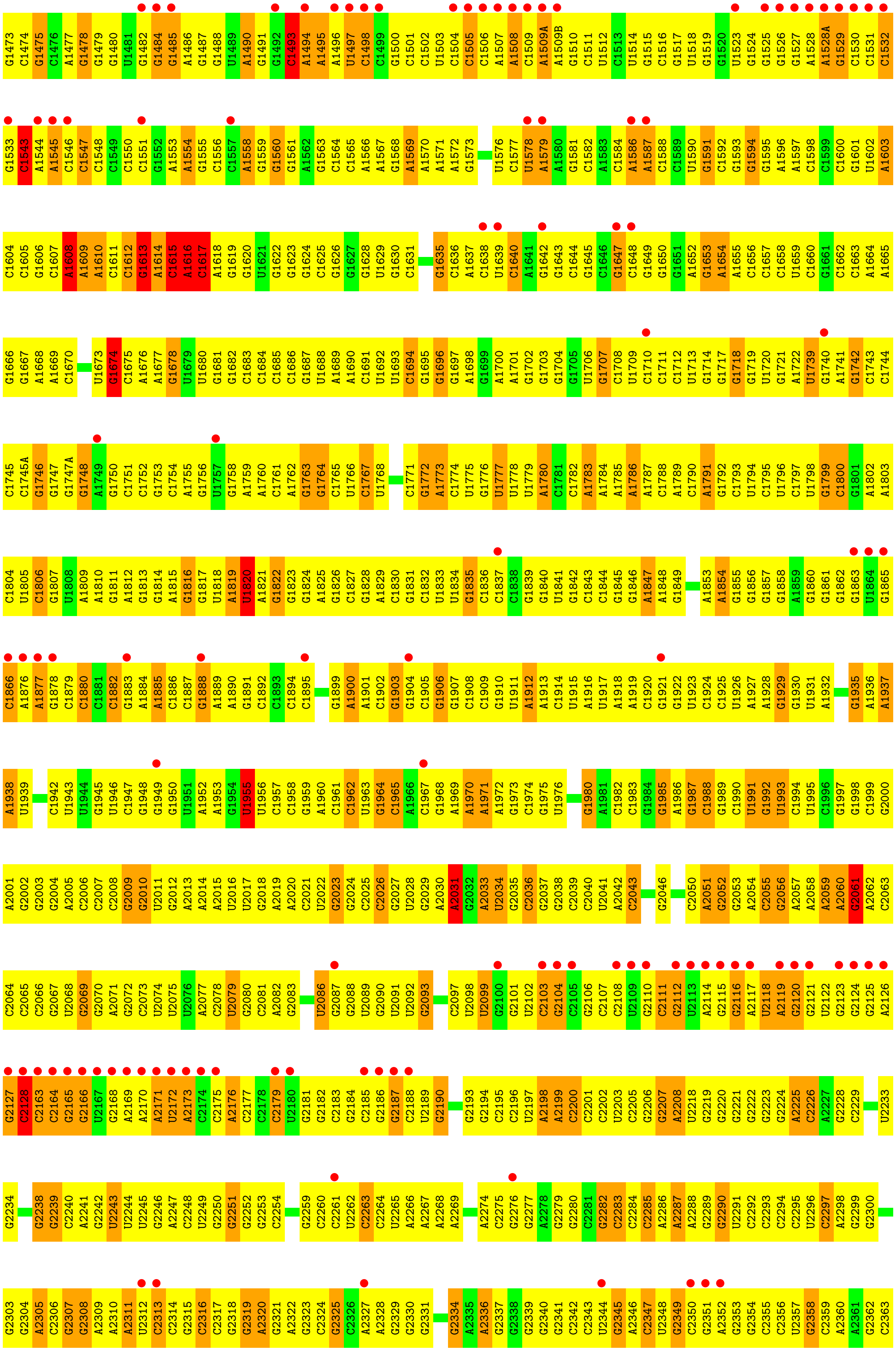
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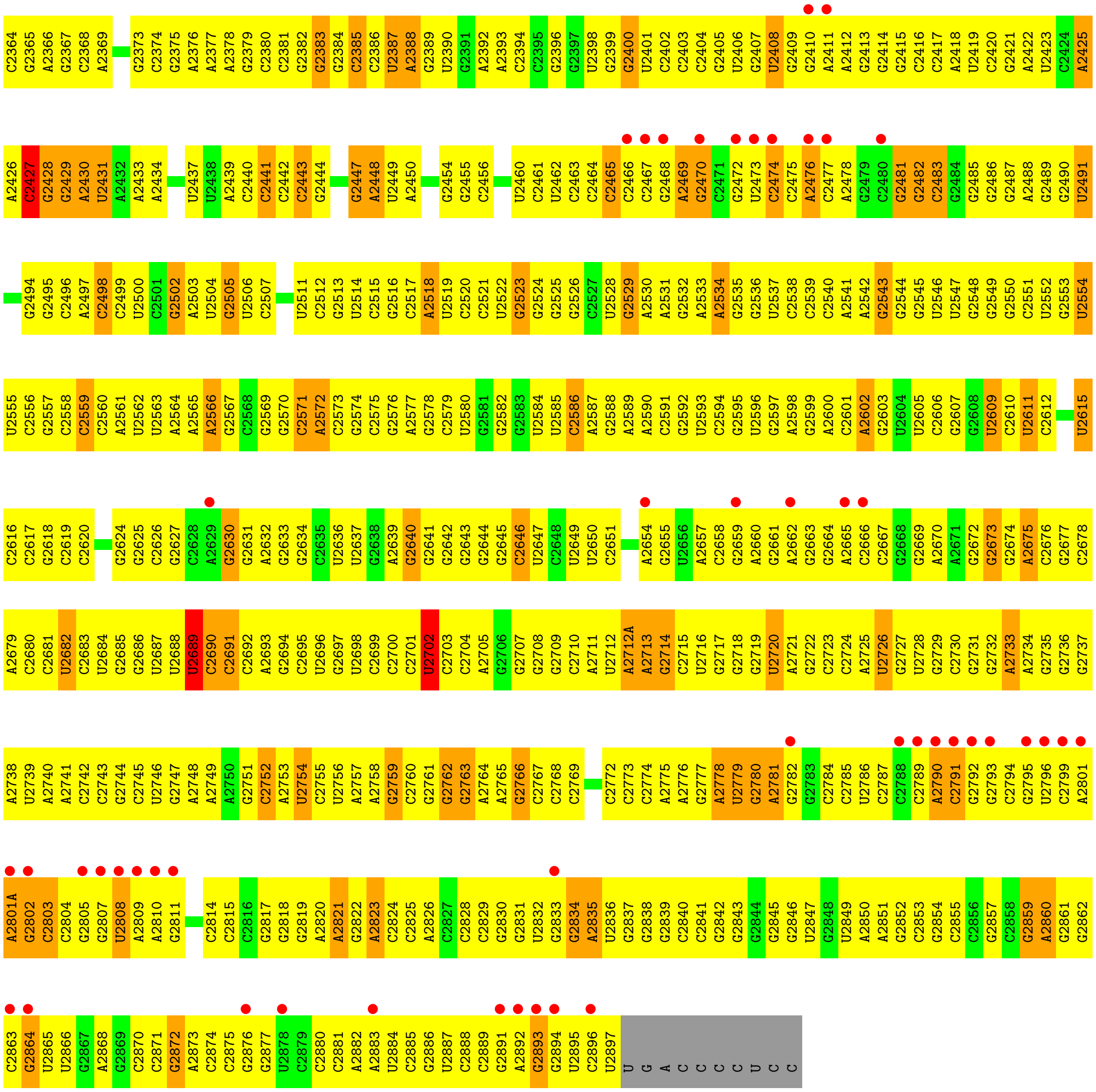
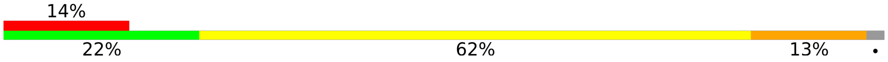
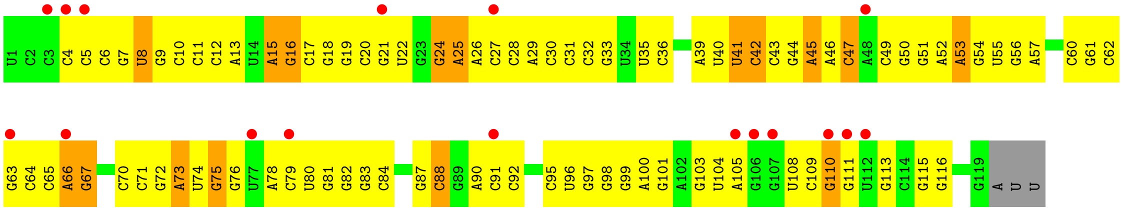
G2234 G2238 G2239 C2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2250 G2251 G2252 G2253 C2254 G2259 C2260 C2261 U2262 C2263 C2264 U2265 A2266 A2267 A2268 A2269 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2281 G2282 C2283 C2284 C2285 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 U2296 C2297 A2298 G2299 G2300
G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 C2316 C2317 G2318 G2319 A2320 G2321 A2322 G2323 C2324 G2325 C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 G2337 G2338 G2339 G2340 G2341 C2342 C2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2351 A2352 G2353 G2354 C2355 C2356 U2357 G2358 C2359 A2360 A2361 G2362 C2363



- Molecule 36: 5S ribosomal RNA

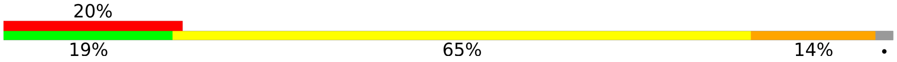
Chain BB:

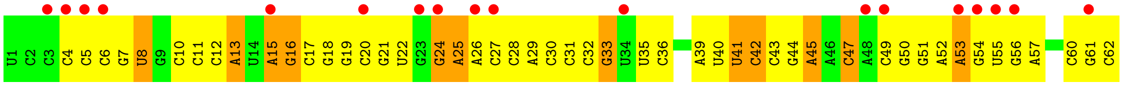


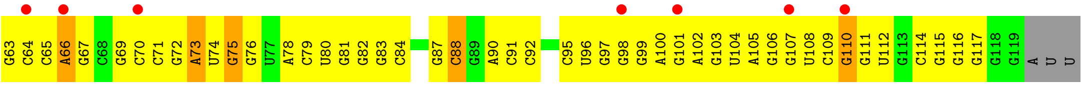


- Molecule 36: 5S ribosomal RNA

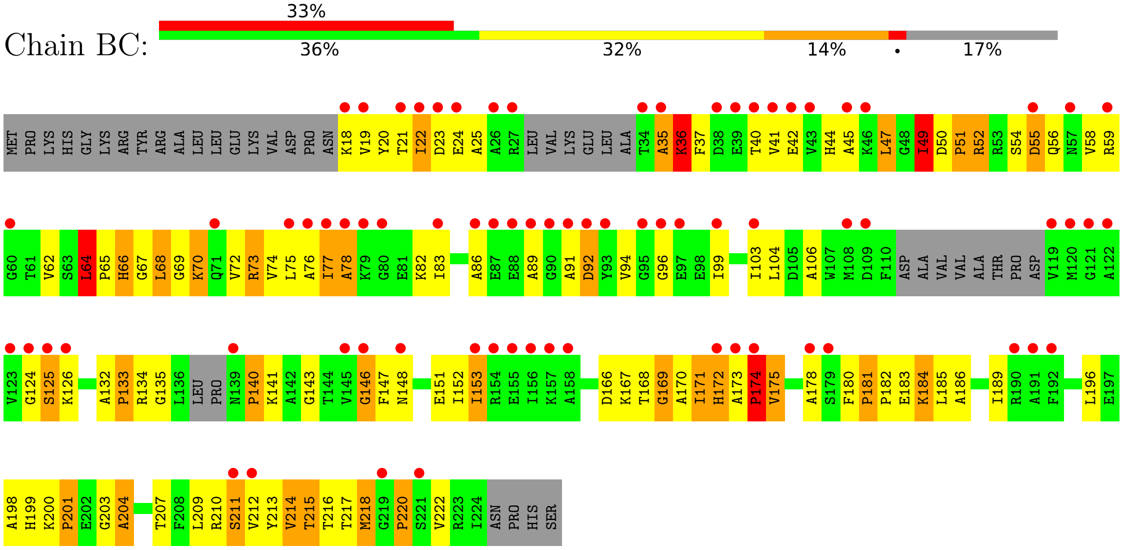
Chain DB:



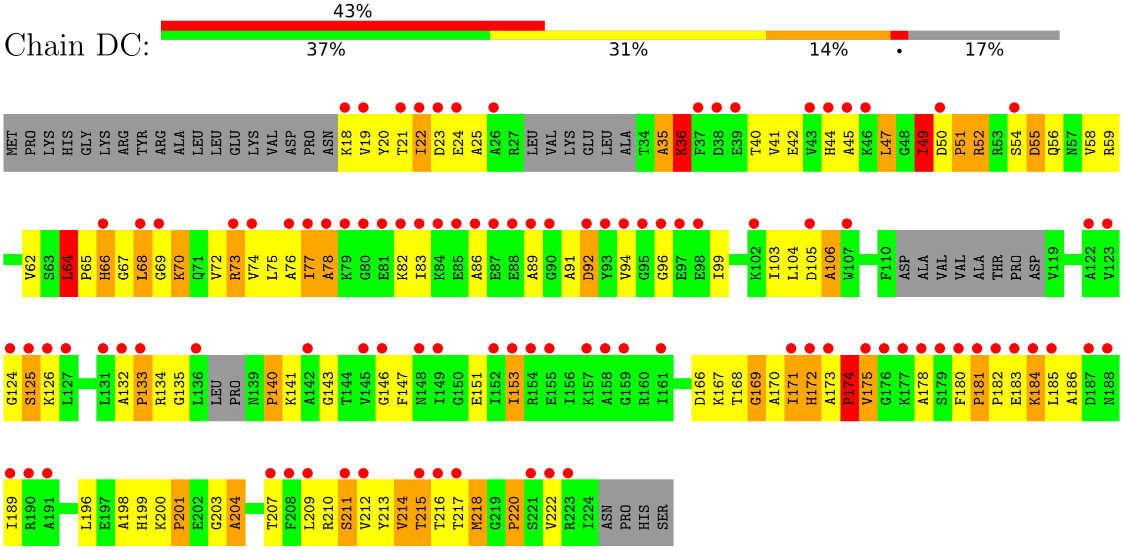




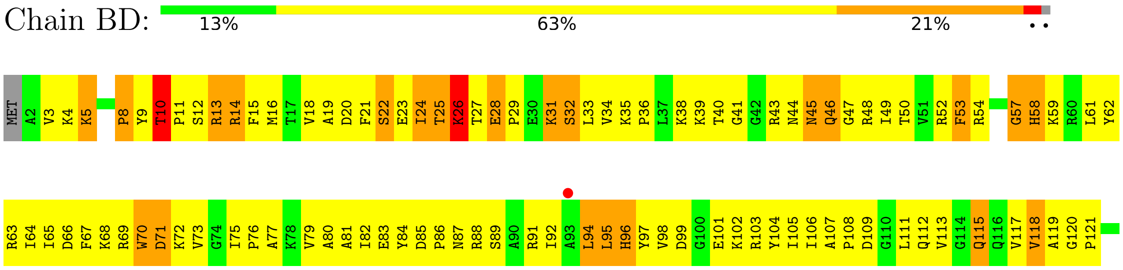
- Molecule 37: 50S RIBOSOMAL PROTEIN L1

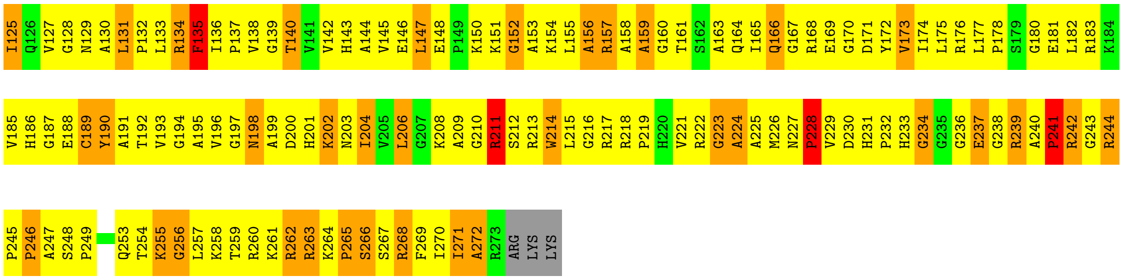


- Molecule 37: 50S RIBOSOMAL PROTEIN L1



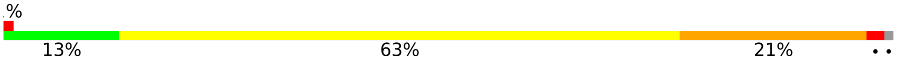
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

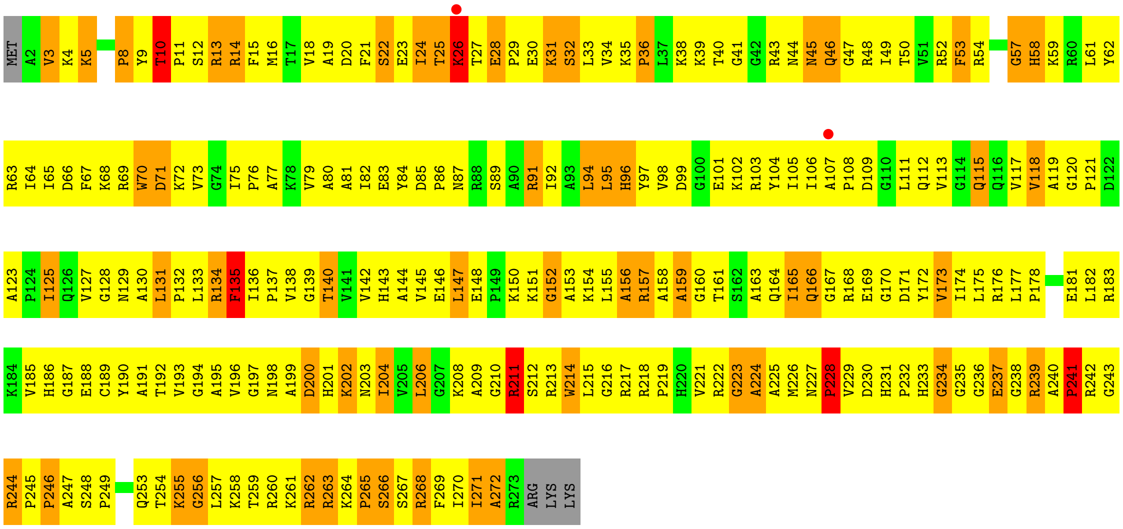




- Molecule 38: 50S RIBOSOMAL PROTEIN L2

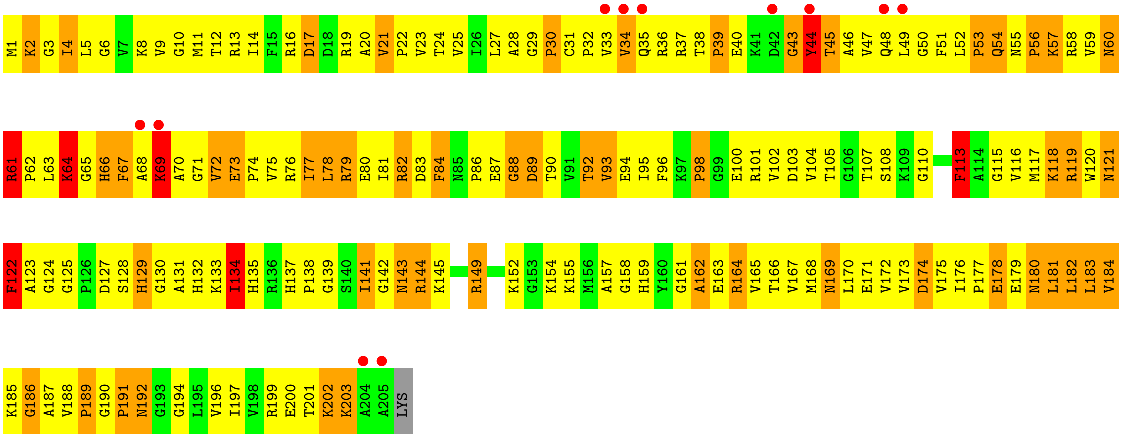
Chain DD:





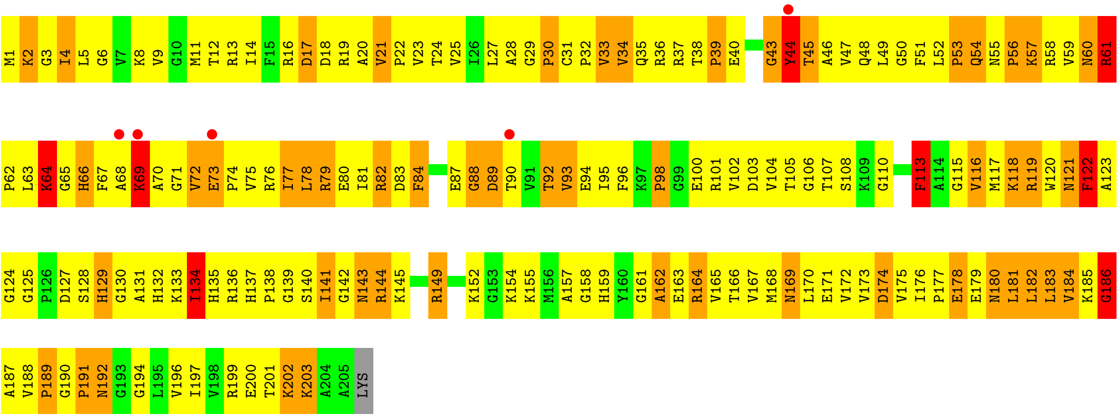
- Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



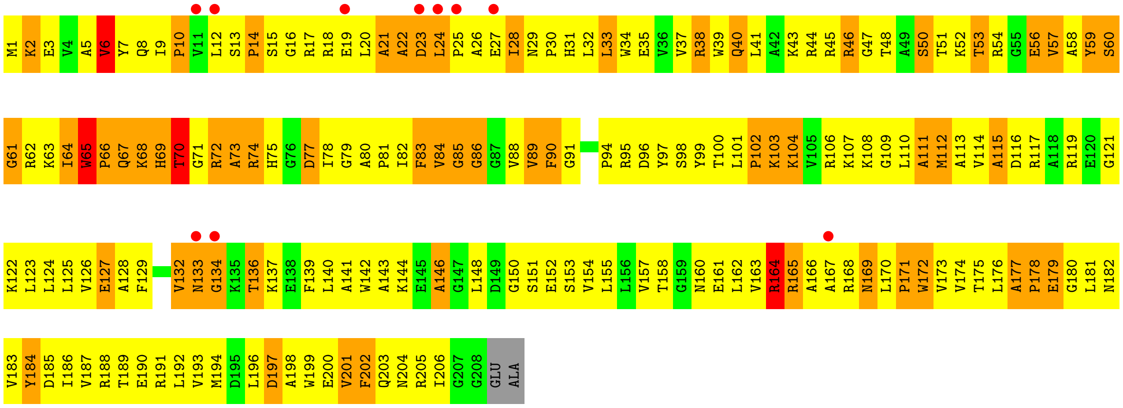
- Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE:



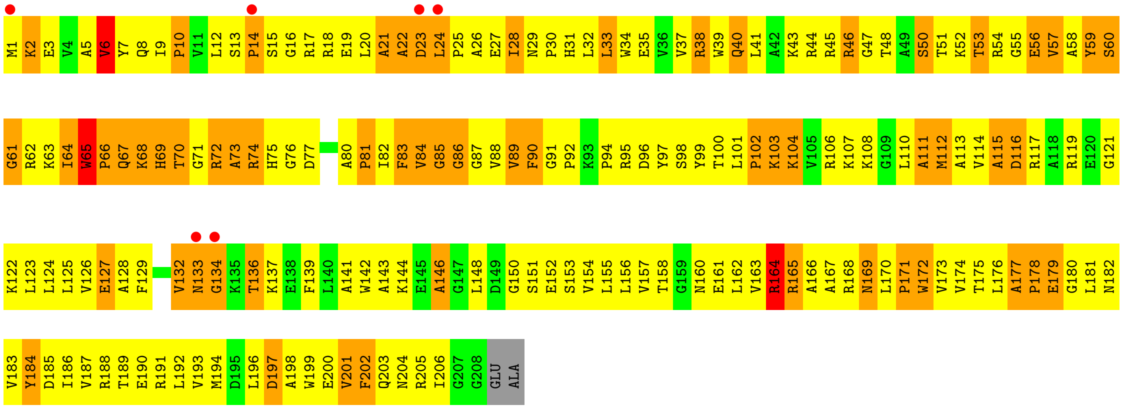
- Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



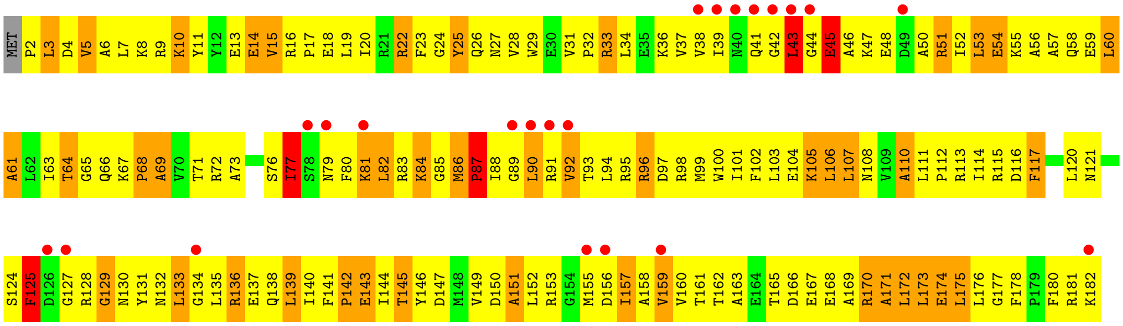
- Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain DF:



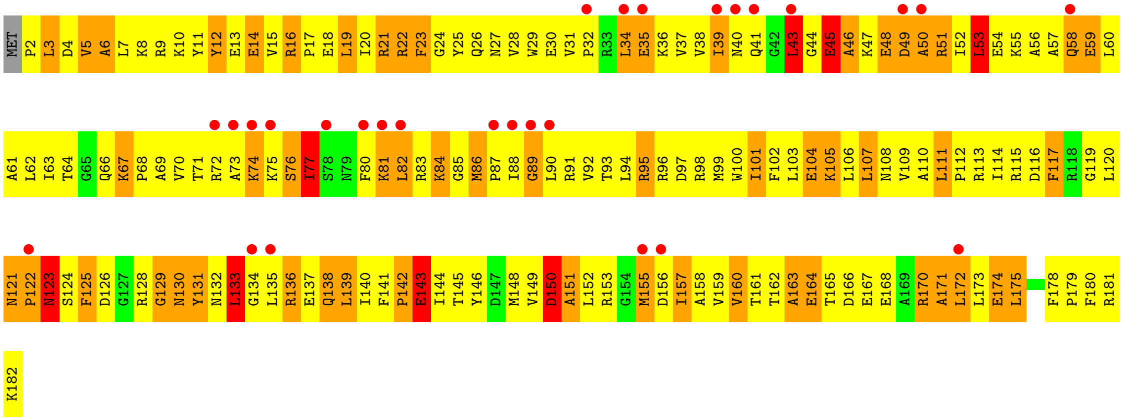
- Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:



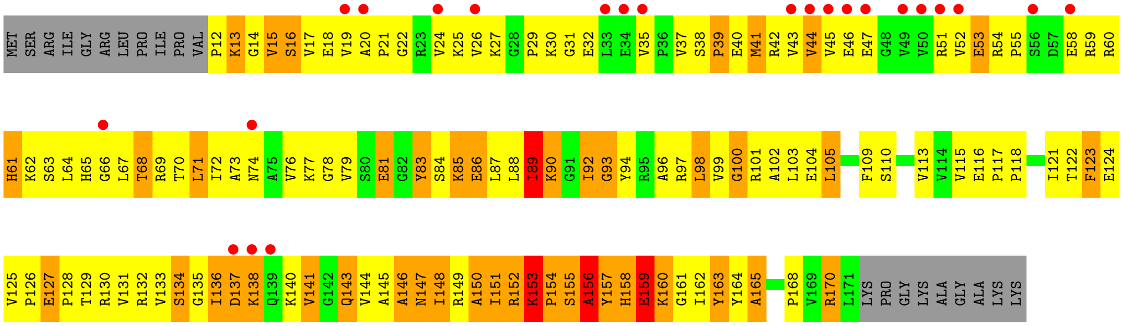
- Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain DG:



