wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 11:06 pm GMT

PDB ID	:	4V51
Title	:	Structure of the Thermus thermophilus 70S ribosome complexed with mRNA, tRNA and paromomycin
Authors	:	Selmer, M.; Dunham, C.M.; Murphy, F.V.; Weixlbaumer, A.; Petry, S.; Weir, J.R.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2006-07-31
Resolution	:	2.80 Å(reported)

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

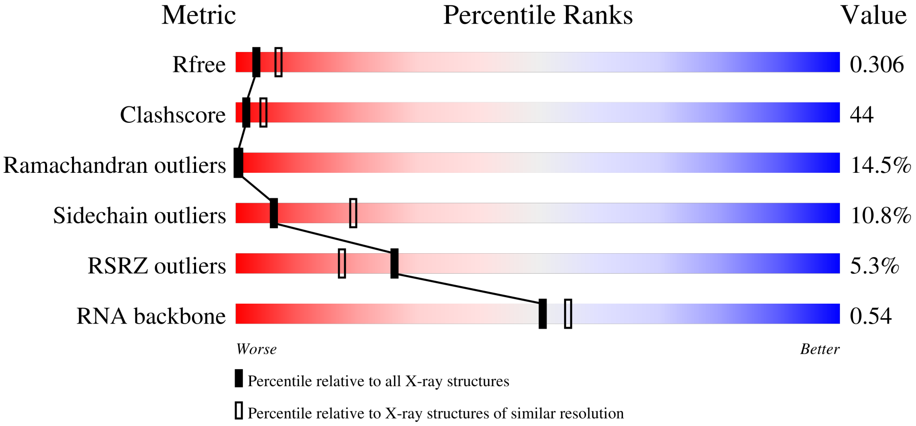
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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

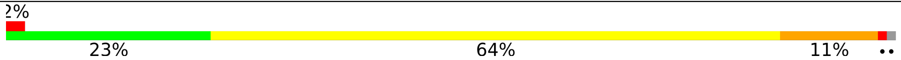
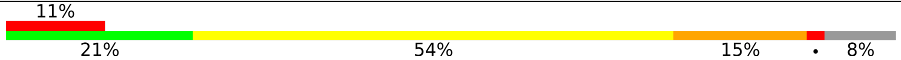
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	
1	CA	1522	
2	AB	256	

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Mol	Chain	Length	Quality of chain
2	CB	256	11% 21% 54% 15% • 8%
3	AC	239	3% 28% 49% 8% • 13%
3	CC	239	5% 29% 48% 8% • 13%
4	AD	209	27% 56% 16% •
4	CD	209	2% 27% 56% 16% •
5	AE	162	% 20% 60% 13% 7%
5	CE	162	% 25% 56% 12% 7%
6	AF	101	3% 33% 58% 8% •
6	CF	101	2% 34% 58% 7% •
7	AG	156	8% 32% 60% 8% •
7	CG	156	15% 33% 59% 7% •
8	AH	138	2% 38% 57% 5%
8	CH	138	3% 38% 57% •
9	AI	128	12% 20% 66% 13% ••
9	CI	128	16% 22% 62% 14% ••
10	AJ	105	16% 26% 56% 12% 6%
10	CJ	105	21% 28% 54% 12% 6%
11	AK	129	2% 31% 56% 5% • 8%
11	CK	129	5% 33% 55% • • 8%
12	AL	135	3% 31% 47% 14% • 7%
12	CL	135	3% 30% 50% 13% • 7%
13	AM	126	12% 19% 63% 17% •
13	CM	126	12% 19% 63% 17% •
14	AN	61	10% 26% 61% 11% •
14	CN	61	7% 28% 61% 10% •

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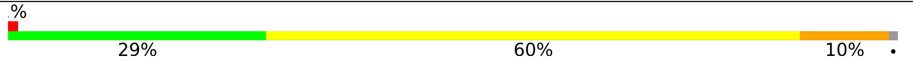
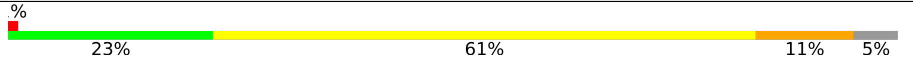
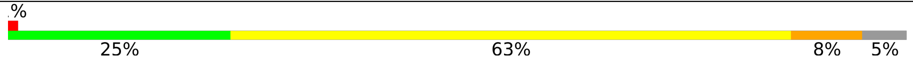
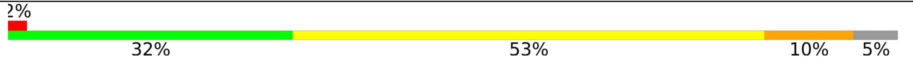
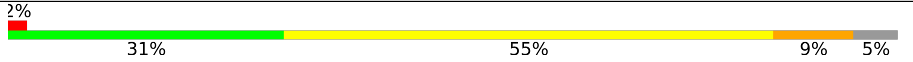
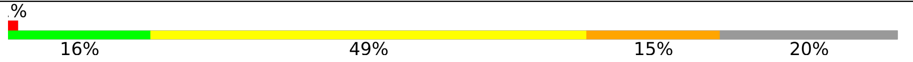
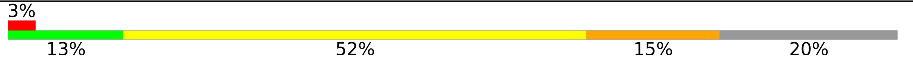
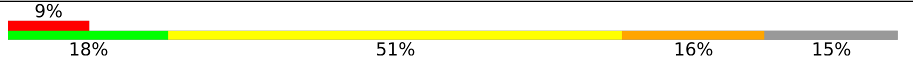
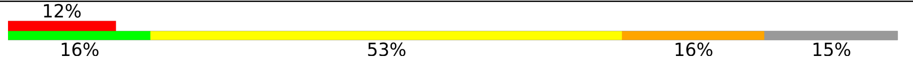
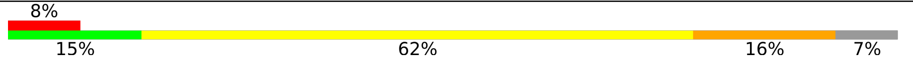
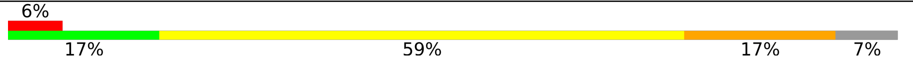
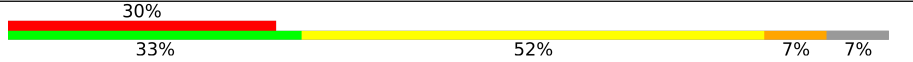
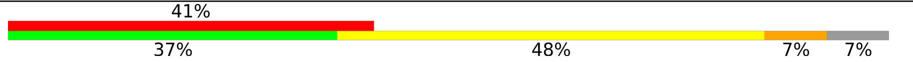
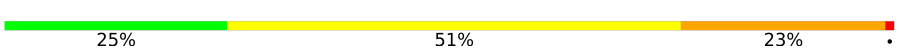
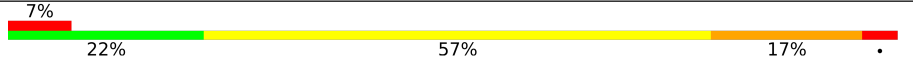
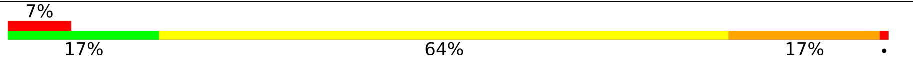
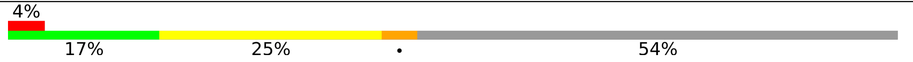
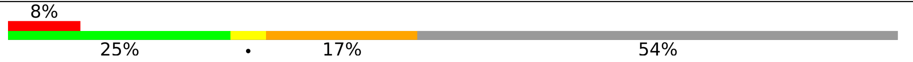
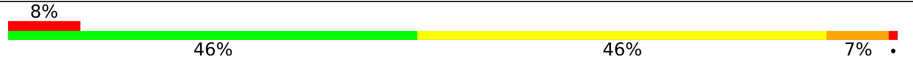
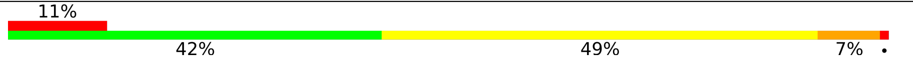
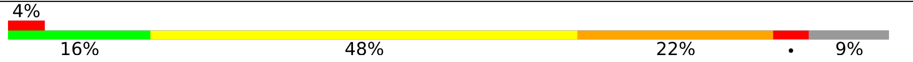
Mol	Chain	Length	Quality of chain
15	AO	89	 30% 58% 10% •
15	CO	89	 % 29% 60% 10% •
16	AP	88	 % 23% 61% 11% 5%
16	CP	88	 % 25% 63% 8% 5%
17	AQ	105	 2% 32% 53% 10% 5%
17	CQ	105	 2% 31% 55% 9% 5%
18	AR	88	 % 16% 49% 15% 20%
18	CR	88	 3% 13% 52% 15% 20%
19	AS	93	 9% 18% 51% 16% 15%
19	CS	93	 12% 16% 53% 16% 15%
20	AT	106	 8% 15% 62% 16% 7%
20	CT	106	 6% 17% 59% 17% 7%
21	AU	27	 30% 33% 52% 7% 7%
21	CU	27	 41% 37% 48% 7% 7%
22	AV	77	 25% 51% 23% •
22	CV	77	 36% 43% 19% •
23	AW	76	 7% 22% 57% 17% •
23	AY	76	 8% 14% • 75%
23	CW	76	 7% 17% 64% 17% •
23	CY	76	 5% 17% • 75%
24	AX	24	 4% 17% 25% • 54%
24	CX	24	 8% 25% • 17% 54%
25	B0	85	 8% 46% 46% 7% •
25	D0	85	 11% 42% 49% 7% •
26	B1	98	 4% 16% 48% 22% • 9%

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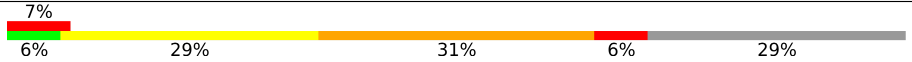
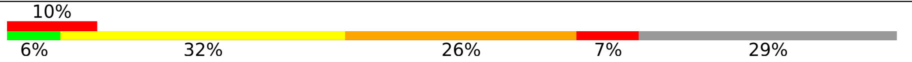
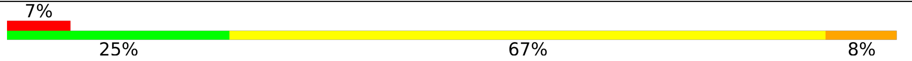
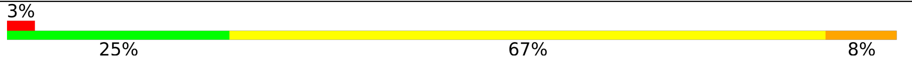
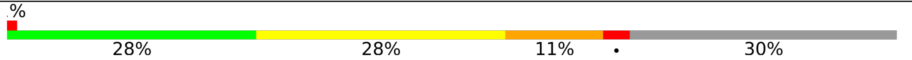
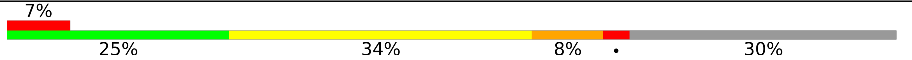
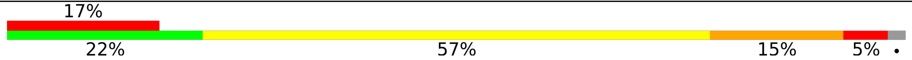
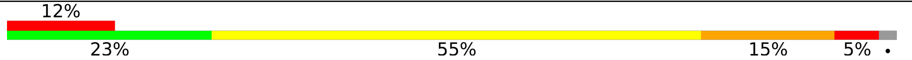
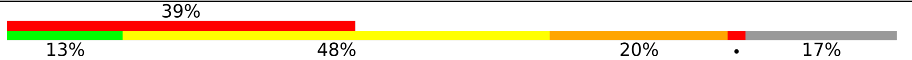
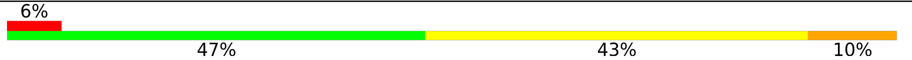
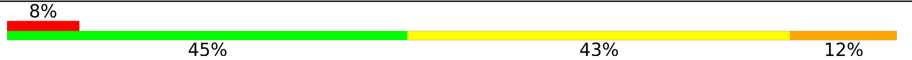
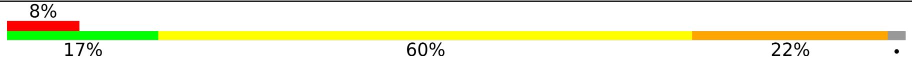
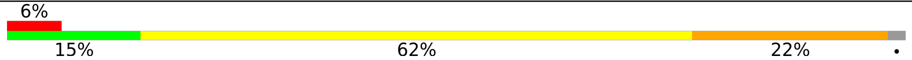
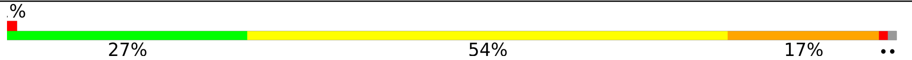
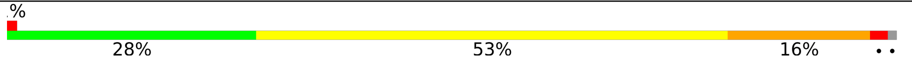
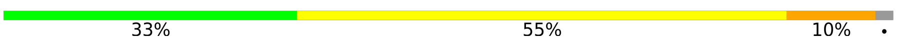
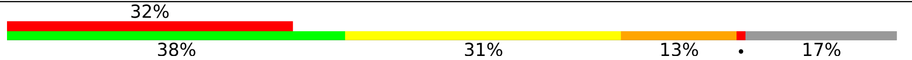
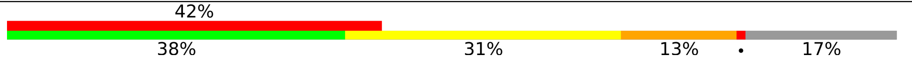
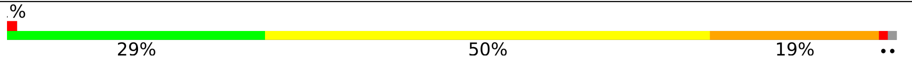
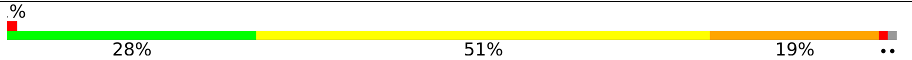
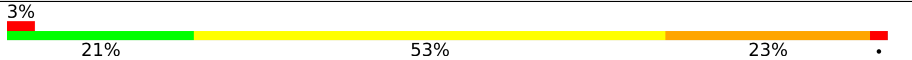
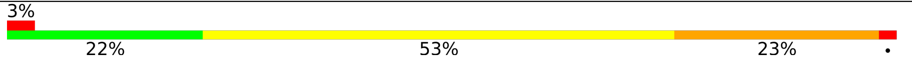
Mol	Chain	Length	Quality of chain
26	D1	98	
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	BA	2787	
34	DA	2787	
35	BB	122	
35	DB	122	
36	BC	229	
36	DC	229	
37	BD	276	
37	DD	276	
38	BE	206	
38	DE	206	

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Mol	Chain	Length	Quality of chain
39	BF	210	4% 26% 60% 13% •
39	DF	210	6% 26% 60% 13% •
40	BG	182	4% 19% 60% 18% • •
40	DG	182	7% 18% 57% 22% • •
41	BH	180	19% 23% 47% 16% • 11%
41	DH	180	16% 22% 48% 16% • 11%
42	BI	148	9% 21% 67% 9% ••
42	DI	148	38% 21% 66% 10% ••
43	BN	140	4% 19% 56% 21% • •
43	DN	140	6% 18% 56% 21% • •
44	BO	122	32% 57% 9% •
44	DO	122	30% 57% 11% •
45	BP	150	2% 13% 54% 26% 5% •
45	DP	150	7% 13% 53% 25% 5% •
46	BQ	141	6% 18% 57% 21% • •
46	DQ	141	8% 19% 56% 21% • •
47	BR	118	% 20% 58% 19% • •
47	DR	118	23% 56% 18% • •
48	BS	112	7% 11% 46% 30% • 12%
48	DS	112	13% 10% 46% 31% • 12%
49	BT	146	6% 15% 54% 21% 5% 5%
49	DT	146	5% 14% 55% 20% 5% 5%
50	BU	118	3% 30% 57% 12% ••
50	DU	118	2% 30% 55% 14% ••
51	BV	101	5% 14% 48% 36% •

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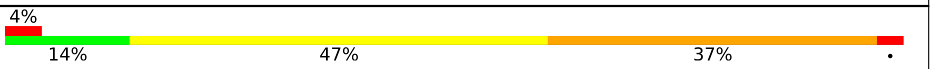
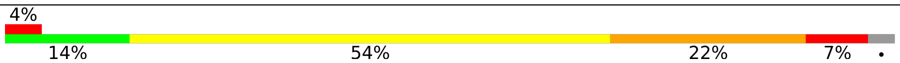
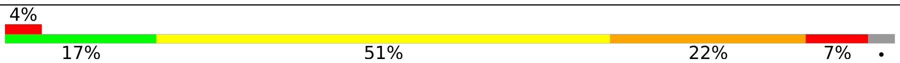
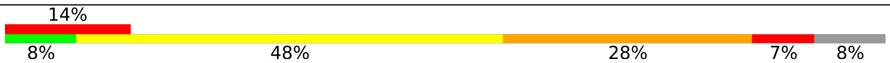
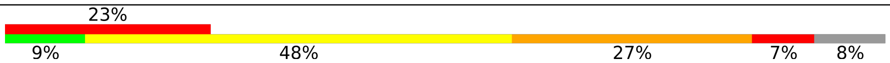
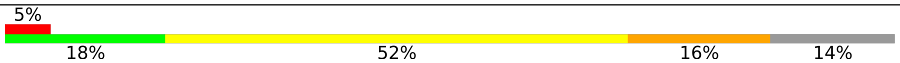
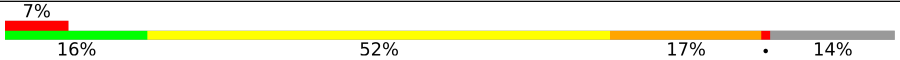
Mol	Chain	Length	Quality of chain
51	DV	101	
52	BW	113	
52	DW	113	
53	BX	96	
53	DX	96	
54	BY	110	
54	DY	110	
55	BZ	206	
55	DZ	206	

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
56	MG	AA	1618	-	-	-	X
56	MG	AA	1633	-	-	-	X
56	MG	AA	1697	-	-	-	X
56	MG	BA	3004	-	-	-	X
56	MG	BA	3403	-	-	-	X
56	MG	BA	3413	-	-	-	X
56	MG	BB	201	-	-	-	X
56	MG	BB	213	-	-	-	X
56	MG	CA	1622	-	-	-	X
56	MG	CA	1637	-	-	-	X
56	MG	CA	1646	-	-	-	X
56	MG	CA	1685	-	-	-	X
56	MG	CA	1719	-	-	-	X
56	MG	CA	1729	-	-	-	X
56	MG	CA	1752	-	-	-	X
56	MG	DA	3004	-	-	-	X
56	MG	DA	3187	-	-	-	X
56	MG	DA	3219	-	-	-	X
56	MG	DA	3255	-	-	-	X
56	MG	DA	3261	-	-	-	X
56	MG	DA	3273	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 291075 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 1147 724 218 201 4	0	0	1
5	CE	151	Total C N O S 1147 724 218 201 4	0	0	1

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

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

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

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

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

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

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

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

- 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 795 499 157 138 1	0	0	1

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AM	125	988	611	206	169	2	0	0	1
13	CM	125	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
			Total	C	N	O	S			
14	AN	60	492	312	104	72	4	0	0	0
14	CN	60	492	312	104	72	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	AV	77	1645	733	297	538	77	0	0	0
22	CV	77	1645	733	297	538	77	0	0	0

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	AW	76	1623	723	290	534	76	0	0	0
23	AY	19	407	183	78	128	18	0	0	0
23	CW	76	1623	723	290	534	76	0	0	0
23	CY	19	407	183	78	128	18	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	235	106	44	74	11	0	0	0
24	CX	11	235	106	44	74	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	B0	85	650	401	137	111	1	0	0	0
25	D0	85	650	401	137	111	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 34 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	2772	Total 59708	C 26573	N 11171	O 19193	P 2771	0	0	0
34	DA	2772	Total 59708	C 26573	N 11171	O 19193	P 2771	0	0	0

- Molecule 35 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	BH	160	Total C N O S 1223 773 229 220 1	0	0	1
41	DH	160	Total C N O S 1223 773 229 220 1	0	0	1

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
42	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	215	Total Mg 215 215	0	0
56	AE	1	Total Mg 1 1	0	0
56	AV	7	Total Mg 7 7	0	0
56	AW	22	Total Mg 22 22	0	0
56	AX	4	Total Mg 4 4	0	0
56	AY	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B1	1	Total Mg 1 1	0	0
56	B2	5	Total Mg 5 5	0	0
56	B3	1	Total Mg 1 1	0	0
56	B5	2	Total Mg 2 2	0	0
56	B7	2	Total Mg 2 2	0	0
56	BA	454	Total Mg 454 454	0	0
56	BB	19	Total Mg 19 19	0	0
56	BE	1	Total Mg 1 1	0	0
56	BF	2	Total Mg 2 2	0	0
56	BN	1	Total Mg 1 1	0	0
56	BO	1	Total Mg 1 1	0	0
56	BV	1	Total Mg 1 1	0	0
56	BX	1	Total Mg 1 1	0	0
56	CA	189	Total Mg 189 189	0	0
56	CF	1	Total Mg 1 1	0	0
56	CJ	1	Total Mg 1 1	0	0
56	CM	1	Total Mg 1 1	0	0
56	CU	1	Total Mg 1 1	0	0
56	CV	4	Total Mg 4 4	0	0
56	CW	13	Total Mg 13 13	0	0
56	CX	6	Total Mg 6 6	0	0

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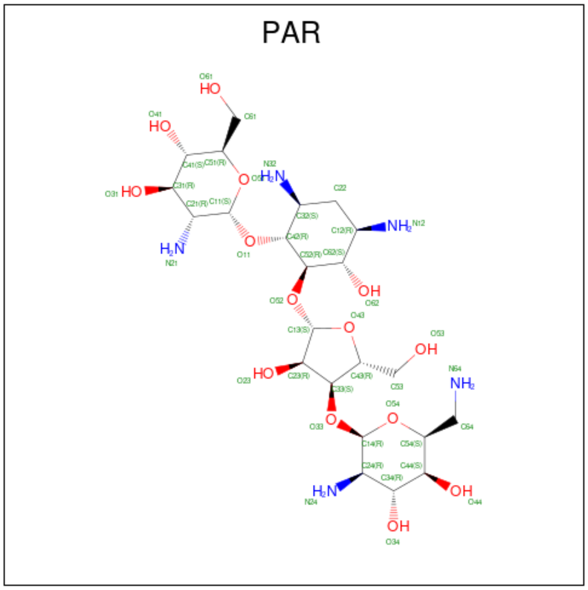
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	D5	2	Total 2	Mg 2	0	0
56	DA	398	Total 398	Mg 398	0	0
56	DB	12	Total 12	Mg 12	0	0
56	DD	2	Total 2	Mg 2	0	0
56	DE	1	Total 1	Mg 1	0	0
56	DF	1	Total 1	Mg 1	0	0
56	DH	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DO	1	Total 1	Mg 1	0	0
56	DS	1	Total 1	Mg 1	0	0
56	DU	1	Total 1	Mg 1	0	0
56	DZ	1	Total 1	Mg 1	0	0

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_{5}O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C N O 42 23 5 14	0	0
57	CA	1	Total C N O 42 23 5 14	0	0

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

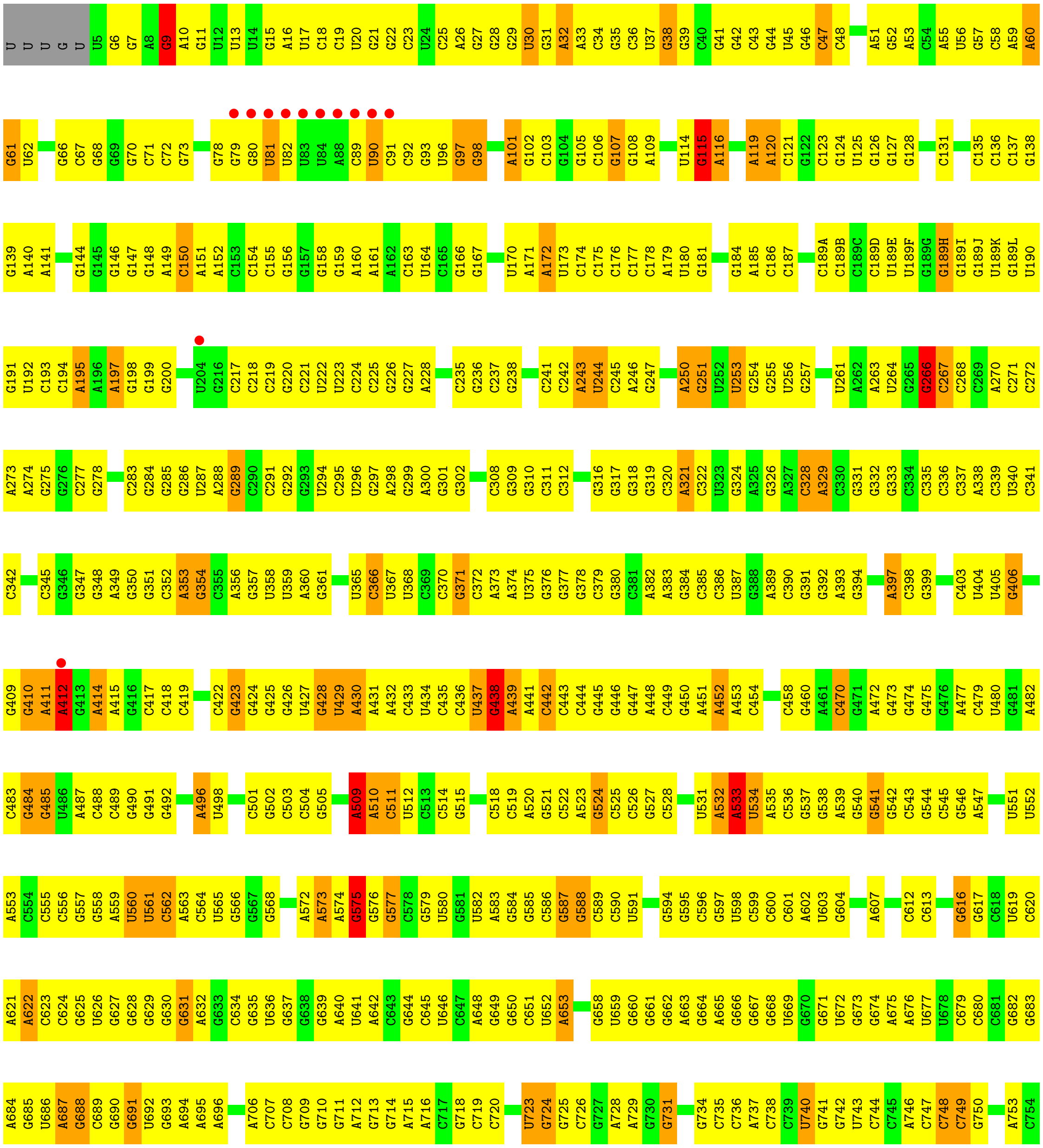
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AD	1	Total Zn 1 1	0	0
58	AN	1	Total Zn 1 1	0	0
58	CD	1	Total Zn 1 1	0	0
58	CN	1	Total Zn 1 1	0	0

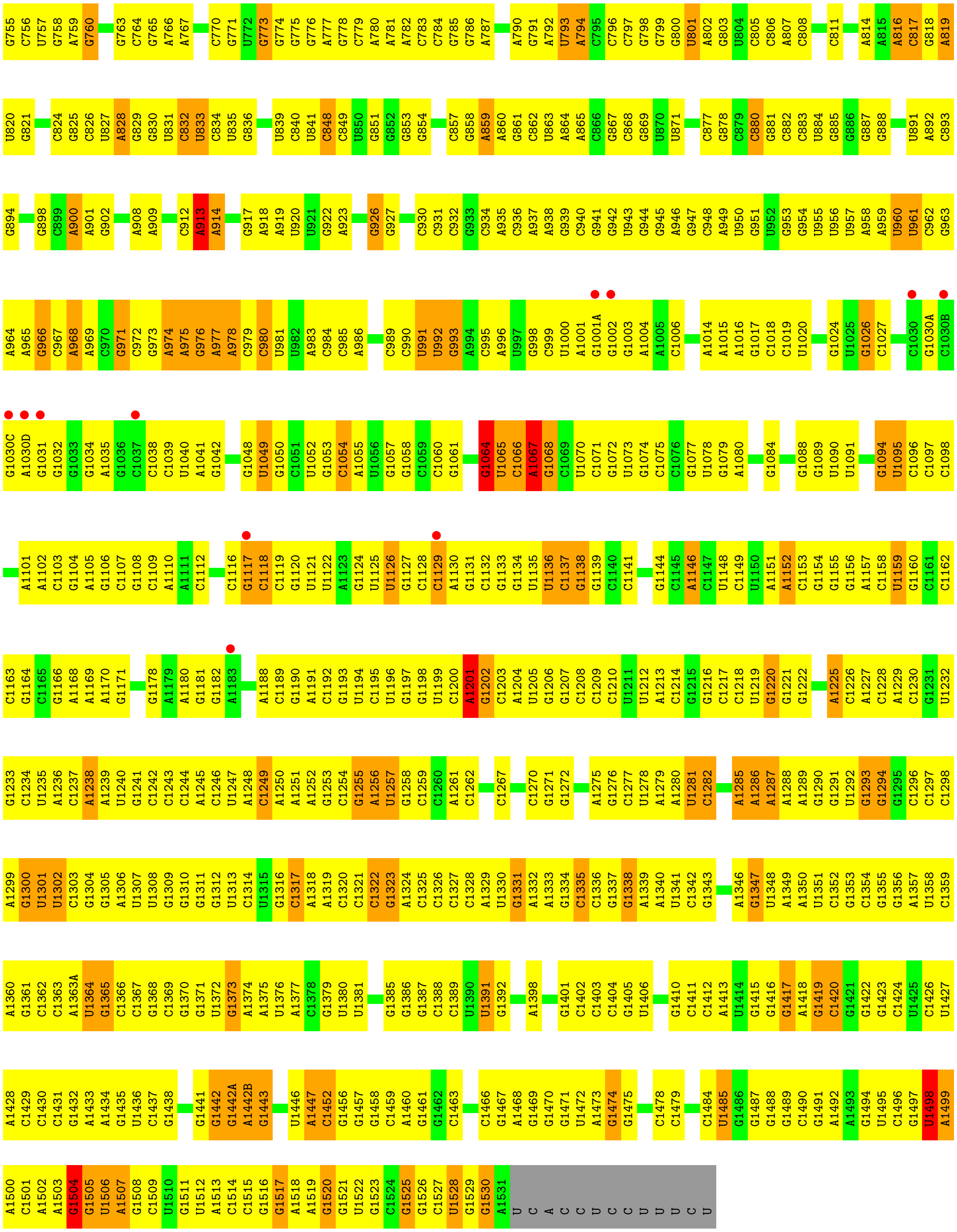
3 Residue-property plots ⓘ

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.

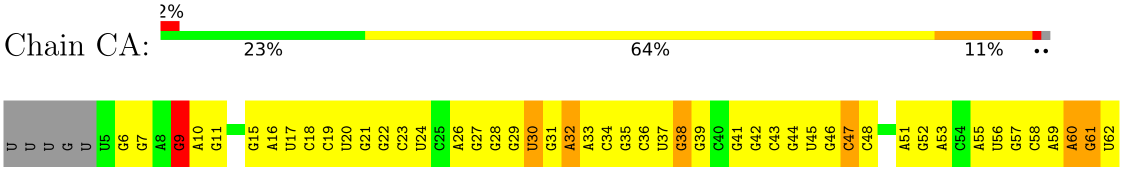
- Molecule 1: 16S ribosomal RNA

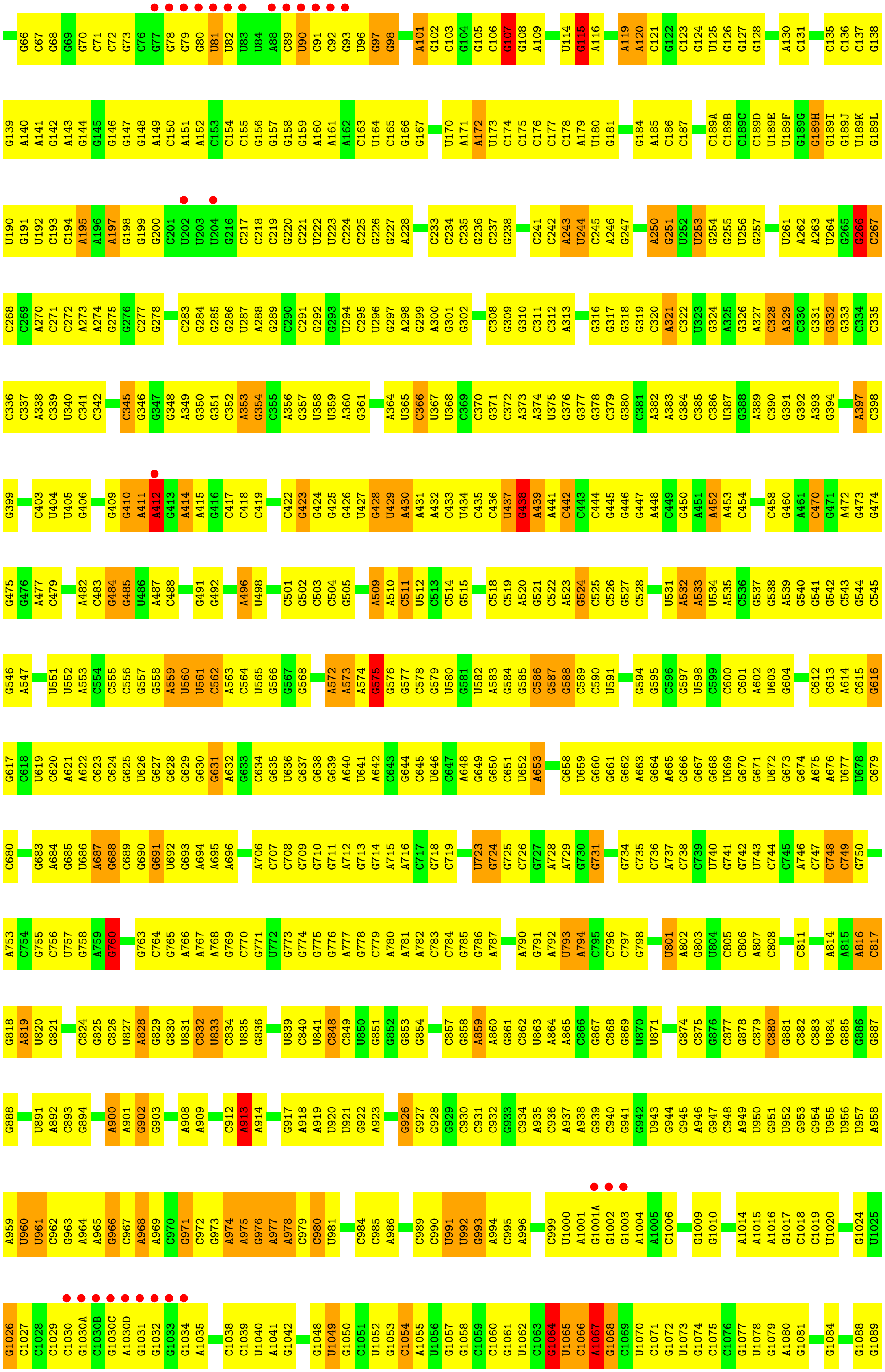
Chain AA:





• Molecule 1: 16S ribosomal RNA

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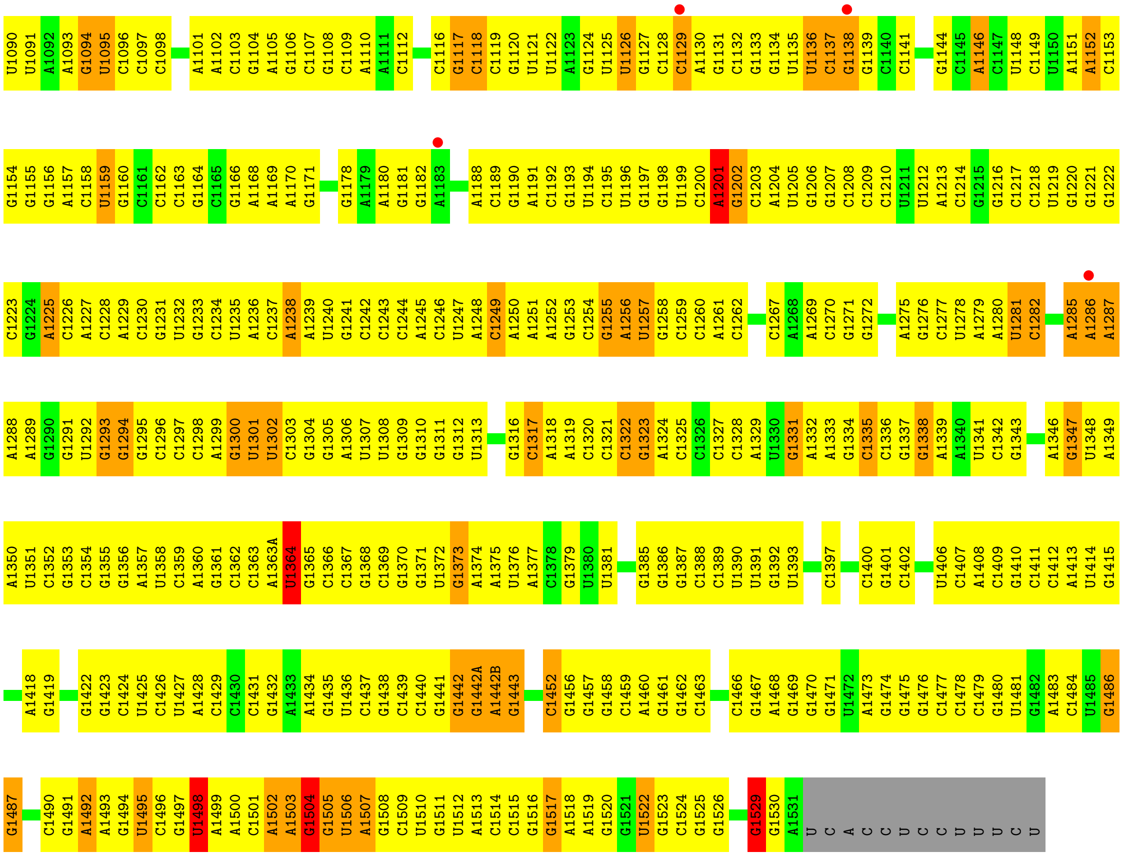
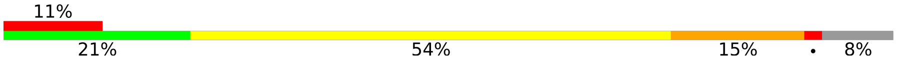
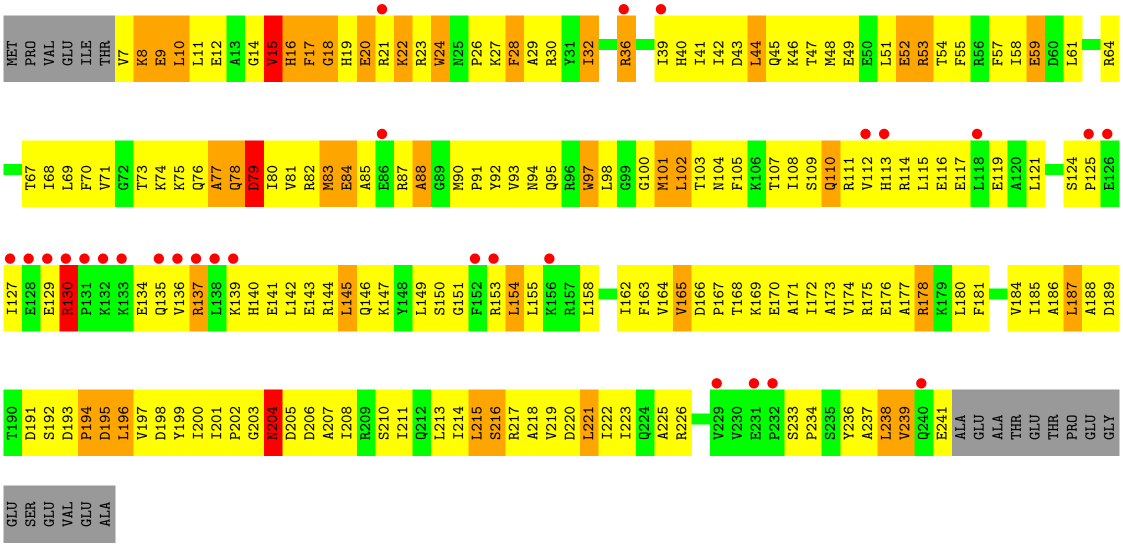


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

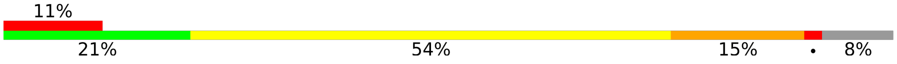
Chain AB:

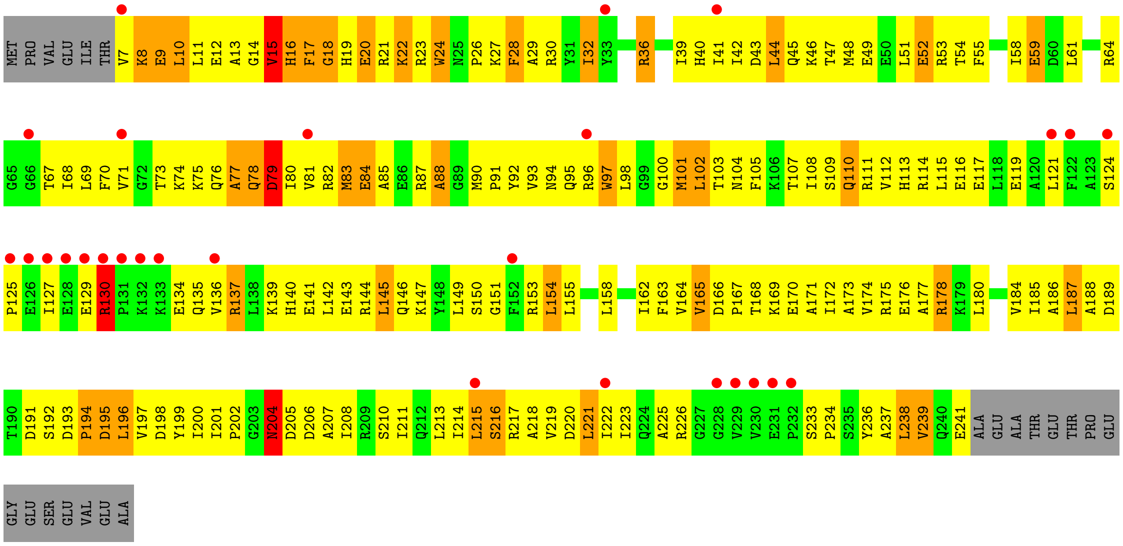




- Molecule 2: 30S RIBOSOMAL PROTEIN S2

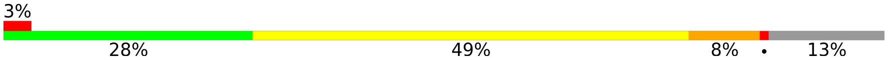
Chain CB:

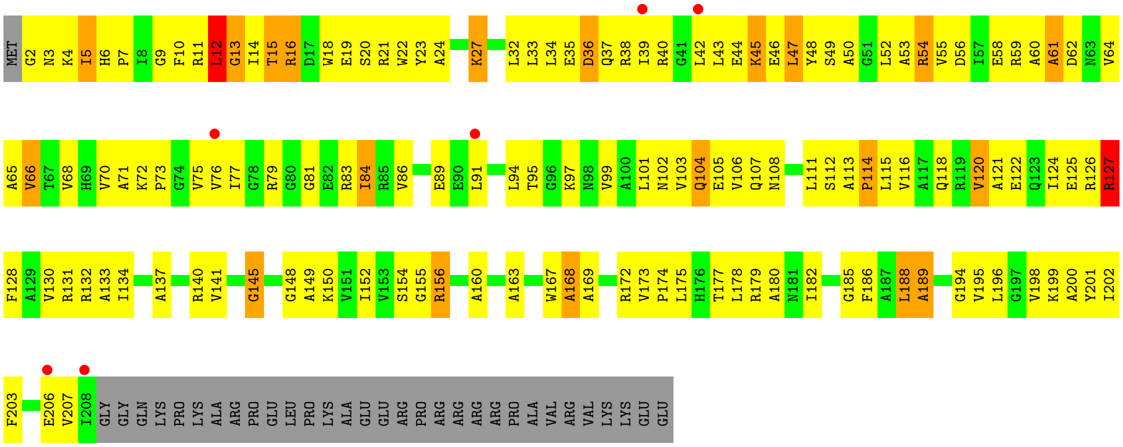




- Molecule 3: 30S RIBOSOMAL PROTEIN S3

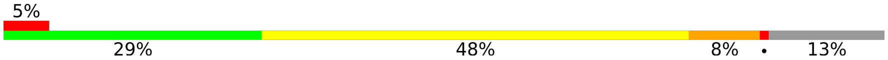
Chain AC:

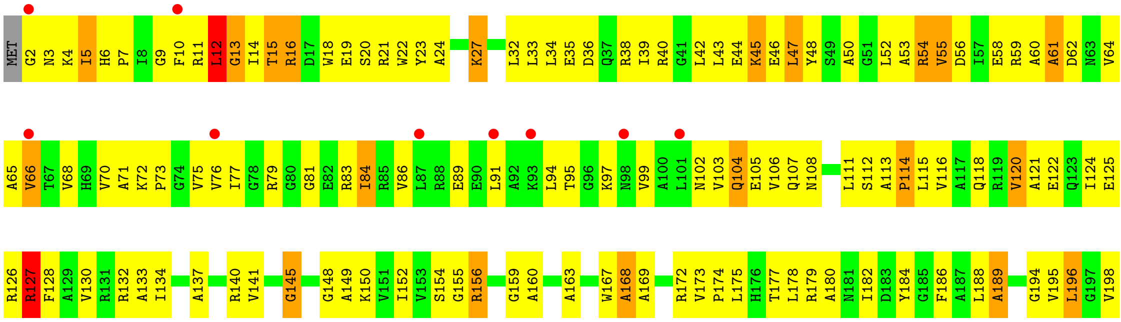


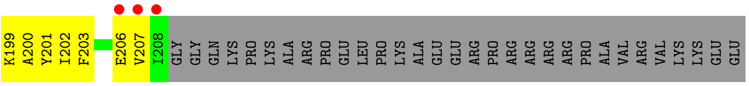


- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:

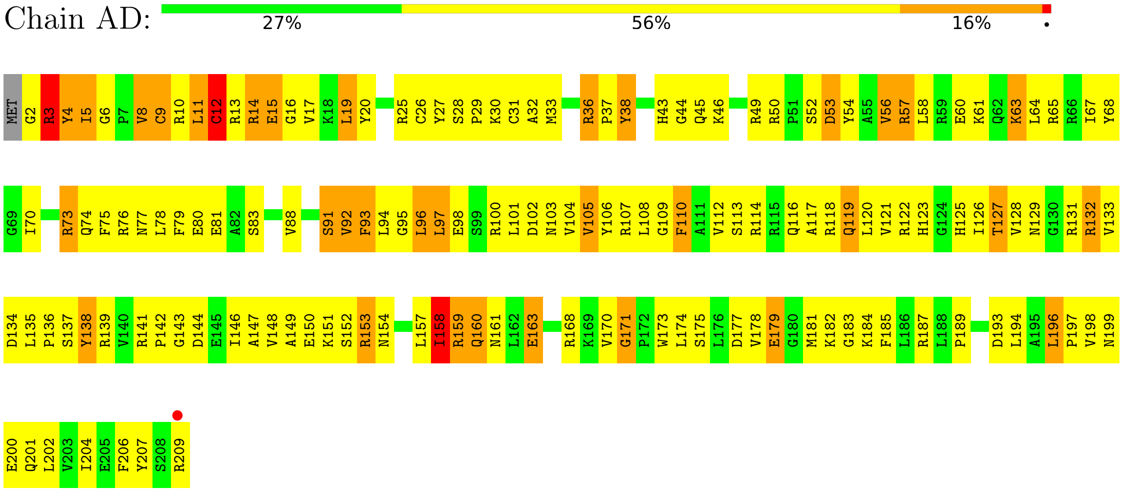






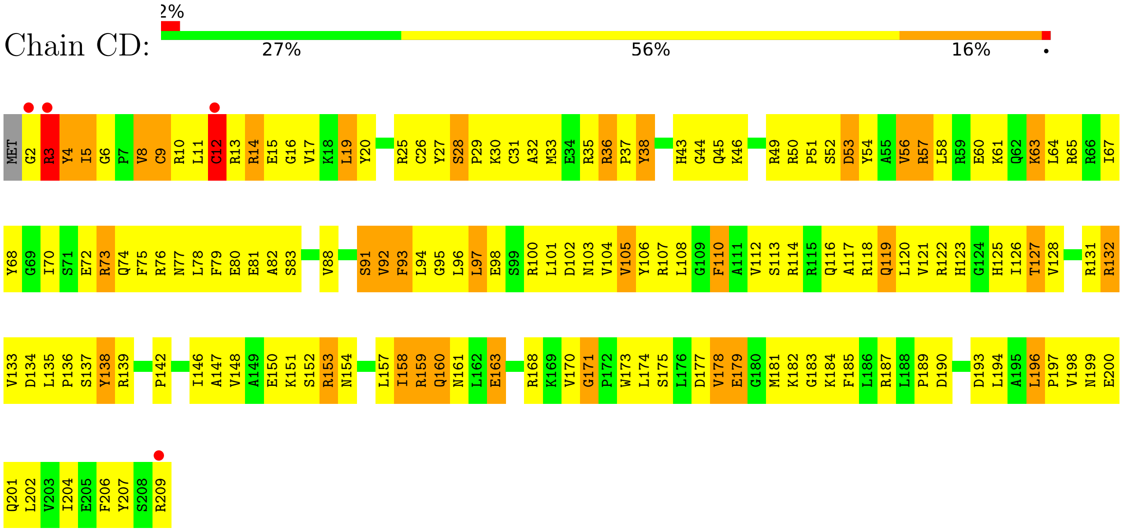
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



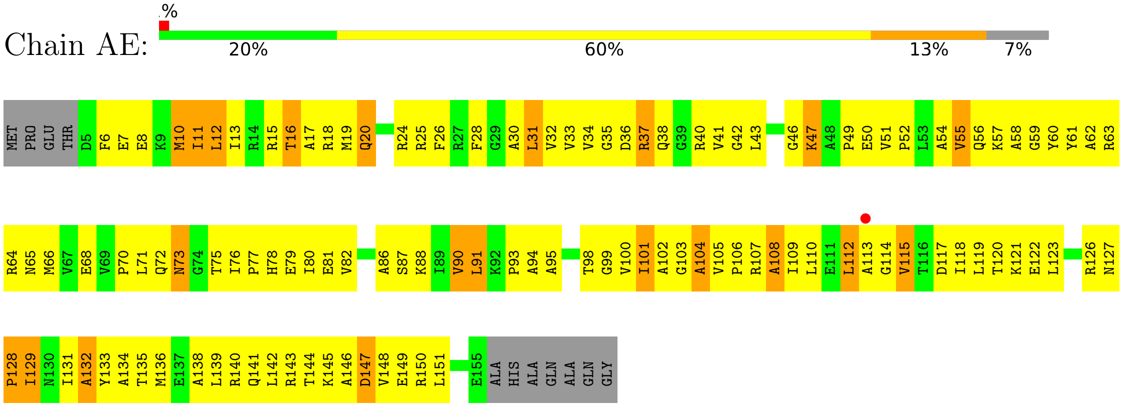
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



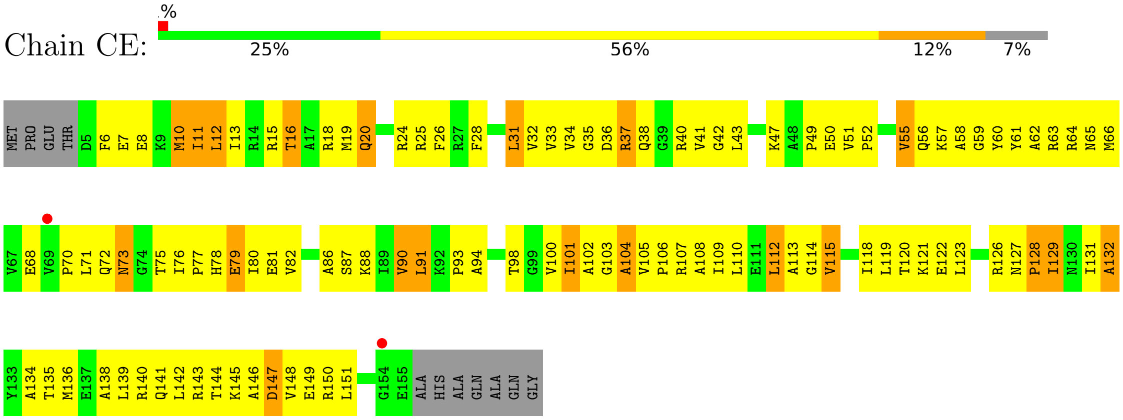
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



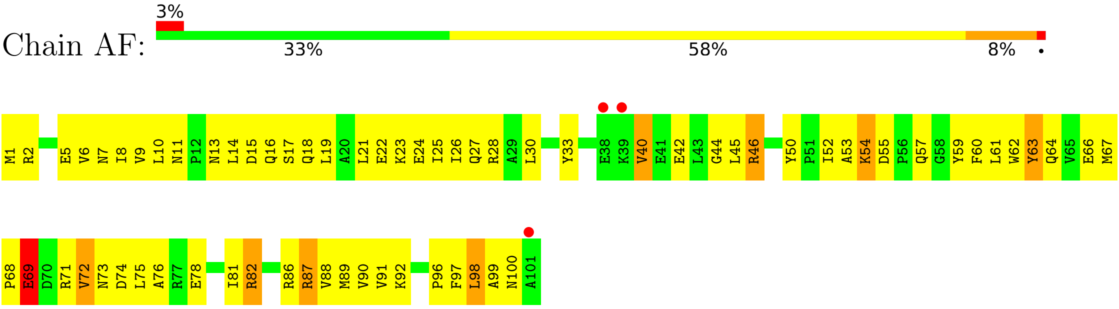
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



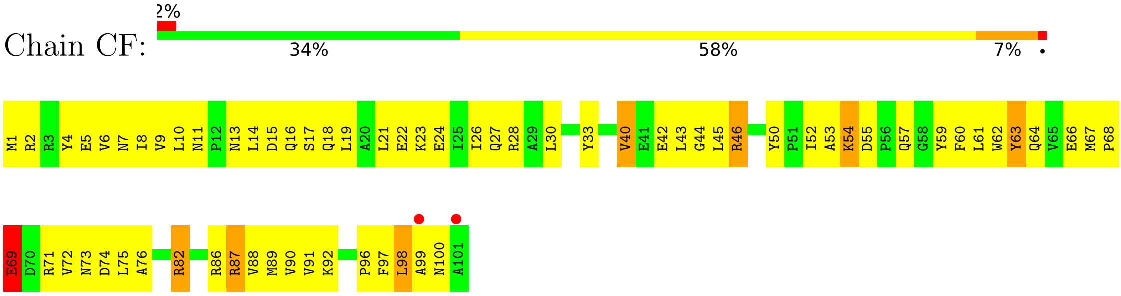
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



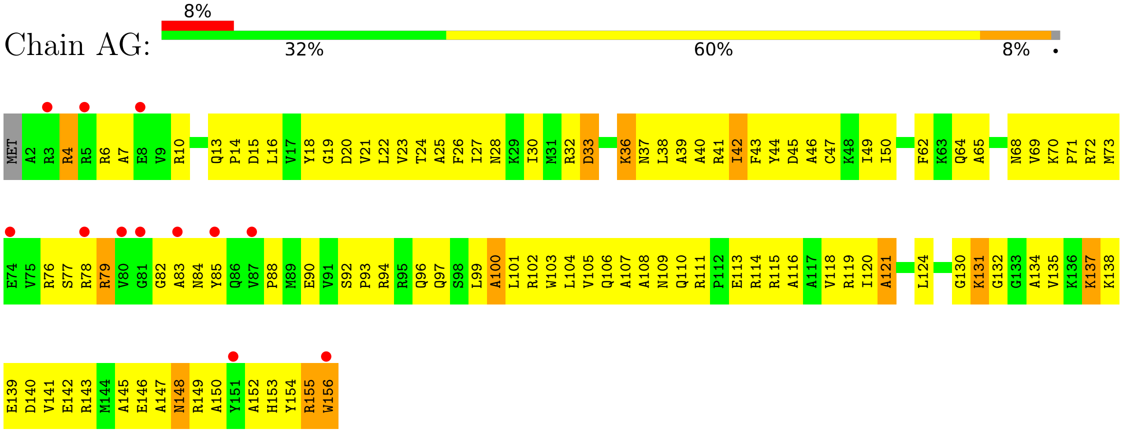
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:

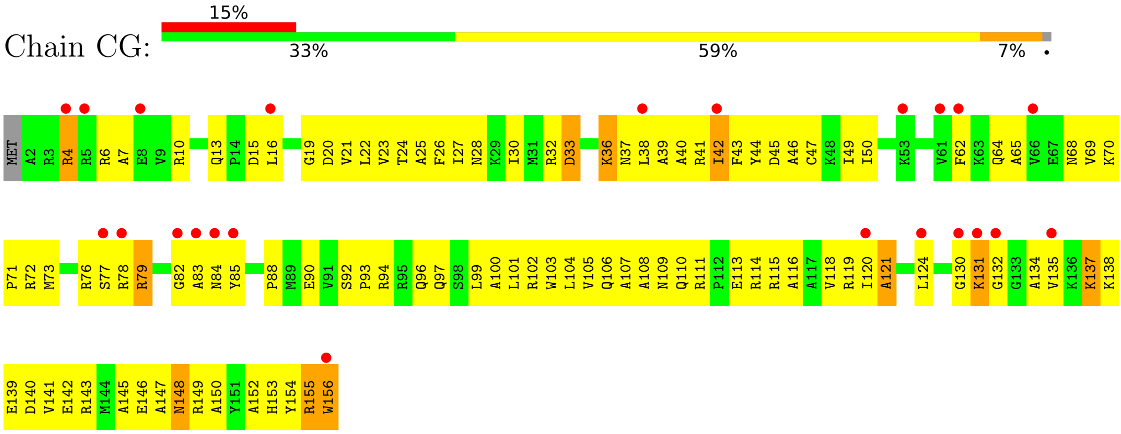


- Molecule 7: 30S RIBOSOMAL PROTEIN S7

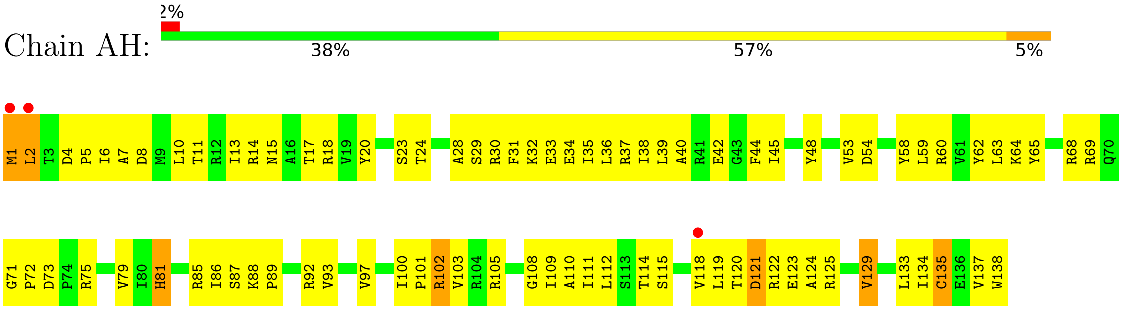
Chain AG:



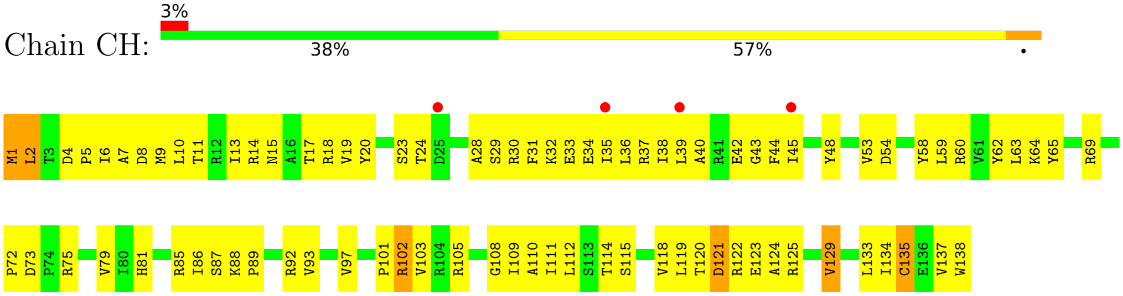
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



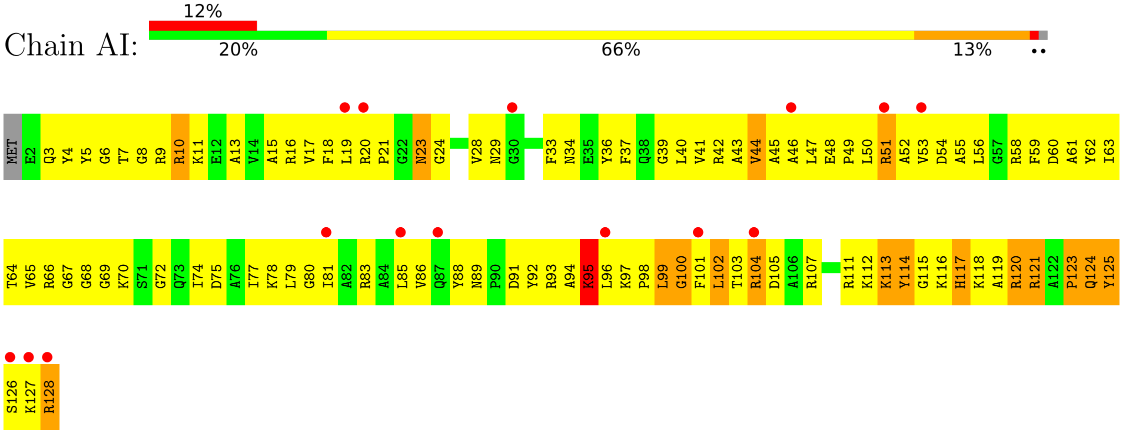
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



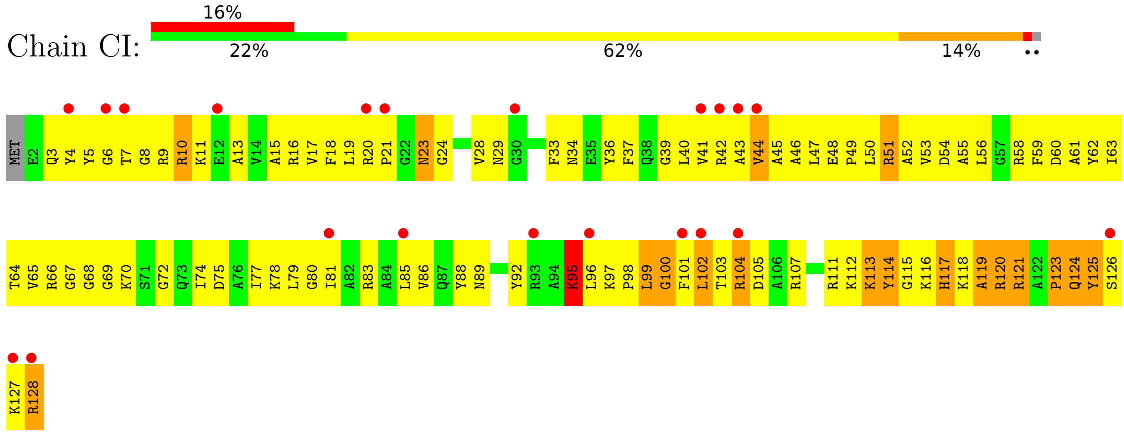
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



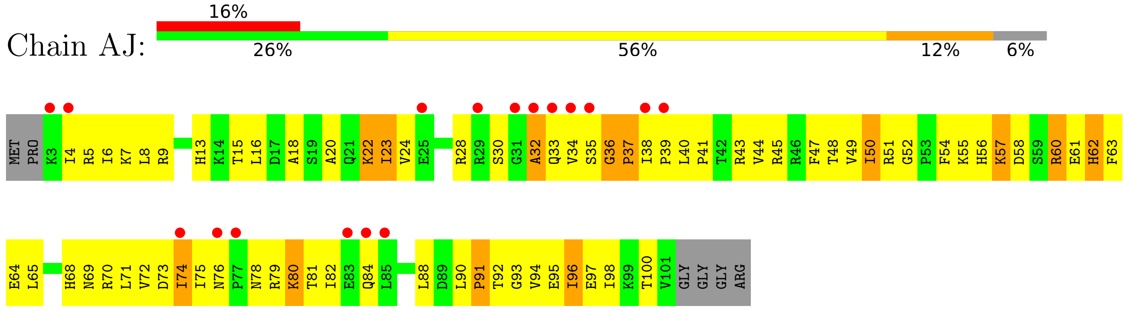
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



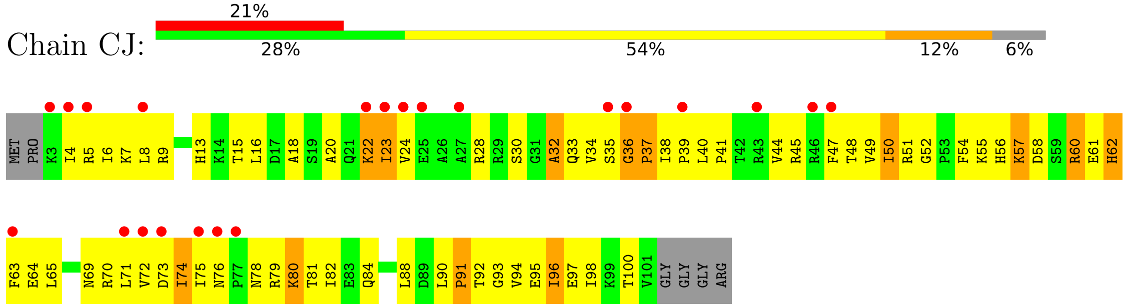
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



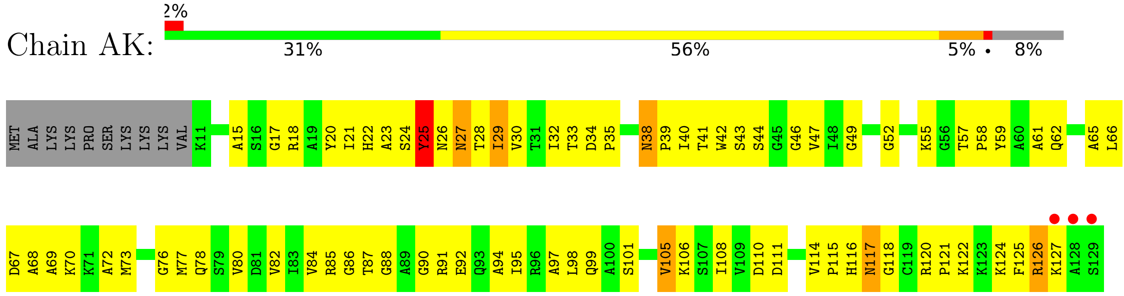
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



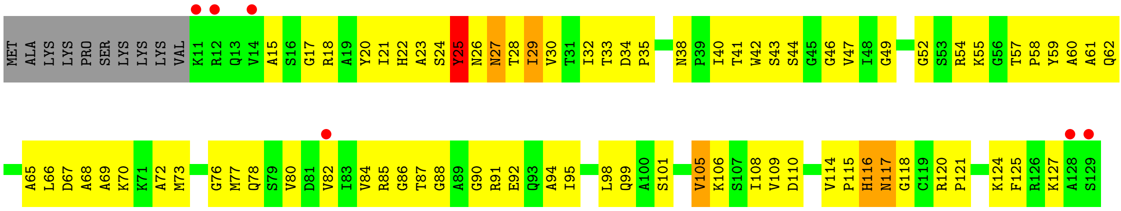
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

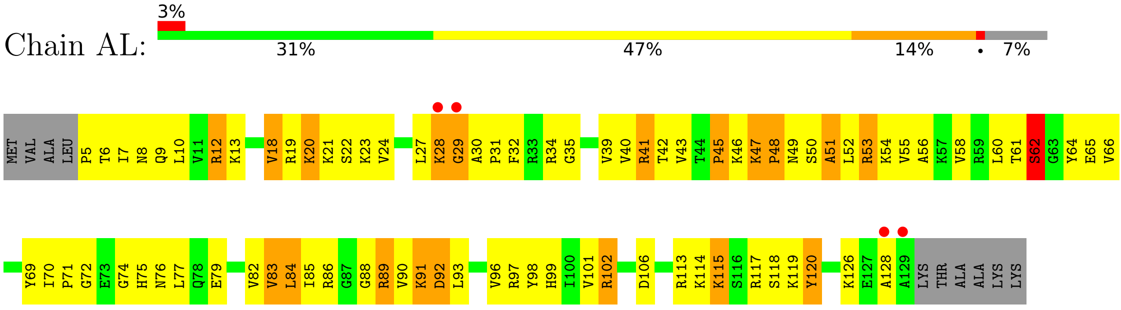


- Molecule 11: 30S RIBOSOMAL PROTEIN S11



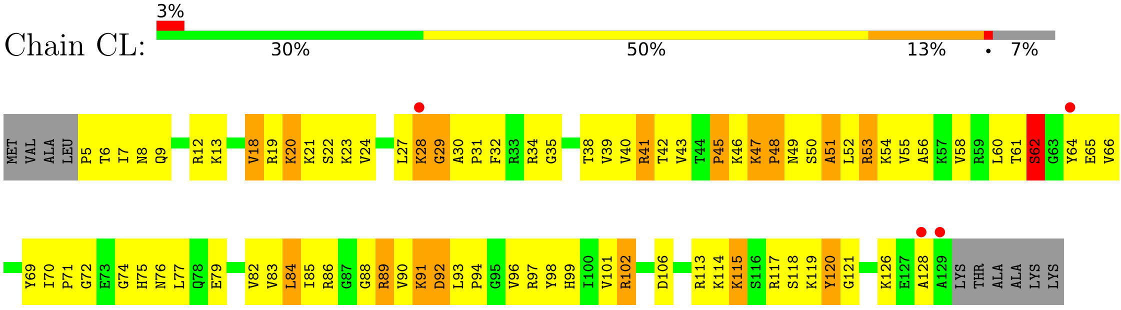
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



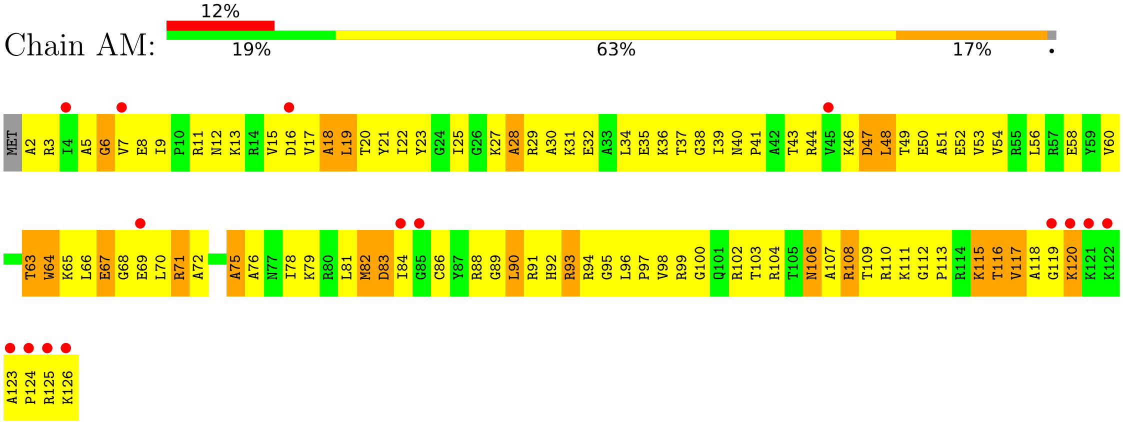
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



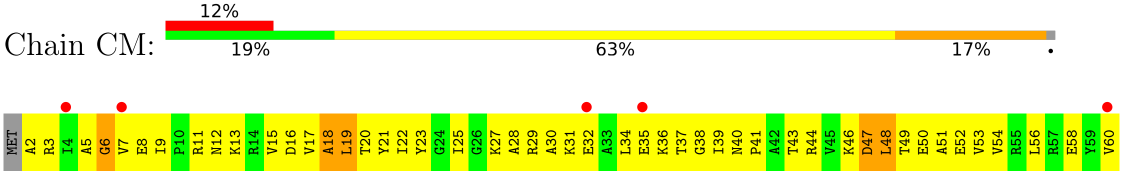
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

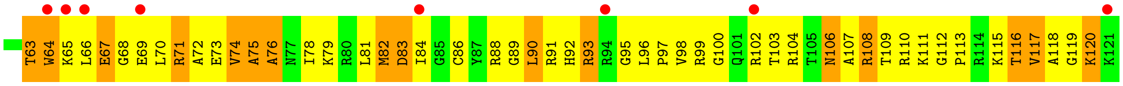
Chain AM:

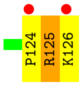


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:

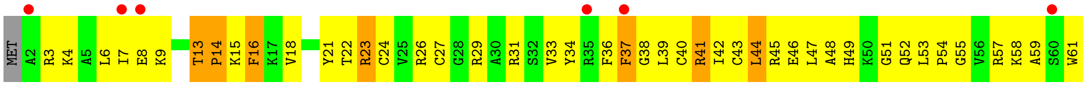






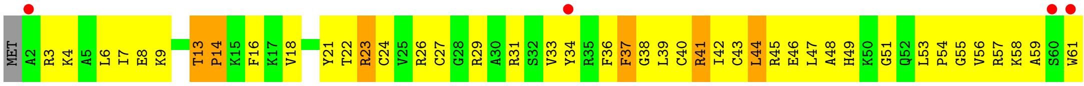
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



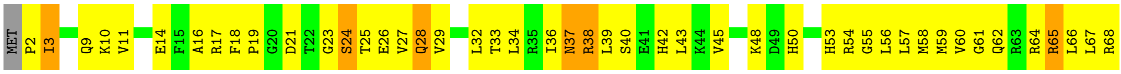
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

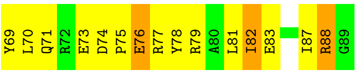
Chain CN:



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

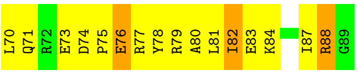
Chain AO:





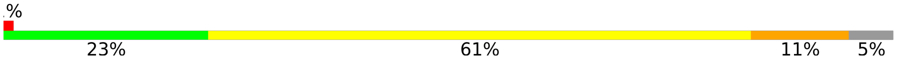
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

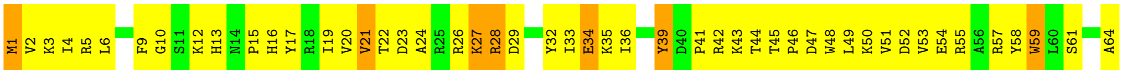
Chain CO:

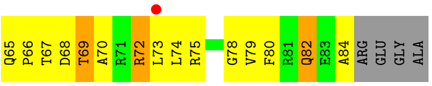


- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:

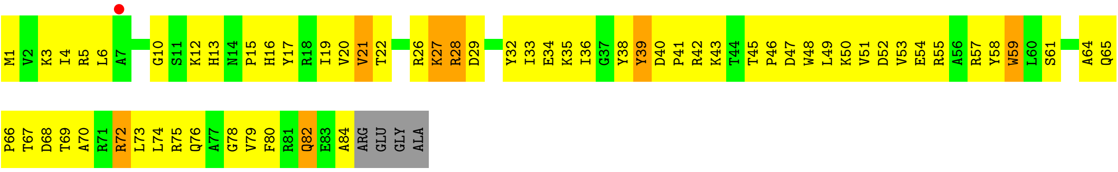






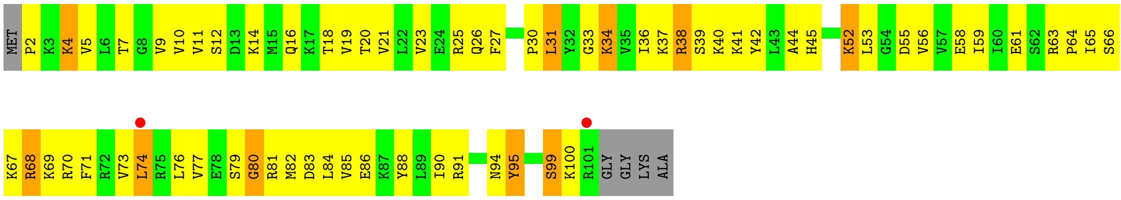
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



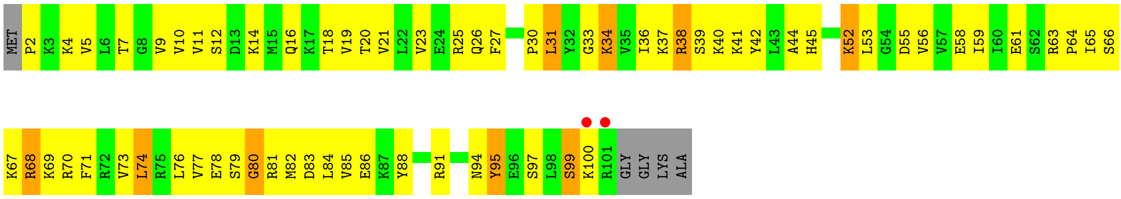
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



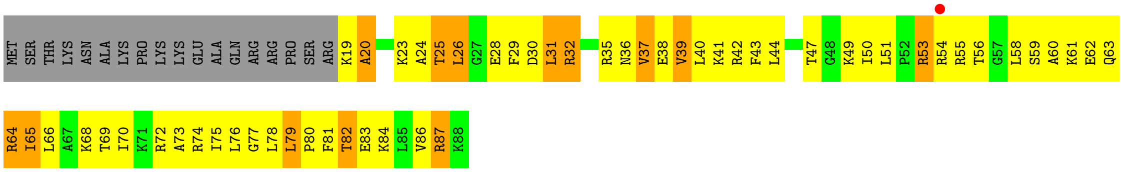
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



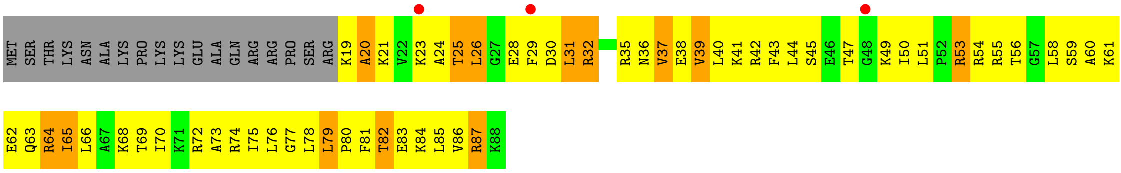
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:

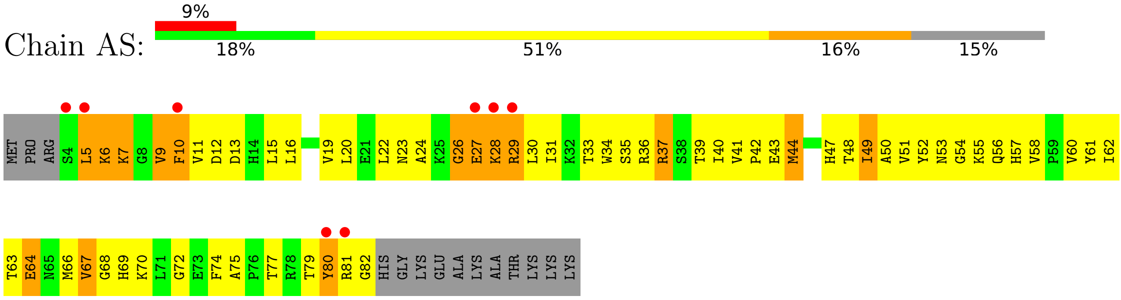


- Molecule 18: 30S RIBOSOMAL PROTEIN S18

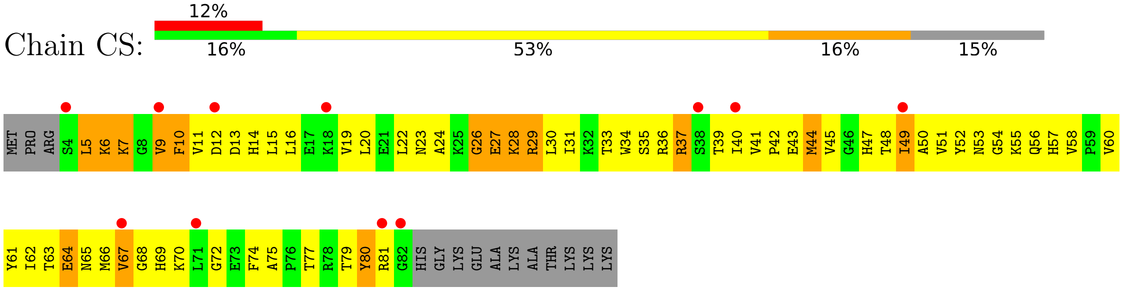
Chain CR:



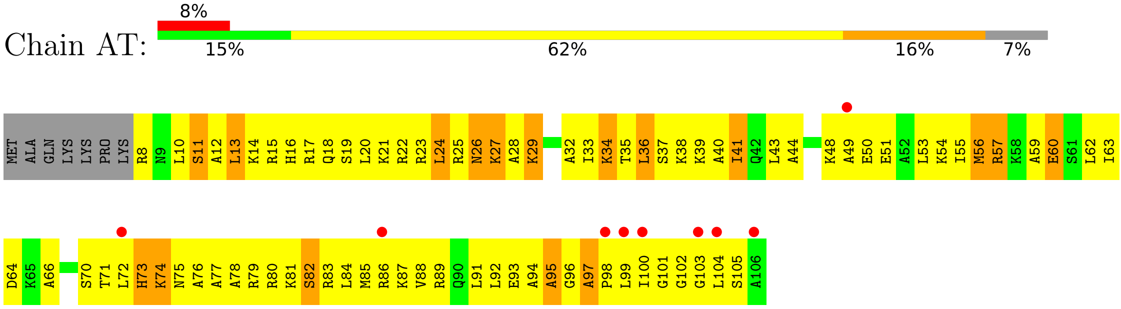
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



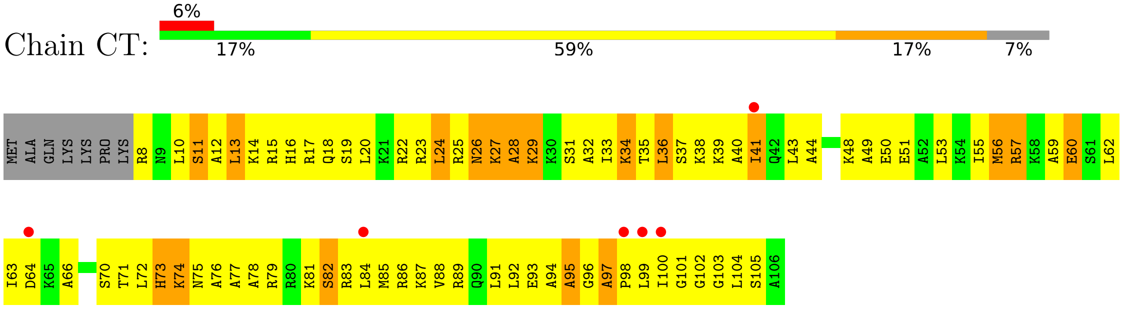
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

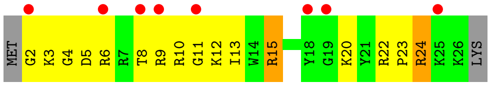


- Molecule 20: 30S RIBOSOMAL PROTEIN S20



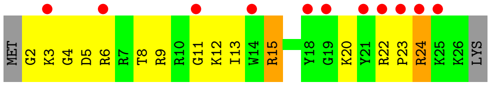
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



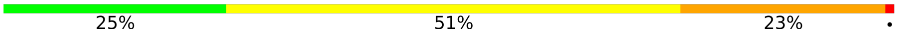
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

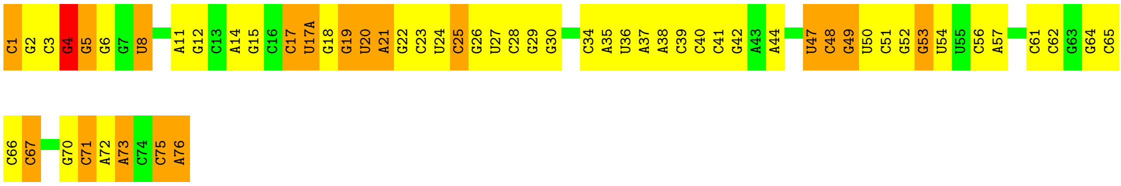
Chain CU:



- Molecule 22: P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

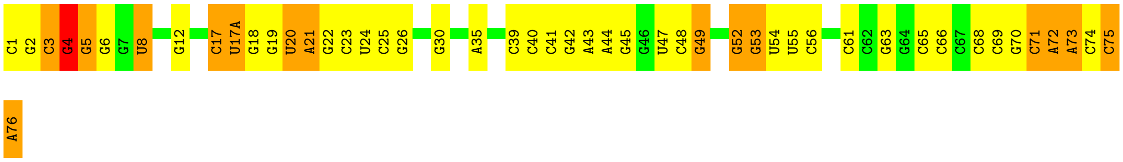
Chain AV:





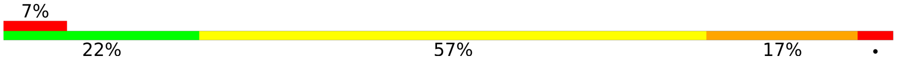
- Molecule 22: P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