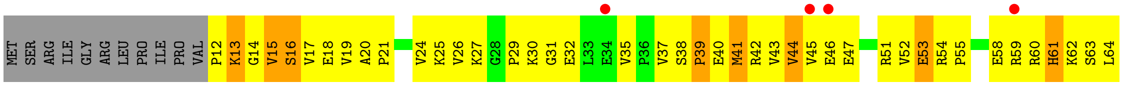
- Molecule 42: 50S RIBOSOMAL PROTEIN L6

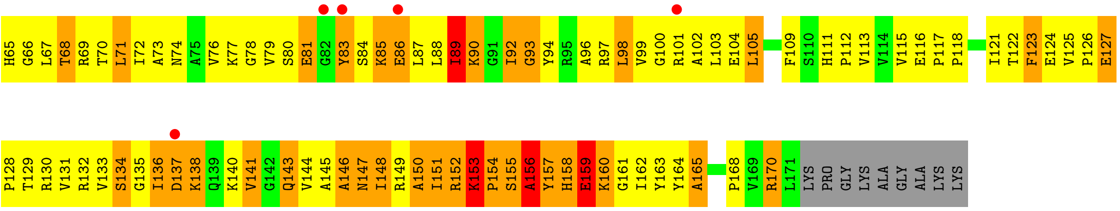
Chain BH:



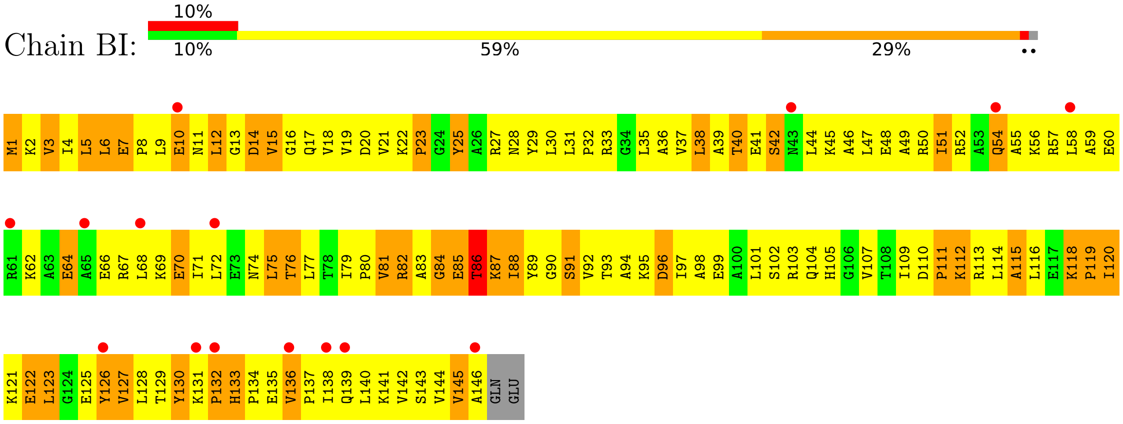
- Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH:

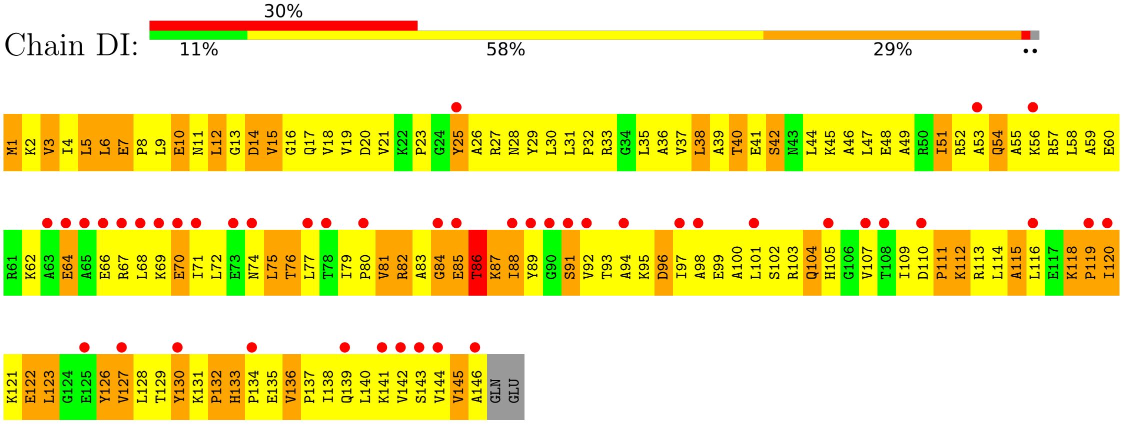




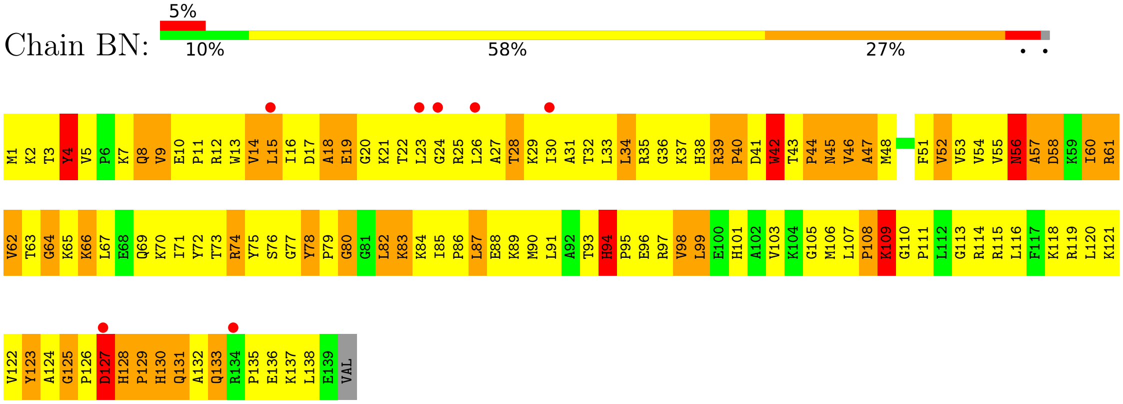
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



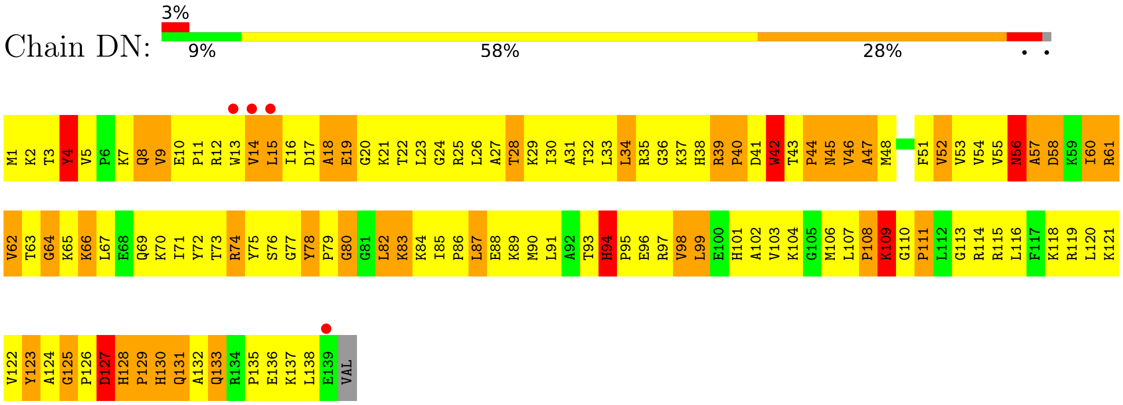
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



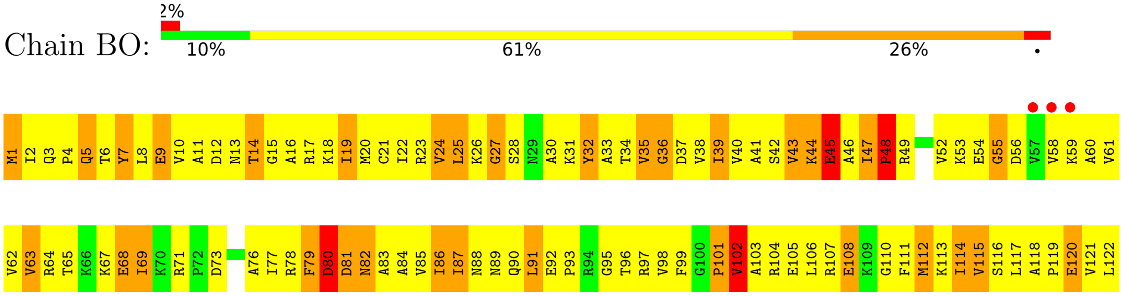
• Molecule 44: 50S RIBOSOMAL PROTEIN L13



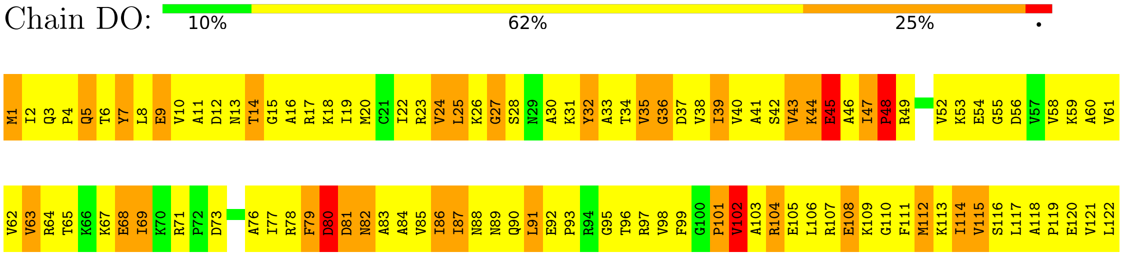
• Molecule 44: 50S RIBOSOMAL PROTEIN L13



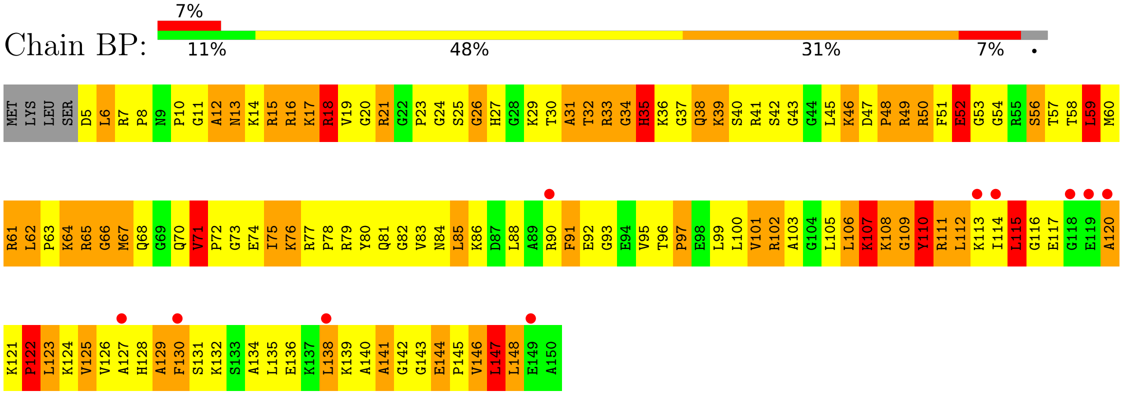
- Molecule 45: 50S RIBOSOMAL PROTEIN L14



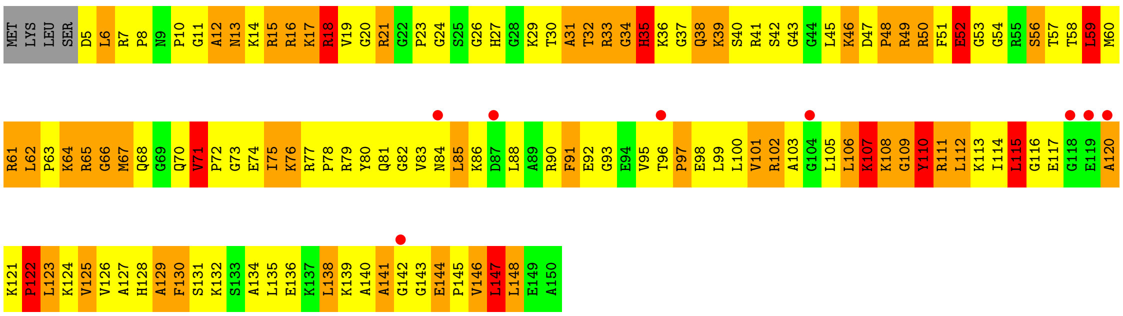
- Molecule 45: 50S RIBOSOMAL PROTEIN L14



- Molecule 46: 50S RIBOSOMAL PROTEIN L15

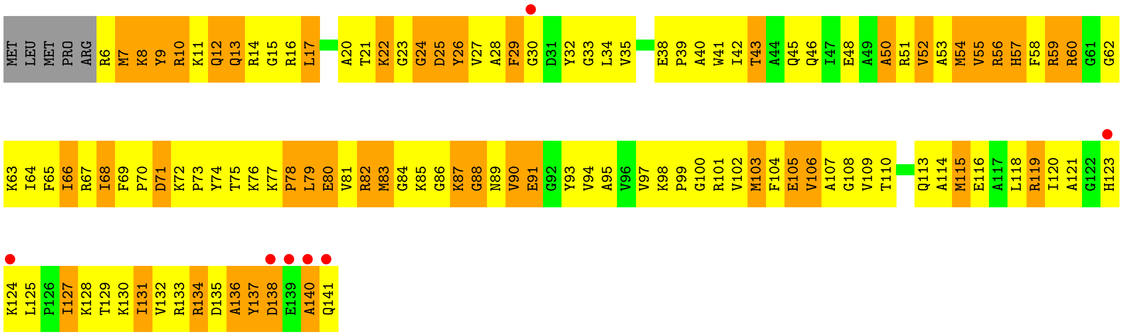


- Molecule 46: 50S RIBOSOMAL PROTEIN L15



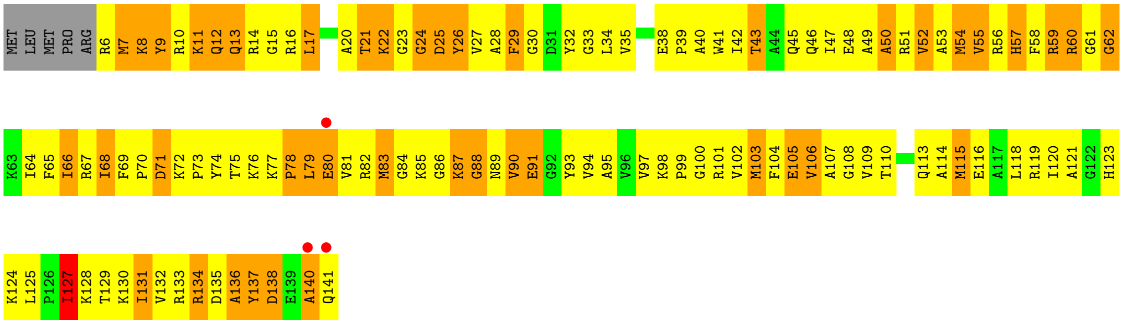
- Molecule 47: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



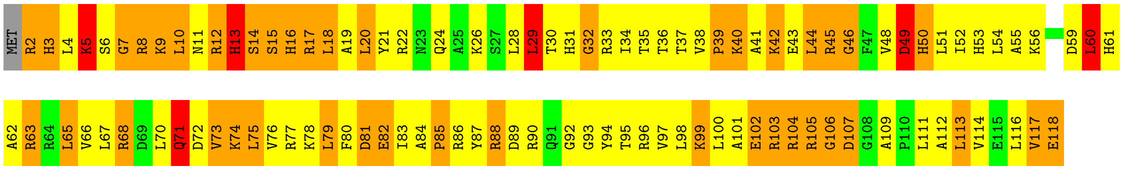
- Molecule 47: 50S RIBOSOMAL PROTEIN L16

Chain DQ:

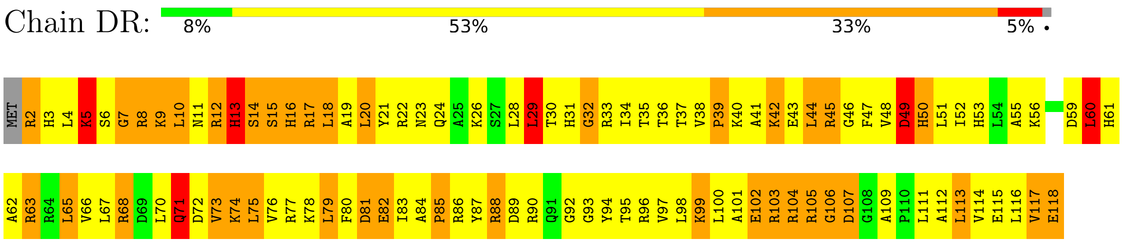


- Molecule 48: 50S RIBOSOMAL PROTEIN L17

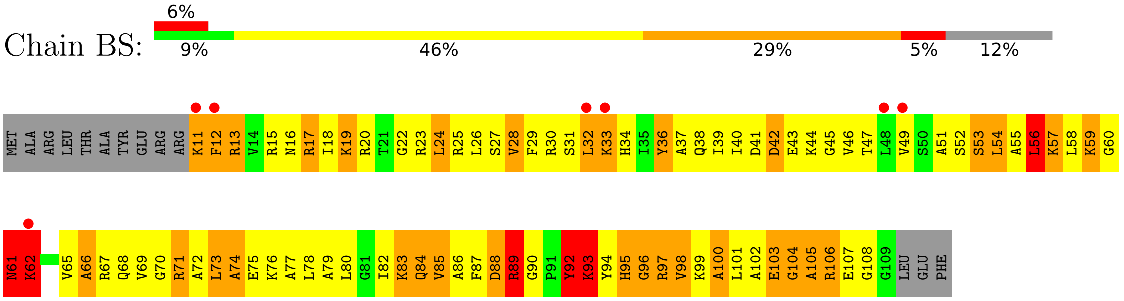
Chain BR:



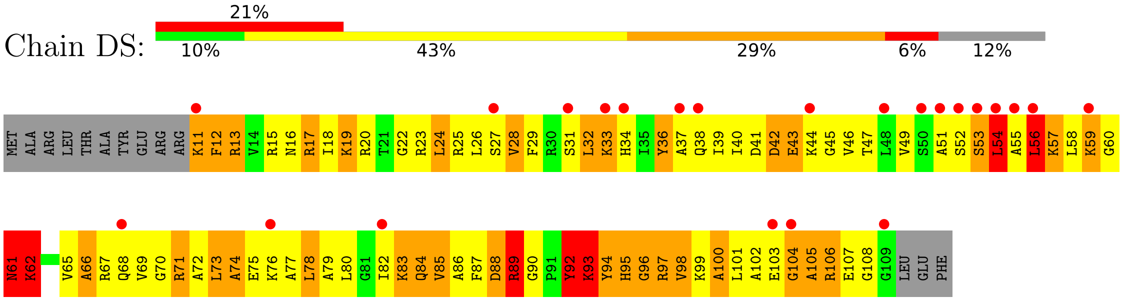
- Molecule 48: 50S RIBOSOMAL PROTEIN L17



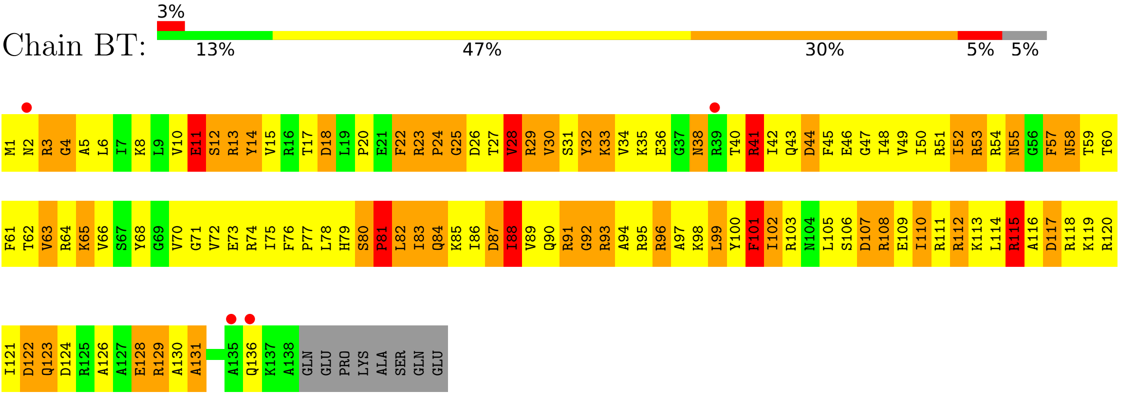
- Molecule 49: 50S RIBOSOMAL PROTEIN L18



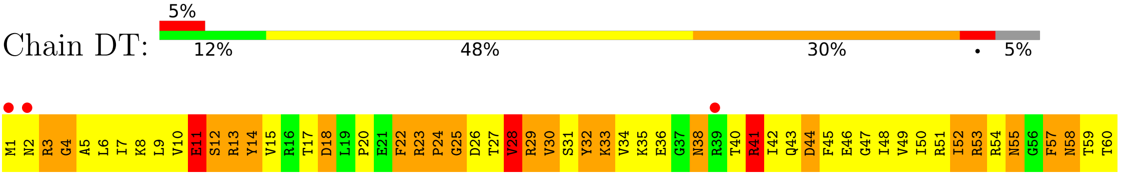
- Molecule 49: 50S RIBOSOMAL PROTEIN L18

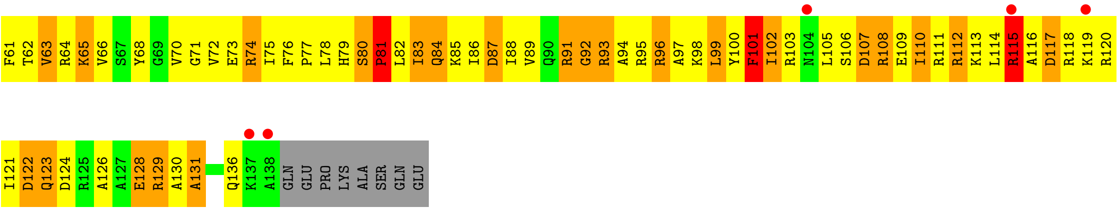


- Molecule 50: 50S RIBOSOMAL PROTEIN L19



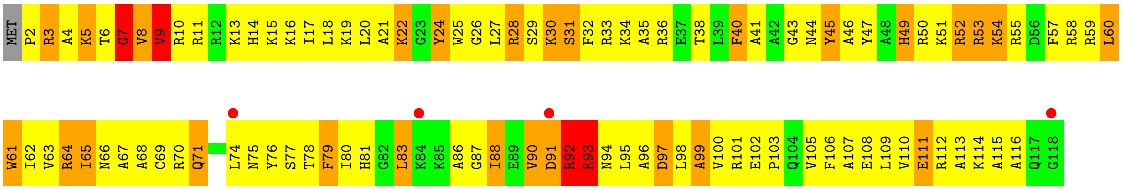
- Molecule 50: 50S RIBOSOMAL PROTEIN L19





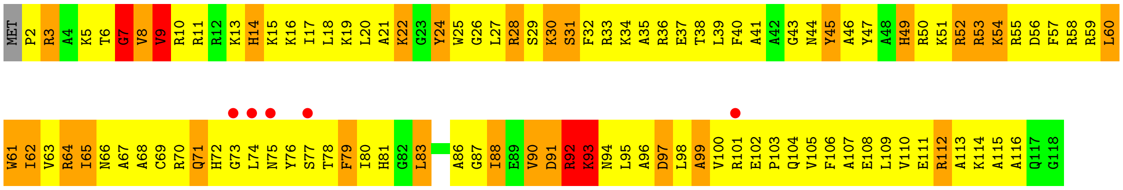
- Molecule 51: 50S RIBOSOMAL PROTEIN L20

Chain BU:



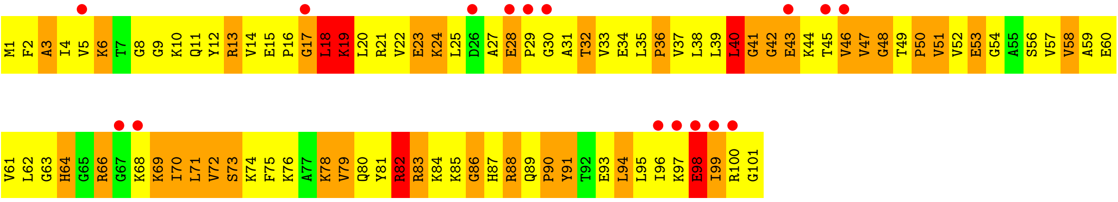
- Molecule 51: 50S RIBOSOMAL PROTEIN L20

Chain DU:



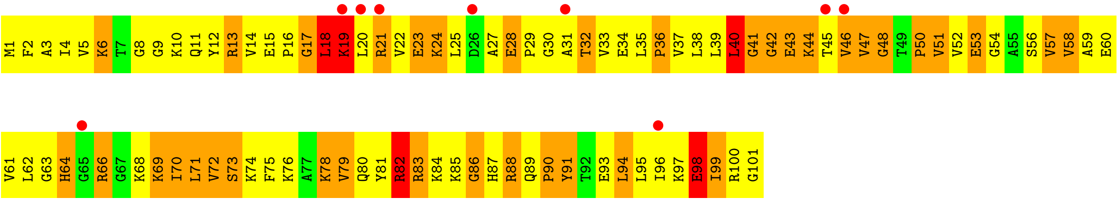
- Molecule 52: 50S RIBOSOMAL PROTEIN L21

Chain BV:



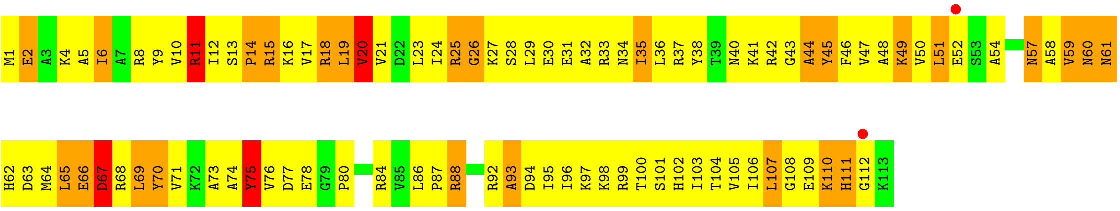
- Molecule 52: 50S RIBOSOMAL PROTEIN L21

Chain DV:



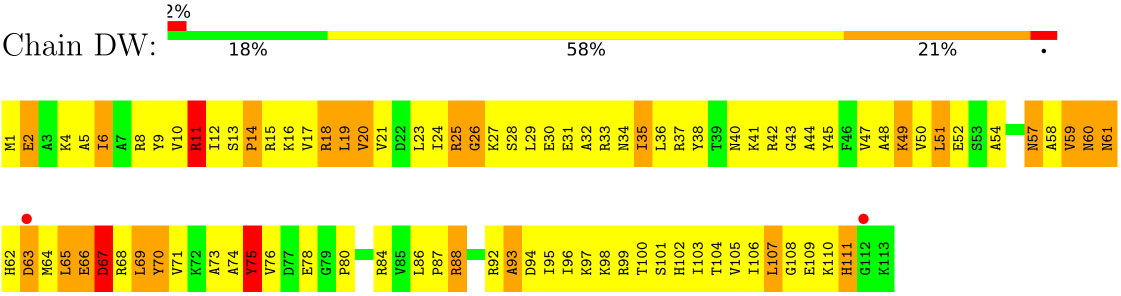
- Molecule 53: 50S RIBOSOMAL PROTEIN L22

Chain BW:



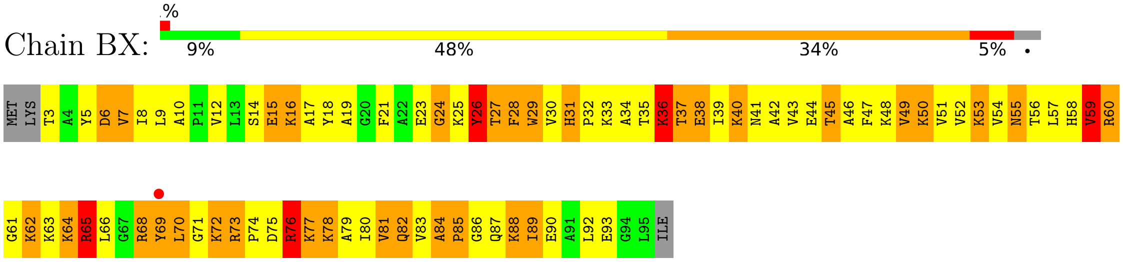
- Molecule 53: 50S RIBOSOMAL PROTEIN L22

Chain DW:



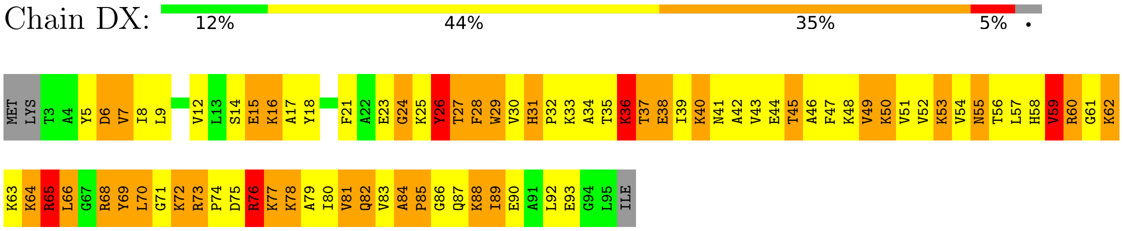
- Molecule 54: 50S RIBOSOMAL PROTEIN L23

Chain BX:



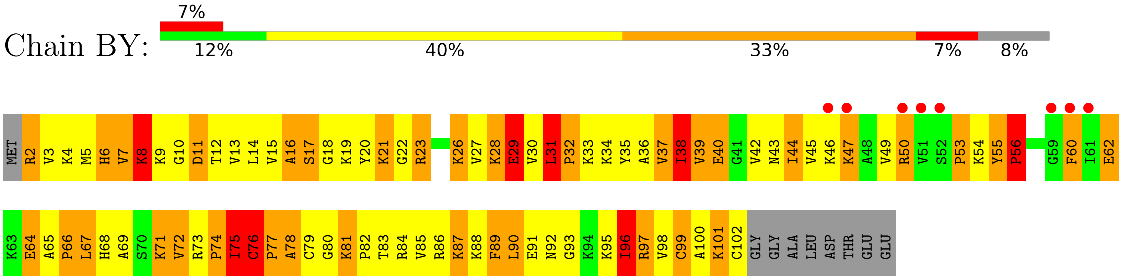
- Molecule 54: 50S RIBOSOMAL PROTEIN L23

Chain DX:



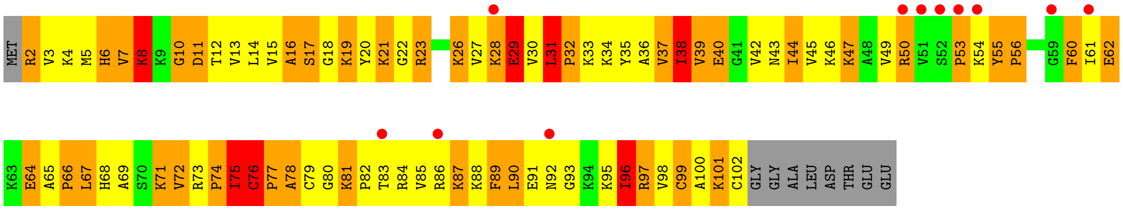
- Molecule 55: 50S RIBOSOMAL PROTEIN L24

Chain BY:



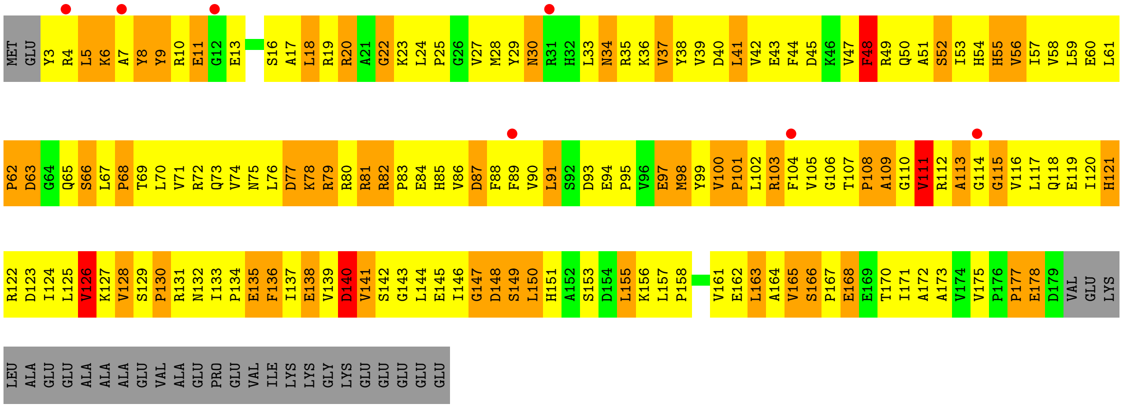
- Molecule 55: 50S RIBOSOMAL PROTEIN L24

Chain DY:



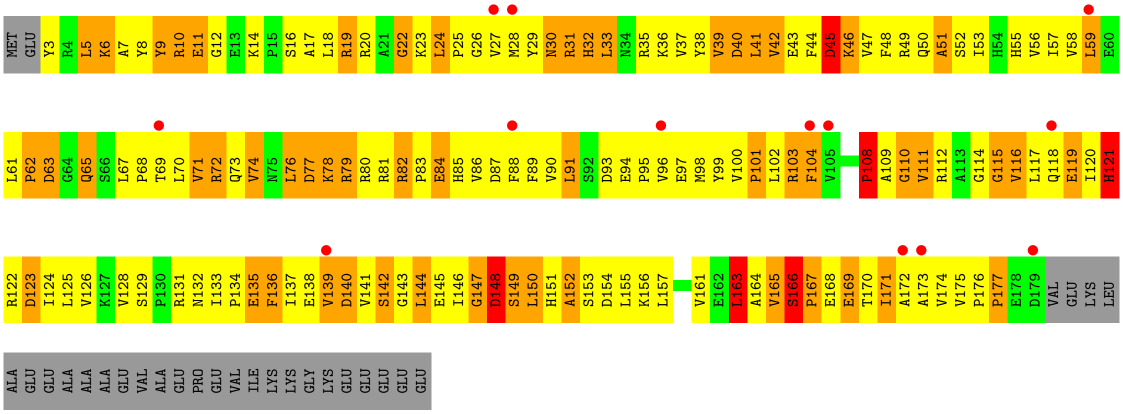
- Molecule 56: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



- Molecule 56: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.41Å 450.11Å 630.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 49.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.50) 98.9 (49.89-3.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.265 , 0.326 0.260 , 0.318	Depositor DCC
R_{free} test set	34086 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å^2)	81.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 94.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	290487	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: 5MU, ZN, 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	0.49	0/36190	0.72	11/56486 (0.0%)
1	CA	0.49	0/36190	0.72	5/56486 (0.0%)
2	AB	0.37	0/1936	0.65	0/2611
2	CB	0.36	0/1936	0.64	0/2611
3	AC	0.37	0/1637	0.63	0/2207
3	CC	0.35	0/1637	0.63	0/2207
4	AD	0.43	0/1733	0.68	0/2318
4	CD	0.42	0/1733	0.68	0/2318
5	AE	0.41	0/1163	0.68	0/1566
5	CE	0.41	0/1163	0.68	0/1566
6	AF	0.36	0/856	0.67	0/1154
6	CF	0.39	0/856	0.68	0/1154
7	AG	0.35	0/1276	0.63	0/1709
7	CG	0.34	0/1276	0.62	0/1709
8	AH	0.36	0/1136	0.66	0/1527
8	CH	0.37	0/1136	0.67	0/1527
9	AI	0.35	0/1027	0.63	0/1372
9	CI	0.34	0/1027	0.62	0/1372
10	AJ	0.38	0/808	0.66	0/1087
10	CJ	0.37	0/808	0.65	0/1087
11	AK	0.37	0/900	0.66	0/1213
11	CK	0.37	0/900	0.67	0/1213
12	AL	0.44	0/987	0.72	0/1322
12	CL	0.42	0/987	0.72	0/1322
13	AM	0.33	0/994	0.59	0/1322
13	CM	0.32	0/994	0.60	0/1322
14	AN	0.39	0/501	0.68	0/664
14	CN	0.37	0/501	0.67	0/664
15	AO	0.36	0/745	0.64	0/992
15	CO	0.36	0/745	0.63	0/992
16	AP	0.47	0/717	0.74	0/965
16	CP	0.43	0/717	0.73	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.41	0/837	0.71	0/1119
17	CQ	0.40	0/837	0.71	0/1119
18	AR	0.39	0/579	0.72	0/768
18	CR	0.41	0/579	0.73	0/768
19	AS	0.36	0/643	0.61	0/867
19	CS	0.36	0/643	0.60	0/867
20	AT	0.34	0/765	0.69	0/1007
20	CT	0.33	0/765	0.69	0/1007
21	AU	0.44	0/213	0.64	0/279
21	CU	0.42	0/213	0.63	0/279
22	AV	0.66	0/405	0.77	0/630
22	CV	0.61	0/405	0.77	1/630 (0.2%)
23	AW	0.43	0/1810	0.73	0/2821
23	CW	0.46	0/1810	0.72	0/2821
24	AX	0.70	0/256	0.93	0/397
24	CX	0.68	0/256	0.91	0/397
25	AY	0.40	0/1497	0.71	0/2017
25	CY	0.44	0/1497	0.72	0/2017
26	B0	0.39	0/660	0.64	0/882
26	D0	0.40	0/660	0.64	0/882
27	B1	0.57	0/700	1.00	1/931 (0.1%)
27	D1	0.55	0/700	0.96	3/931 (0.3%)
28	B2	0.49	0/423	0.97	2/560 (0.4%)
28	D2	0.52	0/423	0.91	1/560 (0.2%)
29	B3	0.39	0/473	0.68	0/636
29	D3	0.40	0/473	0.68	0/636
30	B4	0.43	0/241	0.80	3/334 (0.9%)
30	D4	0.44	0/241	0.80	4/334 (1.2%)
31	B5	0.37	0/473	0.69	0/639
31	D5	0.38	0/473	0.71	0/639
32	B6	0.45	0/387	0.63	0/517
32	D6	0.42	0/387	0.63	0/517
33	B7	0.53	0/427	0.83	0/563
33	D7	0.53	0/427	0.84	1/563 (0.2%)
34	B8	0.51	0/516	0.89	1/681 (0.1%)
34	D8	0.49	0/516	0.88	1/681 (0.1%)
35	BA	0.57	2/66757 (0.0%)	0.76	19/104221 (0.0%)
35	DA	0.61	3/66757 (0.0%)	0.76	19/104221 (0.0%)
36	BB	0.40	0/2853	0.70	0/4451
36	DB	0.39	0/2853	0.70	0/4451
37	BC	0.36	0/1145	0.68	7/1556 (0.4%)
37	DC	0.36	0/1146	0.68	7/1558 (0.4%)
38	BD	0.47	0/2155	0.84	2/2907 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DD	0.49	0/2155	0.84	2/2907 (0.1%)
39	BE	0.44	0/1597	0.78	1/2155 (0.0%)
39	DE	0.47	0/1597	0.79	1/2155 (0.0%)
40	BF	0.46	1/1659 (0.1%)	0.72	0/2246
40	DF	0.46	1/1659 (0.1%)	0.72	0/2246
41	BG	0.39	0/1498	0.76	2/2013 (0.1%)
41	DG	0.38	0/1498	0.76	0/2013
42	BH	0.37	0/1246	0.72	1/1684 (0.1%)
42	DH	0.40	0/1246	0.73	1/1684 (0.1%)
43	BI	0.39	0/1147	0.72	0/1553
43	DI	0.40	0/1147	0.71	0/1553
44	BN	0.40	0/1132	0.74	0/1527
44	DN	0.45	0/1132	0.75	0/1527
45	BO	0.47	0/943	0.78	0/1269
45	DO	0.49	0/943	0.80	0/1269
46	BP	0.42	0/1131	0.94	5/1504 (0.3%)
46	DP	0.40	0/1131	0.94	5/1504 (0.3%)
47	BQ	0.41	0/1100	0.76	0/1470
47	DQ	0.42	0/1100	0.78	0/1470
48	BR	0.39	0/974	0.75	0/1302
48	DR	0.42	0/974	0.77	0/1302
49	BS	0.42	0/779	0.71	0/1038
49	DS	0.39	0/779	0.70	0/1038
50	BT	0.44	0/1156	0.77	1/1544 (0.1%)
50	DT	0.45	0/1156	0.77	1/1544 (0.1%)
51	BU	0.40	0/975	0.75	1/1297 (0.1%)
51	DU	0.46	0/975	0.77	1/1297 (0.1%)
52	BV	0.41	0/789	0.74	1/1054 (0.1%)
52	DV	0.42	0/789	0.75	1/1054 (0.1%)
53	BW	0.42	0/907	0.67	0/1216
53	DW	0.42	0/907	0.66	0/1216
54	BX	0.47	0/740	0.88	2/995 (0.2%)
54	DX	0.47	0/740	0.89	2/995 (0.2%)
55	BY	0.43	0/789	0.78	0/1053
55	DY	0.44	0/789	0.77	0/1053
56	BZ	0.40	0/1436	0.74	0/1951
56	DZ	0.40	0/1436	0.77	1/1951 (0.1%)
All	All	0.51	7/313639 (0.0%)	0.74	117/468340 (0.0%)

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	0	17
1	CA	0	20
22	CV	0	2
23	AW	0	1
24	AX	0	3
35	BA	1	69
35	DA	1	63
All	All	2	175

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1543	C	N1-C2	5.59	1.45	1.40
40	DF	65	TRP	CB-CG	-5.48	1.40	1.50
35	DA	1543	C	N1-C2	5.43	1.45	1.40
35	DA	652	C	C3'-O3'	5.38	1.49	1.42
35	BA	652	C	C3'-O3'	5.30	1.49	1.42

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	DA	2128	C	C2'-C3'-O3'	10.31	132.19	109.50
35	BA	2128	C	C2'-C3'-O3'	10.29	132.14	109.50
46	BP	52	GLU	N-CA-C	8.91	135.05	111.00
46	DP	52	GLU	N-CA-C	8.80	134.76	111.00
38	BD	238	GLY	N-CA-C	-8.62	91.56	113.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	2128	C	C3'
35	DA	2128	C	C3'

5 of 175 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	21	G	Sidechain
1	AA	265	G	Sidechain
1	AA	323	U	Sidechain
1	AA	445	G	Sidechain
1	AA	96	U	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16313	2049	0
1	CA	32329	0	16314	2040	0
2	AB	1901	0	1951	382	0
2	CB	1901	0	1951	378	0
3	AC	1613	0	1677	256	0
3	CC	1613	0	1677	246	0
4	AD	1703	0	1763	346	0
4	CD	1703	0	1764	336	0
5	AE	1147	0	1207	211	0
5	CE	1147	0	1207	202	0
6	AF	843	0	857	151	0
6	CF	843	0	857	157	0
7	AG	1257	0	1296	235	0
7	CG	1257	0	1296	216	0
8	AH	1116	0	1177	231	0
8	CH	1116	0	1177	233	0
9	AI	1011	0	1041	208	0
9	CI	1011	0	1041	209	0
10	AJ	795	0	840	153	0
10	CJ	795	0	840	154	0
11	AK	885	0	904	179	0
11	CK	885	0	904	180	0
12	AL	971	0	1057	210	0
12	CL	971	0	1057	196	0
13	AM	988	0	1055	163	0
13	CM	988	0	1055	156	0
14	AN	492	0	529	95	0
14	CN	492	0	530	89	0
15	AO	734	0	771	111	0
15	CO	734	0	771	117	0
16	AP	701	0	720	157	0
16	CP	701	0	720	146	0
17	AQ	824	0	891	140	0
17	CQ	824	0	891	138	0
18	AR	574	0	644	138	0
18	CR	574	0	644	133	0
19	AS	630	0	652	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	630	0	652	138	0
20	AT	763	0	861	133	0
20	CT	763	0	861	125	0
21	AU	209	0	221	30	0
21	CU	209	0	221	28	0
22	AV	362	0	186	23	0
22	CV	362	0	186	20	0
23	AW	1641	0	836	105	0
23	CW	1641	0	839	72	0
24	AX	230	0	118	12	0
24	CX	230	0	117	16	0
25	AY	1478	0	1526	283	0
25	CY	1478	0	1526	303	0
26	B0	652	0	658	102	0
26	D0	652	0	658	87	0
27	B1	693	0	764	248	0
27	D1	693	0	763	241	0
28	B2	421	0	461	118	0
28	D2	421	0	461	146	0
29	B3	468	0	523	86	0
29	D3	468	0	523	82	0
30	B4	242	0	103	14	0
30	D4	242	0	103	10	0
31	B5	459	0	480	103	0
31	D5	459	0	480	107	0
32	B6	381	0	390	69	0
32	D6	381	0	390	72	0
33	B7	419	0	467	75	0
33	D7	419	0	467	72	0
34	B8	508	0	576	154	0
34	D8	508	0	576	143	0
35	BA	59601	0	30029	3750	1
35	DA	59601	0	30026	3756	0
36	BB	2551	0	1294	137	1
36	DB	2551	0	1294	155	0
37	BC	1142	0	861	85	0
37	DC	1143	0	865	78	0
38	BD	2105	0	2182	497	0
38	DD	2105	0	2182	503	0
39	BE	1564	0	1629	382	0
39	DE	1564	0	1629	393	0
40	BF	1624	0	1677	349	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DF	1624	0	1676	353	0
41	BG	1474	0	1534	336	0
41	DG	1474	0	1534	441	0
42	BH	1223	0	1282	242	0
42	DH	1223	0	1282	245	0
43	BI	1132	0	1218	227	0
43	DI	1132	0	1218	225	0
44	BN	1105	0	1180	277	0
44	DN	1105	0	1180	291	0
45	BO	933	0	996	234	0
45	DO	933	0	996	237	0
46	BP	1114	0	1187	382	0
46	DP	1114	0	1187	378	0
47	BQ	1080	0	1127	274	0
47	DQ	1080	0	1127	259	0
48	BR	960	0	1021	221	0
48	DR	960	0	1021	220	0
49	BS	771	0	832	201	0
49	DS	771	0	832	207	0
50	BT	1142	0	1202	320	0
50	DT	1142	0	1202	325	0
51	BU	958	0	1014	245	0
51	DU	958	0	1014	256	0
52	BV	779	0	851	231	0
52	DV	779	0	851	234	0
53	BW	896	0	953	174	0
53	DW	896	0	953	164	0
54	BX	726	0	778	251	0
54	DX	726	0	777	252	0
55	BY	776	0	870	205	0
55	DY	776	0	870	208	0
56	BZ	1404	0	1432	353	0
56	DZ	1404	0	1432	318	0
57	AA	204	0	0	0	0
57	AD	2	0	0	0	0
57	AE	2	0	0	0	0
57	AG	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	1	0	0	0	0
57	AV	4	0	0	0	0
57	AW	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AX	5	0	0	0	0
57	B1	4	0	0	0	0
57	B2	2	0	0	0	0
57	B3	1	0	0	0	0
57	B5	2	0	0	0	0
57	B7	1	0	0	0	0
57	BA	445	0	0	1	0
57	BB	20	0	0	0	0
57	BD	3	0	0	0	0
57	BE	1	0	0	0	0
57	BF	4	0	0	0	0
57	BG	1	0	0	0	0
57	BN	4	0	0	0	0
57	BO	1	0	0	0	0
57	BP	3	0	0	0	0
57	BU	2	0	0	1	0
57	BX	2	0	0	0	0
57	CA	208	0	0	0	0
57	CE	3	0	0	0	0
57	CG	1	0	0	0	0
57	CL	2	0	0	0	0
57	CN	1	0	0	0	0
57	CV	4	0	0	0	0
57	CW	23	0	0	0	0
57	CX	4	0	0	0	0
57	D1	4	0	0	0	0
57	D2	2	0	0	0	0
57	D3	1	0	0	0	0
57	D5	1	0	0	0	0
57	D7	1	0	0	0	0
57	DA	441	0	0	0	0
57	DB	19	0	0	0	0
57	DD	3	0	0	0	0
57	DE	2	0	0	0	0
57	DF	5	0	0	0	0
57	DG	1	0	0	0	0
57	DH	1	0	0	0	0
57	DN	2	0	0	0	0
57	DP	4	0	0	0	0
57	DS	1	0	0	0	0
57	DU	3	0	0	0	0
57	DV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DX	3	0	0	0	0
58	AD	1	0	0	0	0
58	AN	1	0	0	0	0
58	CD	1	0	0	0	0
58	CN	1	0	0	0	0
All	All	290487	0	197331	30322	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 62.

The worst 5 of 30322 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)
53:BW:29:LEU:HD21	53:BW:33:ARG:HE	1.07	1.20
55:DY:45:VAL:HA	55:DY:62:GLU:HG2	1.20	1.20
35:DA:2758:A:H2'	35:DA:2759:G:H5"	1.25	1.19
1:CA:1442(A):G:H3'	1:CA:1442(B):A:H5"	1.22	1.18
43:BI:91:SER:HB2	43:BI:119:PRO:HB2	1.21	1.18

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:BA:1593:G:O2'	36:BB:54:G:OP1[1_655]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	114 (49%)	69 (30%)	50 (22%)	0	1
2	CB	233/256 (91%)	114 (49%)	68 (29%)	51 (22%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	205/239 (86%)	119 (58%)	50 (24%)	36 (18%)	0	2
3	CC	205/239 (86%)	121 (59%)	47 (23%)	37 (18%)	0	2
4	AD	206/209 (99%)	101 (49%)	62 (30%)	43 (21%)	0	1
4	CD	206/209 (99%)	101 (49%)	61 (30%)	44 (21%)	0	1
5	AE	149/162 (92%)	85 (57%)	44 (30%)	20 (13%)	0	4
5	CE	149/162 (92%)	84 (56%)	45 (30%)	20 (13%)	0	4
6	AF	99/101 (98%)	61 (62%)	23 (23%)	15 (15%)	0	3
6	CF	99/101 (98%)	60 (61%)	24 (24%)	15 (15%)	0	3
7	AG	153/156 (98%)	97 (63%)	31 (20%)	25 (16%)	0	2
7	CG	153/156 (98%)	97 (63%)	31 (20%)	25 (16%)	0	2
8	AH	136/138 (99%)	78 (57%)	39 (29%)	19 (14%)	0	3
8	CH	136/138 (99%)	79 (58%)	37 (27%)	20 (15%)	0	3
9	AI	121/128 (94%)	80 (66%)	27 (22%)	14 (12%)	0	5
9	CI	121/128 (94%)	79 (65%)	27 (22%)	15 (12%)	0	5
10	AJ	97/105 (92%)	64 (66%)	23 (24%)	10 (10%)	0	7
10	CJ	97/105 (92%)	64 (66%)	22 (23%)	11 (11%)	0	6
11	AK	117/129 (91%)	69 (59%)	31 (26%)	17 (14%)	0	3
11	CK	117/129 (91%)	68 (58%)	32 (27%)	17 (14%)	0	3
12	AL	123/135 (91%)	78 (63%)	28 (23%)	17 (14%)	0	3
12	CL	123/135 (91%)	77 (63%)	27 (22%)	19 (15%)	0	3
13	AM	113/126 (90%)	59 (52%)	35 (31%)	19 (17%)	0	2
13	CM	113/126 (90%)	60 (53%)	34 (30%)	19 (17%)	0	2
14	AN	58/61 (95%)	38 (66%)	12 (21%)	8 (14%)	0	3
14	CN	58/61 (95%)	38 (66%)	12 (21%)	8 (14%)	0	3
15	AO	86/89 (97%)	48 (56%)	26 (30%)	12 (14%)	0	3
15	CO	86/89 (97%)	49 (57%)	26 (30%)	11 (13%)	0	4
16	AP	82/88 (93%)	45 (55%)	24 (29%)	13 (16%)	0	2
16	CP	82/88 (93%)	45 (55%)	24 (29%)	13 (16%)	0	2
17	AQ	98/105 (93%)	66 (67%)	19 (19%)	13 (13%)	0	4
17	CQ	98/105 (93%)	65 (66%)	20 (20%)	13 (13%)	0	4
18	AR	68/88 (77%)	38 (56%)	18 (26%)	12 (18%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	68/88 (77%)	37 (54%)	20 (29%)	11 (16%)	0	2
19	AS	77/93 (83%)	49 (64%)	19 (25%)	9 (12%)	0	5
19	CS	77/93 (83%)	49 (64%)	19 (25%)	9 (12%)	0	5
20	AT	97/106 (92%)	46 (47%)	29 (30%)	22 (23%)	0	1
20	CT	97/106 (92%)	46 (47%)	30 (31%)	21 (22%)	0	1
21	AU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	9
21	CU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	9
25	AY	183/185 (99%)	115 (63%)	44 (24%)	24 (13%)	0	4
25	CY	183/185 (99%)	81 (44%)	54 (30%)	48 (26%)	0	0
26	B0	83/85 (98%)	61 (74%)	13 (16%)	9 (11%)	0	6
26	D0	83/85 (98%)	59 (71%)	15 (18%)	9 (11%)	0	6
27	B1	87/98 (89%)	34 (39%)	22 (25%)	31 (36%)	0	0
27	D1	87/98 (89%)	41 (47%)	22 (25%)	24 (28%)	0	0
28	B2	49/72 (68%)	14 (29%)	21 (43%)	14 (29%)	0	0
28	D2	49/72 (68%)	16 (33%)	20 (41%)	13 (26%)	0	0
29	B3	58/60 (97%)	34 (59%)	15 (26%)	9 (16%)	0	3
29	D3	58/60 (97%)	34 (59%)	15 (26%)	9 (16%)	0	3
30	B4	48/71 (68%)	8 (17%)	23 (48%)	17 (35%)	0	0
30	D4	48/71 (68%)	8 (17%)	22 (46%)	18 (38%)	0	0
31	B5	57/60 (95%)	28 (49%)	14 (25%)	15 (26%)	0	0
31	D5	57/60 (95%)	28 (49%)	12 (21%)	17 (30%)	0	0
32	B6	41/54 (76%)	21 (51%)	11 (27%)	9 (22%)	0	1
32	D6	41/54 (76%)	21 (51%)	11 (27%)	9 (22%)	0	1
33	B7	47/49 (96%)	29 (62%)	9 (19%)	9 (19%)	0	2
33	D7	47/49 (96%)	29 (62%)	10 (21%)	8 (17%)	0	2
34	B8	62/65 (95%)	25 (40%)	22 (36%)	15 (24%)	0	0
34	D8	62/65 (95%)	26 (42%)	21 (34%)	15 (24%)	0	0
37	BC	183/229 (80%)	79 (43%)	49 (27%)	55 (30%)	0	0
37	DC	183/229 (80%)	79 (43%)	49 (27%)	55 (30%)	0	0
38	BD	270/276 (98%)	158 (58%)	62 (23%)	50 (18%)	0	2
38	DD	270/276 (98%)	159 (59%)	62 (23%)	49 (18%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BE	203/206 (98%)	110 (54%)	46 (23%)	47 (23%)	0	1
39	DE	203/206 (98%)	111 (55%)	44 (22%)	48 (24%)	0	1
40	BF	206/210 (98%)	109 (53%)	53 (26%)	44 (21%)	0	1
40	DF	206/210 (98%)	108 (52%)	53 (26%)	45 (22%)	0	1
41	BG	177/182 (97%)	89 (50%)	48 (27%)	40 (23%)	0	1
41	DG	177/182 (97%)	89 (50%)	41 (23%)	47 (27%)	0	0
42	BH	158/180 (88%)	78 (49%)	44 (28%)	36 (23%)	0	1
42	DH	158/180 (88%)	80 (51%)	44 (28%)	34 (22%)	0	1
43	BI	144/148 (97%)	80 (56%)	36 (25%)	28 (19%)	0	2
43	DI	144/148 (97%)	80 (56%)	37 (26%)	27 (19%)	0	2
44	BN	137/140 (98%)	64 (47%)	40 (29%)	33 (24%)	0	0
44	DN	137/140 (98%)	65 (47%)	39 (28%)	33 (24%)	0	0
45	BO	120/122 (98%)	73 (61%)	24 (20%)	23 (19%)	0	2
45	DO	120/122 (98%)	74 (62%)	24 (20%)	22 (18%)	0	2
46	BP	144/150 (96%)	77 (54%)	27 (19%)	40 (28%)	0	0
46	DP	144/150 (96%)	75 (52%)	29 (20%)	40 (28%)	0	0
47	BQ	134/141 (95%)	70 (52%)	37 (28%)	27 (20%)	0	1
47	DQ	134/141 (95%)	72 (54%)	35 (26%)	27 (20%)	0	1
48	BR	115/118 (98%)	54 (47%)	26 (23%)	35 (30%)	0	0
48	DR	115/118 (98%)	53 (46%)	29 (25%)	33 (29%)	0	0
49	BS	97/112 (87%)	34 (35%)	27 (28%)	36 (37%)	0	0
49	DS	97/112 (87%)	34 (35%)	28 (29%)	35 (36%)	0	0
50	BT	136/146 (93%)	79 (58%)	26 (19%)	31 (23%)	0	1
50	DT	136/146 (93%)	78 (57%)	29 (21%)	29 (21%)	0	1
51	BU	115/118 (98%)	50 (44%)	39 (34%)	26 (23%)	0	1
51	DU	115/118 (98%)	51 (44%)	38 (33%)	26 (23%)	0	1
52	BV	97/101 (96%)	39 (40%)	21 (22%)	37 (38%)	0	0
52	DV	97/101 (96%)	39 (40%)	22 (23%)	36 (37%)	0	0
53	BW	111/113 (98%)	62 (56%)	27 (24%)	22 (20%)	0	1
53	DW	111/113 (98%)	60 (54%)	34 (31%)	17 (15%)	0	3
54	BX	91/96 (95%)	39 (43%)	24 (26%)	28 (31%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	DX	91/96 (95%)	38 (42%)	25 (28%)	28 (31%)	0	0
55	BY	99/110 (90%)	36 (36%)	29 (29%)	34 (34%)	0	0
55	DY	99/110 (90%)	38 (38%)	25 (25%)	36 (36%)	0	0
56	BZ	175/206 (85%)	87 (50%)	41 (23%)	47 (27%)	0	0
56	DZ	175/206 (85%)	92 (53%)	46 (26%)	37 (21%)	0	1
All	All	11936/12888 (93%)	6356 (53%)	3078 (26%)	2502 (21%)	0	1