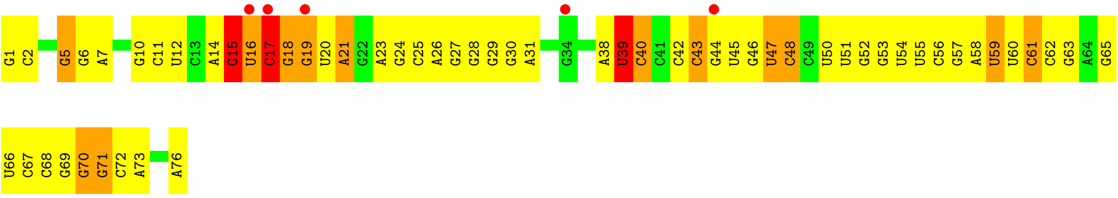
Chain CV:



- Molecule 23: E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES)

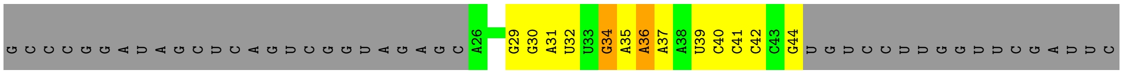
Chain AW:





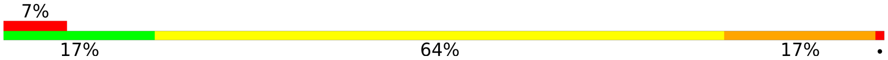
- Molecule 23: E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES)

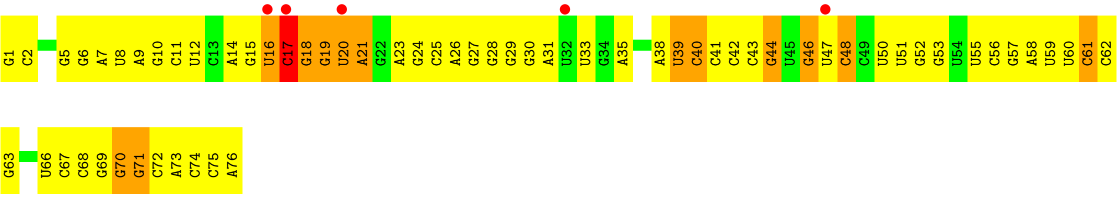
Chain AY:



- Molecule 23: E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES)

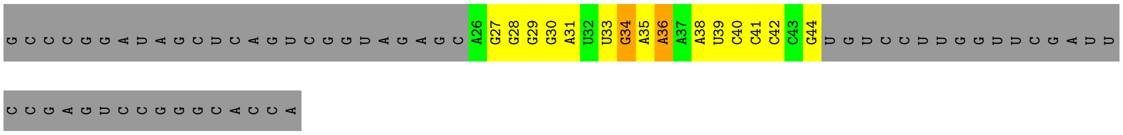
Chain CW:





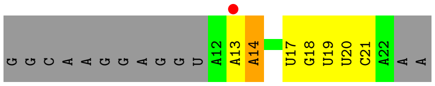
- Molecule 23: E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES)

Chain CY:



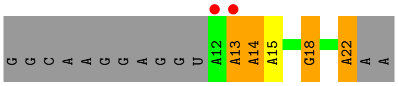
- Molecule 24: MRNA

Chain AX:



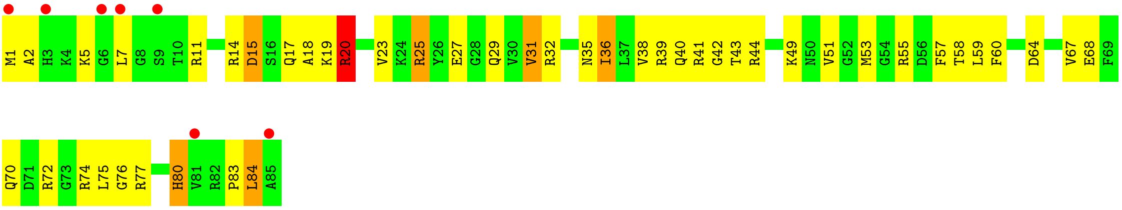
- Molecule 24: MRNA

Chain CX:



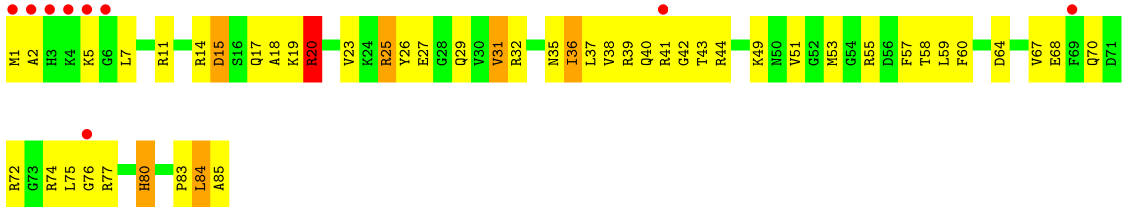
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



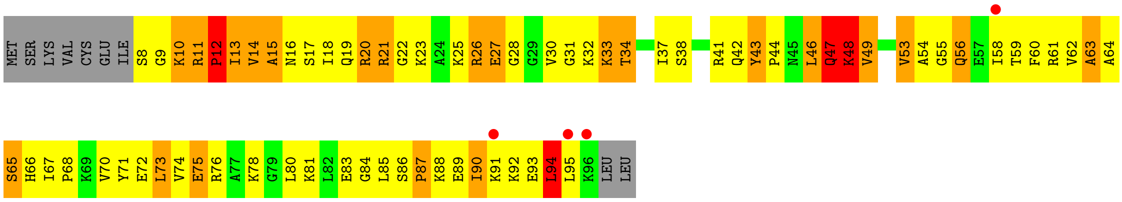
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain D0:



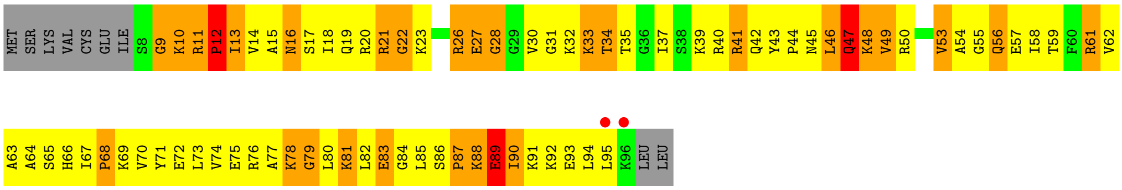
- Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



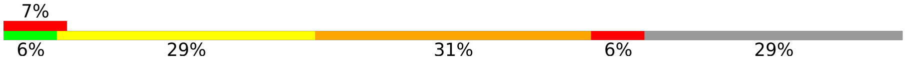
- Molecule 26: 50S RIBOSOMAL PROTEIN L28

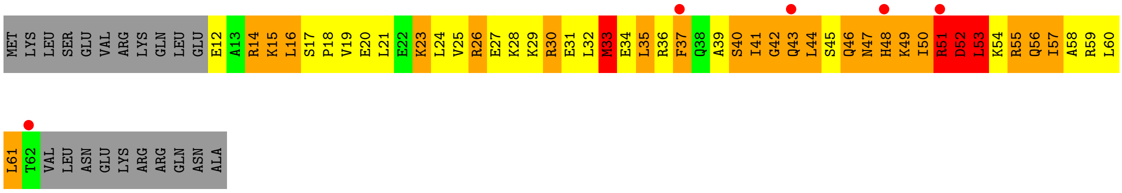
Chain D1:



- Molecule 27: 50S RIBOSOMAL PROTEIN L29

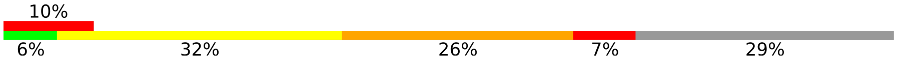
Chain B2:

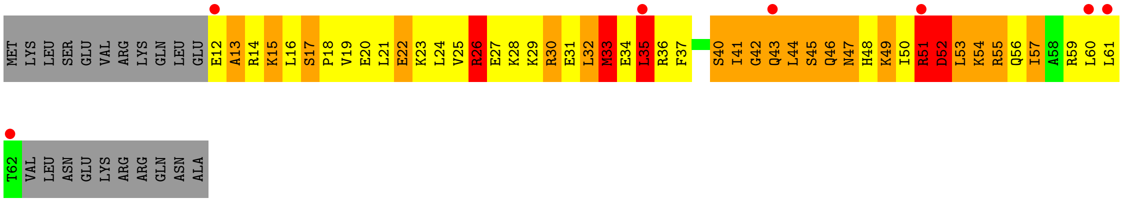




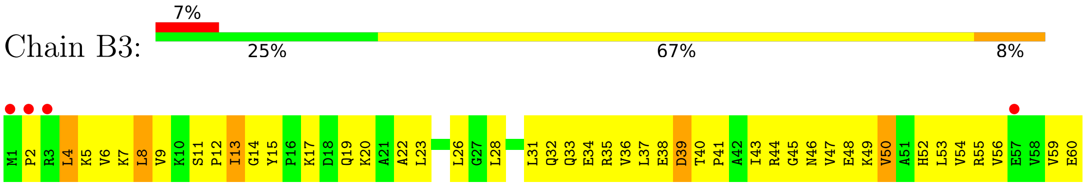
- Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:

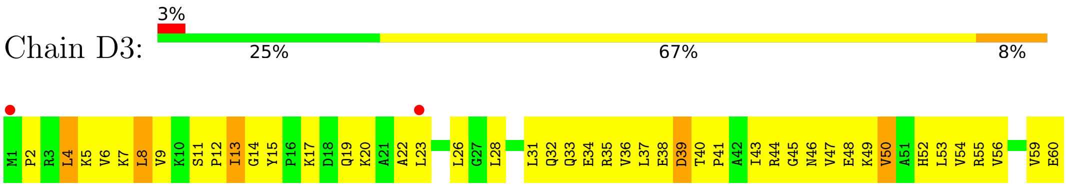




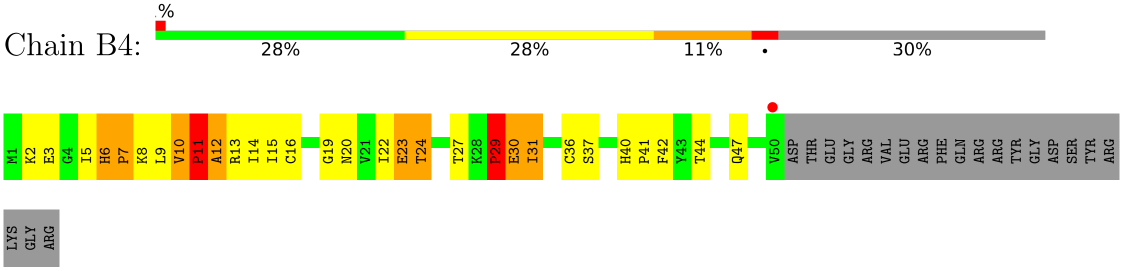
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



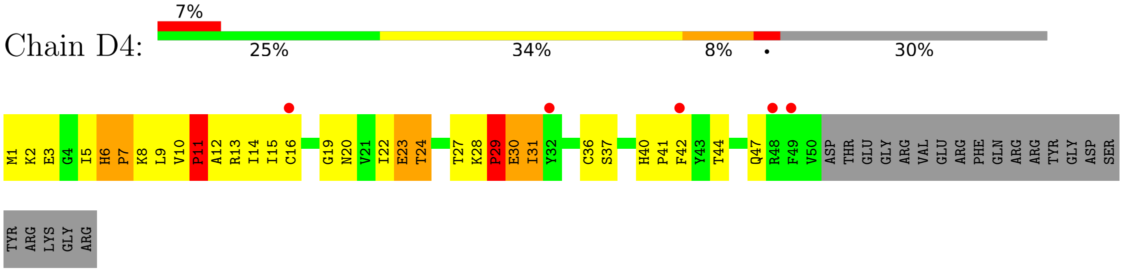
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



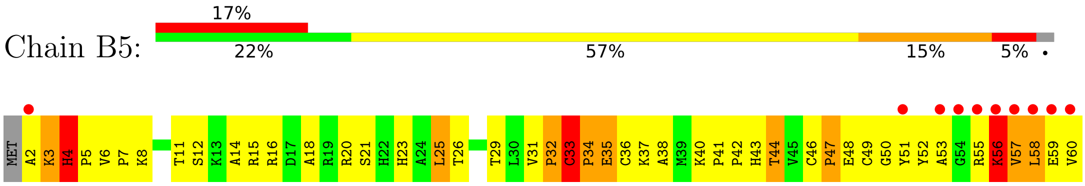
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



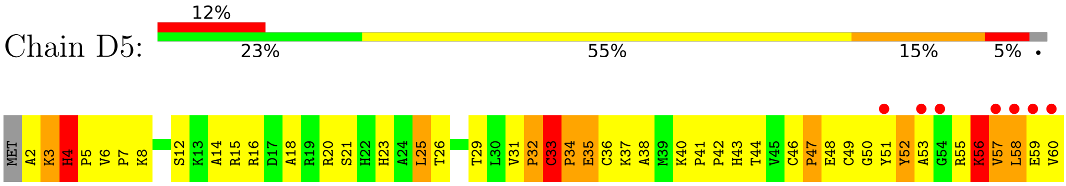
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



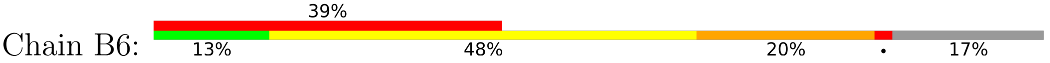
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



- Molecule 30: 50S RIBOSOMAL PROTEIN L32

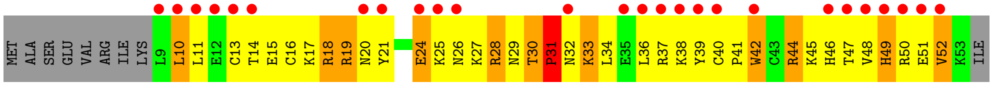


- Molecule 31: 50S RIBOSOMAL PROTEIN L33



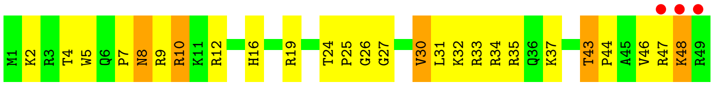
• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6:



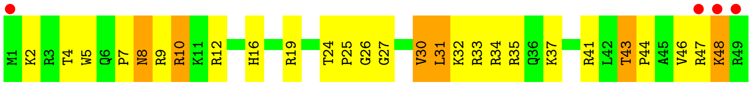
• Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:



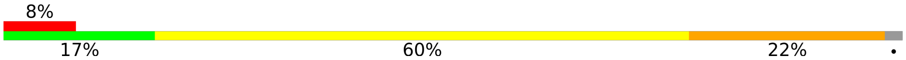
• Molecule 32: 50S RIBOSOMAL PROTEIN L34

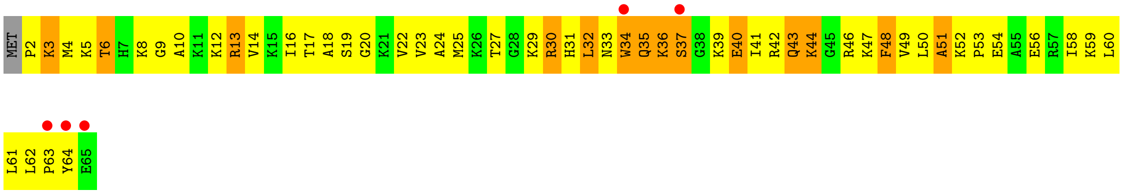
Chain D7:



• Molecule 33: 50S RIBOSOMAL PROTEIN L35

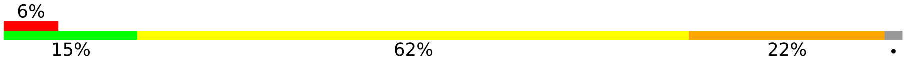
Chain B8:

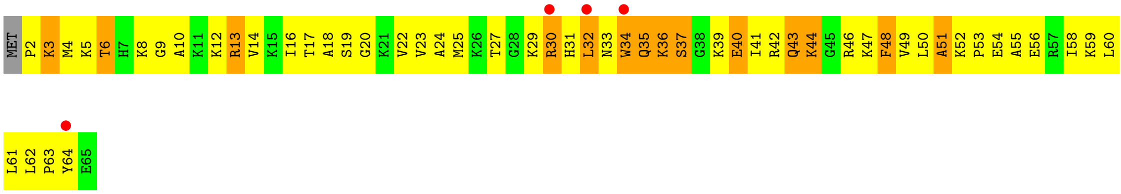




• Molecule 33: 50S RIBOSOMAL PROTEIN L35

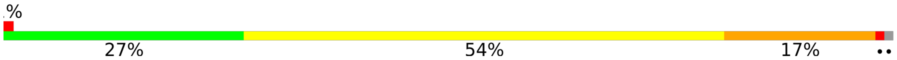
Chain D8:

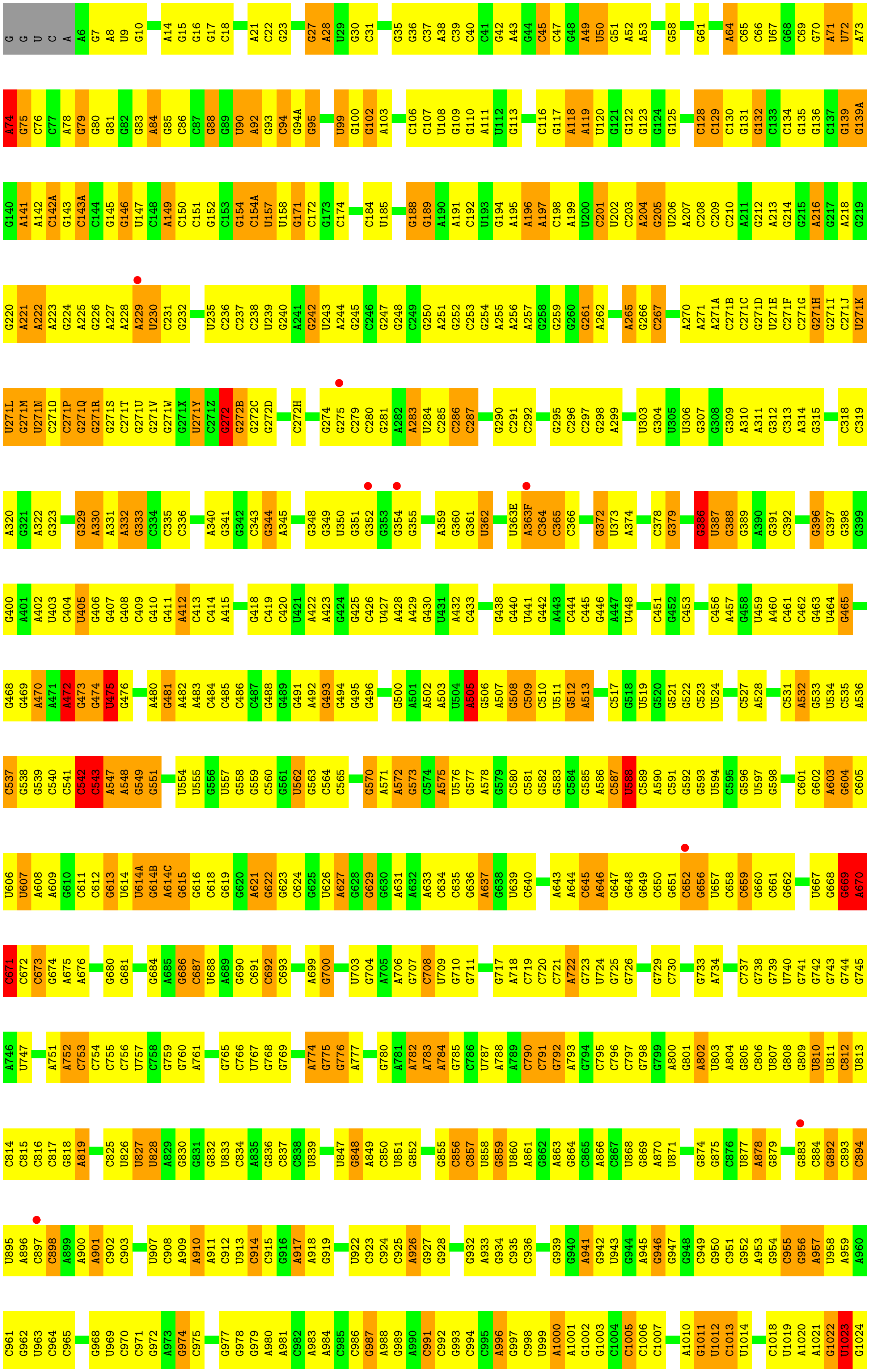




• Molecule 34: 23S RIBOSOMAL RNA

Chain BA:

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A74 G75 C76 C77 A78 G79 G80 G81 G82 G83 A84 G85 C86 C87 G88 G89 U90 A92 G93 C94 G94A G95 U99 G100 G102 A103 C106 C107 U108 G109 G110 A111 U112 G113 C116 G117 A118 A119 U120 G121 G122 G123 G124 G125 C128 C129 C130 G131 G132 C133 C134 G135 G136 C137 G139 G139A
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A746 U747 A751 A752 C753 C754 C755 C756 U757 C758 G759 G760 A761 G765 C766 U767 G768 C769 A774 G775 C776 A777 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 G798 G799 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813
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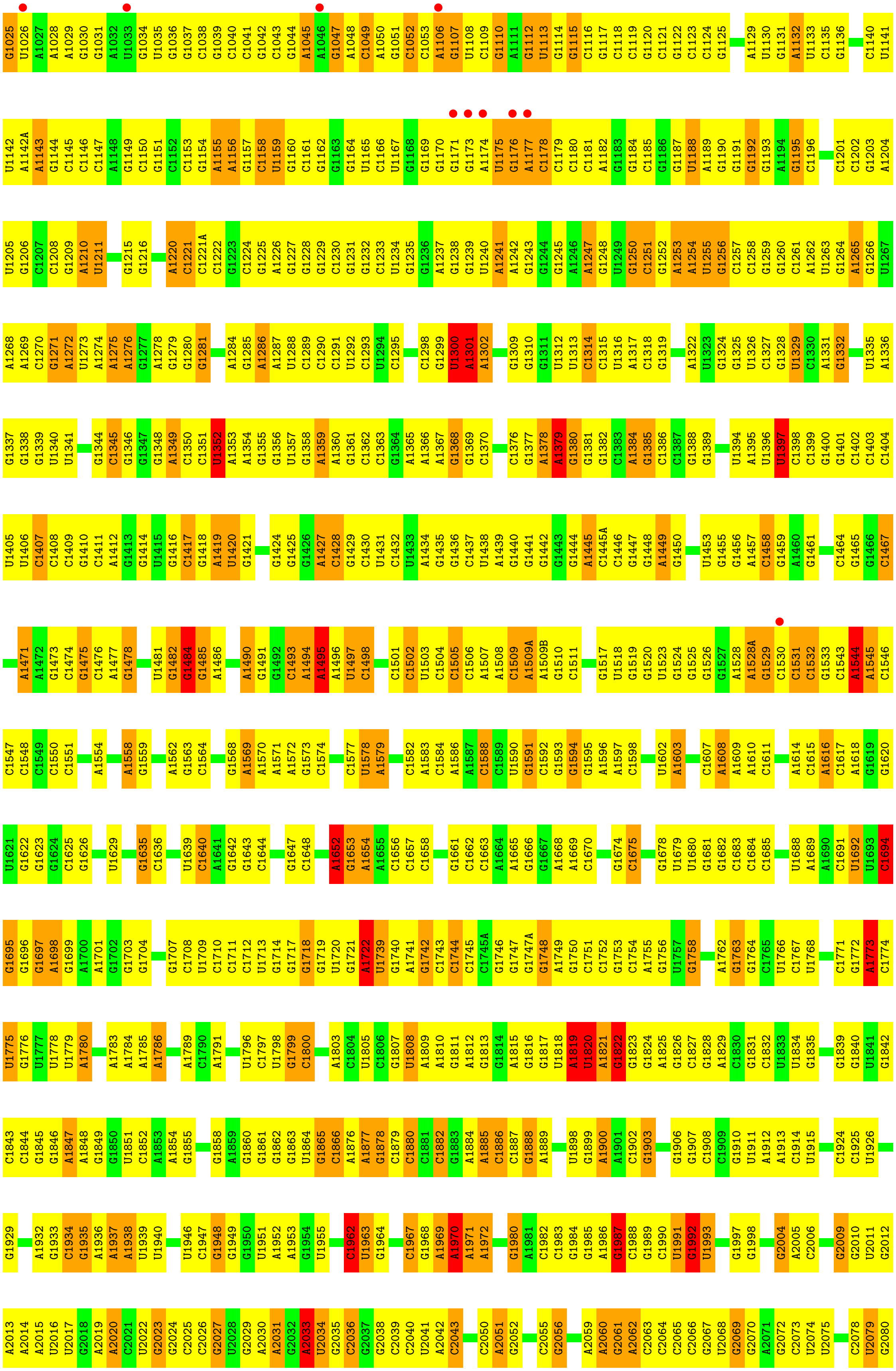
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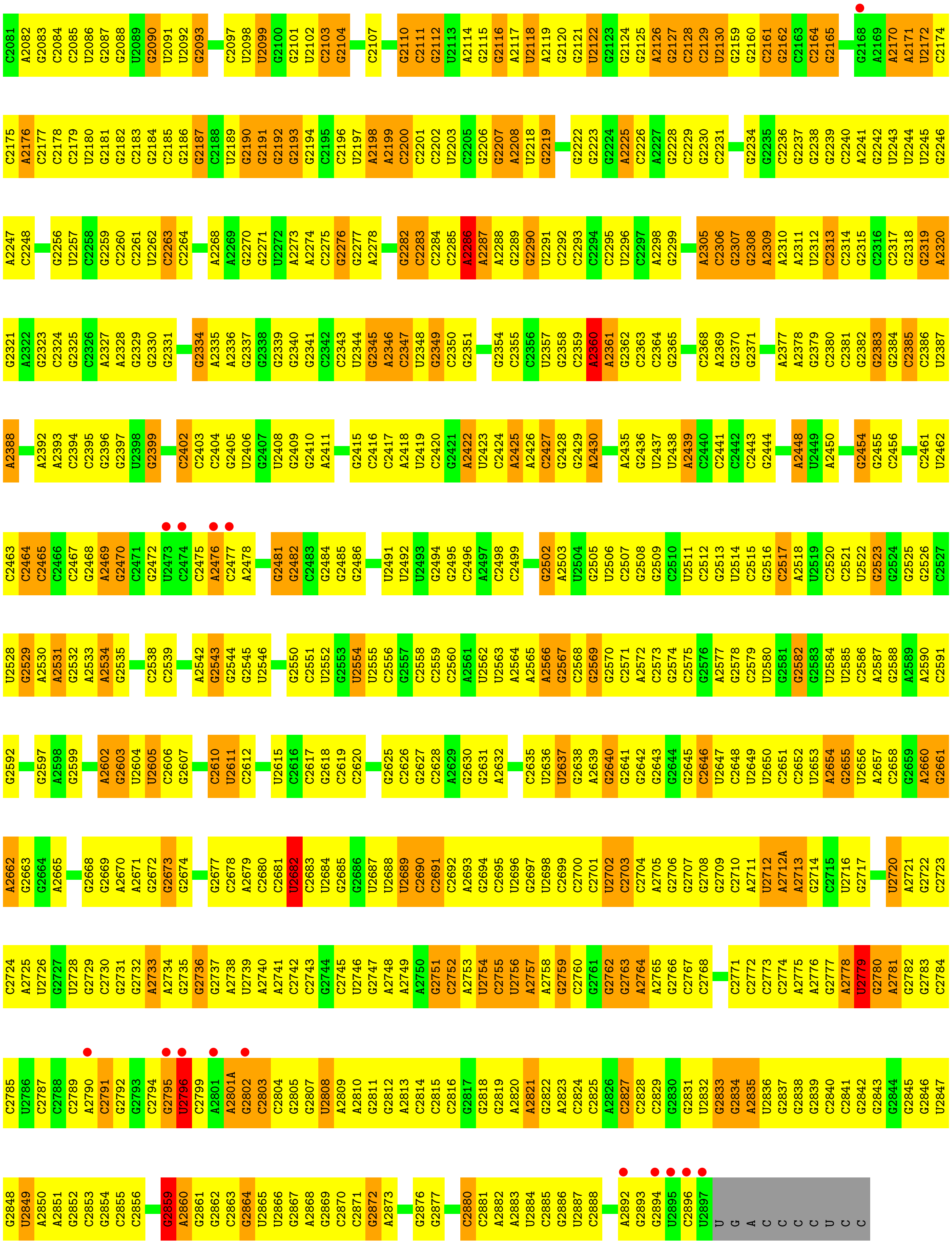

- Molecule 34: 23S RIBOSOMAL RNA

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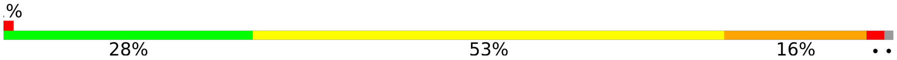