5 of 2502 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	GLU
2	AB	22	LYS
2	AB	29	ALA
2	AB	30	ARG
2	AB	37	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	177 (88%)	25 (12%)	4	23
2	CB	202/220 (92%)	177 (88%)	25 (12%)	4	23
3	AC	160/188 (85%)	142 (89%)	18 (11%)	6	27
3	CC	160/188 (85%)	142 (89%)	18 (11%)	6	27
4	AD	180/181 (99%)	155 (86%)	25 (14%)	3	20
4	CD	180/181 (99%)	156 (87%)	24 (13%)	4	21
5	AE	115/123 (94%)	99 (86%)	16 (14%)	3	20
5	CE	115/123 (94%)	99 (86%)	16 (14%)	3	20
6	AF	90/90 (100%)	86 (96%)	4 (4%)	28	62
6	CF	90/90 (100%)	86 (96%)	4 (4%)	28	62
7	AG	126/127 (99%)	118 (94%)	8 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CG	126/127 (99%)	116 (92%)	10 (8%)	12	41
8	AH	119/119 (100%)	108 (91%)	11 (9%)	9	36
8	CH	119/119 (100%)	108 (91%)	11 (9%)	9	36
9	AI	98/99 (99%)	83 (85%)	15 (15%)	2	17
9	CI	98/99 (99%)	85 (87%)	13 (13%)	4	21
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	12	41
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	12	41
11	AK	90/99 (91%)	80 (89%)	10 (11%)	6	28
11	CK	90/99 (91%)	81 (90%)	9 (10%)	7	32
12	AL	104/111 (94%)	91 (88%)	13 (12%)	4	23
12	CL	104/111 (94%)	93 (89%)	11 (11%)	6	30
13	AM	99/101 (98%)	92 (93%)	7 (7%)	14	46
13	CM	99/101 (98%)	92 (93%)	7 (7%)	14	46
14	AN	49/50 (98%)	45 (92%)	4 (8%)	11	40
14	CN	49/50 (98%)	45 (92%)	4 (8%)	11	40
15	AO	79/80 (99%)	71 (90%)	8 (10%)	7	32
15	CO	79/80 (99%)	70 (89%)	9 (11%)	5	26
16	AP	72/74 (97%)	61 (85%)	11 (15%)	2	17
16	CP	72/74 (97%)	61 (85%)	11 (15%)	2	17
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	17	50
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	17	50
18	AR	61/77 (79%)	56 (92%)	5 (8%)	11	40
18	CR	61/77 (79%)	55 (90%)	6 (10%)	8	33
19	AS	69/80 (86%)	57 (83%)	12 (17%)	2	11
19	CS	69/80 (86%)	56 (81%)	13 (19%)	1	8
20	AT	76/82 (93%)	65 (86%)	11 (14%)	3	18
20	CT	76/82 (93%)	65 (86%)	11 (14%)	3	18
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	55
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	55
25	AY	157/157 (100%)	135 (86%)	22 (14%)	3	19
25	CY	157/157 (100%)	142 (90%)	15 (10%)	8	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	B0	61/67 (91%)	57 (93%)	4 (7%)	16	49
26	D0	61/67 (91%)	57 (93%)	4 (7%)	16	49
27	B1	73/83 (88%)	54 (74%)	19 (26%)	0	3
27	D1	73/83 (88%)	50 (68%)	23 (32%)	0	2
28	B2	46/67 (69%)	31 (67%)	15 (33%)	0	2
28	D2	46/67 (69%)	34 (74%)	12 (26%)	0	3
29	B3	51/52 (98%)	48 (94%)	3 (6%)	19	53
29	D3	51/52 (98%)	48 (94%)	3 (6%)	19	53
31	B5	51/52 (98%)	42 (82%)	9 (18%)	2	10
31	D5	51/52 (98%)	43 (84%)	8 (16%)	2	15
32	B6	43/52 (83%)	34 (79%)	9 (21%)	1	6
32	D6	43/52 (83%)	34 (79%)	9 (21%)	1	6
33	B7	41/42 (98%)	34 (83%)	7 (17%)	2	12
33	D7	41/42 (98%)	34 (83%)	7 (17%)	2	12
34	B8	53/55 (96%)	45 (85%)	8 (15%)	3	17
34	D8	53/55 (96%)	45 (85%)	8 (15%)	3	17
37	BC	61/181 (34%)	56 (92%)	5 (8%)	11	40
37	DC	61/181 (34%)	57 (93%)	4 (7%)	16	49
38	BD	213/218 (98%)	186 (87%)	27 (13%)	4	22
38	DD	213/218 (98%)	186 (87%)	27 (13%)	4	22
39	BE	165/166 (99%)	142 (86%)	23 (14%)	3	20
39	DE	165/166 (99%)	141 (86%)	24 (14%)	3	18
40	BF	165/166 (99%)	142 (86%)	23 (14%)	3	20
40	DF	165/166 (99%)	142 (86%)	23 (14%)	3	20
41	BG	155/156 (99%)	137 (88%)	18 (12%)	5	26
41	DG	155/156 (99%)	127 (82%)	28 (18%)	1	9
42	BH	132/148 (89%)	115 (87%)	17 (13%)	4	22
42	DH	132/148 (89%)	116 (88%)	16 (12%)	5	24
43	BI	122/124 (98%)	103 (84%)	19 (16%)	2	16
43	DI	122/124 (98%)	103 (84%)	19 (16%)	2	16
44	BN	117/119 (98%)	100 (86%)	17 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DN	117/119 (98%)	99 (85%)	18 (15%)	2	16
45	BO	100/100 (100%)	80 (80%)	20 (20%)	1	7
45	DO	100/100 (100%)	79 (79%)	21 (21%)	1	5
46	BP	112/116 (97%)	84 (75%)	28 (25%)	0	4
46	DP	112/116 (97%)	84 (75%)	28 (25%)	0	4
47	BQ	106/111 (96%)	86 (81%)	20 (19%)	1	8
47	DQ	106/111 (96%)	88 (83%)	18 (17%)	2	12
48	BR	100/101 (99%)	80 (80%)	20 (20%)	1	7
48	DR	100/101 (99%)	80 (80%)	20 (20%)	1	7
49	BS	77/88 (88%)	63 (82%)	14 (18%)	1	9
49	DS	77/88 (88%)	62 (80%)	15 (20%)	1	7
50	BT	120/127 (94%)	89 (74%)	31 (26%)	0	3
50	DT	120/127 (94%)	89 (74%)	31 (26%)	0	3
51	BU	92/94 (98%)	80 (87%)	12 (13%)	4	21
51	DU	92/94 (98%)	81 (88%)	11 (12%)	5	24
52	BV	82/82 (100%)	68 (83%)	14 (17%)	2	12
52	DV	82/82 (100%)	68 (83%)	14 (17%)	2	12
53	BW	91/92 (99%)	78 (86%)	13 (14%)	3	19
53	DW	91/92 (99%)	78 (86%)	13 (14%)	3	19
54	BX	74/78 (95%)	59 (80%)	15 (20%)	1	6
54	DX	74/78 (95%)	58 (78%)	16 (22%)	1	5
55	BY	84/91 (92%)	63 (75%)	21 (25%)	0	4
55	DY	84/91 (92%)	63 (75%)	21 (25%)	0	4
56	BZ	155/179 (87%)	134 (86%)	21 (14%)	4	21
56	DZ	155/179 (87%)	124 (80%)	31 (20%)	1	7
All	All	9778/10552 (93%)	8384 (86%)	1394 (14%)	3	19

5 of 1394 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	D1	12	PRO
44	DN	87	LEU
28	D2	30	ARG

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Mol	Chain	Res	Type
26	D0	64	ASP
39	DE	127	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 303 such sidechains are listed below:

Mol	Chain	Res	Type
32	D6	32	ASN
50	DT	84	GLN
38	DD	58	HIS
41	DG	132	ASN
54	DX	55	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	210 (13%)	31 (2%)
1	CA	1503/1522 (98%)	214 (14%)	29 (1%)
22	AV	16/76 (21%)	0	0
22	CV	16/76 (21%)	0	0
23	AW	76/77 (98%)	26 (34%)	0
23	CW	76/77 (98%)	20 (26%)	0
24	AX	10/31 (32%)	3 (30%)	0
24	CX	10/31 (32%)	2 (20%)	0
35	BA	2766/2782 (99%)	577 (20%)	57 (2%)
35	DA	2766/2782 (99%)	580 (20%)	57 (2%)
36	BB	118/122 (96%)	19 (16%)	1 (0%)
36	DB	118/122 (96%)	19 (16%)	1 (0%)
All	All	8978/9220 (97%)	1670 (18%)	176 (1%)

5 of 1670 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 176 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1285	A
35	DA	1176	G
35	DA	49	A
35	DA	474	G
35	DA	1459	G

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

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	$\#\|Z\| > 2$
23	5MU	AW	55	23	19,22,23	0.24	0	28,32,35	0.36	0
23	5MU	CW	55	23	19,22,23	0.30	0	28,32,35	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	AW	55	23	-	0/7/25/26	0/2/2/2
23	5MU	CW	55	23	-	0/7/25/26	0/2/2/2

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	55	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	CW	55	5MU	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1486 ligands modelled in this entry, 1486 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	CI	2
9	AI	2
32	B6	1
32	D6	1
41	DG	1
52	DV	1
52	BV	1
41	BG	1

The worst 5 of 20 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	6.15
1	D6	46:HIS	C	47:THR	N	6.12
1	CI	53:VAL	C	54:ASP	N	5.30
1	AI	53:VAL	C	54:ASP	N	5.29
1	DG	112:PRO	C	113:ARG	N	4.36

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1504/1522 (98%)	0.64	162 (10%)	5	6	15, 82, 177, 200	0
1	CA	1504/1522 (98%)	0.81	195 (12%)	3	4	20, 90, 190, 200	0
2	AB	235/256 (91%)	0.21	22 (9%)	8	9	19, 113, 188, 200	0
2	CB	235/256 (91%)	0.22	21 (8%)	9	10	26, 127, 188, 200	0
3	AC	207/239 (86%)	0.11	14 (6%)	17	16	11, 98, 175, 200	0
3	CC	207/239 (86%)	0.27	16 (7%)	13	13	38, 121, 183, 200	0
4	AD	208/209 (99%)	-0.23	4 (1%)	66	61	13, 75, 145, 200	0
4	CD	208/209 (99%)	-0.23	3 (1%)	75	69	25, 89, 155, 200	0
5	AE	151/162 (93%)	-0.22	3 (1%)	65	60	21, 73, 158, 190	0
5	CE	151/162 (93%)	0.11	6 (3%)	38	33	26, 89, 157, 200	0
6	AF	101/101 (100%)	-0.15	2 (1%)	65	60	19, 100, 151, 189	0
6	CF	101/101 (100%)	-0.24	0	100	100	16, 83, 141, 170	0
7	AG	155/156 (99%)	0.16	16 (10%)	6	7	34, 104, 175, 194	0
7	CG	155/156 (99%)	0.31	18 (11%)	4	5	53, 123, 185, 200	0
8	AH	138/138 (100%)	-0.31	1 (0%)	87	83	33, 81, 145, 190	0
8	CH	138/138 (100%)	-0.37	1 (0%)	87	83	30, 91, 147, 165	0
9	AI	127/128 (99%)	0.00	4 (3%)	49	43	27, 123, 180, 200	0
9	CI	127/128 (99%)	0.80	27 (21%)	0	1	43, 140, 195, 200	0
10	AJ	99/105 (94%)	0.23	5 (5%)	28	25	47, 120, 180, 200	0
10	CJ	99/105 (94%)	1.01	16 (16%)	1	2	65, 140, 189, 200	0
11	AK	119/129 (92%)	0.27	12 (10%)	7	7	13, 78, 163, 187	0
11	CK	119/129 (92%)	0.30	9 (7%)	13	14	30, 86, 164, 200	0
12	AL	125/135 (92%)	-0.36	1 (0%)	86	81	19, 71, 146, 200	0
12	CL	125/135 (92%)	-0.26	1 (0%)	86	81	12, 75, 143, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	125/126 (99%)	0.55	20 (16%) 1 2	56, 124, 183, 200	0
13	CM	125/126 (99%)	0.32	12 (9%) 8 8	41, 140, 199, 200	0
14	AN	60/61 (98%)	-0.12	2 (3%) 46 41	38, 94, 181, 200	0
14	CN	60/61 (98%)	0.06	1 (1%) 70 64	57, 117, 171, 189	0
15	AO	88/89 (98%)	-0.37	1 (1%) 80 75	11, 84, 147, 172	0
15	CO	88/89 (98%)	-0.18	4 (4%) 33 29	18, 88, 146, 167	0
16	AP	84/88 (95%)	-0.23	2 (2%) 59 53	17, 64, 135, 200	0
16	CP	84/88 (95%)	0.21	8 (9%) 8 8	32, 90, 139, 199	0
17	AQ	100/105 (95%)	0.11	11 (11%) 5 6	15, 81, 143, 200	0
17	CQ	100/105 (95%)	0.23	14 (14%) 2 3	20, 84, 134, 200	0
18	AR	70/88 (79%)	0.09	2 (2%) 51 45	33, 87, 156, 200	0
18	CR	70/88 (79%)	0.00	4 (5%) 23 21	17, 79, 137, 170	0
19	AS	79/93 (84%)	0.14	3 (3%) 40 36	60, 134, 200, 200	0
19	CS	79/93 (84%)	0.47	11 (13%) 2 3	76, 140, 200, 200	0
20	AT	99/106 (93%)	0.11	6 (6%) 21 19	21, 91, 178, 200	0
20	CT	99/106 (93%)	-0.03	7 (7%) 16 15	45, 102, 167, 197	0
21	AU	25/27 (92%)	0.06	0 100 100	59, 114, 161, 200	0
21	CU	25/27 (92%)	0.98	5 (20%) 1 1	58, 131, 182, 200	0
22	AV	17/76 (22%)	0.68	2 (11%) 4 5	55, 68, 122, 125	0
22	CV	17/76 (22%)	0.33	1 (5%) 22 20	56, 73, 128, 131	0
23	AW	76/77 (98%)	3.55	45 (59%) 0 0	63, 179, 200, 200	0
23	CW	76/77 (98%)	5.00	61 (80%) 0 0	62, 191, 200, 200	0
24	AX	11/31 (35%)	-0.04	0 100 100	23, 72, 120, 172	0
24	CX	11/31 (35%)	-0.05	0 100 100	41, 63, 93, 196	0
25	AY	185/185 (100%)	0.60	30 (16%) 1 2	27, 99, 167, 200	0
25	CY	185/185 (100%)	0.38	27 (14%) 2 3	9, 93, 166, 198	0
26	B0	85/85 (100%)	0.59	11 (12%) 3 4	21, 80, 184, 199	0
26	D0	85/85 (100%)	0.64	11 (12%) 3 4	39, 95, 174, 200	0
27	B1	89/98 (90%)	-0.30	2 (2%) 62 56	5, 64, 138, 193	0
27	D1	89/98 (90%)	-0.49	2 (2%) 62 56	5, 62, 133, 200	0
28	B2	51/72 (70%)	-0.31	2 (3%) 39 35	44, 103, 157, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	D2	51/72 (70%)	0.13	5 (9%) 7 8	24, 93, 168, 200	0
29	B3	60/60 (100%)	-0.13	1 (1%) 70 64	15, 81, 158, 200	0
29	D3	60/60 (100%)	-0.14	1 (1%) 70 64	21, 85, 167, 200	0
30	B4	50/71 (70%)	-0.18	0 100 100	71, 144, 192, 200	0
30	D4	50/71 (70%)	0.18	5 (10%) 7 8	86, 167, 192, 200	0
31	B5	59/60 (98%)	0.09	4 (6%) 17 16	22, 84, 184, 200	0
31	D5	59/60 (98%)	-0.35	0 100 100	6, 74, 191, 200	0
32	B6	45/54 (83%)	0.83	7 (15%) 2 2	53, 122, 184, 200	0
32	D6	45/54 (83%)	1.44	14 (31%) 0 0	54, 147, 188, 200	0
33	B7	49/49 (100%)	-0.23	0 100 100	5, 47, 114, 200	0
33	D7	49/49 (100%)	-0.38	1 (2%) 65 60	3, 44, 105, 176	0
34	B8	64/65 (98%)	-0.17	1 (1%) 72 66	7, 53, 145, 200	0
34	D8	64/65 (98%)	-0.12	2 (3%) 49 43	27, 73, 140, 185	0
35	BA	2767/2782 (99%)	0.70	328 (11%) 4 5	9, 65, 172, 200	0
35	DA	2767/2782 (99%)	0.70	321 (11%) 4 5	6, 62, 169, 200	0
36	BB	119/122 (97%)	1.06	17 (14%) 2 3	60, 102, 160, 189	0
36	DB	119/122 (97%)	1.13	25 (21%) 1 1	69, 140, 188, 200	0
37	BC	191/229 (83%)	2.09	75 (39%) 0 0	76, 175, 200, 200	0
37	DC	191/229 (83%)	2.60	99 (51%) 0 0	120, 180, 200, 200	0
38	BD	272/276 (98%)	-0.40	1 (0%) 92 90	8, 56, 122, 200	0
38	DD	272/276 (98%)	-0.47	2 (0%) 87 83	1, 47, 114, 200	0
39	BE	205/206 (99%)	0.12	11 (5%) 25 23	10, 75, 160, 200	0
39	DE	205/206 (99%)	-0.14	5 (2%) 59 53	7, 64, 153, 199	0
40	BF	208/210 (99%)	-0.08	10 (4%) 30 27	1, 69, 164, 200	0
40	DF	208/210 (99%)	-0.15	6 (2%) 51 45	6, 75, 170, 200	0
41	BG	181/182 (99%)	0.29	22 (12%) 4 5	36, 107, 171, 200	0
41	DG	181/182 (99%)	0.78	28 (15%) 2 2	45, 135, 191, 200	0
42	BH	160/180 (88%)	0.62	23 (14%) 2 3	47, 145, 200, 200	0
42	DH	160/180 (88%)	0.09	9 (5%) 24 22	36, 110, 180, 200	0
43	BI	146/148 (98%)	0.29	15 (10%) 6 7	25, 112, 184, 200	0
43	DI	146/148 (98%)	1.75	45 (30%) 0 0	17, 134, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	BN	139/140 (99%)	-0.11	7 (5%)	28	25	37, 98, 160, 200	0
44	DN	139/140 (99%)	-0.31	4 (2%)	51	45	19, 76, 152, 195	0
45	BO	122/122 (100%)	-0.25	3 (2%)	57	51	15, 63, 116, 133	0
45	DO	122/122 (100%)	-0.41	0	100	100	10, 49, 100, 128	0
46	BP	146/150 (97%)	0.06	10 (6%)	17	16	6, 84, 167, 200	0
46	DP	146/150 (97%)	0.13	8 (5%)	25	22	18, 93, 168, 199	0
47	BQ	136/141 (96%)	-0.00	7 (5%)	28	25	26, 90, 187, 200	0
47	DQ	136/141 (96%)	-0.25	3 (2%)	62	56	16, 73, 158, 200	0
48	BR	117/118 (99%)	-0.47	0	100	100	8, 66, 138, 198	0
48	DR	117/118 (99%)	-0.43	0	100	100	8, 64, 136, 180	0
49	BS	99/112 (88%)	0.22	7 (7%)	16	15	32, 105, 186, 200	0
49	DS	99/112 (88%)	1.01	23 (23%)	0	0	62, 133, 182, 200	0
50	BT	138/146 (94%)	-0.12	4 (2%)	51	45	21, 96, 190, 200	0
50	DT	138/146 (94%)	-0.07	8 (5%)	23	20	17, 84, 173, 200	0
51	BU	117/118 (99%)	-0.25	4 (3%)	45	40	15, 79, 161, 182	0
51	DU	117/118 (99%)	-0.20	5 (4%)	35	31	12, 65, 141, 194	0
52	BV	101/101 (100%)	0.57	16 (15%)	2	2	26, 106, 188, 200	0
52	DV	101/101 (100%)	0.09	9 (8%)	9	10	29, 100, 178, 200	0
53	BW	113/113 (100%)	-0.45	2 (1%)	68	62	8, 55, 134, 200	0
53	DW	113/113 (100%)	-0.34	2 (1%)	68	62	16, 66, 148, 200	0
54	BX	93/96 (96%)	-0.35	1 (1%)	80	75	12, 83, 163, 200	0
54	DX	93/96 (96%)	-0.35	0	100	100	18, 79, 147, 185	0
55	BY	101/110 (91%)	0.03	8 (7%)	12	13	16, 94, 187, 200	0
55	DY	101/110 (91%)	0.35	11 (10%)	5	6	21, 108, 187, 200	0
56	BZ	177/206 (85%)	-0.12	7 (3%)	38	33	46, 113, 178, 200	0
56	DZ	177/206 (85%)	0.22	13 (7%)	15	15	11, 114, 180, 200	0
All	All	21176/22108 (95%)	0.41	2111 (9%)	7	8	1, 84, 184, 200	0

The worst 5 of 2111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	897	C	19.0
35	DA	2109	U	18.4

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Mol	Chain	Res	Type	RSRZ
35	DA	897	C	18.4
43	DI	143	SER	17.7
23	CW	7	G	14.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	5MU	CW	55	21/22	0.21	0.71	177,200,200,200	0
23	5MU	AW	55	21/22	0.84	0.25	130,173,200,200	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
57	MG	BB	220	1/1	-0.38	1.19	71,71,71,71	1
57	MG	CA	1796	1/1	-0.36	0.27	95,95,95,95	1
57	MG	CW	111	1/1	-0.29	0.56	136,136,136,136	1
57	MG	BA	3423	1/1	-0.04	0.63	54,54,54,54	1
57	MG	BA	3231	1/1	0.01	0.83	102,102,102,102	0
57	MG	CW	110	1/1	0.05	2.15	66,66,66,66	1
57	MG	AW	118	1/1	0.12	0.32	69,69,69,69	1
57	MG	DA	3212	1/1	0.12	0.71	86,86,86,86	1
57	MG	DA	3090	1/1	0.13	0.55	97,97,97,97	0
57	MG	CA	1746	1/1	0.13	0.92	74,74,74,74	0
57	MG	DA	3301	1/1	0.18	1.59	55,55,55,55	1
57	MG	CW	116	1/1	0.24	0.73	107,107,107,107	0
57	MG	DA	3439	1/1	0.28	1.57	85,85,85,85	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1789	1/1	0.29	0.45	111,111,111,111	0
57	MG	CA	1759	1/1	0.31	2.40	108,108,108,108	1
57	MG	AW	112	1/1	0.34	0.23	64,64,64,64	1
57	MG	CW	123	1/1	0.42	0.32	1,1,1,1	1
57	MG	DB	202	1/1	0.42	0.67	33,33,33,33	1
57	MG	BA	3281	1/1	0.43	1.96	43,43,43,43	1
57	MG	CA	1785	1/1	0.43	0.43	112,112,112,112	0
57	MG	AW	111	1/1	0.43	0.32	76,76,76,76	1
57	MG	DA	3329	1/1	0.44	1.32	62,62,62,62	1
57	MG	AA	1706	1/1	0.45	0.57	58,58,58,58	1
57	MG	AA	1780	1/1	0.46	0.68	95,95,95,95	1
57	MG	CW	115	1/1	0.46	0.85	93,93,93,93	1
57	MG	CW	106	1/1	0.47	1.15	47,47,47,47	1
57	MG	DA	3361	1/1	0.49	0.51	88,88,88,88	0
57	MG	CA	1681	1/1	0.50	0.48	96,96,96,96	1
57	MG	AA	1650	1/1	0.51	1.83	20,20,20,20	1
57	MG	BA	3379	1/1	0.51	1.28	50,50,50,50	1
57	MG	CW	109	1/1	0.51	0.36	30,30,30,30	1
57	MG	AA	1799	1/1	0.52	0.37	58,58,58,58	1
57	MG	BA	3018	1/1	0.52	0.26	35,35,35,35	0
57	MG	BA	3412	1/1	0.53	0.50	34,34,34,34	1
57	MG	CA	1731	1/1	0.54	0.49	54,54,54,54	0
57	MG	CW	117	1/1	0.55	0.26	57,57,57,57	1
57	MG	CA	1737	1/1	0.55	0.66	1,1,1,1	1
57	MG	CW	113	1/1	0.55	0.68	68,68,68,68	1
57	MG	DA	3295	1/1	0.57	0.23	79,79,79,79	0
57	MG	BA	3251	1/1	0.57	0.52	64,64,64,64	0
57	MG	CA	1715	1/1	0.58	0.20	55,55,55,55	0
57	MG	BA	3035	1/1	0.58	0.40	67,67,67,67	1
57	MG	BA	3392	1/1	0.58	0.19	70,70,70,70	0
57	MG	D1	104	1/1	0.59	0.55	74,74,74,74	1
57	MG	CA	1786	1/1	0.60	0.49	39,39,39,39	1
57	MG	DA	3127	1/1	0.60	0.54	57,57,57,57	0
57	MG	BA	3227	1/1	0.60	1.36	71,71,71,71	1
57	MG	DA	3273	1/1	0.60	0.44	97,97,97,97	1
57	MG	AA	1798	1/1	0.60	0.70	52,52,52,52	1
57	MG	DA	3221	1/1	0.62	0.79	79,79,79,79	1
57	MG	AA	1743	1/1	0.62	0.65	74,74,74,74	1
57	MG	DA	3371	1/1	0.62	0.19	35,35,35,35	1
57	MG	DA	3422	1/1	0.62	0.22	62,62,62,62	0
57	MG	DA	3176	1/1	0.62	0.62	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	1725	1/1	0.62	0.64	43,43,43,43	1
57	MG	DA	3270	1/1	0.63	1.08	47,47,47,47	1
57	MG	DA	3140	1/1	0.63	0.44	25,25,25,25	0
57	MG	BB	213	1/1	0.64	0.78	33,33,33,33	1
57	MG	CA	1686	1/1	0.65	0.46	49,49,49,49	0
57	MG	DA	3278	1/1	0.65	0.33	36,36,36,36	1
57	MG	AA	1762	1/1	0.66	0.44	58,58,58,58	0
57	MG	BB	210	1/1	0.66	0.89	68,68,68,68	1
57	MG	DB	212	1/1	0.66	0.27	55,55,55,55	0
57	MG	DA	3281	1/1	0.67	0.48	64,64,64,64	0
57	MG	BA	3324	1/1	0.67	0.34	56,56,56,56	0
57	MG	CA	1770	1/1	0.67	1.18	78,78,78,78	1
57	MG	AA	1615	1/1	0.67	1.36	47,47,47,47	0
57	MG	BA	3287	1/1	0.67	0.43	45,45,45,45	1
57	MG	DB	219	1/1	0.67	0.74	56,56,56,56	1
57	MG	DH	201	1/1	0.67	0.53	12,12,12,12	1
57	MG	CA	1673	1/1	0.68	0.11	57,57,57,57	0
57	MG	BA	3014	1/1	0.68	0.76	51,51,51,51	0
57	MG	BA	3101	1/1	0.68	0.43	1,1,1,1	1
57	MG	BA	3207	1/1	0.68	0.75	1,1,1,1	1
57	MG	AA	1716	1/1	0.68	0.26	60,60,60,60	0
57	MG	DA	3241	1/1	0.68	0.86	50,50,50,50	0
57	MG	CA	1658	1/1	0.68	0.99	24,24,24,24	1
57	MG	CE	202	1/1	0.69	0.50	85,85,85,85	1
57	MG	BB	209	1/1	0.69	0.50	108,108,108,108	0
57	MG	DA	3366	1/1	0.69	0.40	46,46,46,46	1
57	MG	AW	123	1/1	0.69	0.47	1,1,1,1	1
57	MG	AW	108	1/1	0.69	1.09	24,24,24,24	1
57	MG	CA	1623	1/1	0.70	0.34	84,84,84,84	1
57	MG	CA	1792	1/1	0.70	0.15	16,16,16,16	1
57	MG	AA	1791	1/1	0.70	1.23	35,35,35,35	1
57	MG	DA	3101	1/1	0.70	0.43	17,17,17,17	1
57	MG	BB	217	1/1	0.70	0.23	49,49,49,49	0
57	MG	CA	1726	1/1	0.70	0.33	36,36,36,36	0
57	MG	DA	3159	1/1	0.70	0.30	21,21,21,21	0
57	MG	BA	3334	1/1	0.70	0.44	51,51,51,51	1
57	MG	CW	118	1/1	0.70	0.43	1,1,1,1	1
57	MG	DA	3370	1/1	0.71	0.47	100,100,100,100	1
57	MG	AV	102	1/1	0.71	0.41	73,73,73,73	0
57	MG	DA	3299	1/1	0.71	0.51	13,13,13,13	1
57	MG	DA	3434	1/1	0.71	0.38	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	1602	1/1	0.71	0.61	72,72,72,72	0
57	MG	DA	3214	1/1	0.71	0.35	64,64,64,64	1
57	MG	DA	3215	1/1	0.71	0.58	17,17,17,17	1
57	MG	DA	3363	1/1	0.71	0.44	13,13,13,13	1
57	MG	BA	3153	1/1	0.71	0.35	35,35,35,35	1
57	MG	CV	102	1/1	0.72	0.45	57,57,57,57	0
57	MG	BA	3397	1/1	0.72	0.41	44,44,44,44	0
57	MG	DA	3367	1/1	0.72	0.56	95,95,95,95	1
57	MG	CV	101	1/1	0.73	0.15	41,41,41,41	0
57	MG	CA	1765	1/1	0.73	0.64	85,85,85,85	0
57	MG	CA	1788	1/1	0.73	0.33	1,1,1,1	1
57	MG	AA	1749	1/1	0.73	0.45	1,1,1,1	1
57	MG	CA	1783	1/1	0.73	0.10	33,33,33,33	1
57	MG	BA	3286	1/1	0.73	0.43	32,32,32,32	1
57	MG	DA	3262	1/1	0.73	1.45	79,79,79,79	1
57	MG	AA	1769	1/1	0.74	1.24	48,48,48,48	0
57	MG	DA	3006	1/1	0.74	0.48	93,93,93,93	0
57	MG	BA	3327	1/1	0.74	0.13	46,46,46,46	1
57	MG	CA	1718	1/1	0.74	0.94	59,59,59,59	0
57	MG	CA	1738	1/1	0.74	0.93	67,67,67,67	0
57	MG	BA	3316	1/1	0.74	0.59	1,1,1,1	1
57	MG	CN	101	1/1	0.74	0.51	65,65,65,65	0
57	MG	DA	3296	1/1	0.75	0.68	33,33,33,33	1
57	MG	BA	3002	1/1	0.75	0.39	16,16,16,16	1
57	MG	CA	1707	1/1	0.75	0.34	32,32,32,32	0
57	MG	DA	3326	1/1	0.75	0.85	96,96,96,96	1
57	MG	CW	104	1/1	0.75	0.21	35,35,35,35	1
57	MG	BA	3322	1/1	0.75	0.77	21,21,21,21	1
57	MG	DN	202	1/1	0.75	0.29	31,31,31,31	1
57	MG	BA	3309	1/1	0.76	0.66	47,47,47,47	0
57	MG	DA	3346	1/1	0.76	0.43	115,115,115,115	0
57	MG	DA	3358	1/1	0.76	0.71	11,11,11,11	1
57	MG	CA	1697	1/1	0.76	0.36	59,59,59,59	1
57	MG	D2	2601	1/1	0.76	0.47	73,73,73,73	1
57	MG	BB	204	1/1	0.76	0.75	76,76,76,76	1
57	MG	DA	3049	1/1	0.76	0.99	43,43,43,43	0
57	MG	CA	1709	1/1	0.76	0.19	46,46,46,46	0
57	MG	CA	1747	1/1	0.76	0.66	19,19,19,19	1
57	MG	CA	1804	1/1	0.76	0.32	45,45,45,45	0
57	MG	BA	3168	1/1	0.76	0.37	29,29,29,29	0
57	MG	AW	103	1/1	0.76	0.29	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	DA	3161	1/1	0.76	0.31	112,112,112,112	0
57	MG	DA	3174	1/1	0.76	0.56	50,50,50,50	1
57	MG	AA	1653	1/1	0.76	0.79	93,93,93,93	1
57	MG	DA	3319	1/1	0.76	0.25	116,116,116,116	1
57	MG	AW	102	1/1	0.76	0.39	82,82,82,82	1
57	MG	BN	204	1/1	0.77	0.36	20,20,20,20	1
57	MG	CA	1736	1/1	0.77	0.45	71,71,71,71	0
57	MG	AW	113	1/1	0.77	0.27	60,60,60,60	0
57	MG	BA	3102	1/1	0.77	0.38	21,21,21,21	1
57	MG	DA	3409	1/1	0.77	1.57	83,83,83,83	1
57	MG	DA	3307	1/1	0.77	0.48	43,43,43,43	0
57	MG	CA	1643	1/1	0.77	1.02	73,73,73,73	1
57	MG	CA	1646	1/1	0.77	0.44	56,56,56,56	0
57	MG	CA	1754	1/1	0.77	0.33	42,42,42,42	0
57	MG	AV	103	1/1	0.77	0.14	70,70,70,70	0
57	MG	BA	3006	1/1	0.77	0.45	77,77,77,77	0
57	MG	CA	1767	1/1	0.77	1.32	94,94,94,94	0
57	MG	BA	3270	1/1	0.77	0.23	6,6,6,6	0
57	MG	DA	3242	1/1	0.78	0.18	100,100,100,100	1
57	MG	BA	3229	1/1	0.78	0.21	39,39,39,39	0
57	MG	DA	3321	1/1	0.78	0.36	85,85,85,85	0
57	MG	DA	3004	1/1	0.78	0.83	64,64,64,64	0
57	MG	CA	1760	1/1	0.78	0.44	40,40,40,40	0
57	MG	CA	1649	1/1	0.78	0.23	14,14,14,14	1
57	MG	AA	1734	1/1	0.78	0.79	36,36,36,36	0
57	MG	AA	1788	1/1	0.78	0.30	40,40,40,40	0
57	MG	AK	201	1/1	0.78	0.44	33,33,33,33	1
57	MG	CA	1758	1/1	0.78	0.39	21,21,21,21	1
57	MG	DA	3152	1/1	0.78	0.66	62,62,62,62	1
57	MG	DA	3135	1/1	0.79	0.86	12,12,12,12	0
57	MG	DA	3355	1/1	0.79	0.19	42,42,42,42	1
57	MG	DA	3139	1/1	0.79	0.59	53,53,53,53	0
57	MG	BA	3289	1/1	0.79	0.37	60,60,60,60	1
57	MG	DA	3271	1/1	0.79	0.51	113,113,113,113	1
57	MG	CW	102	1/1	0.79	0.27	38,38,38,38	1
57	MG	BA	3292	1/1	0.79	0.81	27,27,27,27	1
57	MG	BA	3299	1/1	0.79	1.03	26,26,26,26	1
57	MG	DA	3165	1/1	0.79	0.17	47,47,47,47	0
57	MG	DA	3400	1/1	0.79	0.80	61,61,61,61	1
57	MG	AA	1785	1/1	0.79	0.15	19,19,19,19	0
57	MG	CA	1797	1/1	0.79	1.54	82,82,82,82	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1733	1/1	0.79	0.43	5,5,5,5	1
57	MG	DA	3303	1/1	0.79	0.54	4,4,4,4	0
57	MG	CW	112	1/1	0.79	0.47	24,24,24,24	1
57	MG	BA	3206	1/1	0.79	0.35	1,1,1,1	1
57	MG	DA	3220	1/1	0.79	0.77	86,86,86,86	0
57	MG	CA	1668	1/1	0.79	0.28	43,43,43,43	0
57	MG	BA	3005	1/1	0.79	0.37	25,25,25,25	0
57	MG	DX	103	1/1	0.79	0.35	48,48,48,48	1
57	MG	AA	1720	1/1	0.80	0.48	91,91,91,91	0
57	MG	AW	114	1/1	0.80	0.16	78,78,78,78	0
57	MG	CA	1735	1/1	0.80	0.30	1,1,1,1	1
57	MG	DA	3385	1/1	0.80	0.38	44,44,44,44	0
57	MG	AA	1680	1/1	0.80	0.33	53,53,53,53	0
57	MG	DA	3258	1/1	0.80	0.67	23,23,23,23	1
57	MG	AW	121	1/1	0.80	0.49	63,63,63,63	0
57	MG	AA	1705	1/1	0.80	0.29	38,38,38,38	0
57	MG	DA	3436	1/1	0.80	0.70	41,41,41,41	0
57	MG	BA	3167	1/1	0.80	0.29	50,50,50,50	0
57	MG	DA	3441	1/1	0.80	1.10	44,44,44,44	1
57	MG	AA	1737	1/1	0.80	0.35	30,30,30,30	1
57	MG	DB	209	1/1	0.80	0.40	96,96,96,96	1
57	MG	BA	3189	1/1	0.80	0.92	87,87,87,87	0
57	MG	AW	110	1/1	0.80	0.32	30,30,30,30	1
57	MG	DA	3282	1/1	0.80	0.41	1,1,1,1	1
57	MG	AA	1718	1/1	0.80	0.40	1,1,1,1	1
57	MG	AA	1748	1/1	0.80	0.18	73,73,73,73	0
57	MG	DA	3392	1/1	0.81	0.50	46,46,46,46	0
57	MG	DA	3163	1/1	0.81	0.47	17,17,17,17	1
57	MG	CA	1674	1/1	0.81	0.24	44,44,44,44	1
57	MG	DA	3087	1/1	0.81	0.46	17,17,17,17	1
57	MG	DA	3424	1/1	0.81	0.22	31,31,31,31	1
57	MG	DA	3332	1/1	0.81	0.34	41,41,41,41	1
57	MG	BA	3402	1/1	0.81	0.22	13,13,13,13	1
57	MG	BA	3343	1/1	0.81	0.28	33,33,33,33	0
57	MG	CA	1803	1/1	0.81	0.30	83,83,83,83	0
57	MG	AW	106	1/1	0.81	0.54	26,26,26,26	1
57	MG	BA	3390	1/1	0.81	0.56	24,24,24,24	0
57	MG	CG	201	1/1	0.81	0.35	10,10,10,10	1
57	MG	BA	3325	1/1	0.81	0.26	30,30,30,30	0
57	MG	DA	3154	1/1	0.81	0.41	83,83,83,83	1
57	MG	BA	3337	1/1	0.81	0.69	1,1,1,1	1
57	MG	DA	3016	1/1	0.81	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	AA	1693	1/1	0.82	0.10	80,80,80,80	0
57	MG	DA	3382	1/1	0.82	0.37	71,71,71,71	0
57	MG	CA	1655	1/1	0.82	0.55	69,69,69,69	1
57	MG	DA	3320	1/1	0.82	0.55	75,75,75,75	0
57	MG	AA	1797	1/1	0.82	0.69	9,9,9,9	1
57	MG	CA	1793	1/1	0.82	0.64	74,74,74,74	0
57	MG	BA	3225	1/1	0.82	0.90	67,67,67,67	0
57	MG	DA	3100	1/1	0.82	0.36	63,63,63,63	1
57	MG	DA	3336	1/1	0.82	0.31	60,60,60,60	0
57	MG	DA	3343	1/1	0.82	0.39	1,1,1,1	1
57	MG	DA	3438	1/1	0.82	1.20	48,48,48,48	1
57	MG	DA	3279	1/1	0.82	0.46	75,75,75,75	0
57	MG	CA	1748	1/1	0.82	0.61	97,97,97,97	1
57	MG	CA	1801	1/1	0.82	1.27	2,2,2,2	1
57	MG	DB	208	1/1	0.82	0.17	53,53,53,53	1
57	MG	DA	3360	1/1	0.82	0.09	5,5,5,5	0
57	MG	CW	119	1/1	0.82	0.70	57,57,57,57	1
57	MG	DB	216	1/1	0.82	0.28	54,54,54,54	0
57	MG	DB	218	1/1	0.82	0.25	30,30,30,30	1
57	MG	CA	1802	1/1	0.82	1.35	39,39,39,39	0
57	MG	CW	107	1/1	0.82	0.99	84,84,84,84	0
57	MG	BA	3010	1/1	0.82	0.92	17,17,17,17	1
57	MG	BF	304	1/1	0.82	0.36	9,9,9,9	1
57	MG	AA	1683	1/1	0.83	0.43	1,1,1,1	1
57	MG	BA	3443	1/1	0.83	0.14	49,49,49,49	0
57	MG	BA	3264	1/1	0.83	1.20	66,66,66,66	0
57	MG	AA	1792	1/1	0.83	0.52	56,56,56,56	0
57	MG	CA	1756	1/1	0.83	0.54	56,56,56,56	0
57	MG	CW	101	1/1	0.83	1.79	83,83,83,83	1
57	MG	CA	1684	1/1	0.83	0.35	59,59,59,59	0
57	MG	BA	3188	1/1	0.83	0.16	12,12,12,12	0
57	MG	CA	1692	1/1	0.83	0.32	74,74,74,74	1
57	MG	BA	3285	1/1	0.83	0.54	40,40,40,40	0
57	MG	CA	1704	1/1	0.83	0.82	62,62,62,62	0
57	MG	AA	1715	1/1	0.83	0.98	29,29,29,29	1
57	MG	AA	1679	1/1	0.83	0.46	12,12,12,12	1
57	MG	BA	3365	1/1	0.83	0.35	36,36,36,36	0
57	MG	BA	3369	1/1	0.83	0.15	50,50,50,50	0
57	MG	DA	3316	1/1	0.83	0.41	14,14,14,14	1
57	MG	AA	1640	1/1	0.83	0.33	18,18,18,18	0
57	MG	BA	3103	1/1	0.83	0.95	33,33,33,33	1
57	MG	BA	3141	1/1	0.83	0.25	6,6,6,6	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3181	1/1	0.83	0.36	47,47,47,47	1
57	MG	CA	1794	1/1	0.83	0.70	68,68,68,68	0
57	MG	AA	1764	1/1	0.83	0.26	35,35,35,35	0
57	MG	BA	3315	1/1	0.83	0.56	87,87,87,87	0
57	MG	BA	3158	1/1	0.83	0.35	32,32,32,32	0
57	MG	BA	3418	1/1	0.83	0.39	41,41,41,41	1
57	MG	CA	1743	1/1	0.83	0.33	64,64,64,64	0
57	MG	CA	1744	1/1	0.83	0.18	33,33,33,33	0
57	MG	DA	3252	1/1	0.83	0.34	89,89,89,89	0
57	MG	CA	1640	1/1	0.84	0.27	65,65,65,65	1
57	MG	AW	109	1/1	0.84	0.28	37,37,37,37	1
57	MG	CA	1645	1/1	0.84	0.30	46,46,46,46	0
57	MG	BA	3441	1/1	0.84	0.20	6,6,6,6	1
57	MG	BA	3166	1/1	0.84	0.27	66,66,66,66	0
57	MG	DA	3141	1/1	0.84	0.68	1,1,1,1	1
57	MG	DA	3150	1/1	0.84	0.45	39,39,39,39	1
57	MG	BA	3445	1/1	0.84	0.51	25,25,25,25	1
57	MG	CA	1728	1/1	0.84	0.37	41,41,41,41	1
57	MG	BA	3373	1/1	0.84	0.29	1,1,1,1	1
57	MG	BA	3053	1/1	0.84	0.14	1,1,1,1	0
57	MG	AA	1781	1/1	0.84	0.33	7,7,7,7	1
57	MG	AA	1702	1/1	0.84	0.48	57,57,57,57	0
57	MG	AA	1726	1/1	0.84	0.31	10,10,10,10	0
57	MG	AA	1668	1/1	0.84	0.31	18,18,18,18	0
57	MG	BA	3411	1/1	0.84	0.22	99,99,99,99	1
57	MG	DA	3206	1/1	0.84	0.70	32,32,32,32	1
57	MG	BA	3340	1/1	0.84	0.63	22,22,22,22	1
57	MG	BA	3417	1/1	0.84	0.54	17,17,17,17	1
57	MG	DA	3372	1/1	0.84	0.71	35,35,35,35	1
57	MG	BA	3030	1/1	0.84	0.34	56,56,56,56	1
57	MG	CA	1657	1/1	0.85	0.44	67,67,67,67	0
57	MG	DA	3207	1/1	0.85	0.54	36,36,36,36	1
57	MG	BA	3238	1/1	0.85	0.69	38,38,38,38	1
57	MG	AW	116	1/1	0.85	0.30	61,61,61,61	0
57	MG	DA	3390	1/1	0.85	0.19	34,34,34,34	0
57	MG	AA	1603	1/1	0.85	0.23	20,20,20,20	0
57	MG	AA	1671	1/1	0.85	0.33	47,47,47,47	0
57	MG	DA	3136	1/1	0.85	0.27	9,9,9,9	1
57	MG	DA	3415	1/1	0.85	0.40	3,3,3,3	1
57	MG	DA	3225	1/1	0.85	0.16	35,35,35,35	0
57	MG	CA	1764	1/1	0.85	0.08	49,49,49,49	0
57	MG	DA	3431	1/1	0.85	0.12	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	DA	3325	1/1	0.85	0.26	72,72,72,72	0
57	MG	BB	203	1/1	0.85	0.26	60,60,60,60	0
57	MG	BA	3362	1/1	0.85	0.28	38,38,38,38	0
57	MG	CA	1641	1/1	0.85	0.14	17,17,17,17	0
57	MG	CA	1778	1/1	0.85	0.46	1,1,1,1	1
57	MG	CA	1782	1/1	0.85	0.12	28,28,28,28	0
57	MG	BB	208	1/1	0.85	0.16	38,38,38,38	1
57	MG	CV	104	1/1	0.85	0.35	45,45,45,45	1
57	MG	DA	3275	1/1	0.85	0.89	2,2,2,2	1
57	MG	AA	1666	1/1	0.85	0.41	47,47,47,47	0
57	MG	AA	1696	1/1	0.85	0.41	45,45,45,45	1
57	MG	BA	3330	1/1	0.85	0.14	35,35,35,35	0
57	MG	DF	305	1/1	0.85	0.30	1,1,1,1	1
57	MG	CA	1651	1/1	0.85	0.36	50,50,50,50	1
57	MG	DA	3292	1/1	0.85	0.37	45,45,45,45	0
57	MG	BA	3374	1/1	0.85	0.95	28,28,28,28	1
57	MG	CA	1616	1/1	0.86	0.79	64,64,64,64	0
57	MG	DA	3138	1/1	0.86	0.26	17,17,17,17	0
57	MG	CA	1733	1/1	0.86	0.39	59,59,59,59	0
57	MG	DA	3396	1/1	0.86	0.60	14,14,14,14	0
57	MG	AA	1760	1/1	0.86	0.24	37,37,37,37	0
57	MG	BA	3232	1/1	0.86	0.34	30,30,30,30	0
57	MG	DA	3245	1/1	0.86	0.60	67,67,67,67	0
57	MG	DA	3323	1/1	0.86	0.14	63,63,63,63	1
57	MG	CA	1771	1/1	0.86	0.08	1,1,1,1	1
57	MG	DA	3426	1/1	0.86	0.24	44,44,44,44	0
57	MG	CA	1774	1/1	0.86	0.32	74,74,74,74	0
57	MG	BA	3321	1/1	0.86	0.12	51,51,51,51	0
57	MG	BA	3348	1/1	0.86	1.26	84,84,84,84	0
57	MG	BA	3405	1/1	0.86	0.36	22,22,22,22	0
57	MG	CA	1702	1/1	0.86	0.64	47,47,47,47	0
57	MG	AA	1676	1/1	0.86	0.24	32,32,32,32	0
57	MG	BA	3088	1/1	0.86	0.31	1,1,1,1	1
57	MG	AA	1800	1/1	0.86	0.29	38,38,38,38	0
57	MG	BA	3294	1/1	0.86	0.54	55,55,55,55	0
57	MG	DA	3202	1/1	0.86	0.88	7,7,7,7	1
57	MG	DA	3285	1/1	0.86	0.52	13,13,13,13	1
57	MG	CW	108	1/1	0.86	0.43	28,28,28,28	1
57	MG	BA	3178	1/1	0.86	0.38	38,38,38,38	0
57	MG	BA	3434	1/1	0.86	0.20	60,60,60,60	0
57	MG	BA	3437	1/1	0.86	0.32	64,64,64,64	0
57	MG	BA	3157	1/1	0.86	0.20	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3302	1/1	0.86	0.28	80,80,80,80	1
57	MG	BA	3129	1/1	0.87	0.31	8,8,8,8	1
57	MG	AA	1701	1/1	0.87	0.58	8,8,8,8	1
57	MG	AA	1644	1/1	0.87	0.29	1,1,1,1	0
57	MG	CA	1617	1/1	0.87	0.72	29,29,29,29	0
57	MG	CA	1724	1/1	0.87	0.36	51,51,51,51	0
57	MG	DA	3289	1/1	0.87	0.53	36,36,36,36	0
57	MG	BA	3408	1/1	0.87	0.24	21,21,21,21	0
57	MG	AA	1646	1/1	0.87	0.42	29,29,29,29	0
57	MG	BA	3250	1/1	0.87	0.16	24,24,24,24	0
57	MG	AA	1741	1/1	0.87	0.30	48,48,48,48	0
57	MG	BA	3258	1/1	0.87	0.17	32,32,32,32	0
57	MG	DA	3407	1/1	0.87	0.28	9,9,9,9	0
57	MG	DA	3192	1/1	0.87	0.61	27,27,27,27	0