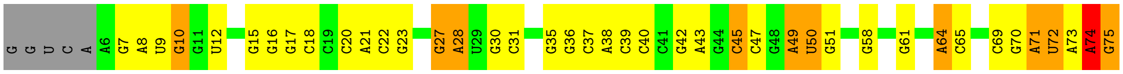

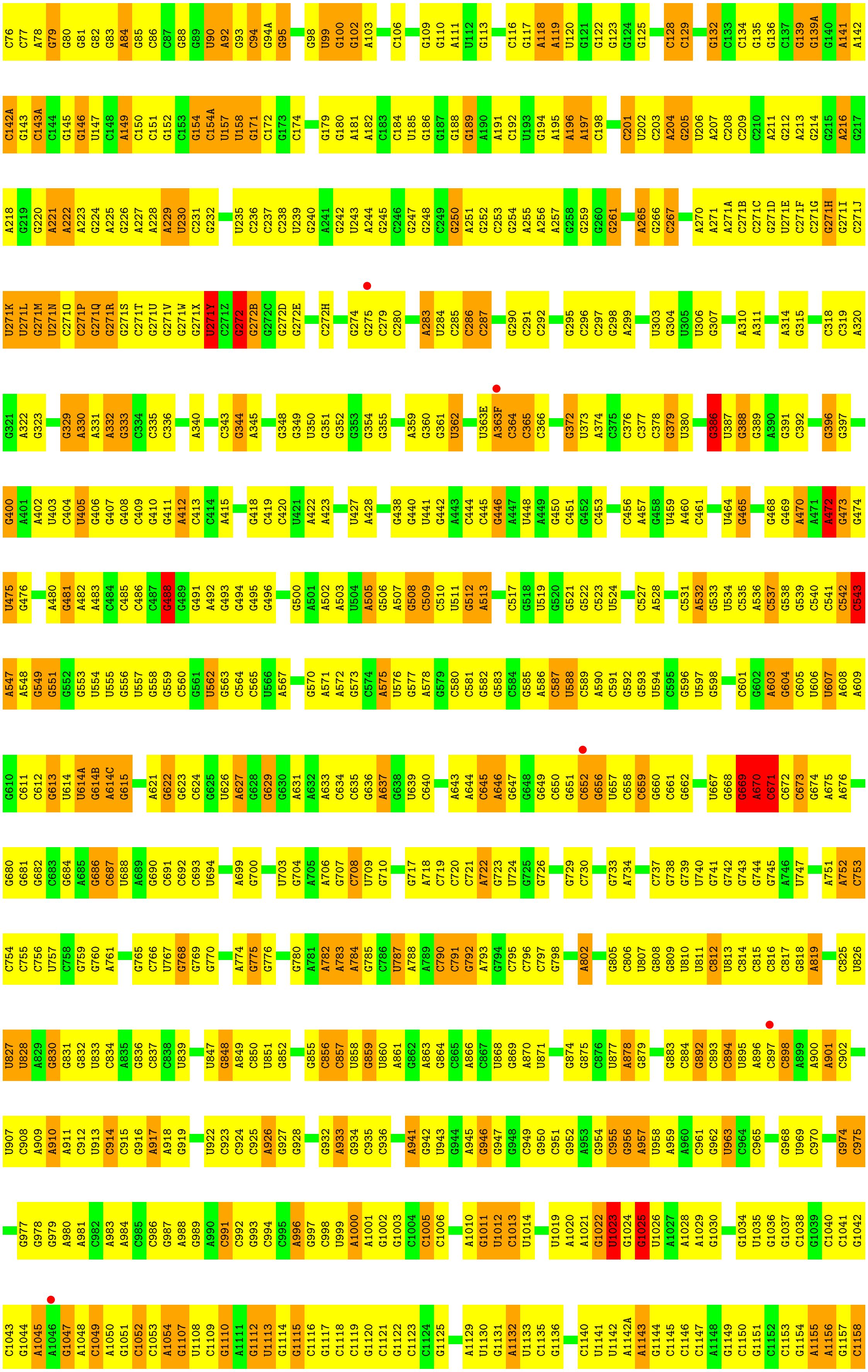
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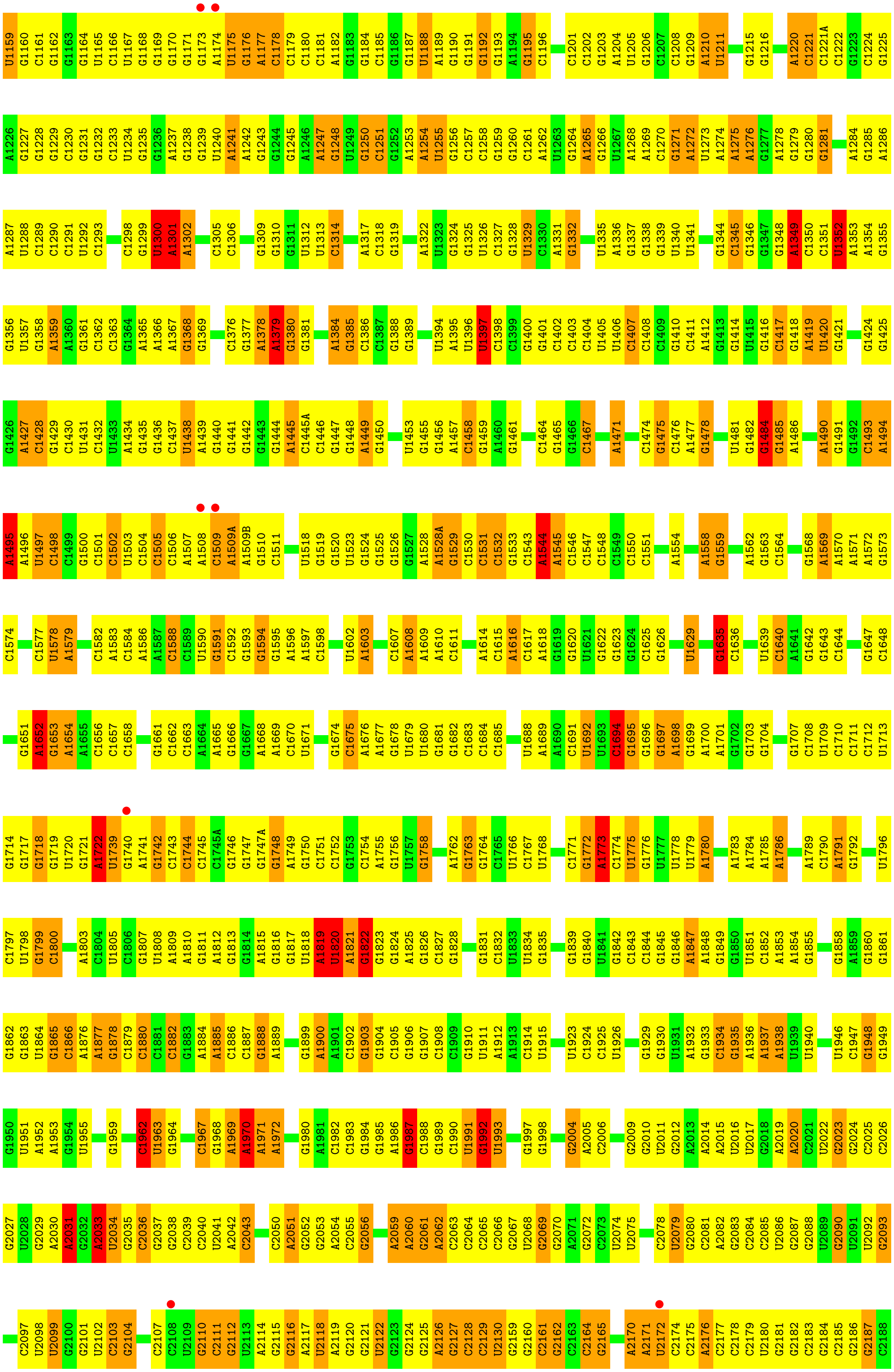
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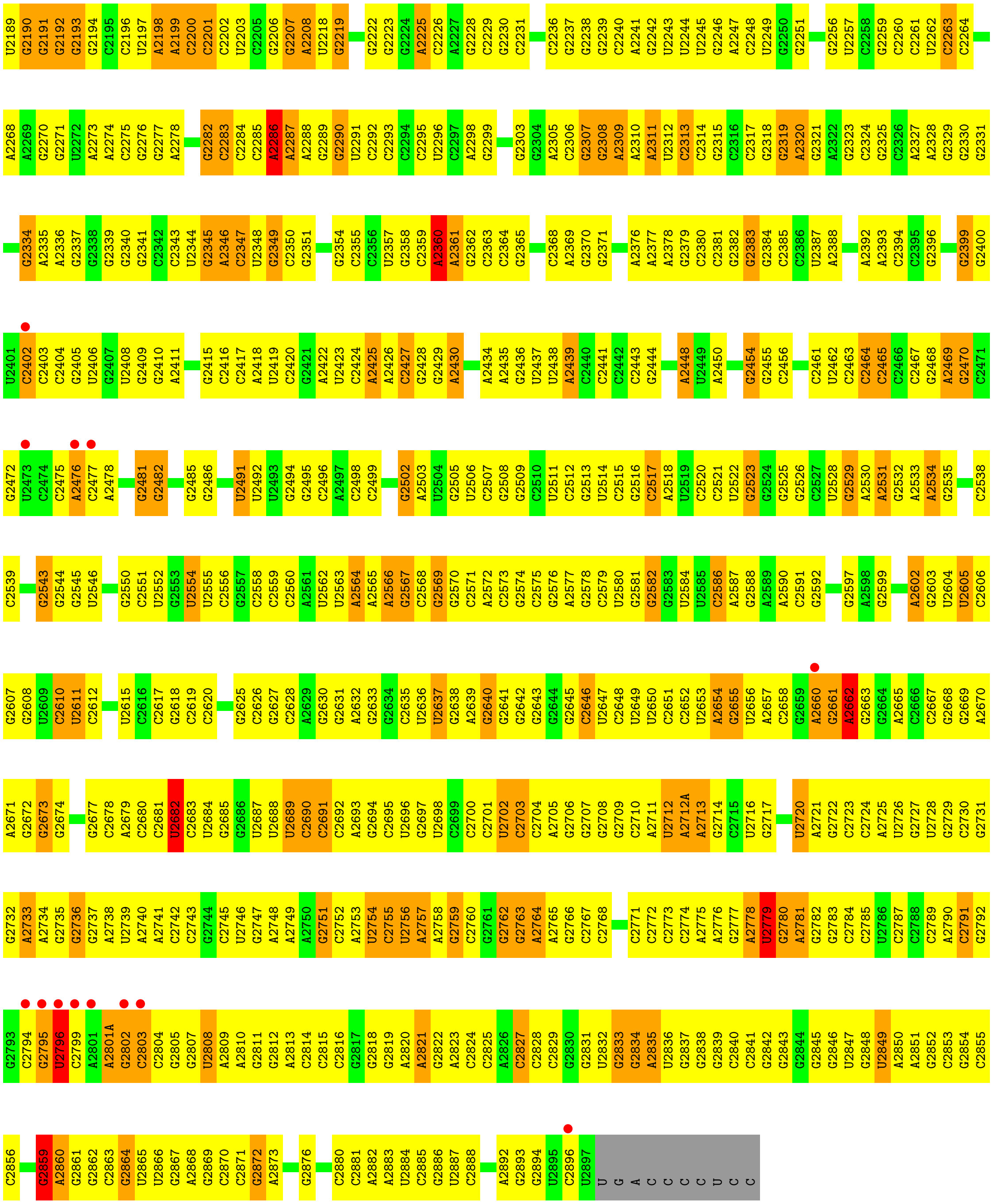
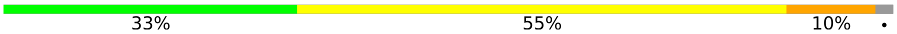
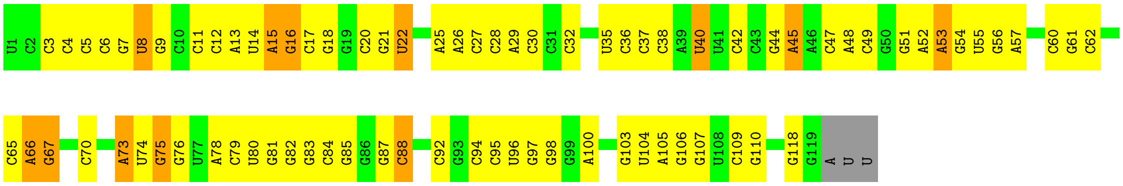


- Molecule 35: 5S RIBOSOMAL RNA

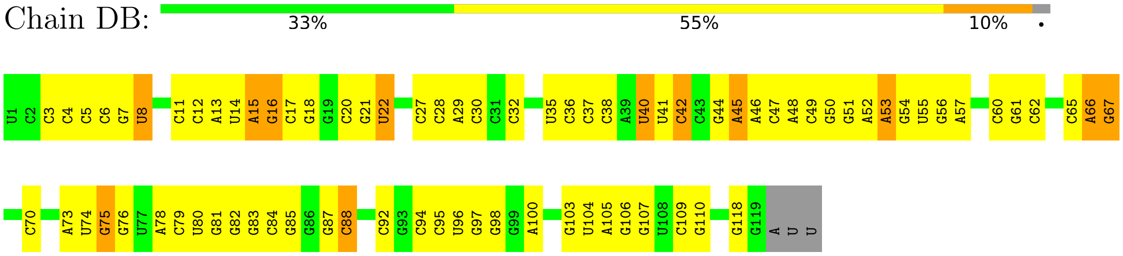
Chain BB:





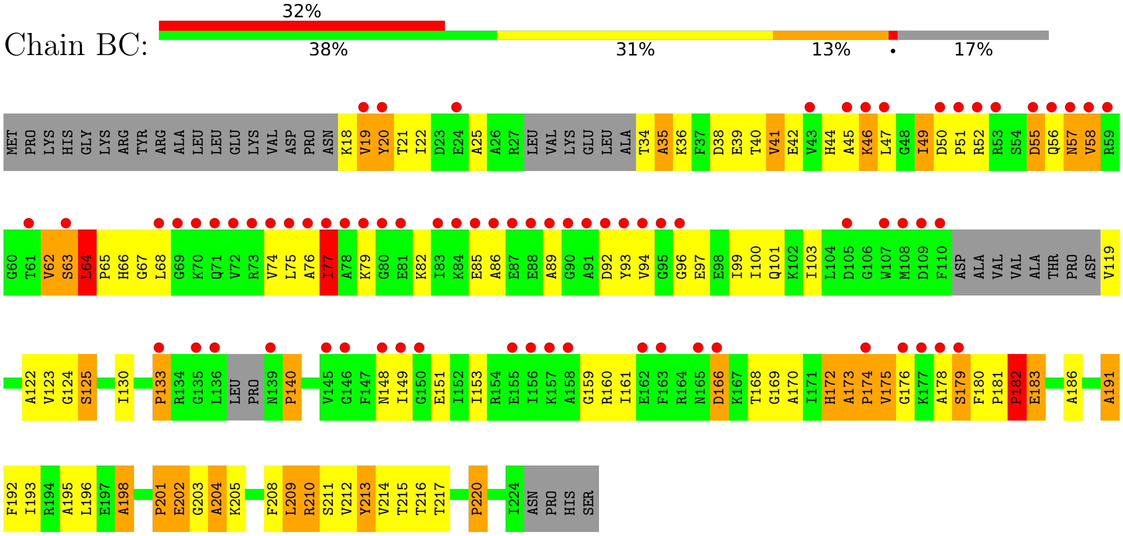
- Molecule 35: 5S RIBOSOMAL RNA

Chain DB:



- Molecule 36: 50S RIBOSOMAL PROTEIN L1

Chain BC:



- Molecule 36: 50S RIBOSOMAL PROTEIN L1

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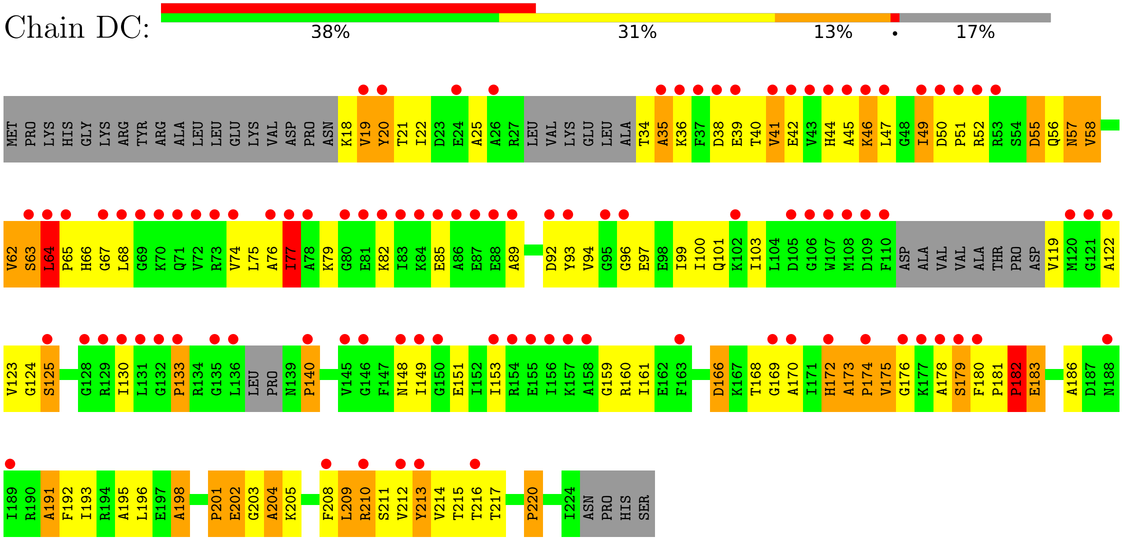
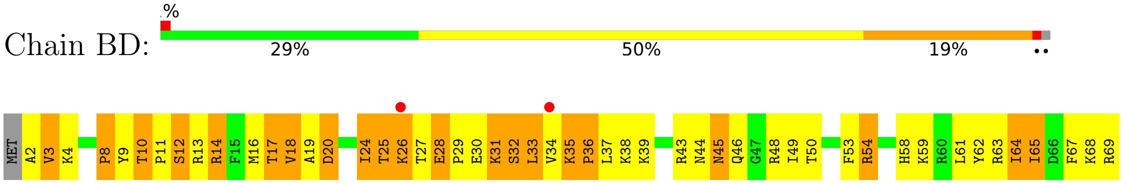
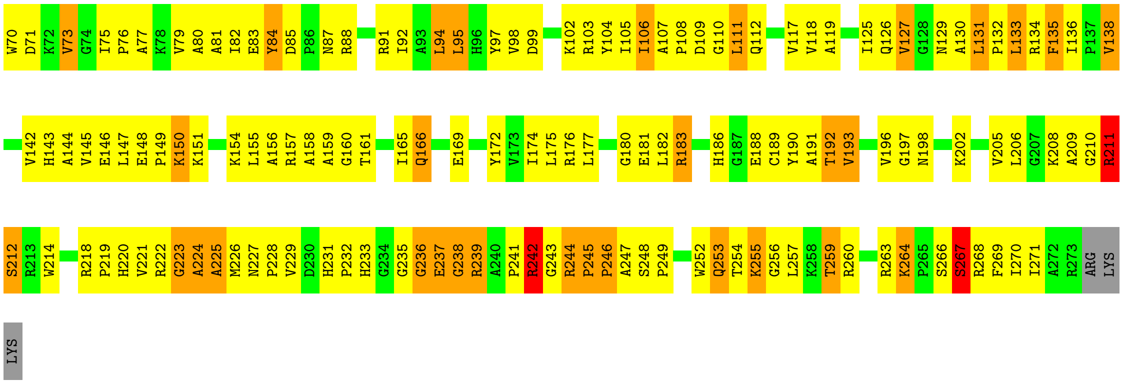


- Molecule 37: 50S RIBOSOMAL PROTEIN L2

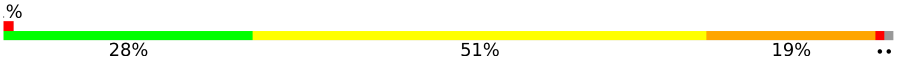
Chain BD:

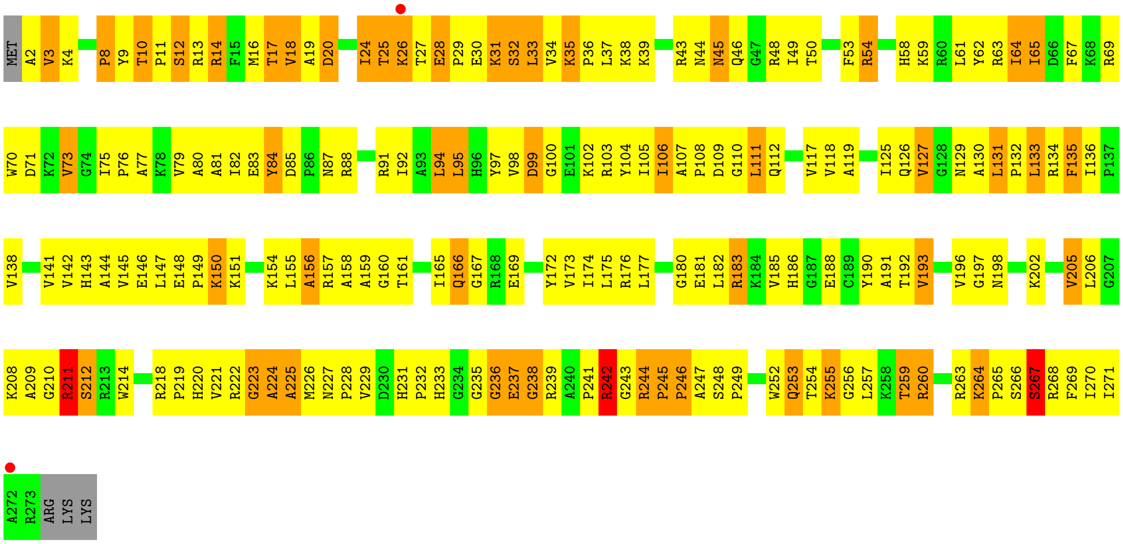




- Molecule 37: 50S RIBOSOMAL PROTEIN L2

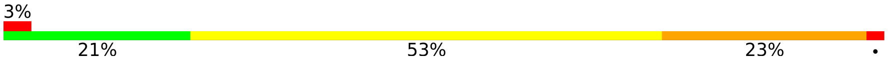
Chain DD:

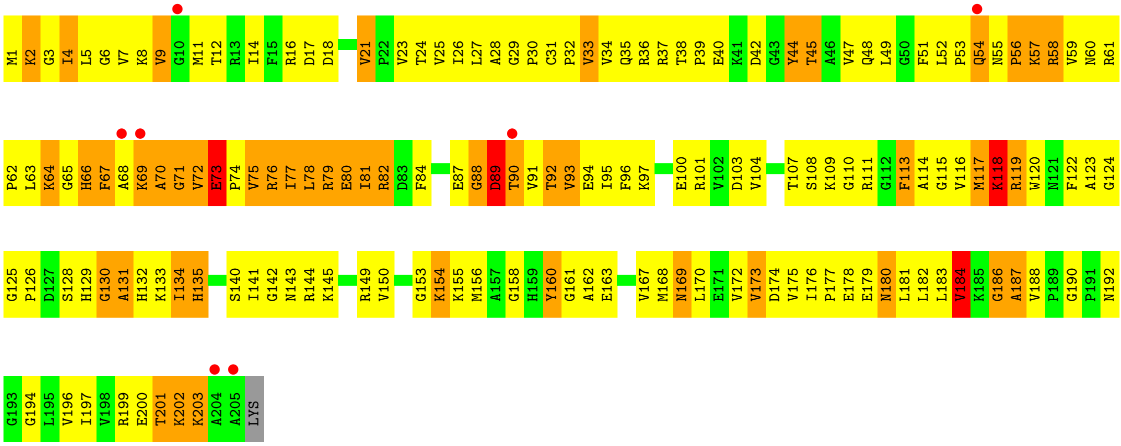




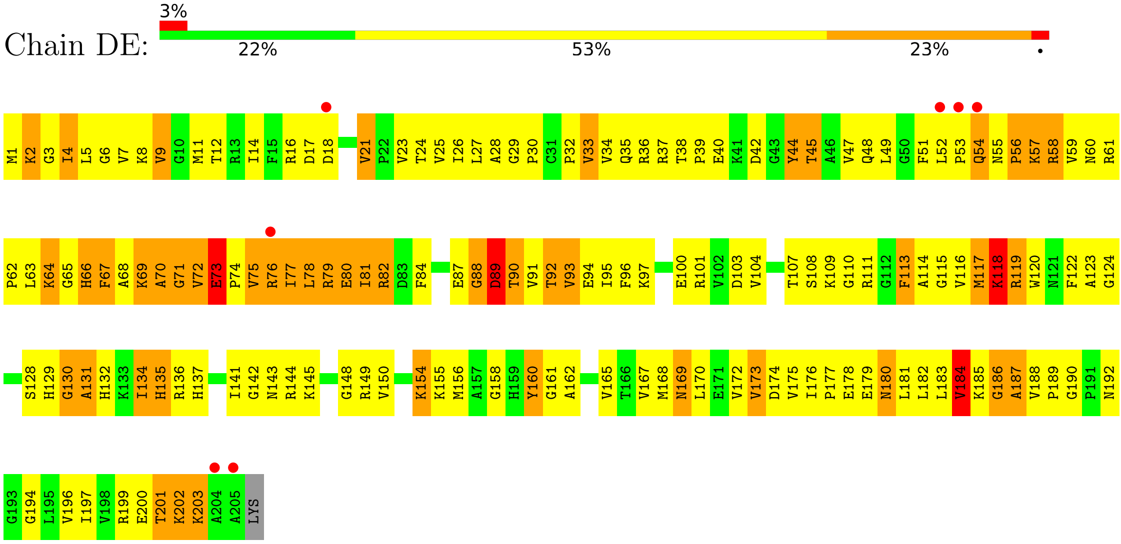
- Molecule 38: 50S RIBOSOMAL PROTEIN L3

Chain BE:

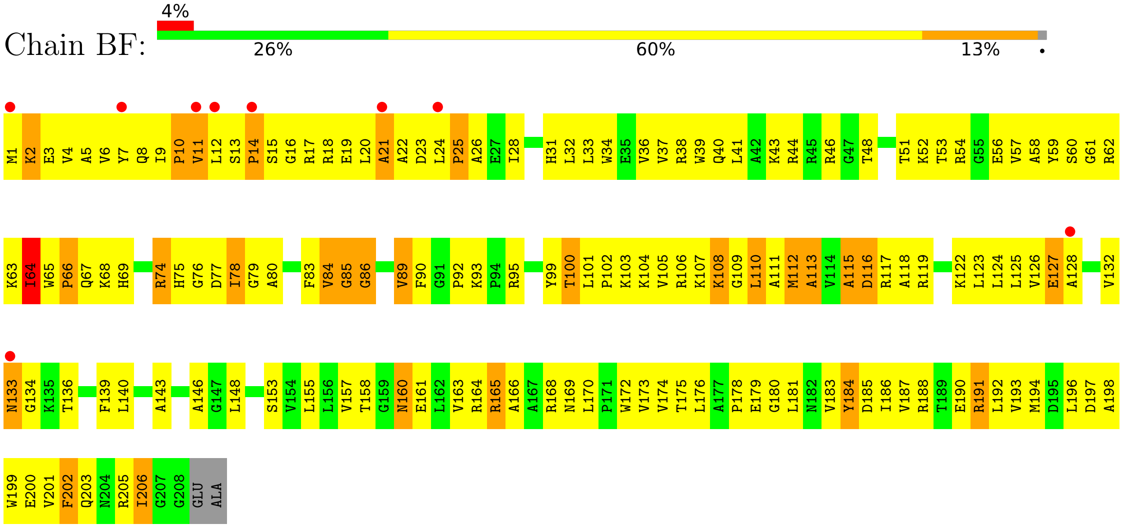




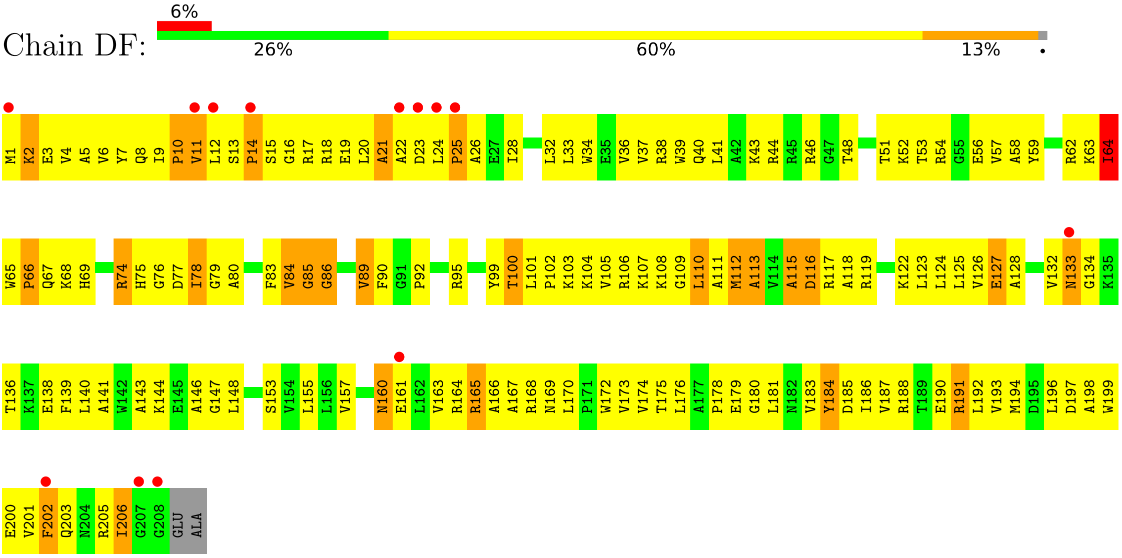
- Molecule 38: 50S RIBOSOMAL PROTEIN L3



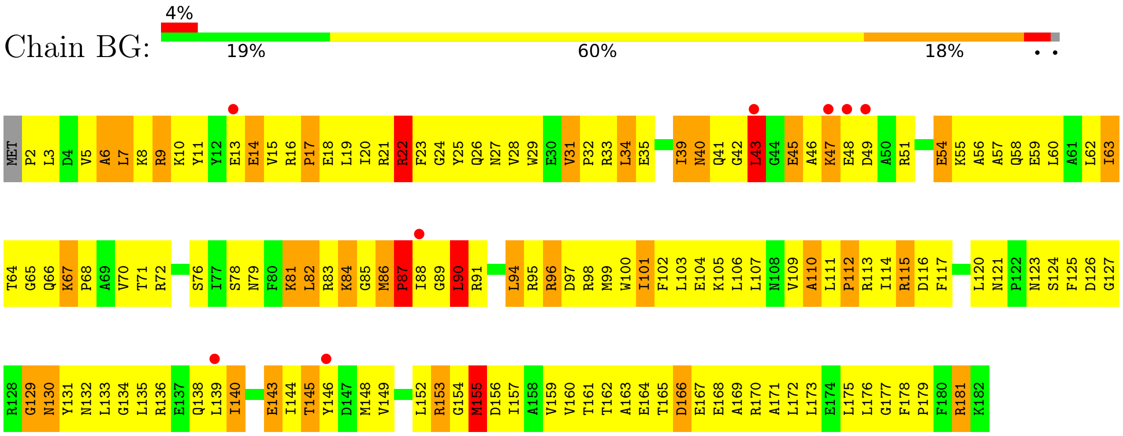
- Molecule 39: 50S RIBOSOMAL PROTEIN L4



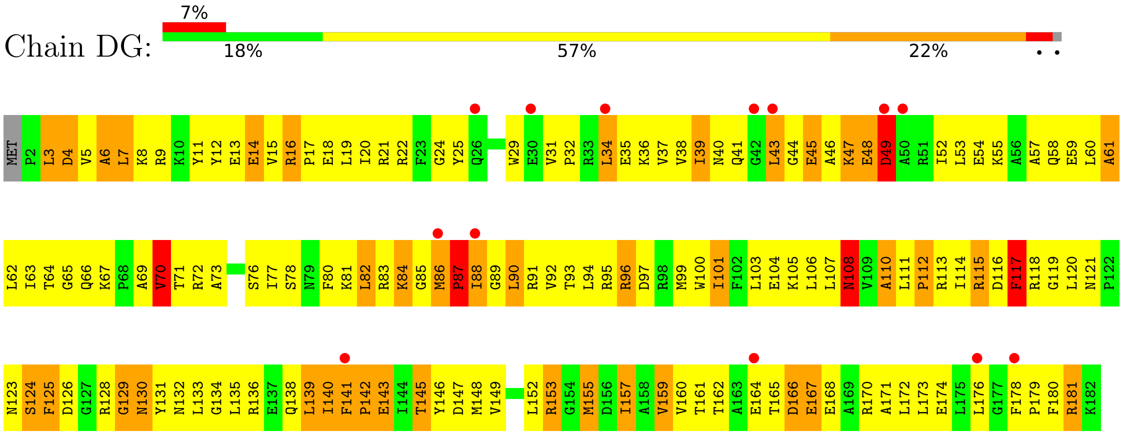
- Molecule 39: 50S RIBOSOMAL PROTEIN L4



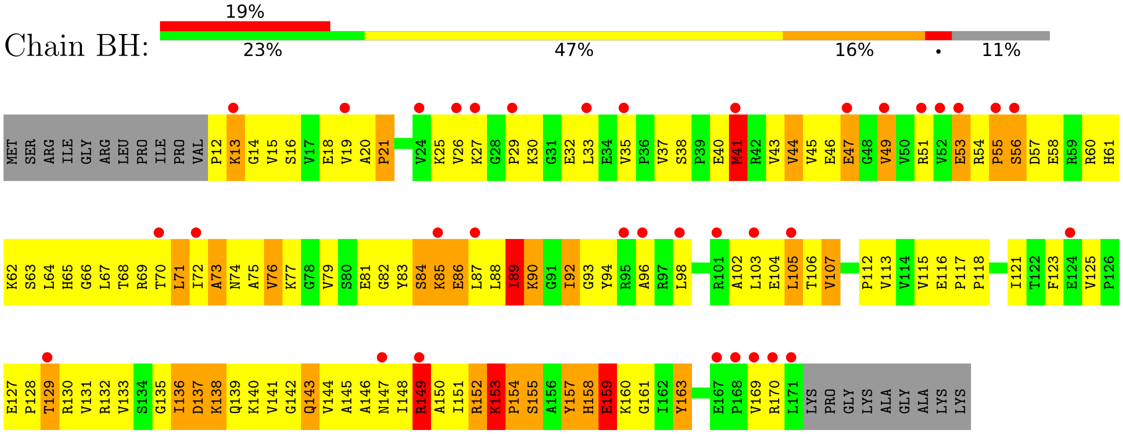
- Molecule 40: 50S RIBOSOMAL PROTEIN L5



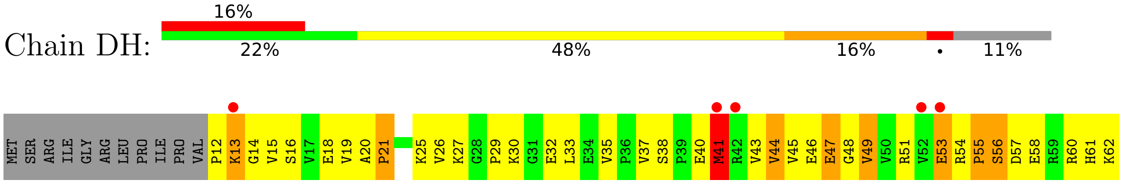
- Molecule 40: 50S RIBOSOMAL PROTEIN L5

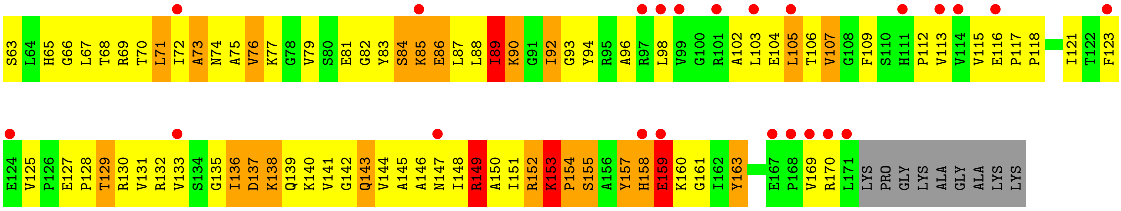


- Molecule 41: 50S RIBOSOMAL PROTEIN L6

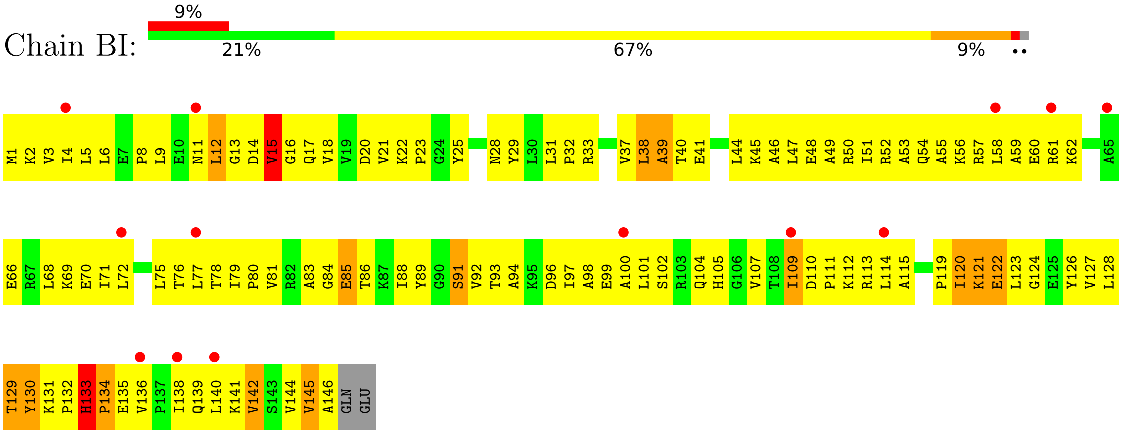


- Molecule 41: 50S RIBOSOMAL PROTEIN L6

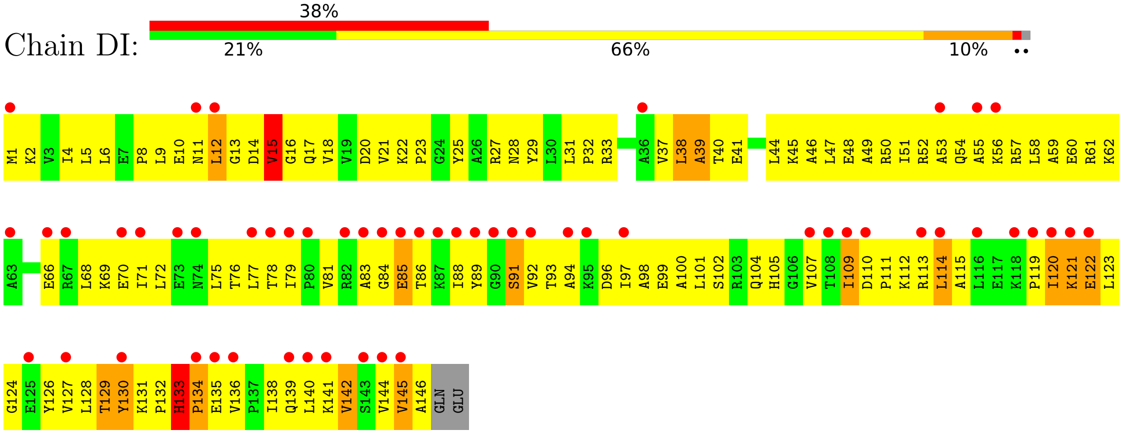




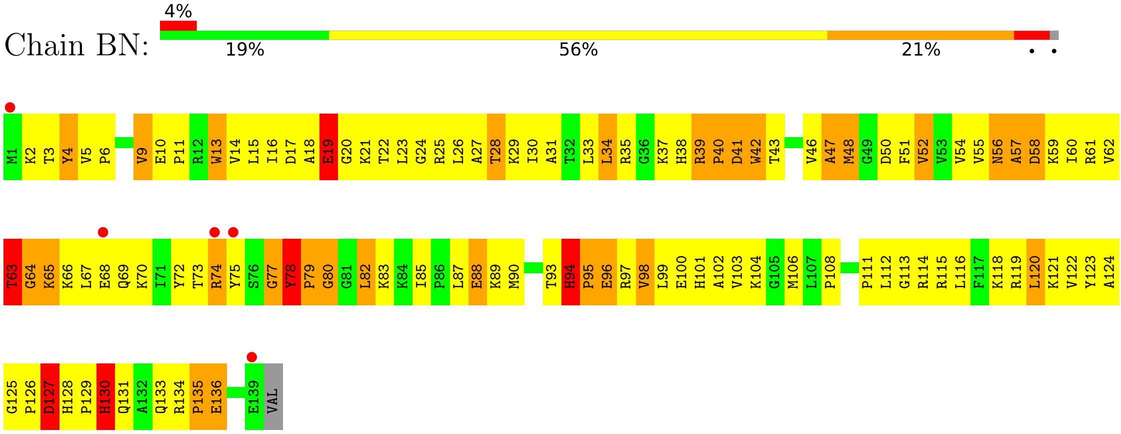
- Molecule 42: 50S RIBOSOMAL PROTEIN L9



- Molecule 42: 50S RIBOSOMAL PROTEIN L9

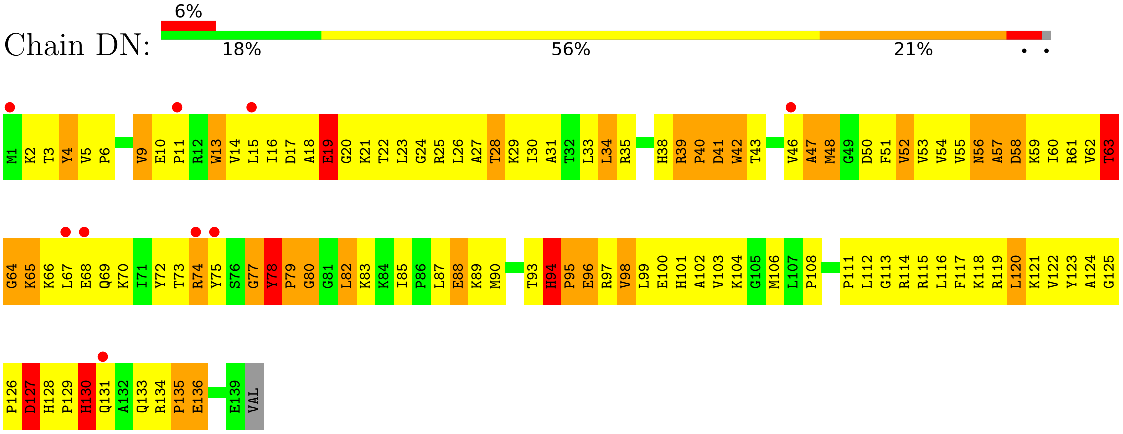


- Molecule 43: 50S RIBOSOMAL PROTEIN L13



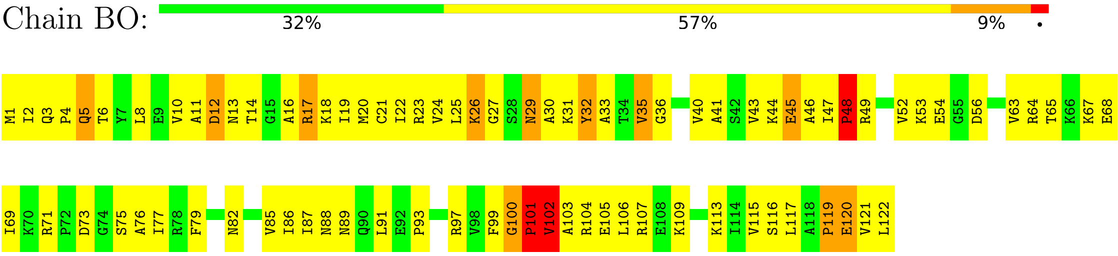
- Molecule 43: 50S RIBOSOMAL PROTEIN L13

Chain DN:



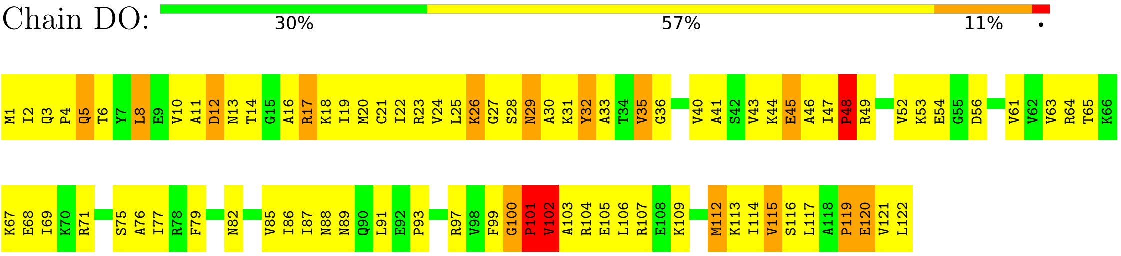
- Molecule 44: 50S RIBOSOMAL PROTEIN L14

Chain BO:



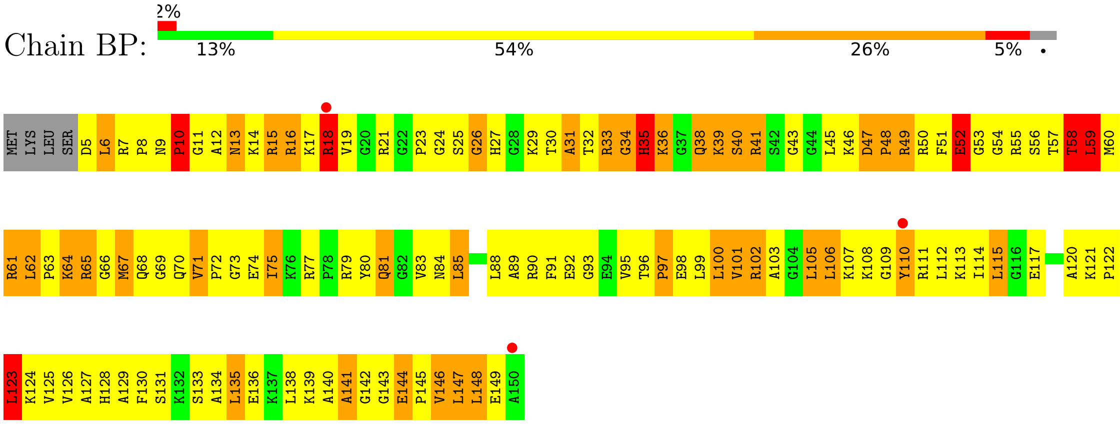
- Molecule 44: 50S RIBOSOMAL PROTEIN L14

Chain DO:



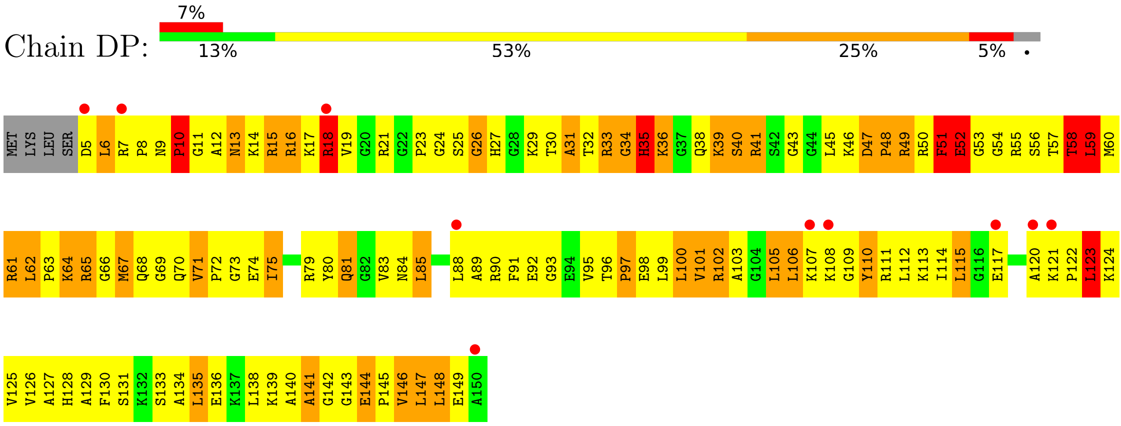
- Molecule 45: 50S RIBOSOMAL PROTEIN L15

Chain BP:



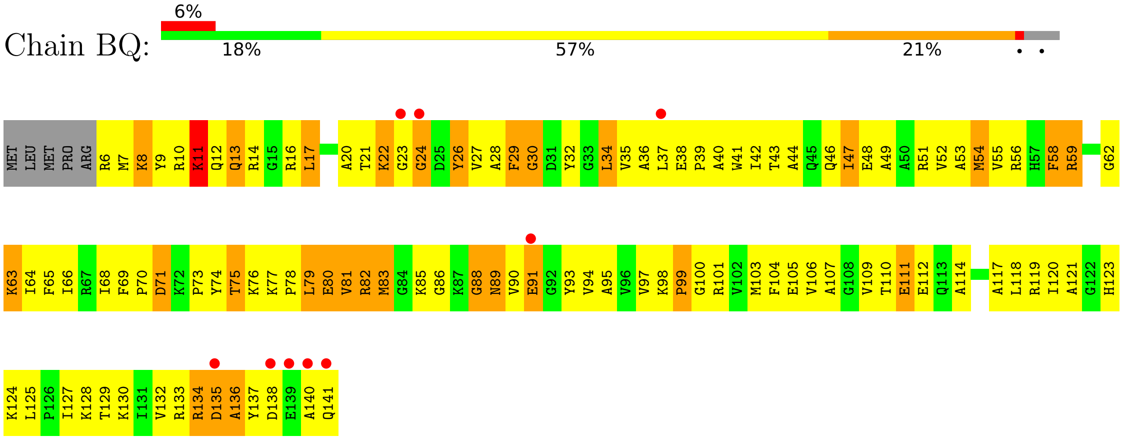
- Molecule 45: 50S RIBOSOMAL PROTEIN L15

Chain DP:



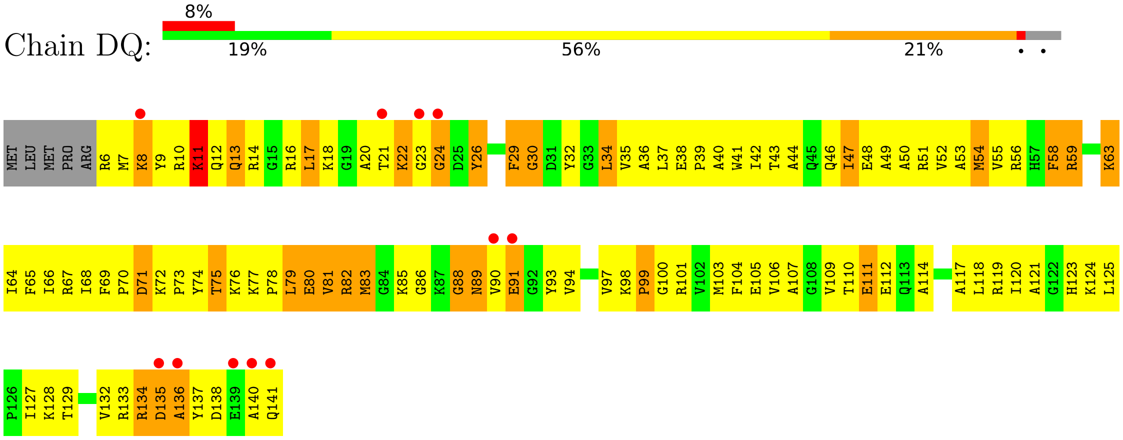
- Molecule 46: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



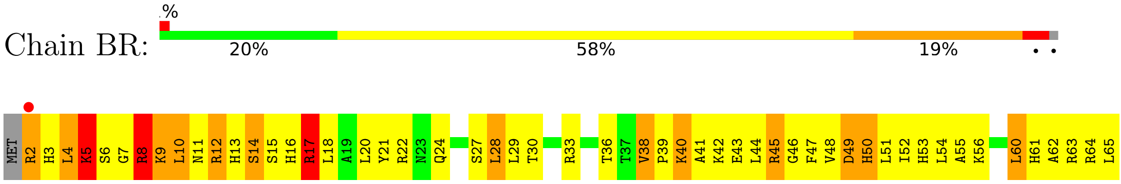
- Molecule 46: 50S RIBOSOMAL PROTEIN L16

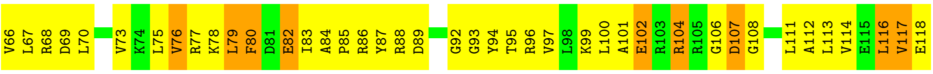
Chain DQ:



- Molecule 47: 50S RIBOSOMAL PROTEIN L17

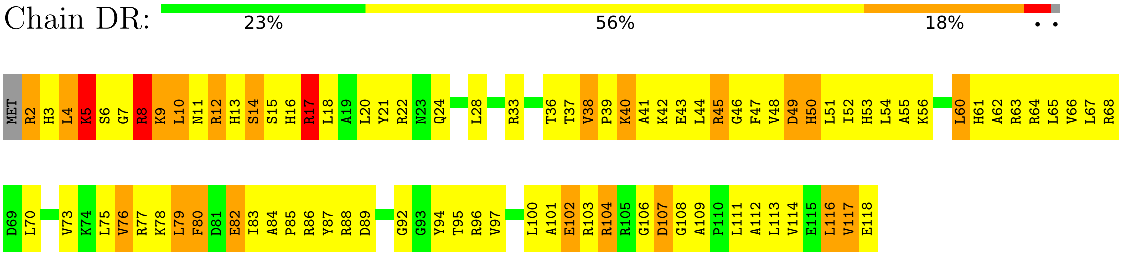
Chain BR:





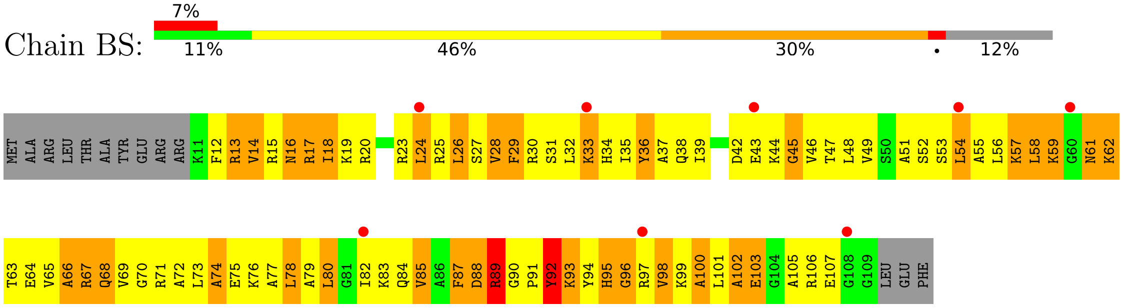
- Molecule 47: 50S RIBOSOMAL PROTEIN L17

Chain DR:



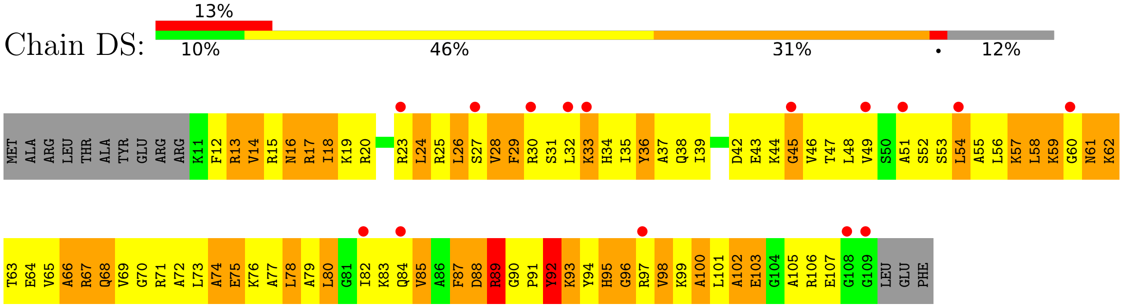
- Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain BS:



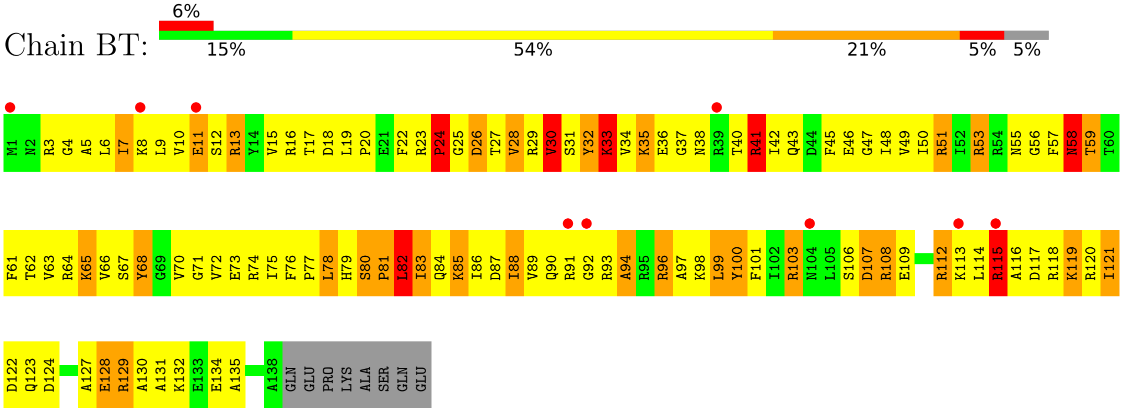
- Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain DS:



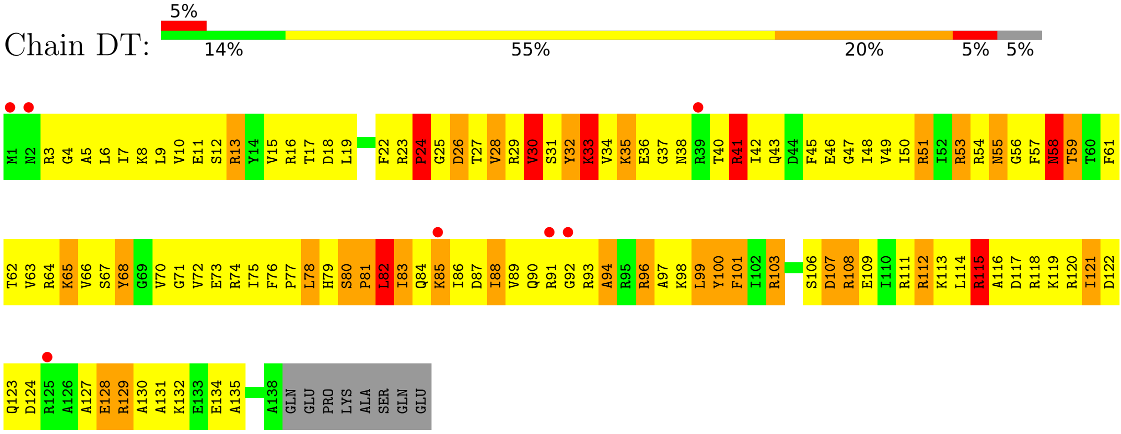
- Molecule 49: 50S RIBOSOMAL PROTEIN L19

Chain BT:



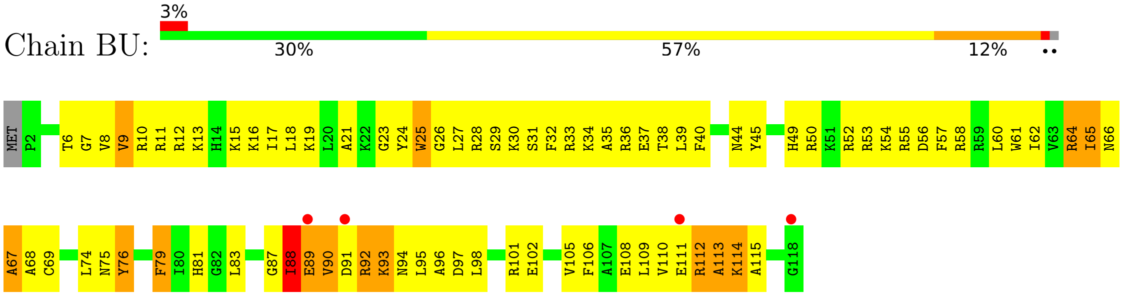
- Molecule 49: 50S RIBOSOMAL PROTEIN L19

Chain DT:



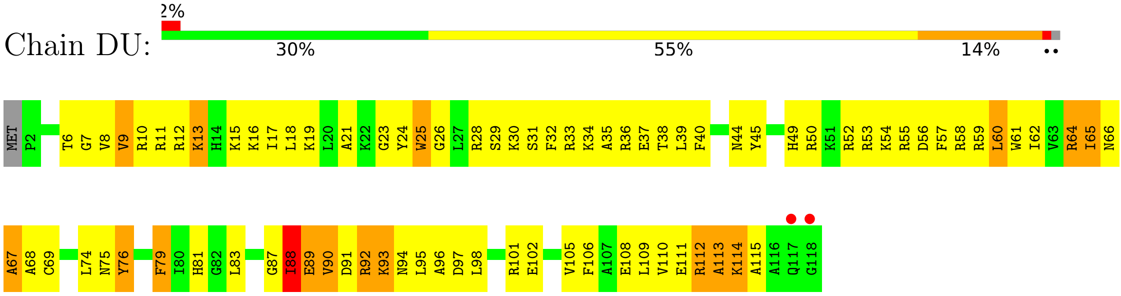
- Molecule 50: 50S RIBOSOMAL PROTEIN L20

Chain BU:



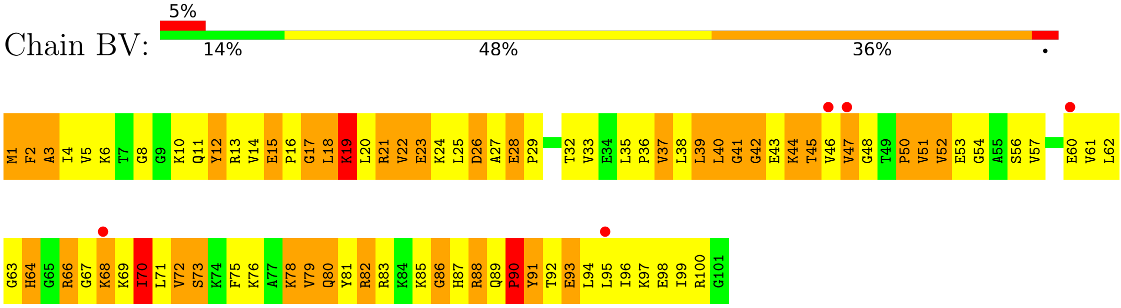
- Molecule 50: 50S RIBOSOMAL PROTEIN L20

Chain DU:



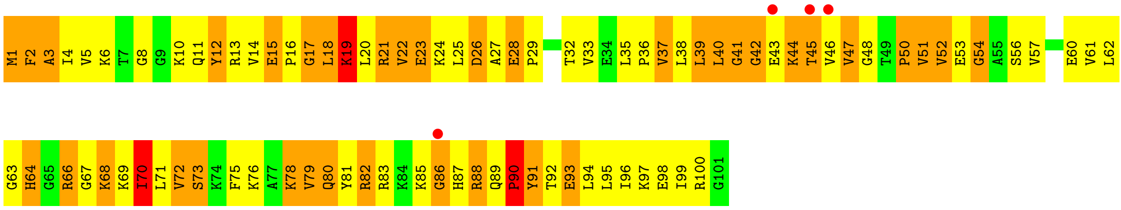
- Molecule 51: 50S RIBOSOMAL PROTEIN L21

Chain BV:



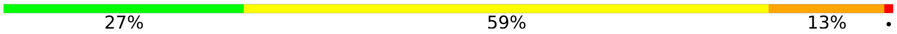
- Molecule 51: 50S RIBOSOMAL PROTEIN L21

Chain DV:



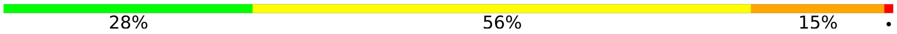
- Molecule 52: 50S RIBOSOMAL PROTEIN L22

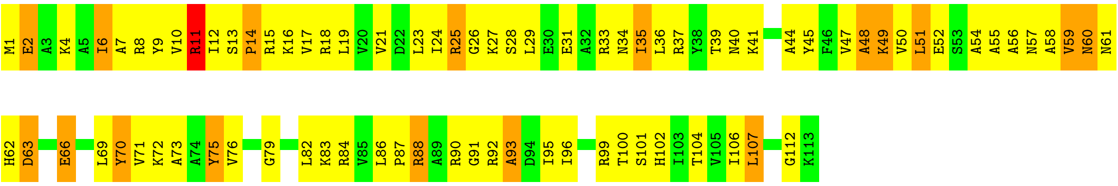
Chain BW:



- Molecule 52: 50S RIBOSOMAL PROTEIN L22

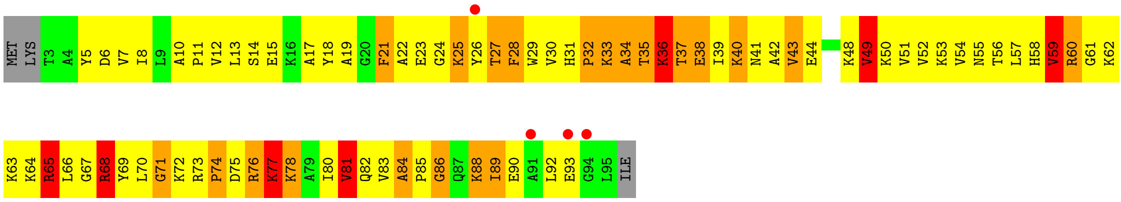
Chain DW:





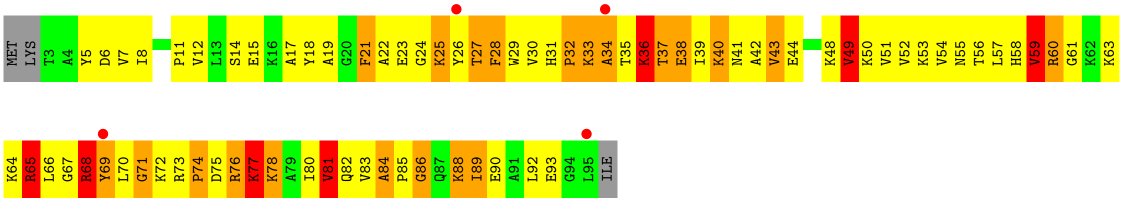
- Molecule 53: 50S RIBOSOMAL PROTEIN L23

Chain BX:

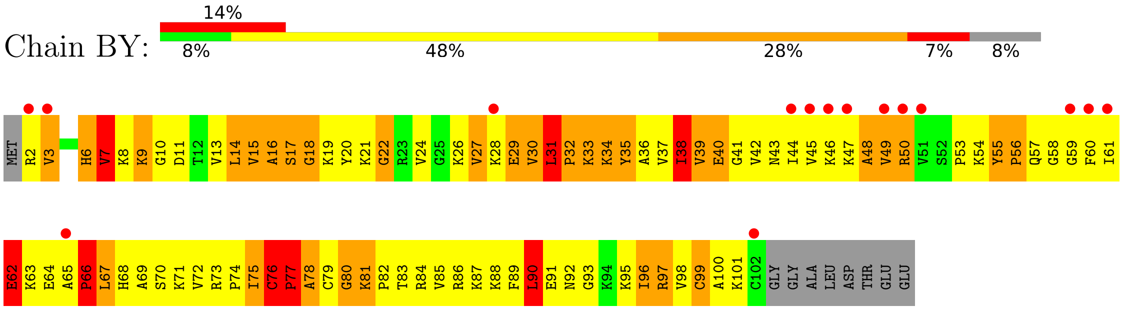


- Molecule 53: 50S RIBOSOMAL PROTEIN L23

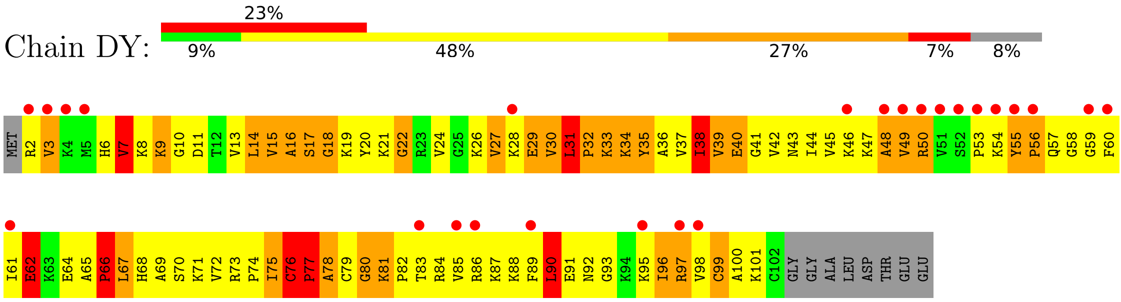
Chain DX:



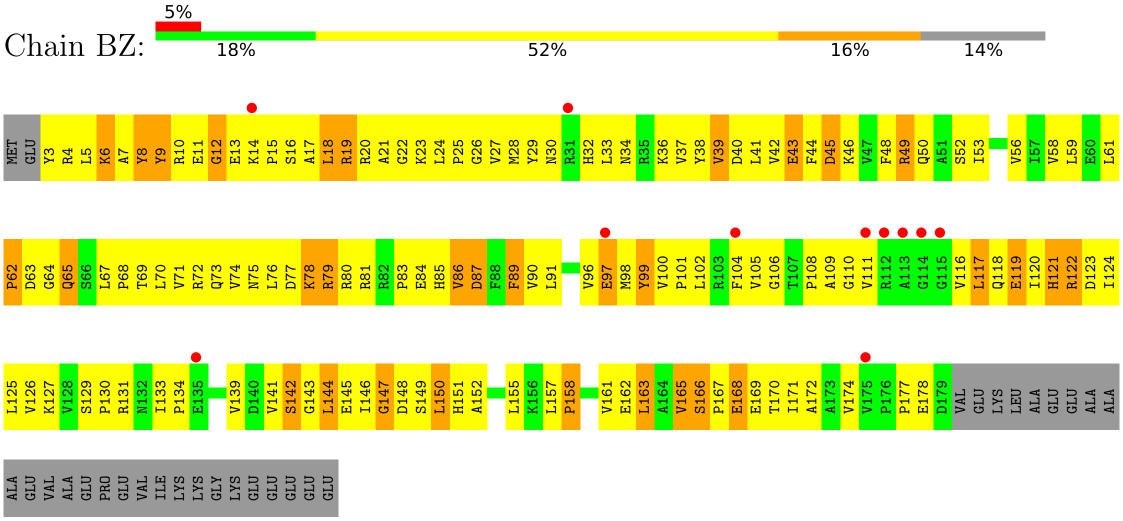
- Molecule 54: 50S RIBOSOMAL PROTEIN L24



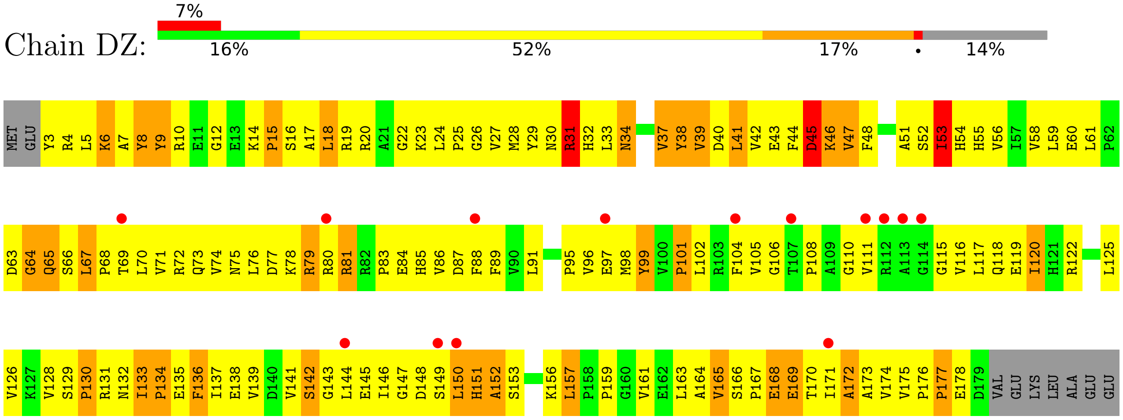
- Molecule 54: 50S RIBOSOMAL PROTEIN L24



- Molecule 55: 50S RIBOSOMAL PROTEIN L25



- Molecule 55: 50S RIBOSOMAL PROTEIN L25

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4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	213.32Å 452.95Å 631.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-2.80) 90.7 (49.96-2.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.272 , 0.313 0.266 , 0.306	Depositor DCC
R_{free} test set	64102 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 81.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	291075	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PAR, 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	0.50	0/36190	0.71	20/56486 (0.0%)
1	CA	0.47	0/36190	0.71	24/56486 (0.0%)
2	AB	0.33	0/1936	0.59	0/2611
2	CB	0.33	0/1936	0.59	0/2611
3	AC	0.35	0/1637	0.58	0/2207
3	CC	0.34	0/1637	0.58	0/2207
4	AD	0.42	0/1733	0.67	0/2318
4	CD	0.41	0/1733	0.66	0/2318
5	AE	0.41	0/1163	0.66	0/1566
5	CE	0.39	0/1163	0.65	0/1566
6	AF	0.37	0/856	0.64	0/1154
6	CF	0.38	0/856	0.65	0/1154
7	AG	0.34	0/1276	0.54	0/1709
7	CG	0.33	0/1276	0.54	0/1709
8	AH	0.35	0/1136	0.62	0/1527
8	CH	0.34	0/1136	0.62	0/1527
9	AI	0.32	0/1027	0.55	0/1372
9	CI	0.32	0/1027	0.55	0/1372
10	AJ	0.36	0/808	0.62	0/1087
10	CJ	0.34	0/808	0.62	0/1087
11	AK	0.38	0/900	0.64	0/1213
11	CK	0.35	0/900	0.63	0/1213
12	AL	0.42	0/987	0.71	0/1322
12	CL	0.43	0/987	0.73	0/1322
13	AM	0.34	0/994	0.62	0/1322
13	CM	0.32	0/994	0.61	0/1322
14	AN	0.39	0/501	0.66	0/664
14	CN	0.38	0/501	0.64	0/664
15	AO	0.38	0/745	0.63	0/992
15	CO	0.36	0/745	0.61	0/992
16	AP	0.43	0/717	0.69	0/965
16	CP	0.42	0/717	0.68	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
17	AQ	0.41	0/837	0.67	0/1119
17	CQ	0.38	0/837	0.66	0/1119
18	AR	0.39	0/579	0.70	0/768
18	CR	0.38	0/579	0.70	0/768
19	AS	0.37	0/643	0.61	0/867
19	CS	0.36	0/643	0.60	0/867
20	AT	0.33	0/765	0.59	0/1007
20	CT	0.32	0/765	0.59	0/1007
21	AU	0.45	0/213	0.56	0/279
21	CU	0.44	0/213	0.55	0/279
22	AV	0.51	1/1814 (0.1%)	0.72	0/2825
22	CV	0.50	1/1814 (0.1%)	0.72	0/2825
23	AW	0.43	1/1813 (0.1%)	0.77	6/2823 (0.2%)
23	AY	0.36	0/456	0.72	0/710
23	CW	0.45	1/1813 (0.1%)	0.76	2/2823 (0.1%)
23	CY	0.35	0/456	0.68	0/710
24	AX	0.58	0/263	0.84	0/407
24	CX	0.58	0/263	0.81	1/407 (0.2%)
25	B0	0.38	0/658	0.65	0/878
25	D0	0.39	0/658	0.65	0/878
26	B1	0.61	0/700	1.04	1/931 (0.1%)
26	D1	0.52	0/700	0.99	1/931 (0.1%)
27	B2	0.45	0/423	0.99	3/560 (0.5%)
27	D2	0.45	0/423	0.89	2/560 (0.4%)
28	B3	0.37	0/473	0.61	0/636
28	D3	0.39	0/473	0.61	0/636
29	B4	0.47	0/241	0.88	4/334 (1.2%)
29	D4	0.44	0/241	0.88	4/334 (1.2%)
30	B5	0.42	0/473	0.74	0/639
30	D5	0.40	0/473	0.73	0/639
31	B6	0.39	0/387	0.62	0/517
31	D6	0.39	0/387	0.62	0/517
32	B7	0.51	0/427	0.73	0/563
32	D7	0.53	0/427	0.70	0/563
33	B8	0.50	0/516	0.81	0/681
33	D8	0.48	0/516	0.80	0/681
34	BA	0.62	4/66876 (0.0%)	0.77	56/104407 (0.1%)
34	DA	0.62	5/66876 (0.0%)	0.77	53/104407 (0.1%)
35	BB	0.39	0/2853	0.70	0/4451
35	DB	0.38	0/2853	0.70	0/4451
36	BC	0.38	0/1145	0.68	7/1556 (0.4%)
36	DC	0.40	0/1145	0.68	7/1556 (0.4%)
37	BD	0.52	0/2155	0.87	3/2907 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DD	0.51	0/2155	0.86	3/2907 (0.1%)
38	BE	0.43	0/1597	0.76	0/2155
38	DE	0.45	0/1597	0.77	0/2155
39	BF	0.45	0/1659	0.70	0/2246
39	DF	0.44	0/1659	0.69	0/2246
40	BG	0.39	0/1498	0.72	1/2013 (0.0%)
40	DG	0.35	0/1498	0.73	0/2013
41	BH	0.33	0/1246	0.69	0/1684
41	DH	0.35	0/1246	0.69	0/1684
42	BI	0.35	0/1147	0.66	0/1553
42	DI	0.34	0/1147	0.66	0/1553
43	BN	0.40	0/1132	0.78	0/1527
43	DN	0.45	0/1132	0.79	0/1527
44	BO	0.48	0/943	0.74	0/1269
44	DO	0.49	0/943	0.75	0/1269
45	BP	0.42	0/1131	1.00	6/1504 (0.4%)
45	DP	0.41	0/1131	1.00	7/1504 (0.5%)
46	BQ	0.37	0/1100	0.72	1/1470 (0.1%)
46	DQ	0.37	0/1100	0.72	1/1470 (0.1%)
47	BR	0.40	0/974	0.74	1/1302 (0.1%)
47	DR	0.38	0/974	0.74	1/1302 (0.1%)
48	BS	0.40	0/779	0.73	0/1038
48	DS	0.39	0/779	0.73	0/1038
49	BT	0.42	0/1156	0.77	2/1544 (0.1%)
49	DT	0.42	0/1156	0.77	1/1544 (0.1%)
50	BU	0.37	0/975	0.68	0/1297
50	DU	0.40	0/975	0.69	0/1297
51	BV	0.38	0/789	0.73	0/1054
51	DV	0.40	0/789	0.73	0/1054
52	BW	0.43	0/907	0.72	0/1216
52	DW	0.45	0/907	0.72	0/1216
53	BX	0.53	0/740	0.89	3/995 (0.3%)
53	DX	0.50	0/740	0.89	3/995 (0.3%)
54	BY	0.41	0/789	0.78	0/1053
54	DY	0.43	0/789	0.78	0/1053
55	BZ	0.35	0/1436	0.64	0/1951
55	DZ	0.36	0/1436	0.62	0/1951
All	All	0.52	13/314628 (0.0%)	0.74	224/470502 (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	2	37
1	CA	2	29
22	AV	0	2
22	CV	0	2
23	AW	3	1
23	CW	2	0
24	CX	0	1
26	B1	0	1
34	BA	30	81
34	DA	28	79
All	All	67	233

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	1	G	OP3-P	-7.25	1.52	1.61
23	AW	1	G	OP3-P	-7.19	1.52	1.61
22	CV	1	C	OP3-P	-7.12	1.52	1.61
22	AV	1	C	OP3-P	-6.95	1.52	1.61
34	BA	783	A	C5-C6	-6.34	1.35	1.41

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	CW	17	C	N1-C1'-C2'	10.99	128.28	114.00
34	DA	1962	C	N1-C1'-C2'	10.90	128.18	114.00
34	BA	1962	C	N1-C1'-C2'	10.48	127.62	114.00
34	BA	669	G	N9-C1'-C2'	10.36	127.47	114.00
34	DA	669	G	N9-C1'-C2'	10.24	127.32	114.00

5 of 67 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	410	G	C3'
1	AA	412	A	C1'
23	AW	17	C	C1'
23	AW	47	U	C1'
23	AW	70	G	C3'

5 of 233 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	107	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	253	U	Sidechain
1	AA	371	G	Sidechain
1	AA	38	G	Sidechain
1	AA	9	G	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	16314	1350	0
1	CA	32329	0	16316	1333	0
2	AB	1901	0	1951	258	0
2	CB	1901	0	1951	256	0
3	AC	1613	0	1677	209	0
3	CC	1613	0	1677	203	0
4	AD	1703	0	1764	192	0
4	CD	1703	0	1766	191	0
5	AE	1147	0	1207	161	0
5	CE	1147	0	1206	159	0
6	AF	843	0	857	98	0
6	CF	843	0	857	101	0
7	AG	1257	0	1296	125	0
7	CG	1257	0	1296	122	0
8	AH	1116	0	1177	128	0
8	CH	1116	0	1177	130	0
9	AI	1011	0	1041	140	0
9	CI	1011	0	1041	140	0
10	AJ	795	0	840	147	0
10	CJ	795	0	840	144	0
11	AK	885	0	904	104	0
11	CK	885	0	904	96	0
12	AL	971	0	1057	122	0
12	CL	971	0	1057	120	0
13	AM	988	0	1055	156	0
13	CM	988	0	1055	151	0
14	AN	492	0	530	62	0
14	CN	492	0	529	61	0
15	AO	734	0	771	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	76	0
16	AP	701	0	720	83	0
16	CP	701	0	720	75	0
17	AQ	824	0	891	91	0
17	CQ	824	0	891	90	0
18	AR	574	0	644	97	0
18	CR	574	0	644	94	0
19	AS	630	0	652	106	0
19	CS	630	0	652	106	0
20	AT	763	0	861	106	0
20	CT	763	0	861	102	0
21	AU	209	0	221	23	0
21	CU	209	0	221	22	0
22	AV	1645	0	838	61	0
22	CV	1645	0	838	51	0
23	AW	1623	0	821	83	0
23	AY	407	0	208	16	0
23	CW	1623	0	821	81	0
23	CY	407	0	208	13	0
24	AX	235	0	119	6	0
24	CX	235	0	119	5	0
25	B0	650	0	654	72	0
25	D0	650	0	654	78	0
26	B1	693	0	764	182	0
26	D1	693	0	764	197	0
27	B2	421	0	460	124	0
27	D2	421	0	461	125	0
28	B3	468	0	523	53	0
28	D3	468	0	523	52	0
29	B4	242	0	103	22	0
29	D4	242	0	103	23	0
30	B5	459	0	480	75	0
30	D5	459	0	480	70	0
31	B6	381	0	390	59	0
31	D6	381	0	390	56	0
32	B7	419	0	467	35	0
32	D7	419	0	467	35	0
33	B8	508	0	576	110	0
33	D8	508	0	576	114	0
34	BA	59708	0	30096	2501	0
34	DA	59708	0	30096	2505	0
35	BB	2551	0	1294	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DB	2551	0	1294	100	0
36	BC	1142	0	865	109	0
36	DC	1142	0	865	106	0
37	BD	2105	0	2182	357	0
37	DD	2105	0	2182	362	0
38	BE	1564	0	1629	325	0
38	DE	1564	0	1629	323	0
39	BF	1624	0	1677	237	0
39	DF	1624	0	1677	235	0
40	BG	1474	0	1534	237	0
40	DG	1474	0	1534	242	0
41	BH	1223	0	1282	199	0
41	DH	1223	0	1282	211	0
42	BI	1132	0	1218	198	0
42	DI	1132	0	1218	200	0
43	BN	1105	0	1180	209	0
43	DN	1105	0	1180	215	0
44	BO	933	0	996	139	0
44	DO	933	0	996	139	0
45	BP	1114	0	1187	322	0
45	DP	1114	0	1187	322	0
46	BQ	1080	0	1127	224	0
46	DQ	1080	0	1127	214	0
47	BR	960	0	1021	171	0
47	DR	960	0	1021	170	0
48	BS	771	0	832	182	0
48	DS	771	0	831	186	0
49	BT	1142	0	1202	219	0
49	DT	1142	0	1202	231	0
50	BU	958	0	1015	183	0
50	DU	958	0	1014	186	0
51	BV	779	0	851	212	0
51	DV	779	0	851	216	0
52	BW	896	0	953	111	0
52	DW	896	0	953	110	0
53	BX	726	0	778	203	0
53	DX	726	0	778	200	0
54	BY	776	0	870	220	0
54	DY	776	0	870	216	0
55	BZ	1404	0	1432	219	0
55	DZ	1404	0	1432	241	0
56	AA	215	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AE	1	0	0	0	0
56	AV	7	0	0	0	0
56	AW	22	0	0	0	0
56	AX	4	0	0	0	0
56	AY	1	0	0	0	0
56	B1	1	0	0	0	0
56	B2	5	0	0	0	0
56	B3	1	0	0	0	0
56	B5	2	0	0	0	0
56	B7	2	0	0	0	0
56	BA	454	0	0	0	0
56	BB	19	0	0	0	0
56	BE	1	0	0	0	0
56	BF	2	0	0	0	0
56	BN	1	0	0	0	0
56	BO	1	0	0	0	0
56	BV	1	0	0	0	0
56	BX	1	0	0	0	0
56	CA	189	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CM	1	0	0	0	0
56	CU	1	0	0	0	0
56	CV	4	0	0	0	0
56	CW	13	0	0	0	0
56	CX	6	0	0	0	0
56	D5	2	0	0	0	0
56	DA	398	0	0	0	0
56	DB	12	0	0	0	0
56	DD	2	0	0	0	0
56	DE	1	0	0	0	0
56	DF	1	0	0	0	0
56	DH	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DS	1	0	0	0	0
56	DU	1	0	0	0	0
56	DZ	1	0	0	0	0
57	AA	42	0	45	3	0
57	CA	42	0	45	0	0
58	AD	1	0	0	0	0
58	AN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	CD	1	0	0	0	0
58	CN	1	0	0	0	0
All	All	291075	0	196199	21274	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

The worst 5 of 21274 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)
51:DV:70:ILE:HB	51:DV:90:PRO:HB2	1.21	1.18
42:BI:79:ILE:HG12	42:BI:140:LEU:HD11	1.21	1.17
3:CC:20:SER:HB2	3:CC:40:ARG:HH22	1.00	1.17
37:DD:35:LYS:HD3	37:DD:63:ARG:HB3	1.24	1.17
34:DA:2491:U:H5’	34:DA:2570:G:H5”	1.26	1.16