57	MG	BA	3422	1/1	0.87	0.20	30,30,30,30	0
57	MG	AA	1742	1/1	0.87	0.14	36,36,36,36	0
57	MG	BA	3269	1/1	0.87	0.21	22,22,22,22	0
57	MG	DA	3317	1/1	0.87	0.40	78,78,78,78	1
57	MG	AV	101	1/1	0.87	0.37	46,46,46,46	0
57	MG	CA	1742	1/1	0.87	0.70	1,1,1,1	1
57	MG	BA	3274	1/1	0.87	0.25	55,55,55,55	0
57	MG	DA	3322	1/1	0.87	0.19	34,34,34,34	1
57	MG	BA	3279	1/1	0.87	0.25	35,35,35,35	1
57	MG	BA	3029	1/1	0.87	0.64	1,1,1,1	1
57	MG	DB	201	1/1	0.87	0.23	22,22,22,22	1
57	MG	BA	3282	1/1	0.87	0.31	72,72,72,72	0
57	MG	DB	204	1/1	0.87	0.43	89,89,89,89	1
57	MG	AA	1682	1/1	0.87	0.23	46,46,46,46	0
57	MG	AW	115	1/1	0.87	0.39	19,19,19,19	1
57	MG	AA	1723	1/1	0.87	0.22	55,55,55,55	0
57	MG	AA	1725	1/1	0.87	0.49	48,48,48,48	0
57	MG	CA	1690	1/1	0.87	0.60	20,20,20,20	1
57	MG	AA	1758	1/1	0.87	0.20	11,11,11,11	0
57	MG	CA	1761	1/1	0.87	0.22	1,1,1,1	1
57	MG	AA	1712	1/1	0.87	0.31	50,50,50,50	0
57	MG	B1	102	1/1	0.87	0.22	7,7,7,7	1
57	MG	BA	3306	1/1	0.87	0.86	50,50,50,50	0
57	MG	AA	1736	1/1	0.88	0.44	20,20,20,20	0
57	MG	BB	206	1/1	0.88	0.69	13,13,13,13	1
57	MG	BA	3241	1/1	0.88	0.51	27,27,27,27	0
57	MG	BA	3203	1/1	0.88	0.27	10,10,10,10	0
57	MG	BA	3204	1/1	0.88	0.26	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3058	1/1	0.88	0.45	3,3,3,3	1
57	MG	BA	3120	1/1	0.88	0.43	38,38,38,38	0
57	MG	BA	3266	1/1	0.88	0.82	65,65,65,65	0
57	MG	BA	3128	1/1	0.88	0.28	1,1,1,1	0
57	MG	DA	3387	1/1	0.88	0.26	33,33,33,33	1
57	MG	BA	3351	1/1	0.88	0.36	68,68,68,68	1
57	MG	CA	1745	1/1	0.88	0.21	112,112,112,112	1
57	MG	CA	1687	1/1	0.88	0.44	42,42,42,42	0
57	MG	BA	3356	1/1	0.88	0.29	3,3,3,3	1
57	MG	DA	3406	1/1	0.88	0.82	57,57,57,57	0
57	MG	CA	1610	1/1	0.88	0.22	15,15,15,15	1
57	MG	DA	3166	1/1	0.88	0.35	43,43,43,43	0
57	MG	CW	121	1/1	0.88	0.37	28,28,28,28	1
57	MG	AA	1686	1/1	0.88	0.24	61,61,61,61	0
57	MG	CX	103	1/1	0.88	0.28	45,45,45,45	1
57	MG	DA	3312	1/1	0.88	0.31	1,1,1,1	0
57	MG	D1	102	1/1	0.88	0.32	51,51,51,51	0
57	MG	BA	3130	1/1	0.88	0.28	1,1,1,1	1
57	MG	DA	3318	1/1	0.88	0.63	7,7,7,7	1
57	MG	BA	3276	1/1	0.88	0.82	34,34,34,34	1
57	MG	D3	101	1/1	0.88	0.27	42,42,42,42	0
57	MG	DA	3440	1/1	0.88	0.41	80,80,80,80	0
57	MG	BA	3439	1/1	0.88	0.37	25,25,25,25	0
57	MG	BA	3440	1/1	0.88	0.13	33,33,33,33	0
57	MG	BA	3230	1/1	0.88	0.22	22,22,22,22	0
57	MG	DA	3042	1/1	0.88	0.22	17,17,17,17	1
57	MG	DA	3048	1/1	0.88	0.84	56,56,56,56	1
57	MG	DA	3328	1/1	0.88	0.63	63,63,63,63	0
57	MG	CA	1763	1/1	0.88	0.48	15,15,15,15	0
57	MG	DA	3236	1/1	0.88	0.40	14,14,14,14	0
57	MG	DA	3069	1/1	0.88	0.35	21,21,21,21	0
57	MG	BA	3137	1/1	0.88	0.72	7,7,7,7	0
57	MG	BA	3323	1/1	0.88	0.35	74,74,74,74	0
57	MG	DG	201	1/1	0.88	0.21	38,38,38,38	0
57	MG	AW	119	1/1	0.88	1.01	71,71,71,71	1
57	MG	CA	1650	1/1	0.88	0.25	98,98,98,98	1
57	MG	DS	201	1/1	0.88	0.21	1,1,1,1	1
57	MG	DA	3102	1/1	0.88	0.17	3,3,3,3	0
57	MG	BA	3320	1/1	0.89	0.23	37,37,37,37	1
57	MG	AE	202	1/1	0.89	0.21	37,37,37,37	0
57	MG	CW	103	1/1	0.89	0.76	61,61,61,61	1
57	MG	BB	215	1/1	0.89	0.25	49,49,49,49	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3395	1/1	0.89	0.28	1,1,1,1	1
57	MG	AA	1669	1/1	0.89	0.42	5,5,5,5	0
57	MG	BF	303	1/1	0.89	0.18	36,36,36,36	0
57	MG	AA	1738	1/1	0.89	0.42	18,18,18,18	1
57	MG	AX	101	1/1	0.89	0.28	15,15,15,15	1
57	MG	DA	3290	1/1	0.89	0.49	21,21,21,21	0
57	MG	BA	3150	1/1	0.89	0.25	22,22,22,22	0
57	MG	BA	3409	1/1	0.89	0.40	5,5,5,5	0
57	MG	CA	1711	1/1	0.89	0.44	37,37,37,37	1
57	MG	CA	1615	1/1	0.89	0.23	42,42,42,42	0
57	MG	CA	1716	1/1	0.89	0.81	75,75,75,75	0
57	MG	BA	3216	1/1	0.89	0.09	49,49,49,49	0
57	MG	AA	1694	1/1	0.89	0.24	13,13,13,13	1
57	MG	BA	3154	1/1	0.89	0.19	56,56,56,56	0
57	MG	BA	3284	1/1	0.89	0.29	12,12,12,12	1
57	MG	BA	3156	1/1	0.89	0.63	12,12,12,12	1
57	MG	CA	1729	1/1	0.89	0.57	63,63,63,63	0
57	MG	DA	3435	1/1	0.89	0.25	48,48,48,48	0
57	MG	DA	3194	1/1	0.89	0.40	57,57,57,57	0
57	MG	BA	3060	1/1	0.89	0.23	42,42,42,42	0
57	MG	AA	1665	1/1	0.89	0.44	21,21,21,21	0
57	MG	BA	3163	1/1	0.89	0.21	33,33,33,33	0
57	MG	AA	1625	1/1	0.89	0.43	31,31,31,31	0
57	MG	AA	1613	1/1	0.89	0.49	11,11,11,11	1
57	MG	AA	1687	1/1	0.89	0.14	61,61,61,61	0
57	MG	BA	3176	1/1	0.89	0.57	21,21,21,21	1
57	MG	DA	3018	1/1	0.89	0.39	12,12,12,12	0
57	MG	DA	3022	1/1	0.89	0.26	28,28,28,28	1
57	MG	DA	3331	1/1	0.89	0.22	79,79,79,79	1
57	MG	BA	3372	1/1	0.89	0.34	20,20,20,20	1
57	MG	CA	1808	1/1	0.89	0.40	43,43,43,43	1
57	MG	AW	117	1/1	0.89	0.20	19,19,19,19	1
57	MG	BA	3263	1/1	0.89	0.28	29,29,29,29	0
57	MG	BA	3375	1/1	0.89	0.13	62,62,62,62	0
57	MG	AA	1754	1/1	0.89	0.29	49,49,49,49	1
57	MG	CA	1680	1/1	0.89	0.23	75,75,75,75	1
57	MG	DP	202	1/1	0.89	0.32	1,1,1,1	1
57	MG	DA	3268	1/1	0.89	0.22	24,24,24,24	0
57	MG	BA	3388	1/1	0.89	0.56	4,4,4,4	1
57	MG	CA	1739	1/1	0.90	0.27	32,32,32,32	0
57	MG	AA	1698	1/1	0.90	0.15	1,1,1,1	0
57	MG	AA	1609	1/1	0.90	0.33	7,7,7,7	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3369	1/1	0.90	0.45	142,142,142,142	1
57	MG	AA	1765	1/1	0.90	0.13	41,41,41,41	0
57	MG	BA	3367	1/1	0.90	0.44	37,37,37,37	0
57	MG	CA	1659	1/1	0.90	0.15	34,34,34,34	1
57	MG	BA	3368	1/1	0.90	0.20	1,1,1,1	1
57	MG	AD	302	1/1	0.90	0.44	28,28,28,28	0
57	MG	BA	3297	1/1	0.90	0.26	12,12,12,12	0
57	MG	CW	105	1/1	0.90	0.99	79,79,79,79	1
57	MG	AA	1767	1/1	0.90	0.27	21,21,21,21	0
57	MG	AA	1631	1/1	0.90	0.22	1,1,1,1	1
57	MG	AA	1773	1/1	0.90	0.81	16,16,16,16	1
57	MG	DA	3402	1/1	0.90	0.24	45,45,45,45	1
57	MG	AA	1777	1/1	0.90	0.13	6,6,6,6	0
57	MG	AW	122	1/1	0.90	0.34	47,47,47,47	0
57	MG	AA	1703	1/1	0.90	0.12	22,22,22,22	0
57	MG	AA	1688	1/1	0.90	0.44	12,12,12,12	1
57	MG	CA	1694	1/1	0.90	0.13	59,59,59,59	0
57	MG	DA	3423	1/1	0.90	0.23	49,49,49,49	0
57	MG	BB	218	1/1	0.90	0.11	18,18,18,18	0
57	MG	AA	1782	1/1	0.90	0.29	47,47,47,47	0
57	MG	BA	3191	1/1	0.90	0.19	23,23,23,23	0
57	MG	DA	3177	1/1	0.90	0.49	22,22,22,22	0
57	MG	CA	1706	1/1	0.90	0.42	47,47,47,47	1
57	MG	AA	1645	1/1	0.90	0.22	14,14,14,14	1
57	MG	AA	1707	1/1	0.90	0.52	53,53,53,53	0
57	MG	BA	3407	1/1	0.90	0.40	10,10,10,10	0
57	MG	AA	1752	1/1	0.90	0.29	42,42,42,42	1
57	MG	BA	3328	1/1	0.90	0.13	33,33,33,33	0
57	MG	AA	1659	1/1	0.90	0.53	27,27,27,27	0
57	MG	BA	3280	1/1	0.90	0.22	72,72,72,72	0
57	MG	CA	1622	1/1	0.90	0.23	39,39,39,39	0
57	MG	BA	3416	1/1	0.90	0.35	13,13,13,13	0
57	MG	CA	1631	1/1	0.90	0.23	57,57,57,57	0
57	MG	DA	3224	1/1	0.90	0.24	65,65,65,65	1
57	MG	DB	213	1/1	0.90	0.16	28,28,28,28	1
57	MG	DB	215	1/1	0.90	0.34	63,63,63,63	1
57	MG	BA	3213	1/1	0.90	0.42	49,49,49,49	1
57	MG	AA	1735	1/1	0.90	0.24	15,15,15,15	0
57	MG	DA	3339	1/1	0.90	0.50	1,1,1,1	1
57	MG	BA	3219	1/1	0.90	0.63	1,1,1,1	1
57	MG	BA	3346	1/1	0.90	0.38	43,43,43,43	0
57	MG	BA	3152	1/1	0.90	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	CA	1806	1/1	0.90	0.29	35,35,35,35	0
57	MG	DP	201	1/1	0.90	0.68	1,1,1,1	1
57	MG	BA	3435	1/1	0.90	0.39	85,85,85,85	0
57	MG	AA	1663	1/1	0.90	0.58	36,36,36,36	0
57	MG	DU	203	1/1	0.90	0.26	49,49,49,49	1
57	MG	DA	3362	1/1	0.90	0.27	15,15,15,15	0
57	MG	AA	1674	1/1	0.91	0.21	30,30,30,30	1
57	MG	CA	1672	1/1	0.91	0.27	44,44,44,44	0
57	MG	BF	302	1/1	0.91	0.76	15,15,15,15	1
57	MG	BA	3370	1/1	0.91	0.31	37,37,37,37	0
57	MG	BA	3020	1/1	0.91	0.24	21,21,21,21	0
57	MG	BA	3331	1/1	0.91	0.14	11,11,11,11	1
57	MG	CA	1741	1/1	0.91	0.22	1,1,1,1	1
57	MG	DA	3395	1/1	0.91	0.64	1,1,1,1	0
57	MG	BA	3332	1/1	0.91	0.37	64,64,64,64	0
57	MG	CA	1798	1/1	0.91	0.37	43,43,43,43	1
57	MG	BA	3431	1/1	0.91	0.58	12,12,12,12	0
57	MG	BA	3333	1/1	0.91	0.10	41,41,41,41	0
57	MG	BA	3145	1/1	0.91	0.29	4,4,4,4	0
57	MG	BA	3335	1/1	0.91	0.36	1,1,1,1	1
57	MG	DA	3310	1/1	0.91	0.86	7,7,7,7	1
57	MG	BA	3389	1/1	0.91	0.65	31,31,31,31	0
57	MG	DA	3195	1/1	0.91	0.16	15,15,15,15	0
57	MG	BA	3107	1/1	0.91	0.17	23,23,23,23	0
57	MG	BA	3391	1/1	0.91	0.33	30,30,30,30	0
57	MG	BA	3112	1/1	0.91	0.23	34,34,34,34	1
57	MG	CL	202	1/1	0.91	0.33	5,5,5,5	1
57	MG	DA	3026	1/1	0.91	0.67	1,1,1,1	0
57	MG	AA	1746	1/1	0.91	0.39	29,29,29,29	0
57	MG	DA	3218	1/1	0.91	0.42	12,12,12,12	0
57	MG	DA	3324	1/1	0.91	0.15	40,40,40,40	0
57	MG	AA	1724	1/1	0.91	0.22	34,34,34,34	1
57	MG	BA	3182	1/1	0.91	0.30	13,13,13,13	0
57	MG	BA	3252	1/1	0.91	0.31	23,23,23,23	0
57	MG	DA	3086	1/1	0.91	0.45	1,1,1,1	1
57	MG	DA	3330	1/1	0.91	0.30	73,73,73,73	0
57	MG	DB	206	1/1	0.91	0.22	72,72,72,72	0
57	MG	DA	3227	1/1	0.91	0.43	73,73,73,73	0
57	MG	BA	3406	1/1	0.91	0.45	19,19,19,19	0
57	MG	BA	3257	1/1	0.91	0.23	42,42,42,42	0
57	MG	BA	3222	1/1	0.91	0.14	1,1,1,1	0
57	MG	CA	1653	1/1	0.91	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3344	1/1	0.91	0.15	20,20,20,20	0
57	MG	CA	1768	1/1	0.91	0.59	5,5,5,5	1
57	MG	BA	3224	1/1	0.91	1.25	80,80,80,80	0
57	MG	DE	302	1/1	0.91	0.37	50,50,50,50	0
57	MG	BA	3100	1/1	0.91	0.33	1,1,1,1	1
57	MG	CA	1772	1/1	0.91	0.18	60,60,60,60	0
57	MG	DA	3269	1/1	0.91	0.52	57,57,57,57	1
57	MG	CA	1727	1/1	0.91	1.14	92,92,92,92	0
57	MG	AA	1755	1/1	0.91	0.25	47,47,47,47	0
57	MG	BA	3415	1/1	0.91	0.17	18,18,18,18	1
57	MG	CA	1664	1/1	0.91	0.10	54,54,54,54	1
57	MG	DA	3144	1/1	0.91	0.21	1,1,1,1	0
57	MG	DA	3149	1/1	0.91	0.69	27,27,27,27	0
57	MG	BA	3245	1/1	0.92	0.09	52,52,52,52	1
57	MG	AA	1803	1/1	0.92	0.24	9,9,9,9	0
57	MG	DA	3338	1/1	0.92	0.29	16,16,16,16	1
57	MG	AD	301	1/1	0.92	0.21	15,15,15,15	1
57	MG	DA	3340	1/1	0.92	0.15	59,59,59,59	0
57	MG	AA	1651	1/1	0.92	0.16	32,32,32,32	0
57	MG	AE	201	1/1	0.92	0.19	28,28,28,28	0
57	MG	DA	3345	1/1	0.92	0.15	2,2,2,2	1
57	MG	BA	3169	1/1	0.92	0.33	33,33,33,33	0
57	MG	DA	3354	1/1	0.92	0.24	6,6,6,6	1
57	MG	CA	1632	1/1	0.92	0.22	36,36,36,36	0
57	MG	AA	1608	1/1	0.92	0.06	3,3,3,3	0
57	MG	AA	1655	1/1	0.92	0.33	31,31,31,31	0
57	MG	BA	3179	1/1	0.92	0.18	30,30,30,30	0
57	MG	BA	3267	1/1	0.92	0.24	34,34,34,34	0
57	MG	AA	1753	1/1	0.92	0.41	48,48,48,48	0
57	MG	AA	1634	1/1	0.92	0.11	28,28,28,28	0
57	MG	BA	3421	1/1	0.92	0.69	39,39,39,39	1
57	MG	DA	3368	1/1	0.92	0.36	78,78,78,78	0
57	MG	BA	3338	1/1	0.92	0.17	46,46,46,46	0
57	MG	AA	1602	1/1	0.92	0.15	64,64,64,64	0
57	MG	BA	3429	1/1	0.92	0.16	32,32,32,32	0
57	MG	BA	3275	1/1	0.92	0.14	37,37,37,37	0
57	MG	BA	3117	1/1	0.92	0.18	8,8,8,8	0
57	MG	BA	3197	1/1	0.92	0.20	25,25,25,25	1
57	MG	BA	3001	1/1	0.92	0.38	8,8,8,8	0
57	MG	DA	3389	1/1	0.92	0.26	33,33,33,33	1
57	MG	CA	1666	1/1	0.92	0.28	1,1,1,1	0
57	MG	BA	3353	1/1	0.92	0.54	41,41,41,41	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3125	1/1	0.92	0.45	1,1,1,1	0
57	MG	DA	3005	1/1	0.92	0.11	22,22,22,22	0
57	MG	DA	3264	1/1	0.92	0.24	25,25,25,25	0
57	MG	AA	1787	1/1	0.92	0.19	53,53,53,53	1
57	MG	DA	3403	1/1	0.92	0.47	47,47,47,47	1
57	MG	DA	3012	1/1	0.92	0.41	1,1,1,1	0
57	MG	AA	1616	1/1	0.92	0.12	24,24,24,24	1
57	MG	CA	1675	1/1	0.92	0.84	47,47,47,47	1
57	MG	DA	3414	1/1	0.92	0.18	16,16,16,16	0
57	MG	BA	3209	1/1	0.92	0.08	18,18,18,18	0
57	MG	DA	3420	1/1	0.92	0.26	14,14,14,14	1
57	MG	AA	1621	1/1	0.92	0.12	3,3,3,3	0
57	MG	DA	3037	1/1	0.92	0.17	1,1,1,1	0
57	MG	CA	1683	1/1	0.92	0.45	19,19,19,19	0
57	MG	BA	3132	1/1	0.92	0.12	24,24,24,24	1
57	MG	BA	3009	1/1	0.92	0.35	1,1,1,1	0
57	MG	DA	3057	1/1	0.92	0.19	3,3,3,3	0
57	MG	AA	1790	1/1	0.92	0.28	35,35,35,35	0
57	MG	BA	3143	1/1	0.92	0.45	1,1,1,1	1
57	MG	AA	1761	1/1	0.92	0.19	13,13,13,13	0
57	MG	AA	1739	1/1	0.92	0.44	44,44,44,44	0
57	MG	AA	1794	1/1	0.92	0.29	40,40,40,40	0
57	MG	CA	1700	1/1	0.92	0.25	10,10,10,10	0
57	MG	BA	3380	1/1	0.92	0.17	63,63,63,63	0
57	MG	DA	3107	1/1	0.92	0.38	34,34,34,34	0
57	MG	DA	3126	1/1	0.92	0.20	1,1,1,1	0
57	MG	DB	205	1/1	0.92	0.40	5,5,5,5	1
57	MG	BA	3387	1/1	0.92	0.15	42,42,42,42	0
57	MG	DA	3309	1/1	0.92	0.34	44,44,44,44	0
57	MG	BA	3308	1/1	0.92	0.97	30,30,30,30	1
57	MG	AA	1721	1/1	0.92	0.43	44,44,44,44	0
57	MG	AA	1623	1/1	0.92	0.23	16,16,16,16	0
57	MG	AA	1704	1/1	0.92	0.20	11,11,11,11	0
57	MG	CA	1712	1/1	0.92	0.50	19,19,19,19	0
57	MG	CA	1713	1/1	0.92	0.25	40,40,40,40	1
57	MG	BG	201	1/1	0.92	0.09	17,17,17,17	0
57	MG	BN	202	1/1	0.92	0.62	3,3,3,3	1
57	MG	BN	203	1/1	0.92	0.17	56,56,56,56	1
57	MG	CA	1721	1/1	0.92	0.20	17,17,17,17	1
57	MG	BA	3038	1/1	0.92	0.34	22,22,22,22	1
57	MG	BA	3239	1/1	0.92	0.20	14,14,14,14	1
57	MG	CA	1607	1/1	0.92	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1611	1/1	0.92	0.12	24,24,24,24	0
57	MG	CA	1612	1/1	0.92	0.28	75,75,75,75	0
57	MG	CA	1613	1/1	0.92	0.70	10,10,10,10	1
57	MG	CA	1730	1/1	0.92	0.23	1,1,1,1	0
57	MG	BA	3401	1/1	0.93	0.68	42,42,42,42	0
57	MG	BU	201	1/1	0.93	0.24	12,12,12,12	1
57	MG	BX	102	1/1	0.93	0.18	1,1,1,1	1
57	MG	AA	1648	1/1	0.93	0.16	3,3,3,3	1
57	MG	BA	3404	1/1	0.93	0.19	108,108,108,108	0
57	MG	BA	3336	1/1	0.93	0.19	8,8,8,8	1
57	MG	AA	1710	1/1	0.93	0.38	113,113,113,113	1
57	MG	AA	1695	1/1	0.93	0.45	42,42,42,42	0
57	MG	DA	3145	1/1	0.93	0.46	56,56,56,56	1
57	MG	DA	3147	1/1	0.93	0.21	22,22,22,22	0
57	MG	CA	1717	1/1	0.93	0.15	1,1,1,1	0
57	MG	BA	3339	1/1	0.93	0.39	3,3,3,3	0
57	MG	CA	1719	1/1	0.93	0.20	56,56,56,56	1
57	MG	DA	3337	1/1	0.93	0.32	92,92,92,92	0
57	MG	BA	3246	1/1	0.93	0.30	23,23,23,23	1
57	MG	DA	3156	1/1	0.93	0.21	21,21,21,21	0
57	MG	BA	3290	1/1	0.93	1.13	33,33,33,33	1
57	MG	BA	3345	1/1	0.93	0.84	1,1,1,1	1
57	MG	AA	1656	1/1	0.93	0.26	31,31,31,31	0
57	MG	CA	1629	1/1	0.93	0.11	2,2,2,2	1
57	MG	AA	1802	1/1	0.93	0.21	18,18,18,18	0
57	MG	DA	3170	1/1	0.93	0.33	26,26,26,26	1
57	MG	BA	3349	1/1	0.93	0.34	86,86,86,86	0
57	MG	CA	1639	1/1	0.93	0.44	34,34,34,34	0
57	MG	BA	3350	1/1	0.93	0.35	70,70,70,70	0
57	MG	DA	3179	1/1	0.93	0.40	52,52,52,52	1
57	MG	DA	3180	1/1	0.93	0.39	47,47,47,47	0
57	MG	BA	3295	1/1	0.93	0.12	1,1,1,1	0
57	MG	BA	3205	1/1	0.93	0.15	23,23,23,23	0
57	MG	CA	1644	1/1	0.93	0.24	31,31,31,31	0
57	MG	BA	3253	1/1	0.93	0.38	56,56,56,56	1
57	MG	DA	3201	1/1	0.93	0.14	15,15,15,15	0
57	MG	BA	3425	1/1	0.93	0.12	23,23,23,23	0
57	MG	BA	3359	1/1	0.93	0.39	21,21,21,21	1
57	MG	BA	3303	1/1	0.93	0.40	8,8,8,8	1
57	MG	DA	3373	1/1	0.93	0.26	74,74,74,74	0
57	MG	DA	3376	1/1	0.93	0.22	1,1,1,1	0
57	MG	DA	3377	1/1	0.93	0.84	62,62,62,62	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	BA	3364	1/1	0.93	0.19	12,12,12,12	0
57	MG	CA	1652	1/1	0.93	0.49	1,1,1,1	1
57	MG	CW	114	1/1	0.93	0.17	4,4,4,4	1
57	MG	DA	3388	1/1	0.93	0.74	39,39,39,39	0
57	MG	AA	1629	1/1	0.93	0.10	22,22,22,22	0
57	MG	DA	3219	1/1	0.93	0.70	21,21,21,21	1
57	MG	CA	1654	1/1	0.93	0.24	1,1,1,1	0
57	MG	BA	3366	1/1	0.93	0.52	38,38,38,38	1
57	MG	DA	3223	1/1	0.93	0.61	12,12,12,12	1
57	MG	AA	1717	1/1	0.93	0.19	12,12,12,12	1
57	MG	BA	3123	1/1	0.93	0.58	35,35,35,35	0
57	MG	CW	120	1/1	0.93	0.27	20,20,20,20	1
57	MG	DA	3405	1/1	0.93	0.36	30,30,30,30	1
57	MG	DA	3231	1/1	0.93	0.43	14,14,14,14	0
57	MG	DA	3233	1/1	0.93	0.29	1,1,1,1	1
57	MG	BA	3310	1/1	0.93	0.26	5,5,5,5	1
57	MG	CW	122	1/1	0.93	0.22	70,70,70,70	0
57	MG	CA	1660	1/1	0.93	0.16	8,8,8,8	0
57	MG	DA	3419	1/1	0.93	0.59	58,58,58,58	0
57	MG	CA	1757	1/1	0.93	0.65	35,35,35,35	0
57	MG	BA	3159	1/1	0.93	0.40	1,1,1,1	0
57	MG	AA	1728	1/1	0.93	0.15	34,34,34,34	0
57	MG	AA	1684	1/1	0.93	0.11	25,25,25,25	0
57	MG	BA	3086	1/1	0.93	0.52	1,1,1,1	0
57	MG	DA	3428	1/1	0.93	0.55	17,17,17,17	0
57	MG	DA	3265	1/1	0.93	0.52	70,70,70,70	0
57	MG	DA	3432	1/1	0.93	0.41	50,50,50,50	0
57	MG	AW	120	1/1	0.93	0.32	58,58,58,58	1
57	MG	BA	3272	1/1	0.93	0.15	1,1,1,1	1
57	MG	BA	3089	1/1	0.93	0.56	6,6,6,6	1
57	MG	DA	3008	1/1	0.93	0.41	1,1,1,1	0
57	MG	CA	1679	1/1	0.93	0.21	22,22,22,22	0
57	MG	DA	3014	1/1	0.93	0.24	14,14,14,14	0
57	MG	DA	3276	1/1	0.93	0.23	47,47,47,47	0
57	MG	BA	3383	1/1	0.93	0.96	39,39,39,39	1
57	MG	CA	1769	1/1	0.93	0.23	28,28,28,28	0
57	MG	BA	3385	1/1	0.93	0.16	7,7,7,7	0
57	MG	BB	214	1/1	0.93	0.15	34,34,34,34	0
57	MG	DA	3028	1/1	0.93	0.11	59,59,59,59	1
57	MG	DA	3286	1/1	0.93	0.40	12,12,12,12	0
57	MG	BA	3386	1/1	0.93	0.14	13,13,13,13	0
57	MG	BA	3091	1/1	0.93	0.17	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3045	1/1	0.93	0.21	10,10,10,10	0
57	MG	CA	1775	1/1	0.93	0.22	1,1,1,1	1
57	MG	BA	3228	1/1	0.93	0.24	50,50,50,50	0
57	MG	CA	1780	1/1	0.93	0.72	31,31,31,31	1
57	MG	BA	3277	1/1	0.93	0.21	28,28,28,28	1
57	MG	DA	3071	1/1	0.93	0.38	1,1,1,1	0
57	MG	DA	3084	1/1	0.93	0.22	13,13,13,13	0
57	MG	BA	3139	1/1	0.93	0.38	8,8,8,8	1
57	MG	CA	1784	1/1	0.93	0.23	1,1,1,1	1
57	MG	CA	1693	1/1	0.93	0.08	14,14,14,14	1
57	MG	BA	3140	1/1	0.93	0.24	24,24,24,24	1
57	MG	BA	3093	1/1	0.93	0.14	1,1,1,1	0
57	MG	BA	3393	1/1	0.93	0.22	14,14,14,14	0
57	MG	BA	3184	1/1	0.93	0.11	44,44,44,44	0
57	MG	AA	1719	1/1	0.93	0.26	1,1,1,1	1
57	MG	BA	3085	1/1	0.94	0.19	1,1,1,1	0
57	MG	AA	1610	1/1	0.94	0.19	29,29,29,29	0
57	MG	DA	3164	1/1	0.94	0.09	72,72,72,72	0
57	MG	AA	1793	1/1	0.94	0.19	6,6,6,6	1
57	MG	B5	102	1/1	0.94	0.36	48,48,48,48	0
57	MG	BA	3291	1/1	0.94	0.15	7,7,7,7	0
57	MG	CA	1648	1/1	0.94	0.50	14,14,14,14	1
57	MG	BA	3360	1/1	0.94	0.27	10,10,10,10	0
57	MG	AA	1747	1/1	0.94	0.27	5,5,5,5	0
57	MG	AA	1766	1/1	0.94	0.19	1,1,1,1	1
57	MG	BA	3094	1/1	0.94	0.15	25,25,25,25	1
57	MG	BA	3099	1/1	0.94	0.28	45,45,45,45	1
57	MG	DA	3341	1/1	0.94	0.55	20,20,20,20	0
57	MG	DA	3187	1/1	0.94	0.72	83,83,83,83	1
57	MG	DA	3189	1/1	0.94	0.17	59,59,59,59	0
57	MG	AA	1691	1/1	0.94	0.28	69,69,69,69	0
57	MG	AA	1713	1/1	0.94	0.14	25,25,25,25	0
57	MG	DA	3349	1/1	0.94	0.21	10,10,10,10	1
57	MG	CA	1656	1/1	0.94	0.16	19,19,19,19	1
57	MG	BA	3442	1/1	0.94	0.16	33,33,33,33	0
57	MG	DA	3357	1/1	0.94	0.07	52,52,52,52	0
57	MG	BA	3164	1/1	0.94	0.45	56,56,56,56	0
57	MG	DA	3359	1/1	0.94	0.17	40,40,40,40	0
57	MG	DA	3205	1/1	0.94	0.08	13,13,13,13	0
57	MG	BA	3444	1/1	0.94	0.65	15,15,15,15	1
57	MG	CA	1755	1/1	0.94	0.30	1,1,1,1	0
57	MG	DA	3210	1/1	0.94	0.12	93,93,93,93	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	DA	3365	1/1	0.94	0.21	24,24,24,24	1
57	MG	BA	3307	1/1	0.94	0.36	35,35,35,35	0
57	MG	BB	202	1/1	0.94	0.18	9,9,9,9	1
57	MG	AA	1639	1/1	0.94	0.29	8,8,8,8	1
57	MG	DA	3217	1/1	0.94	0.25	31,31,31,31	0
57	MG	AA	1652	1/1	0.94	0.44	11,11,11,11	0
57	MG	BA	3011	1/1	0.94	0.43	15,15,15,15	0
57	MG	BA	3109	1/1	0.94	0.45	3,3,3,3	0
57	MG	CA	1762	1/1	0.94	0.29	7,7,7,7	1
57	MG	BA	3248	1/1	0.94	0.18	10,10,10,10	0
57	MG	BA	3318	1/1	0.94	0.32	1,1,1,1	0
57	MG	CA	1677	1/1	0.94	0.20	36,36,36,36	0
57	MG	DA	3226	1/1	0.94	0.34	48,48,48,48	0
57	MG	BA	3175	1/1	0.94	0.12	21,21,21,21	0
57	MG	DA	3228	1/1	0.94	0.56	41,41,41,41	0
57	MG	DA	3010	1/1	0.94	0.17	1,1,1,1	0
57	MG	AA	1779	1/1	0.94	0.26	1,1,1,1	1
57	MG	AA	1633	1/1	0.94	0.30	26,26,26,26	0
57	MG	DA	3238	1/1	0.94	0.40	1,1,1,1	0
57	MG	BA	3118	1/1	0.94	0.24	33,33,33,33	1
57	MG	BA	3180	1/1	0.94	0.45	1,1,1,1	1
57	MG	BB	219	1/1	0.94	0.45	73,73,73,73	1
57	MG	DA	3247	1/1	0.94	0.30	13,13,13,13	0
57	MG	DA	3248	1/1	0.94	0.33	5,5,5,5	1
57	MG	AA	1740	1/1	0.94	0.13	35,35,35,35	0
57	MG	DA	3253	1/1	0.94	0.52	25,25,25,25	0
57	MG	BA	3026	1/1	0.94	0.16	8,8,8,8	0
57	MG	DA	3033	1/1	0.94	0.20	13,13,13,13	0
57	MG	CA	1776	1/1	0.94	0.21	32,32,32,32	0
57	MG	AA	1757	1/1	0.94	0.33	51,51,51,51	1
57	MG	AA	1643	1/1	0.94	0.24	43,43,43,43	0
57	MG	DA	3046	1/1	0.94	0.41	1,1,1,1	0
57	MG	AA	1759	1/1	0.94	0.14	20,20,20,20	0
57	MG	CA	1695	1/1	0.94	0.25	1,1,1,1	1
57	MG	BA	3394	1/1	0.94	0.36	7,7,7,7	1
57	MG	DA	3274	1/1	0.94	0.05	65,65,65,65	0
57	MG	DA	3430	1/1	0.94	0.21	13,13,13,13	0
57	MG	CA	1698	1/1	0.94	0.11	22,22,22,22	0
57	MG	AA	1732	1/1	0.94	0.28	31,31,31,31	0
57	MG	DA	3277	1/1	0.94	0.17	22,22,22,22	0
57	MG	BA	3396	1/1	0.94	0.56	15,15,15,15	0
57	MG	CA	1703	1/1	0.94	0.27	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BO	201	1/1	0.94	0.42	1,1,1,1	1
57	MG	CA	1705	1/1	0.94	0.11	5,5,5,5	0
57	MG	DA	3284	1/1	0.94	0.38	18,18,18,18	0
57	MG	BA	3198	1/1	0.94	0.26	4,4,4,4	0
57	MG	BA	3399	1/1	0.94	0.22	56,56,56,56	1
57	MG	BA	3271	1/1	0.94	0.21	9,9,9,9	0
57	MG	DA	3103	1/1	0.94	0.30	1,1,1,1	0
57	MG	BA	3201	1/1	0.94	0.20	31,31,31,31	0
57	MG	DA	3115	1/1	0.94	0.41	6,6,6,6	0
57	MG	DB	207	1/1	0.94	0.26	16,16,16,16	1
57	MG	DA	3117	1/1	0.94	0.34	5,5,5,5	0
57	MG	BA	3040	1/1	0.94	0.09	16,16,16,16	0
57	MG	DB	210	1/1	0.94	0.22	49,49,49,49	1
57	MG	BA	3135	1/1	0.94	0.17	38,38,38,38	0
57	MG	BA	3043	1/1	0.94	0.19	26,26,26,26	0
57	MG	CA	1805	1/1	0.94	0.38	1,1,1,1	0
57	MG	AA	1667	1/1	0.94	0.38	17,17,17,17	0
57	MG	AA	1744	1/1	0.94	0.42	22,22,22,22	0
57	MG	CE	201	1/1	0.94	0.66	78,78,78,78	0
57	MG	DD	303	1/1	0.94	0.20	1,1,1,1	0
57	MG	BA	3341	1/1	0.94	0.16	4,4,4,4	1
57	MG	CA	1620	1/1	0.94	0.13	34,34,34,34	0
57	MG	CA	1720	1/1	0.94	0.14	4,4,4,4	1
57	MG	AA	1763	1/1	0.94	0.64	40,40,40,40	1
57	MG	BA	3073	1/1	0.94	0.47	1,1,1,1	0
57	MG	BA	3413	1/1	0.94	0.37	21,21,21,21	1
57	MG	BA	3214	1/1	0.94	0.16	106,106,106,106	1
57	MG	BA	3347	1/1	0.94	0.50	1,1,1,1	0
57	MG	BA	3215	1/1	0.94	0.72	38,38,38,38	1
57	MG	BA	3144	1/1	0.94	0.18	40,40,40,40	0
57	MG	BA	3044	1/1	0.95	0.38	36,36,36,36	0
57	MG	BA	3126	1/1	0.95	0.33	1,1,1,1	0
57	MG	DA	3356	1/1	0.95	0.17	57,57,57,57	0
57	MG	AA	1729	1/1	0.95	0.10	19,19,19,19	0
57	MG	DA	3058	1/1	0.95	0.22	42,42,42,42	0
57	MG	DA	3059	1/1	0.95	0.18	1,1,1,1	0
57	MG	DA	3067	1/1	0.95	0.32	1,1,1,1	0
57	MG	DA	3068	1/1	0.95	0.26	24,24,24,24	0
57	MG	CA	1669	1/1	0.95	0.41	32,32,32,32	0
57	MG	CE	203	1/1	0.95	0.45	38,38,38,38	1
57	MG	CA	1670	1/1	0.95	0.13	23,23,23,23	0
57	MG	CA	1671	1/1	0.95	0.33	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3235	1/1	0.95	0.44	22,22,22,22	0
57	MG	AA	1709	1/1	0.95	0.18	3,3,3,3	0
57	MG	AL	201	1/1	0.95	0.15	1,1,1,1	1
57	MG	BA	3004	1/1	0.95	0.20	31,31,31,31	1
57	MG	BA	3079	1/1	0.95	0.20	1,1,1,1	0
57	MG	CA	1678	1/1	0.95	0.10	4,4,4,4	0
57	MG	BA	3301	1/1	0.95	0.12	24,24,24,24	0
57	MG	DA	3260	1/1	0.95	0.31	8,8,8,8	1
57	MG	BX	101	1/1	0.95	0.21	26,26,26,26	1
57	MG	BA	3358	1/1	0.95	0.30	22,22,22,22	0
57	MG	AA	1796	1/1	0.95	0.19	9,9,9,9	0
57	MG	AA	1617	1/1	0.95	0.11	6,6,6,6	1
57	MG	DA	3131	1/1	0.95	0.13	22,22,22,22	0
57	MG	BA	3008	1/1	0.95	0.34	19,19,19,19	0
57	MG	BA	3192	1/1	0.95	0.44	15,15,15,15	0
57	MG	DA	3391	1/1	0.95	0.12	19,19,19,19	0
57	MG	AA	1642	1/1	0.95	0.14	26,26,26,26	0
57	MG	DA	3394	1/1	0.95	0.17	30,30,30,30	1
57	MG	AW	101	1/1	0.95	1.05	51,51,51,51	1
57	MG	BA	3312	1/1	0.95	0.22	1,1,1,1	0
57	MG	DA	3398	1/1	0.95	0.18	13,13,13,13	1
57	MG	BA	3426	1/1	0.95	0.20	27,27,27,27	0
57	MG	BA	3199	1/1	0.95	0.46	5,5,5,5	1
57	MG	AA	1601	1/1	0.95	0.15	21,21,21,21	0
57	MG	DA	3146	1/1	0.95	0.16	3,3,3,3	0
57	MG	DA	3280	1/1	0.95	0.16	24,24,24,24	1
57	MG	BA	3260	1/1	0.95	0.45	1,1,1,1	0
57	MG	DA	3408	1/1	0.95	0.28	1,1,1,1	0
57	MG	DA	3148	1/1	0.95	0.21	26,26,26,26	0
57	MG	DA	3410	1/1	0.95	0.16	31,31,31,31	1
57	MG	DA	3411	1/1	0.95	0.17	19,19,19,19	0
57	MG	CA	1624	1/1	0.95	0.69	40,40,40,40	0
57	MG	AA	1638	1/1	0.95	0.41	39,39,39,39	0
57	MG	DA	3418	1/1	0.95	0.62	24,24,24,24	1
57	MG	BA	3015	1/1	0.95	0.15	6,6,6,6	0
57	MG	AA	1614	1/1	0.95	0.59	11,11,11,11	0
57	MG	CA	1634	1/1	0.95	0.42	25,25,25,25	0
57	MG	CA	1635	1/1	0.95	0.06	6,6,6,6	0
57	MG	BA	3019	1/1	0.95	0.48	1,1,1,1	0
57	MG	DA	3425	1/1	0.95	0.26	19,19,19,19	0
57	MG	DA	3162	1/1	0.95	0.14	2,2,2,2	1
57	MG	AA	1772	1/1	0.95	0.57	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1681	1/1	0.95	0.31	14,14,14,14	0
57	MG	CA	1779	1/1	0.95	0.43	34,34,34,34	0
57	MG	BA	3326	1/1	0.95	0.19	23,23,23,23	1
57	MG	CA	1781	1/1	0.95	0.21	1,1,1,1	1
57	MG	DA	3001	1/1	0.95	0.23	49,49,49,49	0
57	MG	BA	3210	1/1	0.95	1.17	10,10,10,10	1
57	MG	DA	3437	1/1	0.95	0.27	59,59,59,59	1
57	MG	AA	1775	1/1	0.95	0.17	14,14,14,14	1
57	MG	BA	3329	1/1	0.95	0.56	61,61,61,61	0
57	MG	DA	3007	1/1	0.95	0.16	14,14,14,14	0
57	MG	CA	1647	1/1	0.95	0.42	82,82,82,82	0
57	MG	DA	3009	1/1	0.95	0.27	1,1,1,1	1
57	MG	AX	105	1/1	0.95	0.14	35,35,35,35	0
57	MG	B1	101	1/1	0.95	0.30	27,27,27,27	0
57	MG	DA	3013	1/1	0.95	0.51	7,7,7,7	1
57	MG	BA	3160	1/1	0.95	0.38	6,6,6,6	0
57	MG	DA	3199	1/1	0.95	0.23	5,5,5,5	0
57	MG	BA	3217	1/1	0.95	0.33	35,35,35,35	0
57	MG	BA	3113	1/1	0.95	0.29	1,1,1,1	0
57	MG	DA	3203	1/1	0.95	0.41	1,1,1,1	1
57	MG	DB	211	1/1	0.95	0.15	1,1,1,1	1
57	MG	BA	3037	1/1	0.95	0.25	27,27,27,27	0
57	MG	AA	1700	1/1	0.95	0.41	34,34,34,34	0
57	MG	B1	103	1/1	0.95	0.15	1,1,1,1	0
57	MG	DA	3032	1/1	0.95	0.19	23,23,23,23	0
57	MG	DA	3333	1/1	0.95	0.10	15,15,15,15	0
57	MG	DA	3211	1/1	0.95	0.17	39,39,39,39	1
57	MG	BA	3226	1/1	0.95	0.32	1,1,1,1	1
57	MG	DA	3213	1/1	0.95	0.24	24,24,24,24	0
57	MG	DF	302	1/1	0.95	0.21	15,15,15,15	0
57	MG	DF	303	1/1	0.95	0.61	4,4,4,4	1
57	MG	DA	3035	1/1	0.95	0.10	48,48,48,48	0
57	MG	BA	3121	1/1	0.95	0.35	30,30,30,30	0
57	MG	DA	3216	1/1	0.95	0.10	28,28,28,28	1
57	MG	DN	201	1/1	0.95	0.18	21,21,21,21	1
57	MG	DA	3040	1/1	0.95	0.13	1,1,1,1	0
57	MG	DA	3041	1/1	0.95	0.12	24,24,24,24	0
57	MG	B2	602	1/1	0.95	0.24	1,1,1,1	1
57	MG	DP	203	1/1	0.95	0.17	1,1,1,1	1
57	MG	DP	204	1/1	0.95	0.13	15,15,15,15	1
57	MG	BA	3174	1/1	0.95	0.19	1,1,1,1	1
57	MG	BA	3288	1/1	0.95	0.22	44,44,44,44	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3352	1/1	0.95	0.27	123,123,123,123	1
57	MG	CA	1628	1/1	0.96	0.68	35,35,35,35	0
57	MG	BA	3033	1/1	0.96	0.31	20,20,20,20	0
57	MG	CA	1630	1/1	0.96	0.33	40,40,40,40	0
57	MG	DA	3155	1/1	0.96	0.37	21,21,21,21	0
57	MG	AA	1774	1/1	0.96	0.30	23,23,23,23	0
57	MG	BA	3114	1/1	0.96	0.27	1,1,1,1	0
57	MG	AA	1627	1/1	0.96	0.48	9,9,9,9	0
57	MG	BA	3293	1/1	0.96	0.10	19,19,19,19	0
57	MG	CA	1636	1/1	0.96	0.23	1,1,1,1	0
57	MG	CA	1637	1/1	0.96	0.15	47,47,47,47	0
57	MG	CA	1638	1/1	0.96	0.11	6,6,6,6	0
57	MG	CA	1734	1/1	0.96	0.21	46,46,46,46	1
57	MG	DA	3168	1/1	0.96	0.87	36,36,36,36	1
57	MG	AW	105	1/1	0.96	0.51	82,82,82,82	0
57	MG	DA	3171	1/1	0.96	0.18	33,33,33,33	0
57	MG	BA	3171	1/1	0.96	0.17	1,1,1,1	1
57	MG	BA	3427	1/1	0.96	0.29	99,99,99,99	1
57	MG	CA	1642	1/1	0.96	0.13	2,2,2,2	0
57	MG	AA	1776	1/1	0.96	0.20	33,33,33,33	1
57	MG	CA	1740	1/1	0.96	0.35	44,44,44,44	0
57	MG	BA	3430	1/1	0.96	0.29	1,1,1,1	1
57	MG	BA	3361	1/1	0.96	0.29	1,1,1,1	1
57	MG	BA	3432	1/1	0.96	0.33	47,47,47,47	0
57	MG	DA	3191	1/1	0.96	0.19	5,5,5,5	1
57	MG	AA	1673	1/1	0.96	0.12	12,12,12,12	1
57	MG	BA	3363	1/1	0.96	0.12	90,90,90,90	0
57	MG	BA	3300	1/1	0.96	0.28	1,1,1,1	1
57	MG	DA	3196	1/1	0.96	0.35	7,7,7,7	1
57	MG	BA	3233	1/1	0.96	0.30	1,1,1,1	0
57	MG	BA	3302	1/1	0.96	0.05	19,19,19,19	1
57	MG	CA	1750	1/1	0.96	0.36	14,14,14,14	0
57	MG	CA	1751	1/1	0.96	0.31	10,10,10,10	0
57	MG	DA	3364	1/1	0.96	0.27	42,42,42,42	0
57	MG	DA	3003	1/1	0.96	0.09	1,1,1,1	1
57	MG	CA	1752	1/1	0.96	0.23	85,85,85,85	0
57	MG	AA	1685	1/1	0.96	0.13	12,12,12,12	0
57	MG	BA	3305	1/1	0.96	0.09	37,37,37,37	0
57	MG	BA	3177	1/1	0.96	0.26	36,36,36,36	1
57	MG	AA	1612	1/1	0.96	0.26	36,36,36,36	0
57	MG	BA	3003	1/1	0.96	0.34	68,68,68,68	1
57	MG	AA	1731	1/1	0.96	0.12	79,79,79,79	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	BA	3181	1/1	0.96	0.08	17,17,17,17	0
57	MG	DA	3374	1/1	0.96	0.15	28,28,28,28	0
57	MG	BA	3063	1/1	0.96	0.13	6,6,6,6	0
57	MG	BA	3377	1/1	0.96	0.26	95,95,95,95	0
57	MG	DA	3379	1/1	0.96	0.16	47,47,47,47	0
57	MG	BB	207	1/1	0.96	0.04	11,11,11,11	0
57	MG	DA	3384	1/1	0.96	0.16	1,1,1,1	1
57	MG	DA	3017	1/1	0.96	0.07	11,11,11,11	0
57	MG	BA	3378	1/1	0.96	0.15	31,31,31,31	0
57	MG	BA	3183	1/1	0.96	0.76	52,52,52,52	0
57	MG	DA	3024	1/1	0.96	0.32	32,32,32,32	0
57	MG	BA	3066	1/1	0.96	0.14	20,20,20,20	0
57	MG	BB	212	1/1	0.96	0.15	1,1,1,1	1
57	MG	BA	3070	1/1	0.96	0.27	24,24,24,24	0
57	MG	BA	3133	1/1	0.96	0.22	1,1,1,1	0
57	MG	DA	3034	1/1	0.96	0.29	33,33,33,33	0
57	MG	BA	3255	1/1	0.96	0.17	25,25,25,25	0
57	MG	DA	3232	1/1	0.96	0.42	1,1,1,1	0
57	MG	DA	3399	1/1	0.96	0.14	19,19,19,19	0
57	MG	DA	3036	1/1	0.96	0.46	13,13,13,13	1
57	MG	BA	3190	1/1	0.96	0.14	17,17,17,17	0
57	MG	DA	3237	1/1	0.96	0.34	22,22,22,22	0
57	MG	DA	3404	1/1	0.96	0.25	43,43,43,43	0
57	MG	AA	1804	1/1	0.96	0.26	20,20,20,20	0
57	MG	AA	1607	1/1	0.96	0.16	1,1,1,1	0
57	MG	BA	3196	1/1	0.96	0.44	19,19,19,19	0
57	MG	BE	301	1/1	0.96	0.22	1,1,1,1	1
57	MG	BF	301	1/1	0.96	0.38	14,14,14,14	0
57	MG	AA	1677	1/1	0.96	0.12	42,42,42,42	0
57	MG	DA	3249	1/1	0.96	0.11	1,1,1,1	0
57	MG	DA	3250	1/1	0.96	0.18	1,1,1,1	0
57	MG	CA	1682	1/1	0.96	0.24	9,9,9,9	0
57	MG	DA	3051	1/1	0.96	0.18	1,1,1,1	0
57	MG	DA	3055	1/1	0.96	0.08	1,1,1,1	0
57	MG	AA	1690	1/1	0.96	0.15	40,40,40,40	0
57	MG	AA	1624	1/1	0.96	0.24	9,9,9,9	0
57	MG	CA	1685	1/1	0.96	0.22	25,25,25,25	1
57	MG	DA	3065	1/1	0.96	0.26	1,1,1,1	1
57	MG	DA	3266	1/1	0.96	0.20	17,17,17,17	1
57	MG	BA	3268	1/1	0.96	0.44	30,30,30,30	0
57	MG	AG	201	1/1	0.96	0.22	5,5,5,5	1
57	MG	BA	3202	1/1	0.96	0.21	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	CA	1790	1/1	0.96	0.18	19,19,19,19	0
57	MG	DA	3081	1/1	0.96	0.14	11,11,11,11	0
57	MG	DA	3433	1/1	0.96	0.18	28,28,28,28	1
57	MG	AA	1619	1/1	0.96	0.16	25,25,25,25	0
57	MG	BA	3398	1/1	0.96	0.10	11,11,11,11	0
57	MG	BP	201	1/1	0.96	0.28	11,11,11,11	1
57	MG	BP	202	1/1	0.96	0.54	9,9,9,9	1
57	MG	DA	3094	1/1	0.96	0.59	1,1,1,1	1
57	MG	AA	1635	1/1	0.96	0.24	2,2,2,2	0
57	MG	BA	3400	1/1	0.96	0.22	1,1,1,1	0
57	MG	BA	3146	1/1	0.96	0.13	1,1,1,1	0
57	MG	CA	1701	1/1	0.96	0.24	3,3,3,3	0
57	MG	DA	3283	1/1	0.96	0.21	7,7,7,7	1
57	MG	BA	3149	1/1	0.96	0.18	36,36,36,36	0
57	MG	DA	3113	1/1	0.96	0.14	1,1,1,1	0
57	MG	CA	1604	1/1	0.96	0.10	41,41,41,41	0
57	MG	DA	3287	1/1	0.96	0.14	28,28,28,28	0
57	MG	DA	3288	1/1	0.96	0.26	7,7,7,7	1
57	MG	CA	1606	1/1	0.96	0.43	29,29,29,29	0
57	MG	DA	3118	1/1	0.96	0.20	9,9,9,9	0
57	MG	DA	3124	1/1	0.96	0.22	24,24,24,24	0
57	MG	DA	3293	1/1	0.96	0.32	1,1,1,1	1
57	MG	DA	3294	1/1	0.96	0.18	73,73,73,73	1
57	MG	DB	214	1/1	0.96	0.95	25,25,25,25	1
57	MG	AL	202	1/1	0.96	0.19	1,1,1,1	0
57	MG	AM	201	1/1	0.96	0.12	28,28,28,28	0
57	MG	DB	217	1/1	0.96	0.05	53,53,53,53	1
57	MG	DA	3298	1/1	0.96	0.08	22,22,22,22	0
57	MG	CA	1611	1/1	0.96	0.10	22,22,22,22	0
57	MG	DA	3300	1/1	0.96	0.19	38,38,38,38	0
57	MG	DA	3133	1/1	0.96	0.16	9,9,9,9	0
57	MG	DF	301	1/1	0.96	0.19	38,38,38,38	1
57	MG	DA	3134	1/1	0.96	0.31	8,8,8,8	0
57	MG	AA	1708	1/1	0.96	0.19	37,37,37,37	0
57	MG	DA	3306	1/1	0.96	0.14	1,1,1,1	0
57	MG	BA	3025	1/1	0.96	0.31	3,3,3,3	0
57	MG	BA	3155	1/1	0.96	0.16	37,37,37,37	0
57	MG	CL	201	1/1	0.96	0.09	1,1,1,1	0
57	MG	AA	1771	1/1	0.96	0.17	9,9,9,9	0
57	MG	BA	3028	1/1	0.96	0.41	1,1,1,1	0
57	MG	AA	1626	1/1	0.96	0.09	1,1,1,1	0
57	MG	AA	1756	1/1	0.96	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CV	103	1/1	0.96	0.05	44,44,44,44	0
57	MG	BA	3110	1/1	0.96	0.19	32,32,32,32	1
57	MG	DU	202	1/1	0.96	0.68	1,1,1,1	1
57	MG	BA	3111	1/1	0.96	0.06	1,1,1,1	0
57	MG	DV	201	1/1	0.96	0.15	1,1,1,1	0
57	MG	DX	102	1/1	0.96	0.26	23,23,23,23	1
57	MG	CA	1625	1/1	0.96	0.17	23,23,23,23	0
57	MG	DA	3313	1/1	0.97	0.28	5,5,5,5	0
57	MG	DA	3314	1/1	0.97	0.37	1,1,1,1	1
57	MG	CA	1708	1/1	0.97	0.15	99,99,99,99	0
57	MG	AW	104	1/1	0.97	0.09	14,14,14,14	1
57	MG	AX	102	1/1	0.97	0.19	4,4,4,4	0
57	MG	BA	3022	1/1	0.97	0.47	1,1,1,1	0
57	MG	BA	3098	1/1	0.97	0.15	1,1,1,1	0
57	MG	CA	1714	1/1	0.97	0.10	53,53,53,53	0
57	MG	BA	3023	1/1	0.97	0.10	1,1,1,1	1
57	MG	CA	1614	1/1	0.97	0.33	6,6,6,6	0
57	MG	BA	3403	1/1	0.97	0.22	55,55,55,55	1
57	MG	AA	1784	1/1	0.97	0.42	43,43,43,43	1
57	MG	AA	1768	1/1	0.97	0.23	7,7,7,7	0
57	MG	DA	3327	1/1	0.97	0.07	2,2,2,2	1
57	MG	BA	3242	1/1	0.97	0.11	1,1,1,1	0
57	MG	DA	3151	1/1	0.97	0.20	1,1,1,1	1
57	MG	CA	1621	1/1	0.97	0.16	31,31,31,31	0
57	MG	AW	107	1/1	0.97	0.77	57,57,57,57	0
57	MG	AA	1786	1/1	0.97	0.12	1,1,1,1	1
57	MG	BA	3104	1/1	0.97	0.10	1,1,1,1	0
57	MG	DA	3157	1/1	0.97	0.25	37,37,37,37	0
57	MG	DA	3158	1/1	0.97	0.13	23,23,23,23	0
57	MG	BA	3410	1/1	0.97	0.20	6,6,6,6	1
57	MG	BA	3106	1/1	0.97	0.17	19,19,19,19	1
57	MG	BA	3172	1/1	0.97	0.29	100,100,100,100	1
57	MG	BA	3173	1/1	0.97	0.29	24,24,24,24	0
57	MG	B1	104	1/1	0.97	0.18	62,62,62,62	0
57	MG	BA	3108	1/1	0.97	0.09	25,25,25,25	0
57	MG	CA	1633	1/1	0.97	0.07	2,2,2,2	0
57	MG	DA	3167	1/1	0.97	0.10	12,12,12,12	0
57	MG	BA	3256	1/1	0.97	0.18	1,1,1,1	1
57	MG	B2	601	1/1	0.97	0.51	22,22,22,22	0
57	MG	AA	1618	1/1	0.97	0.17	1,1,1,1	0
57	MG	BA	3036	1/1	0.97	0.40	18,18,18,18	0
57	MG	B5	101	1/1	0.97	0.23	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CX	102	1/1	0.97	0.17	1,1,1,1	1
57	MG	AA	1722	1/1	0.97	0.12	37,37,37,37	0
57	MG	D1	101	1/1	0.97	0.46	55,55,55,55	0
57	MG	BA	3039	1/1	0.97	0.09	1,1,1,1	0
57	MG	DA	3186	1/1	0.97	0.17	24,24,24,24	0
57	MG	BA	3342	1/1	0.97	0.16	26,26,26,26	1
57	MG	BA	3428	1/1	0.97	0.11	1,1,1,1	0
57	MG	DA	3190	1/1	0.97	0.41	32,32,32,32	0
57	MG	BA	3115	1/1	0.97	0.11	3,3,3,3	0
57	MG	D5	101	1/1	0.97	0.11	20,20,20,20	0
57	MG	DA	3193	1/1	0.97	0.12	1,1,1,1	1
57	MG	D7	101	1/1	0.97	0.12	93,93,93,93	1
57	MG	B7	101	1/1	0.97	0.08	8,8,8,8	0
57	MG	AA	1745	1/1	0.97	0.35	79,79,79,79	0
57	MG	BA	3185	1/1	0.97	0.09	1,1,1,1	0
57	MG	DA	3200	1/1	0.97	0.17	2,2,2,2	0
57	MG	BA	3433	1/1	0.97	0.14	33,33,33,33	0
57	MG	CA	1749	1/1	0.97	0.10	49,49,49,49	1
57	MG	BA	3186	1/1	0.97	0.17	5,5,5,5	1
57	MG	BA	3119	1/1	0.97	0.18	4,4,4,4	0
57	MG	AA	1672	1/1	0.97	0.17	24,24,24,24	0
57	MG	CA	1753	1/1	0.97	0.20	7,7,7,7	1
57	MG	DA	3383	1/1	0.97	0.15	42,42,42,42	1
57	MG	DA	3209	1/1	0.97	0.24	1,1,1,1	1
57	MG	BA	3438	1/1	0.97	0.09	44,44,44,44	0
57	MG	DA	3386	1/1	0.97	0.14	19,19,19,19	0
57	MG	BA	3046	1/1	0.97	0.12	15,15,15,15	0
57	MG	BA	3352	1/1	0.97	0.94	44,44,44,44	1
57	MG	BA	3122	1/1	0.97	0.20	1,1,1,1	1
57	MG	BA	3354	1/1	0.97	0.14	58,58,58,58	0
57	MG	BA	3047	1/1	0.97	0.25	1,1,1,1	0
57	MG	BA	3193	1/1	0.97	0.14	1,1,1,1	0
57	MG	DA	3393	1/1	0.97	0.14	1,1,1,1	1
57	MG	DA	3023	1/1	0.97	0.41	1,1,1,1	0
57	MG	BA	3194	1/1	0.97	0.42	19,19,19,19	0
57	MG	DA	3025	1/1	0.97	0.19	5,5,5,5	0
57	MG	BA	3049	1/1	0.97	0.20	17,17,17,17	0
57	MG	DA	3027	1/1	0.97	0.48	55,55,55,55	1
57	MG	BA	3051	1/1	0.97	0.56	1,1,1,1	0
57	MG	DA	3401	1/1	0.97	0.29	49,49,49,49	1
57	MG	DA	3029	1/1	0.97	0.14	1,1,1,1	0
57	MG	DA	3031	1/1	0.97	0.28	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	CA	1662	1/1	0.97	0.44	1,1,1,1	0
57	MG	BA	3127	1/1	0.97	0.44	3,3,3,3	1
57	MG	CA	1766	1/1	0.97	0.16	1,1,1,1	0
57	MG	AA	1664	1/1	0.97	0.21	4,4,4,4	0
57	MG	BA	3054	1/1	0.97	0.14	20,20,20,20	0
57	MG	AA	1606	1/1	0.97	0.15	1,1,1,1	0
57	MG	DA	3039	1/1	0.97	0.14	2,2,2,2	0
57	MG	BA	3131	1/1	0.97	0.12	1,1,1,1	0
57	MG	DA	3413	1/1	0.97	0.10	10,10,10,10	1
57	MG	BA	3059	1/1	0.97	0.12	9,9,9,9	0
57	MG	DA	3240	1/1	0.97	0.13	72,72,72,72	0
57	MG	BB	211	1/1	0.97	0.31	44,44,44,44	1
57	MG	DA	3043	1/1	0.97	0.17	6,6,6,6	0
57	MG	AA	1636	1/1	0.97	0.06	16,16,16,16	0
57	MG	BA	3061	1/1	0.97	0.21	3,3,3,3	0
57	MG	BA	3136	1/1	0.97	0.29	1,1,1,1	0
57	MG	CA	1777	1/1	0.97	0.12	47,47,47,47	0
57	MG	CA	1676	1/1	0.97	0.21	43,43,43,43	1
57	MG	DA	3052	1/1	0.97	0.16	1,1,1,1	0
57	MG	DA	3427	1/1	0.97	0.22	1,1,1,1	0
57	MG	DA	3053	1/1	0.97	0.28	3,3,3,3	0
57	MG	DA	3429	1/1	0.97	0.76	36,36,36,36	1
57	MG	BA	3208	1/1	0.97	0.21	23,23,23,23	1
57	MG	DA	3056	1/1	0.97	0.24	11,11,11,11	0
57	MG	DA	3261	1/1	0.97	0.37	30,30,30,30	0
57	MG	AA	1750	1/1	0.97	0.12	42,42,42,42	0
57	MG	BA	3065	1/1	0.97	0.18	7,7,7,7	0
57	MG	BA	3296	1/1	0.97	0.26	11,11,11,11	0
57	MG	DA	3063	1/1	0.97	0.44	1,1,1,1	0
57	MG	AA	1795	1/1	0.97	0.16	1,1,1,1	0
57	MG	BD	301	1/1	0.97	0.27	1,1,1,1	0
57	MG	BD	303	1/1	0.97	0.39	13,13,13,13	1
57	MG	AA	1778	1/1	0.97	0.09	16,16,16,16	1
57	MG	DA	3070	1/1	0.97	0.35	40,40,40,40	1
57	MG	CA	1787	1/1	0.97	0.48	11,11,11,11	0
57	MG	BA	3072	1/1	0.97	0.34	100,100,100,100	0
57	MG	DB	203	1/1	0.97	0.29	60,60,60,60	0
57	MG	AA	1637	1/1	0.97	0.22	11,11,11,11	0
57	MG	CA	1791	1/1	0.97	0.13	1,1,1,1	1
57	MG	BA	3382	1/1	0.97	0.06	38,38,38,38	0
57	MG	DA	3088	1/1	0.97	0.51	1,1,1,1	1
57	MG	CA	1688	1/1	0.97	0.37	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3092	1/1	0.97	0.41	1,1,1,1	0
57	MG	DA	3093	1/1	0.97	0.10	9,9,9,9	0
57	MG	BA	3075	1/1	0.97	0.35	6,6,6,6	1
57	MG	DA	3097	1/1	0.97	0.12	55,55,55,55	1
57	MG	CA	1691	1/1	0.97	0.09	1,1,1,1	0
57	MG	BA	3076	1/1	0.97	0.20	1,1,1,1	0
57	MG	BA	3304	1/1	0.97	0.14	24,24,24,24	0
57	MG	BA	3221	1/1	0.97	0.16	49,49,49,49	0
57	MG	BA	3148	1/1	0.97	0.28	8,8,8,8	0
57	MG	DA	3110	1/1	0.97	0.15	1,1,1,1	1
57	MG	DA	3291	1/1	0.97	0.16	1,1,1,1	1
57	MG	DA	3112	1/1	0.97	0.41	1,1,1,1	0
57	MG	AA	1658	1/1	0.97	0.24	1,1,1,1	0
57	MG	DA	3114	1/1	0.97	0.13	1,1,1,1	0
57	MG	BA	3082	1/1	0.97	0.17	1,1,1,1	1
57	MG	CA	1699	1/1	0.97	0.50	6,6,6,6	1
57	MG	DA	3297	1/1	0.97	0.35	11,11,11,11	1
57	MG	BA	3012	1/1	0.97	0.12	38,38,38,38	0
57	MG	AA	1699	1/1	0.97	0.07	1,1,1,1	1
57	MG	BU	202	1/1	0.97	0.25	18,18,18,18	1
57	MG	AA	1628	1/1	0.97	0.14	1,1,1,1	1
57	MG	DA	3128	1/1	0.97	0.12	1,1,1,1	1
57	MG	DA	3129	1/1	0.97	0.18	1,1,1,1	0
57	MG	DA	3304	1/1	0.97	0.46	1,1,1,1	1
57	MG	DA	3130	1/1	0.97	0.09	33,33,33,33	0
57	MG	BA	3313	1/1	0.97	0.40	18,18,18,18	0
57	MG	DU	201	1/1	0.97	0.29	77,77,77,77	1
57	MG	DA	3308	1/1	0.97	0.58	3,3,3,3	0
57	MG	BA	3314	1/1	0.97	0.48	23,23,23,23	0
57	MG	AA	1801	1/1	0.97	0.35	1,1,1,1	0
57	MG	DA	3311	1/1	0.97	0.22	11,11,11,11	1
57	MG	BA	3090	1/1	0.97	0.25	24,24,24,24	1
57	MG	BA	3357	1/1	0.98	0.17	105,105,105,105	1
57	MG	CA	1789	1/1	0.98	0.25	73,73,73,73	0
57	MG	BA	3042	1/1	0.98	0.18	1,1,1,1	0
57	MG	DA	3178	1/1	0.98	0.15	1,1,1,1	1
57	MG	AA	1678	1/1	0.98	0.07	13,13,13,13	0
57	MG	AA	1647	1/1	0.98	0.10	17,17,17,17	1
57	MG	CA	1626	1/1	0.98	0.09	23,23,23,23	0
57	MG	DA	3334	1/1	0.98	0.21	30,30,30,30	0
57	MG	DA	3335	1/1	0.98	0.12	7,7,7,7	1
57	MG	DA	3184	1/1	0.98	0.19	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	1627	1/1	0.98	0.09	5,5,5,5	0
57	MG	BA	3045	1/1	0.98	0.24	1,1,1,1	1
57	MG	DA	3188	1/1	0.98	0.19	26,26,26,26	0
57	MG	CA	1710	1/1	0.98	0.18	16,16,16,16	0
57	MG	BA	3234	1/1	0.98	0.18	12,12,12,12	0
57	MG	CA	1799	1/1	0.98	0.29	39,39,39,39	1
57	MG	DA	3047	1/1	0.98	0.14	1,1,1,1	0
57	MG	BA	3092	1/1	0.98	0.17	5,5,5,5	0
57	MG	BA	3237	1/1	0.98	0.13	8,8,8,8	1
57	MG	DA	3348	1/1	0.98	0.12	9,9,9,9	1
57	MG	DA	3050	1/1	0.98	0.44	136,136,136,136	1
57	MG	DA	3350	1/1	0.98	0.55	73,73,73,73	1
57	MG	DA	3351	1/1	0.98	0.28	11,11,11,11	1
57	MG	B3	101	1/1	0.98	0.20	14,14,14,14	0
57	MG	DA	3353	1/1	0.98	0.25	107,107,107,107	1
57	MG	DA	3197	1/1	0.98	0.24	3,3,3,3	0
57	MG	DA	3198	1/1	0.98	0.16	11,11,11,11	0
57	MG	AA	1751	1/1	0.98	0.23	14,14,14,14	0
57	MG	BA	3240	1/1	0.98	0.20	8,8,8,8	0
57	MG	DA	3054	1/1	0.98	0.10	1,1,1,1	0
57	MG	BA	3138	1/1	0.98	0.21	12,12,12,12	0
57	MG	BA	3097	1/1	0.98	0.10	1,1,1,1	0
57	MG	DA	3204	1/1	0.98	0.21	51,51,51,51	1
57	MG	BA	3187	1/1	0.98	0.09	1,1,1,1	0
57	MG	BA	3371	1/1	0.98	0.28	53,53,53,53	1
57	MG	BA	3048	1/1	0.98	0.46	1,1,1,1	0
57	MG	DA	3060	1/1	0.98	0.23	1,1,1,1	0
57	MG	DA	3062	1/1	0.98	0.54	21,21,21,21	0
57	MG	CA	1722	1/1	0.98	0.09	1,1,1,1	1
57	MG	CA	1723	1/1	0.98	0.19	10,10,10,10	1
57	MG	DA	3066	1/1	0.98	0.31	1,1,1,1	0
57	MG	BA	3021	1/1	0.98	0.16	2,2,2,2	0
57	MG	BA	3249	1/1	0.98	0.40	58,58,58,58	0
57	MG	BA	3311	1/1	0.98	0.12	1,1,1,1	0
57	MG	BA	3142	1/1	0.98	0.15	67,67,67,67	0
57	MG	AA	1692	1/1	0.98	0.19	3,3,3,3	1
57	MG	DA	3375	1/1	0.98	0.52	74,74,74,74	1
57	MG	DA	3074	1/1	0.98	0.07	2,2,2,2	0
57	MG	DA	3075	1/1	0.98	0.15	1,1,1,1	0
57	MG	DA	3076	1/1	0.98	0.33	1,1,1,1	0
57	MG	DA	3380	1/1	0.98	0.10	16,16,16,16	1
57	MG	DA	3077	1/1	0.98	0.11	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	AA	1641	1/1	0.98	0.14	26,26,26,26	0
57	MG	DA	3082	1/1	0.98	0.14	20,20,20,20	0
57	MG	BA	3024	1/1	0.98	0.46	44,44,44,44	1
57	MG	DA	3085	1/1	0.98	0.17	1,1,1,1	0
57	MG	BA	3254	1/1	0.98	0.06	5,5,5,5	0
57	MG	DA	3229	1/1	0.98	0.24	1,1,1,1	0
57	MG	DA	3230	1/1	0.98	0.13	35,35,35,35	0
57	MG	CA	1732	1/1	0.98	0.27	10,10,10,10	0
57	MG	BA	3317	1/1	0.98	0.12	60,60,60,60	0
57	MG	DA	3089	1/1	0.98	0.21	3,3,3,3	0
57	MG	BA	3384	1/1	0.98	0.15	1,1,1,1	1
57	MG	DA	3091	1/1	0.98	0.14	1,1,1,1	0
57	MG	BA	3055	1/1	0.98	0.16	1,1,1,1	0
57	MG	BA	3147	1/1	0.98	0.72	1,1,1,1	1
57	MG	DA	3397	1/1	0.98	0.31	1,1,1,1	0
57	MG	AA	1660	1/1	0.98	0.32	17,17,17,17	0
57	MG	DA	3096	1/1	0.98	0.29	1,1,1,1	0
57	MG	DA	3244	1/1	0.98	0.13	57,57,57,57	0
57	MG	BA	3105	1/1	0.98	0.17	1,1,1,1	0
57	MG	DA	3246	1/1	0.98	0.23	57,57,57,57	0
57	MG	DA	3098	1/1	0.98	0.13	5,5,5,5	0
57	MG	DA	3099	1/1	0.98	0.29	1,1,1,1	1
57	MG	BA	3259	1/1	0.98	0.08	1,1,1,1	1
57	MG	AA	1670	1/1	0.98	0.20	22,22,22,22	0
57	MG	BA	3261	1/1	0.98	0.43	1,1,1,1	0
57	MG	BA	3200	1/1	0.98	0.14	5,5,5,5	1
57	MG	DA	3254	1/1	0.98	0.24	109,109,109,109	1
57	MG	DA	3255	1/1	0.98	0.07	1,1,1,1	0
57	MG	DA	3256	1/1	0.98	0.38	1,1,1,1	0
57	MG	DA	3412	1/1	0.98	0.29	12,12,12,12	0
57	MG	DA	3104	1/1	0.98	0.14	9,9,9,9	1
57	MG	DA	3105	1/1	0.98	0.10	26,26,26,26	0
57	MG	DA	3106	1/1	0.98	0.36	1,1,1,1	0
57	MG	DA	3416	1/1	0.98	0.14	1,1,1,1	1
57	MG	BA	3151	1/1	0.98	0.26	1,1,1,1	0
57	MG	DA	3108	1/1	0.98	0.19	13,13,13,13	0
57	MG	DA	3109	1/1	0.98	0.08	17,17,17,17	0
57	MG	BA	3265	1/1	0.98	0.11	37,37,37,37	0
57	MG	DA	3111	1/1	0.98	0.14	4,4,4,4	0
57	MG	BD	302	1/1	0.98	0.26	1,1,1,1	0
57	MG	CA	1661	1/1	0.98	0.43	17,17,17,17	0
57	MG	BA	3027	1/1	0.98	0.26	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3272	1/1	0.98	0.17	5,5,5,5	0
57	MG	CA	1663	1/1	0.98	0.56	15,15,15,15	1
57	MG	AA	1661	1/1	0.98	0.09	10,10,10,10	1
57	MG	CA	1665	1/1	0.98	0.48	34,34,34,34	0
57	MG	DA	3119	1/1	0.98	0.31	1,1,1,1	0
57	MG	AA	1697	1/1	0.98	0.21	17,17,17,17	1
57	MG	CA	1667	1/1	0.98	0.26	8,8,8,8	0
57	MG	BA	3064	1/1	0.98	0.30	1,1,1,1	0
57	MG	AA	1662	1/1	0.98	0.09	41,41,41,41	1
57	MG	CX	104	1/1	0.98	0.14	39,39,39,39	0
57	MG	BA	3032	1/1	0.98	0.15	1,1,1,1	0
57	MG	AA	1727	1/1	0.98	0.14	63,63,63,63	0
57	MG	DA	3132	1/1	0.98	0.08	34,34,34,34	0
57	MG	BN	201	1/1	0.98	0.19	47,47,47,47	1
57	MG	BA	3071	1/1	0.98	0.14	20,20,20,20	0
57	MG	D2	2602	1/1	0.98	0.34	6,6,6,6	1
57	MG	BA	3034	1/1	0.98	0.14	15,15,15,15	0
57	MG	DA	3137	1/1	0.98	0.15	5,5,5,5	1
57	MG	BA	3211	1/1	0.98	0.17	50,50,50,50	1
57	MG	BA	3116	1/1	0.98	0.13	13,13,13,13	0
57	MG	BA	3278	1/1	0.98	0.07	8,8,8,8	0
57	MG	AX	103	1/1	0.98	0.09	1,1,1,1	1
57	MG	DA	3142	1/1	0.98	0.28	21,21,21,21	0
57	MG	DA	3143	1/1	0.98	0.39	24,24,24,24	0
57	MG	BP	203	1/1	0.98	0.31	1,1,1,1	1
57	MG	BA	3165	1/1	0.98	0.09	4,4,4,4	1
57	MG	AA	1654	1/1	0.98	0.36	65,65,65,65	0
57	MG	BA	3344	1/1	0.98	0.17	1,1,1,1	1
57	MG	AA	1714	1/1	0.98	0.18	23,23,23,23	0
57	MG	BA	3077	1/1	0.98	0.14	1,1,1,1	0
57	MG	CA	1603	1/1	0.98	0.21	77,77,77,77	0
57	MG	AA	1605	1/1	0.98	0.43	3,3,3,3	0
57	MG	BA	3414	1/1	0.98	0.17	20,20,20,20	0
57	MG	DA	3305	1/1	0.98	0.21	1,1,1,1	0
57	MG	DA	3153	1/1	0.98	0.15	1,1,1,1	0
57	MG	CA	1773	1/1	0.98	0.30	9,9,9,9	0
57	MG	BA	3080	1/1	0.98	0.23	26,26,26,26	0
57	MG	CA	1689	1/1	0.98	0.09	87,87,87,87	0
57	MG	CA	1608	1/1	0.98	0.11	17,17,17,17	0
57	MG	DF	304	1/1	0.98	0.23	66,66,66,66	0
57	MG	DA	3021	1/1	0.98	0.19	2,2,2,2	1
57	MG	BA	3223	1/1	0.98	0.22	9,9,9,9	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3160	1/1	0.98	0.18	1,1,1,1	1
57	MG	AA	1632	1/1	0.98	0.19	4,4,4,4	0
57	MG	DA	3315	1/1	0.98	0.32	6,6,6,6	0
57	MG	BA	3083	1/1	0.98	0.15	18,18,18,18	0
57	MG	BA	3419	1/1	0.98	0.07	57,57,57,57	1
57	MG	BA	3084	1/1	0.98	0.17	1,1,1,1	1
57	MG	AA	1657	1/1	0.98	0.16	8,8,8,8	1
57	MG	BA	3041	1/1	0.98	0.18	46,46,46,46	1
57	MG	BA	3424	1/1	0.98	0.15	37,37,37,37	0
57	MG	CA	1619	1/1	0.98	0.07	3,3,3,3	0
57	MG	DA	3169	1/1	0.98	0.34	1,1,1,1	1
57	MG	BA	3355	1/1	0.98	0.10	37,37,37,37	0
57	MG	DX	101	1/1	0.98	0.10	52,52,52,52	1
57	MG	BA	3087	1/1	0.98	0.09	18,18,18,18	0
57	MG	DA	3173	1/1	0.98	0.35	52,52,52,52	1
58	ZN	CN	102	1/1	0.98	0.14	114,114,114,114	0
57	MG	DA	3079	1/1	0.99	0.09	5,5,5,5	0
57	MG	DA	3080	1/1	0.99	0.09	1,1,1,1	1
57	MG	DA	3378	1/1	0.99	0.21	18,18,18,18	1
57	MG	BA	3162	1/1	0.99	0.22	54,54,54,54	1
57	MG	DA	3002	1/1	0.99	0.12	6,6,6,6	1
57	MG	DA	3381	1/1	0.99	0.16	65,65,65,65	0
57	MG	DA	3083	1/1	0.99	0.23	22,22,22,22	0
57	MG	DA	3172	1/1	0.99	0.15	17,17,17,17	1
57	MG	BA	3096	1/1	0.99	0.32	1,1,1,1	1
57	MG	AA	1675	1/1	0.99	0.29	41,41,41,41	1
57	MG	DA	3175	1/1	0.99	0.26	43,43,43,43	1
57	MG	BA	3243	1/1	0.99	0.25	1,1,1,1	0
57	MG	CA	1795	1/1	0.99	0.14	34,34,34,34	0
57	MG	BA	3244	1/1	0.99	0.14	1,1,1,1	0
57	MG	BA	3067	1/1	0.99	0.12	1,1,1,1	1
57	MG	CA	1618	1/1	0.99	0.07	22,22,22,22	1
57	MG	BB	201	1/1	0.99	0.06	32,32,32,32	1
57	MG	DA	3182	1/1	0.99	0.19	1,1,1,1	1
57	MG	DA	3183	1/1	0.99	0.11	11,11,11,11	0
57	MG	DA	3011	1/1	0.99	0.11	42,42,42,42	0
57	MG	DA	3185	1/1	0.99	0.16	19,19,19,19	0
57	MG	CA	1800	1/1	0.99	0.09	9,9,9,9	0
57	MG	BA	3068	1/1	0.99	0.20	1,1,1,1	0
57	MG	DA	3095	1/1	0.99	0.09	1,1,1,1	0
57	MG	BA	3247	1/1	0.99	0.27	26,26,26,26	1
57	MG	DA	3015	1/1	0.99	0.05	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	BA	3069	1/1	0.99	0.27	1,1,1,1	0
57	MG	BB	205	1/1	0.99	0.10	6,6,6,6	1
57	MG	AA	1770	1/1	0.99	0.10	16,16,16,16	1
57	MG	DA	3019	1/1	0.99	0.10	23,23,23,23	0
57	MG	DA	3020	1/1	0.99	0.48	1,1,1,1	0
57	MG	BA	3134	1/1	0.99	0.07	1,1,1,1	0
57	MG	CA	1807	1/1	0.99	0.21	1,1,1,1	0
57	MG	BA	3298	1/1	0.99	0.17	1,1,1,1	1
57	MG	BA	3170	1/1	0.99	0.08	1,1,1,1	1
57	MG	AA	1620	1/1	0.99	0.17	3,3,3,3	0
57	MG	AA	1689	1/1	0.99	0.14	6,6,6,6	0
57	MG	AA	1783	1/1	0.99	0.09	39,39,39,39	1
57	MG	BA	3074	1/1	0.99	0.08	1,1,1,1	1
57	MG	BA	3212	1/1	0.99	0.06	2,2,2,2	0
57	MG	DA	3030	1/1	0.99	0.19	2,2,2,2	0
57	MG	BA	3013	1/1	0.99	0.28	1,1,1,1	0
57	MG	BB	216	1/1	0.99	0.35	1,1,1,1	1
57	MG	BA	3031	1/1	0.99	0.30	1,1,1,1	0
57	MG	DA	3421	1/1	0.99	0.44	40,40,40,40	0
57	MG	DA	3116	1/1	0.99	0.40	1,1,1,1	1
57	MG	BA	3050	1/1	0.99	0.14	1,1,1,1	1
57	MG	CA	1696	1/1	0.99	0.66	52,52,52,52	0
57	MG	BA	3078	1/1	0.99	0.17	1,1,1,1	0
57	MG	DA	3120	1/1	0.99	0.19	1,1,1,1	1
57	MG	DA	3121	1/1	0.99	0.37	20,20,20,20	0
57	MG	DA	3122	1/1	0.99	0.19	8,8,8,8	0
57	MG	DA	3123	1/1	0.99	0.22	1,1,1,1	0
57	MG	AV	104	1/1	0.99	0.08	58,58,58,58	1
57	MG	DA	3125	1/1	0.99	0.39	4,4,4,4	1
57	MG	DA	3038	1/1	0.99	0.20	3,3,3,3	1
57	MG	BA	3262	1/1	0.99	0.18	32,32,32,32	1
57	MG	DA	3222	1/1	0.99	0.23	3,3,3,3	1
57	MG	BA	3218	1/1	0.99	0.08	50,50,50,50	0
57	MG	BA	3052	1/1	0.99	0.10	51,51,51,51	0
57	MG	BA	3220	1/1	0.99	0.16	16,16,16,16	1
57	MG	BA	3081	1/1	0.99	0.14	1,1,1,1	0
57	MG	DA	3044	1/1	0.99	0.27	60,60,60,60	0
57	MG	AA	1711	1/1	0.99	0.14	21,21,21,21	1
57	MG	BA	3016	1/1	0.99	0.14	31,31,31,31	1
57	MG	BA	3017	1/1	0.99	0.12	3,3,3,3	1
57	MG	BA	3056	1/1	0.99	0.09	1,1,1,1	0
57	MG	BA	3319	1/1	0.99	0.11	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	BA	3420	1/1	0.99	0.12	10,10,10,10	0
57	MG	DA	3234	1/1	0.99	0.11	88,88,88,88	1
57	MG	DA	3235	1/1	0.99	0.12	7,7,7,7	1
57	MG	BA	3057	1/1	0.99	0.16	7,7,7,7	0
57	MG	AA	1630	1/1	0.99	0.16	19,19,19,19	0
57	MG	BA	3273	1/1	0.99	0.14	57,57,57,57	1
57	MG	DA	3342	1/1	0.99	0.22	1,1,1,1	1
57	MG	DA	3239	1/1	0.99	0.14	4,4,4,4	0
57	MG	AX	104	1/1	0.99	0.11	55,55,55,55	1
57	MG	AA	1604	1/1	0.99	0.08	3,3,3,3	0
57	MG	AA	1730	1/1	0.99	0.13	1,1,1,1	1
57	MG	DA	3347	1/1	0.99	0.32	35,35,35,35	1
57	MG	DA	3243	1/1	0.99	0.09	18,18,18,18	0
57	MG	BA	3062	1/1	0.99	0.24	1,1,1,1	0
57	MG	BA	3376	1/1	0.99	0.05	15,15,15,15	0
57	MG	AA	1622	1/1	0.99	0.08	1,1,1,1	1
57	MG	DD	301	1/1	0.99	0.19	1,1,1,1	0
57	MG	DD	302	1/1	0.99	0.13	2,2,2,2	0
57	MG	BA	3124	1/1	0.99	0.09	7,7,7,7	0
57	MG	DE	301	1/1	0.99	0.20	1,1,1,1	1
57	MG	DA	3061	1/1	0.99	0.08	31,31,31,31	0
57	MG	CX	101	1/1	0.99	0.08	56,56,56,56	1
57	MG	CA	1601	1/1	0.99	0.12	21,21,21,21	1
57	MG	DA	3251	1/1	0.99	0.23	10,10,10,10	1
57	MG	DA	3064	1/1	0.99	0.09	18,18,18,18	0
57	MG	AA	1649	1/1	0.99	0.09	56,56,56,56	0
57	MG	BA	3195	1/1	0.99	0.13	39,39,39,39	1
57	MG	BA	3381	1/1	0.99	0.11	23,23,23,23	0
57	MG	CA	1605	1/1	0.99	0.08	18,18,18,18	0
57	MG	DA	3257	1/1	0.99	0.15	54,54,54,54	0
57	MG	D1	103	1/1	0.99	0.08	33,33,33,33	0
57	MG	DA	3259	1/1	0.99	0.18	22,22,22,22	0
57	MG	BA	3236	1/1	0.99	0.14	1,1,1,1	0
57	MG	BA	3283	1/1	0.99	0.16	2,2,2,2	0
57	MG	DA	3072	1/1	0.99	0.09	1,1,1,1	1
57	MG	DA	3263	1/1	0.99	0.15	16,16,16,16	0
57	MG	DA	3073	1/1	0.99	0.21	1,1,1,1	1
57	MG	BA	3007	1/1	0.99	0.09	37,37,37,37	0
57	MG	CA	1609	1/1	0.99	0.21	62,62,62,62	0
57	MG	DA	3267	1/1	0.99	0.24	28,28,28,28	1
57	MG	BA	3095	1/1	0.99	0.12	1,1,1,1	0
57	MG	BA	3161	1/1	0.99	0.19	7,7,7,7	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	ZN	AN	101	1/1	0.99	0.23	143,143,143,143	0
57	MG	DA	3078	1/1	0.99	0.16	58,58,58,58	1
57	MG	DA	3417	1/1	1.00	0.10	71,71,71,71	0
58	ZN	AD	303	1/1	1.00	0.20	26,26,26,26	0
57	MG	BA	3436	1/1	1.00	0.18	6,6,6,6	1
58	ZN	CD	301	1/1	1.00	0.22	35,35,35,35	0
57	MG	DA	3208	1/1	1.00	0.11	14,14,14,14	0

6.5 Other polymers

There are no such residues in this entry.