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	147 (63%)	54 (23%)	32 (14%)	0	0
2	CB	233/256 (91%)	149 (64%)	52 (22%)	32 (14%)	0	0
3	AC	205/239 (86%)	130 (63%)	55 (27%)	20 (10%)	0	1
3	CC	205/239 (86%)	130 (63%)	57 (28%)	18 (9%)	1	1
4	AD	206/209 (99%)	130 (63%)	51 (25%)	25 (12%)	0	1
4	CD	206/209 (99%)	128 (62%)	54 (26%)	24 (12%)	0	1
5	AE	149/162 (92%)	108 (72%)	28 (19%)	13 (9%)	1	1
5	CE	149/162 (92%)	107 (72%)	30 (20%)	12 (8%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	99/101 (98%)	72 (73%)	21 (21%)	6 (6%)	1	4
6	CF	99/101 (98%)	72 (73%)	22 (22%)	5 (5%)	2	6
7	AG	153/156 (98%)	100 (65%)	41 (27%)	12 (8%)	1	2
7	CG	153/156 (98%)	100 (65%)	42 (28%)	11 (7%)	1	2
8	AH	136/138 (99%)	103 (76%)	28 (21%)	5 (4%)	3	11
8	CH	136/138 (99%)	102 (75%)	29 (21%)	5 (4%)	3	11
9	AI	121/128 (94%)	80 (66%)	30 (25%)	11 (9%)	1	1
9	CI	121/128 (94%)	81 (67%)	28 (23%)	12 (10%)	0	1
10	AJ	97/105 (92%)	70 (72%)	18 (19%)	9 (9%)	0	1
10	CJ	97/105 (92%)	70 (72%)	18 (19%)	9 (9%)	0	1
11	AK	117/129 (91%)	87 (74%)	25 (21%)	5 (4%)	2	8
11	CK	117/129 (91%)	88 (75%)	24 (20%)	5 (4%)	2	8
12	AL	123/135 (91%)	83 (68%)	22 (18%)	18 (15%)	0	0
12	CL	123/135 (91%)	84 (68%)	20 (16%)	19 (15%)	0	0
13	AM	113/126 (90%)	68 (60%)	26 (23%)	19 (17%)	0	0
13	CM	113/126 (90%)	69 (61%)	23 (20%)	21 (19%)	0	0
14	AN	58/61 (95%)	35 (60%)	17 (29%)	6 (10%)	0	1
14	CN	58/61 (95%)	35 (60%)	17 (29%)	6 (10%)	0	1
15	AO	86/89 (97%)	48 (56%)	34 (40%)	4 (5%)	2	7
15	CO	86/89 (97%)	50 (58%)	31 (36%)	5 (6%)	1	4
16	AP	82/88 (93%)	53 (65%)	24 (29%)	5 (6%)	1	4
16	CP	82/88 (93%)	53 (65%)	25 (30%)	4 (5%)	2	7
17	AQ	98/105 (93%)	74 (76%)	15 (15%)	9 (9%)	1	1
17	CQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	2
18	AR	68/88 (77%)	38 (56%)	21 (31%)	9 (13%)	0	0
18	CR	68/88 (77%)	38 (56%)	21 (31%)	9 (13%)	0	0
19	AS	77/93 (83%)	52 (68%)	14 (18%)	11 (14%)	0	0
19	CS	77/93 (83%)	51 (66%)	15 (20%)	11 (14%)	0	0
20	AT	97/106 (92%)	54 (56%)	29 (30%)	14 (14%)	0	0
20	CT	97/106 (92%)	56 (58%)	27 (28%)	14 (14%)	0	0
21	AU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	CU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	8
25	B0	83/85 (98%)	62 (75%)	16 (19%)	5 (6%)	1	4
25	D0	83/85 (98%)	63 (76%)	15 (18%)	5 (6%)	1	4
26	B1	87/98 (89%)	43 (49%)	25 (29%)	19 (22%)	0	0
26	D1	87/98 (89%)	42 (48%)	21 (24%)	24 (28%)	0	0
27	B2	49/72 (68%)	16 (33%)	16 (33%)	17 (35%)	0	0
27	D2	49/72 (68%)	15 (31%)	15 (31%)	19 (39%)	0	0
28	B3	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	1	3
28	D3	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	1	3
29	B4	48/71 (68%)	14 (29%)	11 (23%)	23 (48%)	0	0
29	D4	48/71 (68%)	14 (29%)	11 (23%)	23 (48%)	0	0
30	B5	57/60 (95%)	37 (65%)	13 (23%)	7 (12%)	0	1
30	D5	57/60 (95%)	38 (67%)	12 (21%)	7 (12%)	0	1
31	B6	41/54 (76%)	18 (44%)	16 (39%)	7 (17%)	0	0
31	D6	41/54 (76%)	18 (44%)	16 (39%)	7 (17%)	0	0
32	B7	47/49 (96%)	36 (77%)	10 (21%)	1 (2%)	7	23
32	D7	47/49 (96%)	37 (79%)	8 (17%)	2 (4%)	2	8
33	B8	62/65 (95%)	38 (61%)	13 (21%)	11 (18%)	0	0
33	D8	62/65 (95%)	37 (60%)	14 (23%)	11 (18%)	0	0
36	BC	183/229 (80%)	88 (48%)	52 (28%)	43 (24%)	0	0
36	DC	183/229 (80%)	87 (48%)	53 (29%)	43 (24%)	0	0
37	BD	270/276 (98%)	193 (72%)	51 (19%)	26 (10%)	0	1
37	DD	270/276 (98%)	194 (72%)	50 (18%)	26 (10%)	0	1
38	BE	203/206 (98%)	116 (57%)	49 (24%)	38 (19%)	0	0
38	DE	203/206 (98%)	116 (57%)	49 (24%)	38 (19%)	0	0
39	BF	206/210 (98%)	142 (69%)	40 (19%)	24 (12%)	0	1
39	DF	206/210 (98%)	142 (69%)	41 (20%)	23 (11%)	0	1
40	BG	177/182 (97%)	93 (52%)	56 (32%)	28 (16%)	0	0
40	DG	177/182 (97%)	101 (57%)	45 (25%)	31 (18%)	0	0
41	BH	158/180 (88%)	100 (63%)	31 (20%)	27 (17%)	0	0
41	DH	158/180 (88%)	100 (63%)	31 (20%)	27 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BI	144/148 (97%)	98 (68%)	36 (25%)	10 (7%)	1	3
42	DI	144/148 (97%)	97 (67%)	36 (25%)	11 (8%)	1	2
43	BN	137/140 (98%)	75 (55%)	35 (26%)	27 (20%)	0	0
43	DN	137/140 (98%)	77 (56%)	33 (24%)	27 (20%)	0	0
44	BO	120/122 (98%)	92 (77%)	17 (14%)	11 (9%)	1	1
44	DO	120/122 (98%)	90 (75%)	18 (15%)	12 (10%)	0	1
45	BP	144/150 (96%)	72 (50%)	37 (26%)	35 (24%)	0	0
45	DP	144/150 (96%)	72 (50%)	38 (26%)	34 (24%)	0	0
46	BQ	134/141 (95%)	81 (60%)	34 (25%)	19 (14%)	0	0
46	DQ	134/141 (95%)	79 (59%)	35 (26%)	20 (15%)	0	0
47	BR	115/118 (98%)	74 (64%)	20 (17%)	21 (18%)	0	0
47	DR	115/118 (98%)	72 (63%)	23 (20%)	20 (17%)	0	0
48	BS	97/112 (87%)	49 (50%)	19 (20%)	29 (30%)	0	0
48	DS	97/112 (87%)	49 (50%)	18 (19%)	30 (31%)	0	0
49	BT	136/146 (93%)	77 (57%)	34 (25%)	25 (18%)	0	0
49	DT	136/146 (93%)	79 (58%)	33 (24%)	24 (18%)	0	0
50	BU	115/118 (98%)	61 (53%)	42 (36%)	12 (10%)	0	1
50	DU	115/118 (98%)	61 (53%)	40 (35%)	14 (12%)	0	1
51	BV	97/101 (96%)	47 (48%)	23 (24%)	27 (28%)	0	0
51	DV	97/101 (96%)	47 (48%)	23 (24%)	27 (28%)	0	0
52	BW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	1
52	DW	111/113 (98%)	77 (69%)	19 (17%)	15 (14%)	0	0
53	BX	91/96 (95%)	45 (50%)	23 (25%)	23 (25%)	0	0
53	DX	91/96 (95%)	45 (50%)	23 (25%)	23 (25%)	0	0
54	BY	99/110 (90%)	41 (41%)	24 (24%)	34 (34%)	0	0
54	DY	99/110 (90%)	41 (41%)	24 (24%)	34 (34%)	0	0
55	BZ	175/206 (85%)	99 (57%)	48 (27%)	28 (16%)	0	0
55	DZ	175/206 (85%)	109 (62%)	33 (19%)	33 (19%)	0	0
All	All	11570/12518 (92%)	7170 (62%)	2726 (24%)	1674 (14%)	0	0

5 of 1674 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	52	GLU
2	AB	77	ALA
2	AB	84	GLU
2	AB	154	LEU

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%)	182 (90%)	20 (10%)	8	23
2	CB	202/220 (92%)	182 (90%)	20 (10%)	8	23
3	AC	160/188 (85%)	151 (94%)	9 (6%)	21	51
3	CC	160/188 (85%)	150 (94%)	10 (6%)	18	46
4	AD	180/181 (99%)	159 (88%)	21 (12%)	5	16
4	CD	180/181 (99%)	161 (89%)	19 (11%)	6	20
5	AE	115/123 (94%)	102 (89%)	13 (11%)	6	18
5	CE	115/123 (94%)	103 (90%)	12 (10%)	7	21
6	AF	90/90 (100%)	84 (93%)	6 (7%)	16	43
6	CF	90/90 (100%)	84 (93%)	6 (7%)	16	43
7	AG	126/127 (99%)	122 (97%)	4 (3%)	39	73
7	CG	126/127 (99%)	122 (97%)	4 (3%)	39	73
8	AH	119/119 (100%)	114 (96%)	5 (4%)	30	63
8	CH	119/119 (100%)	114 (96%)	5 (4%)	30	63
9	AI	98/99 (99%)	88 (90%)	10 (10%)	7	22
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	22
10	AJ	88/92 (96%)	82 (93%)	6 (7%)	16	42
10	CJ	88/92 (96%)	82 (93%)	6 (7%)	16	42
11	AK	90/99 (91%)	85 (94%)	5 (6%)	21	51
11	CK	90/99 (91%)	86 (96%)	4 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/111 (94%)	95 (91%)	9 (9%)	10	30
12	CL	104/111 (94%)	96 (92%)	8 (8%)	13	35
13	AM	99/101 (98%)	93 (94%)	6 (6%)	18	48
13	CM	99/101 (98%)	93 (94%)	6 (6%)	18	48
14	AN	49/50 (98%)	47 (96%)	2 (4%)	30	64
14	CN	49/50 (98%)	47 (96%)	2 (4%)	30	64
15	AO	79/80 (99%)	74 (94%)	5 (6%)	18	46
15	CO	79/80 (99%)	74 (94%)	5 (6%)	18	46
16	AP	72/74 (97%)	65 (90%)	7 (10%)	8	24
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	24
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	53	84
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	53	84
18	AR	61/77 (79%)	55 (90%)	6 (10%)	8	24
18	CR	61/77 (79%)	55 (90%)	6 (10%)	8	24
19	AS	69/80 (86%)	62 (90%)	7 (10%)	7	22
19	CS	69/80 (86%)	62 (90%)	7 (10%)	7	22
20	AT	76/82 (93%)	65 (86%)	11 (14%)	3	9
20	CT	76/82 (93%)	65 (86%)	11 (14%)	3	9
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	20
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	20
25	B0	61/67 (91%)	54 (88%)	7 (12%)	5	17
25	D0	61/67 (91%)	54 (88%)	7 (12%)	5	17
26	B1	73/83 (88%)	62 (85%)	11 (15%)	3	9
26	D1	73/83 (88%)	63 (86%)	10 (14%)	3	11
27	B2	46/67 (69%)	35 (76%)	11 (24%)	0	2
27	D2	46/67 (69%)	35 (76%)	11 (24%)	0	2
28	B3	51/52 (98%)	49 (96%)	2 (4%)	32	66
28	D3	51/52 (98%)	49 (96%)	2 (4%)	32	66
30	B5	51/52 (98%)	41 (80%)	10 (20%)	1	4
30	D5	51/52 (98%)	41 (80%)	10 (20%)	1	4
31	B6	43/52 (83%)	36 (84%)	7 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D6	43/52 (83%)	36 (84%)	7 (16%)	2	7
32	B7	41/42 (98%)	37 (90%)	4 (10%)	8	24
32	D7	41/42 (98%)	37 (90%)	4 (10%)	8	24
33	B8	53/55 (96%)	45 (85%)	8 (15%)	3	9
33	D8	53/55 (96%)	45 (85%)	8 (15%)	3	9
36	BC	61/181 (34%)	54 (88%)	7 (12%)	5	17
36	DC	61/181 (34%)	54 (88%)	7 (12%)	5	17
37	BD	213/218 (98%)	179 (84%)	34 (16%)	2	7
37	DD	213/218 (98%)	181 (85%)	32 (15%)	3	9
38	BE	165/166 (99%)	145 (88%)	20 (12%)	5	15
38	DE	165/166 (99%)	145 (88%)	20 (12%)	5	15
39	BF	165/166 (99%)	153 (93%)	12 (7%)	14	38
39	DF	165/166 (99%)	153 (93%)	12 (7%)	14	38
40	BG	155/156 (99%)	135 (87%)	20 (13%)	4	13
40	DG	155/156 (99%)	132 (85%)	23 (15%)	3	9
41	BH	132/148 (89%)	117 (89%)	15 (11%)	5	18
41	DH	132/148 (89%)	117 (89%)	15 (11%)	5	18
42	BI	122/124 (98%)	113 (93%)	9 (7%)	13	37
42	DI	122/124 (98%)	113 (93%)	9 (7%)	13	37
43	BN	117/119 (98%)	98 (84%)	19 (16%)	2	7
43	DN	117/119 (98%)	97 (83%)	20 (17%)	2	6
44	BO	100/100 (100%)	92 (92%)	8 (8%)	12	34
44	DO	100/100 (100%)	91 (91%)	9 (9%)	9	28
45	BP	112/116 (97%)	92 (82%)	20 (18%)	2	5
45	DP	112/116 (97%)	91 (81%)	21 (19%)	1	5
46	BQ	106/111 (96%)	93 (88%)	13 (12%)	4	15
46	DQ	106/111 (96%)	93 (88%)	13 (12%)	4	15
47	BR	100/101 (99%)	91 (91%)	9 (9%)	9	28
47	DR	100/101 (99%)	91 (91%)	9 (9%)	9	28
48	BS	77/88 (88%)	65 (84%)	12 (16%)	2	8
48	DS	77/88 (88%)	65 (84%)	12 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BT	120/127 (94%)	99 (82%)	21 (18%)	2	6
49	DT	120/127 (94%)	99 (82%)	21 (18%)	2	6
50	BU	92/94 (98%)	85 (92%)	7 (8%)	13	36
50	DU	92/94 (98%)	85 (92%)	7 (8%)	13	36
51	BV	82/82 (100%)	64 (78%)	18 (22%)	1	2
51	DV	82/82 (100%)	64 (78%)	18 (22%)	1	2
52	BW	91/92 (99%)	85 (93%)	6 (7%)	16	44
52	DW	91/92 (99%)	84 (92%)	7 (8%)	13	35
53	BX	74/78 (95%)	59 (80%)	15 (20%)	1	4
53	DX	74/78 (95%)	60 (81%)	14 (19%)	1	5
54	BY	84/91 (92%)	67 (80%)	17 (20%)	1	4
54	DY	84/91 (92%)	67 (80%)	17 (20%)	1	4
55	BZ	155/179 (87%)	144 (93%)	11 (7%)	14	39
55	DZ	155/179 (87%)	141 (91%)	14 (9%)	9	28
All	All	9464/10238 (92%)	8444 (89%)	1020 (11%)	6	19

5 of 1020 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BW	75	TYR
45	DP	144	GLU
6	CF	82	ARG
45	DP	61	ARG
50	DU	88	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 275 such sidechains are listed below:

Mol	Chain	Res	Type
42	DI	133	HIS
45	DP	13	ASN
50	DU	75	ASN
45	BP	9	ASN
43	BN	128	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	200 (13%)	36 (2%)
1	CA	1503/1522 (98%)	204 (13%)	36 (2%)
22	AV	76/77 (98%)	18 (23%)	0
22	CV	76/77 (98%)	20 (26%)	0
23	AW	75/76 (98%)	15 (20%)	3 (4%)
23	AY	18/76 (23%)	2 (11%)	0
23	CW	75/76 (98%)	16 (21%)	3 (4%)
23	CY	18/76 (23%)	3 (16%)	0
24	AX	10/24 (41%)	2 (20%)	0
24	CX	10/24 (41%)	2 (20%)	0
34	BA	2771/2787 (99%)	563 (20%)	76 (2%)
34	DA	2771/2787 (99%)	560 (20%)	76 (2%)
35	BB	118/122 (96%)	14 (11%)	1 (0%)
35	DB	118/122 (96%)	14 (11%)	1 (0%)
All	All	9142/9368 (97%)	1633 (17%)	232 (2%)

5 of 1633 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 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BB	66	A
34	DA	2481	G
1	CA	1065	U
34	DA	2282	G
34	DA	1694	C

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	$\#\|Z\| > 2$
22	5MU	CV	54	22	19,22,23	0.24	0	28,32,35	0.37	0
22	5MU	AV	54	22	19,22,23	0.23	0	28,32,35	0.38	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
22	5MU	CV	54	22	-	0/7/25/26	0/2/2/2
22	5MU	AV	54	22	-	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
22	CV	54	5MU	2	0
22	AV	54	5MU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1385 ligands modelled in this entry, 1383 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	PAR	CA	1790	-	45,45,45	1.56	10 (22%)	64,67,67	1.30	7 (10%)
57	PAR	AA	1816	-	45,45,45	1.59	8 (17%)	64,67,67	1.20	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	CA	1790	-	-	4/18/94/94	0/4/4/4
57	PAR	AA	1816	-	-	5/18/94/94	0/4/4/4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	1816	PAR	C64-C54	5.15	1.59	1.52
57	CA	1790	PAR	C64-C54	4.38	1.58	1.52
57	CA	1790	PAR	C34-C24	4.37	1.59	1.53
57	AA	1816	PAR	C52-C42	3.08	1.58	1.52
57	AA	1816	PAR	O54-C14	2.82	1.49	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	AA	1816	PAR	O33-C14-C24	4.79	116.47	108.22
57	CA	1790	PAR	O33-C14-C24	4.44	115.86	108.22
57	CA	1790	PAR	O54-C54-C64	3.85	113.18	106.01
57	CA	1790	PAR	C14-O54-C54	3.51	120.57	113.69
57	AA	1816	PAR	O52-C13-C23	3.34	114.89	107.96

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	CA	1790	PAR	O43-C43-C53-O53
57	CA	1790	PAR	C33-C43-C53-O53
57	AA	1816	PAR	O43-C13-O52-C52
57	AA	1816	PAR	C23-C13-O52-C52

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Mol	Chain	Res	Type	Atoms
57	AA	1816	PAR	O54-C54-C64-N64

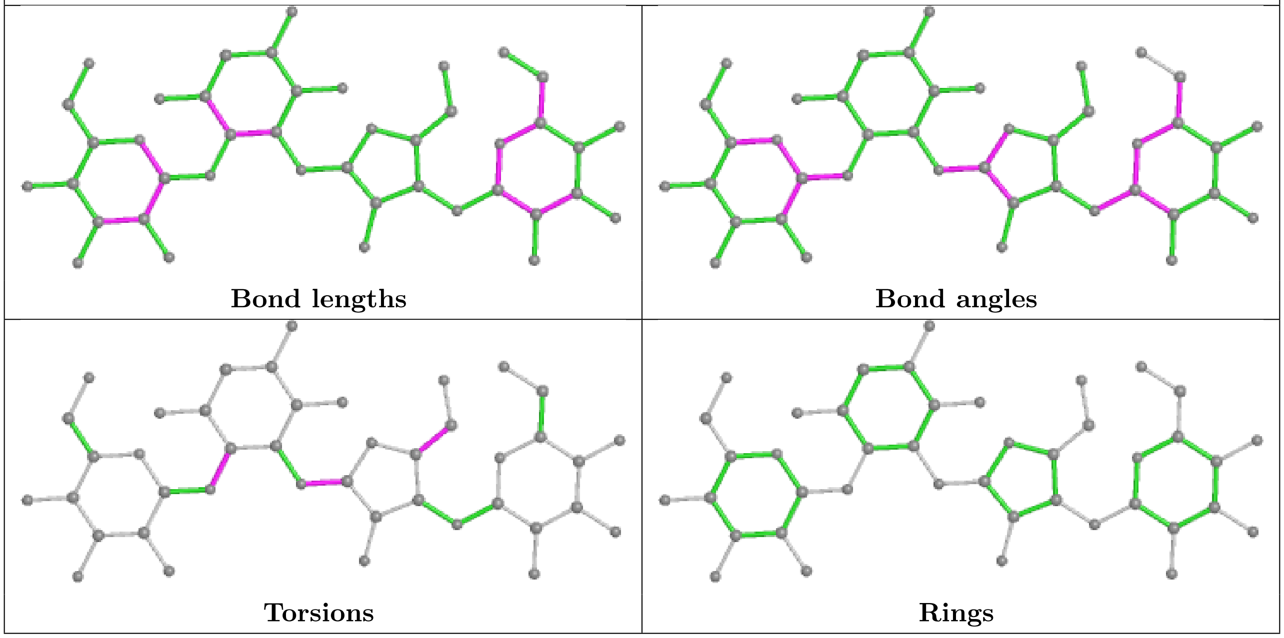
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1816	PAR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAR CA 1790



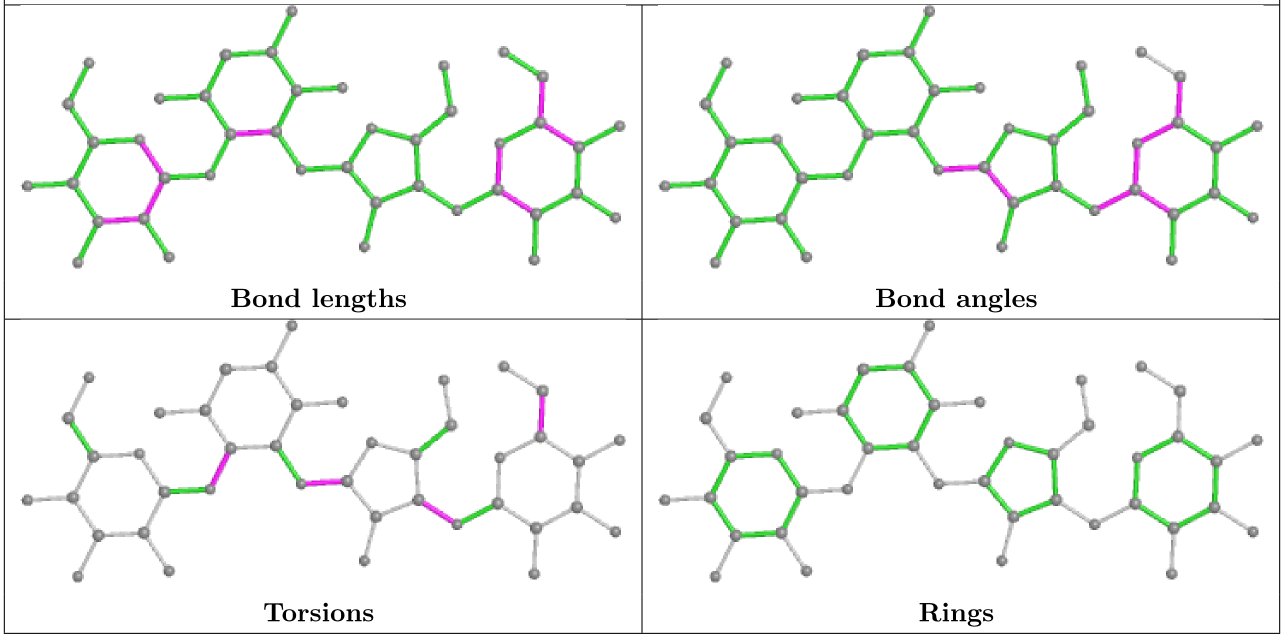
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR AA 1816



Bond lengths

Bond angles

Torsions

Rings

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	AM	5
13	CM	5
9	CI	2
9	AI	2
31	B6	1
31	D6	1
40	BG	1
40	DG	1
51	BV	1
51	DV	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	4.89
1	D6	46:HIS	C	47:THR	N	4.87
1	AM	69:GLU	C	70:LEU	N	4.66

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	4.66
1	CI	53:VAL	C	54:ASP	N	4.02

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1504/1522 (98%)	-0.41	23 (1%) 73 68	2, 42, 165, 200	0
1	CA	1504/1522 (98%)	-0.33	32 (2%) 63 54	3, 50, 172, 200	0
2	AB	235/256 (91%)	0.26	28 (11%) 4 2	17, 94, 183, 200	0
2	CB	235/256 (91%)	0.38	28 (11%) 4 2	17, 104, 187, 200	0
3	AC	207/239 (86%)	-0.15	6 (2%) 51 41	17, 70, 156, 200	0
3	CC	207/239 (86%)	0.14	12 (5%) 23 15	19, 84, 149, 190	0
4	AD	208/209 (99%)	-0.32	1 (0%) 91 88	1, 43, 127, 198	0
4	CD	208/209 (99%)	-0.25	4 (1%) 66 59	4, 51, 133, 182	0
5	AE	151/162 (93%)	-0.32	1 (0%) 87 84	4, 51, 128, 177	0
5	CE	151/162 (93%)	-0.09	2 (1%) 77 72	3, 56, 140, 185	0
6	AF	101/101 (100%)	-0.36	3 (2%) 50 40	5, 48, 131, 156	0
6	CF	101/101 (100%)	-0.37	2 (1%) 65 56	2, 54, 130, 151	0
7	AG	155/156 (99%)	0.07	12 (7%) 13 7	8, 68, 151, 184	0
7	CG	155/156 (99%)	0.61	23 (14%) 2 1	15, 87, 155, 190	0
8	AH	138/138 (100%)	-0.24	3 (2%) 62 52	3, 52, 120, 173	0
8	CH	138/138 (100%)	-0.14	4 (2%) 51 41	16, 58, 138, 152	0
9	AI	127/128 (99%)	0.66	15 (11%) 4 2	26, 97, 171, 200	0
9	CI	127/128 (99%)	0.66	21 (16%) 1 1	28, 111, 175, 200	0
10	AJ	99/105 (94%)	0.75	17 (17%) 1 1	17, 105, 178, 200	0
10	CJ	99/105 (94%)	1.11	22 (22%) 0 0	34, 123, 176, 197	0
11	AK	119/129 (92%)	-0.29	3 (2%) 57 47	8, 46, 151, 192	0
11	CK	119/129 (92%)	0.06	6 (5%) 28 19	16, 61, 147, 200	0
12	AL	125/135 (92%)	-0.12	4 (3%) 47 37	5, 38, 133, 200	0
12	CL	125/135 (92%)	-0.08	4 (3%) 47 37	1, 38, 132, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AM	125/126 (99%)	0.37	15 (12%)	4	2	13, 74, 159, 196	0
13	CM	125/126 (99%)	0.43	15 (12%)	4	2	19, 91, 160, 191	0
14	AN	60/61 (98%)	0.47	6 (10%)	7	4	14, 66, 161, 184	0
14	CN	60/61 (98%)	0.20	4 (6%)	17	10	19, 73, 143, 182	0
15	AO	88/89 (98%)	-0.54	0	100	100	2, 42, 129, 141	0
15	CO	88/89 (98%)	-0.36	1 (1%)	80	75	2, 56, 124, 167	0
16	AP	84/88 (95%)	-0.21	1 (1%)	79	73	6, 36, 104, 190	0
16	CP	84/88 (95%)	-0.06	1 (1%)	79	73	6, 49, 121, 199	0
17	AQ	100/105 (95%)	-0.33	2 (2%)	65	56	1, 45, 110, 193	0
17	CQ	100/105 (95%)	0.17	2 (2%)	65	56	18, 60, 105, 194	0
18	AR	70/88 (79%)	-0.13	1 (1%)	75	70	10, 50, 140, 172	0
18	CR	70/88 (79%)	0.19	3 (4%)	35	25	7, 56, 144, 179	0
19	AS	79/93 (84%)	0.26	8 (10%)	7	4	22, 79, 186, 200	0
19	CS	79/93 (84%)	0.68	11 (13%)	2	1	25, 83, 175, 197	0
20	AT	99/106 (93%)	0.30	9 (9%)	9	5	5, 60, 152, 180	0
20	CT	99/106 (93%)	0.21	6 (6%)	21	13	17, 77, 141, 183	0
21	AU	25/27 (92%)	1.42	8 (32%)	0	0	27, 72, 128, 141	0
21	CU	25/27 (92%)	2.31	11 (44%)	0	0	40, 74, 127, 139	0
22	AV	76/77 (98%)	-0.64	0	100	100	14, 53, 143, 194	0
22	CV	76/77 (98%)	-0.53	0	100	100	21, 55, 146, 198	0
23	AW	76/76 (100%)	-0.23	5 (6%)	18	11	30, 103, 164, 199	0
23	AY	19/76 (25%)	-0.27	0	100	100	23, 72, 190, 196	0
23	CW	76/76 (100%)	-0.03	5 (6%)	18	11	35, 116, 165, 196	0
23	CY	19/76 (25%)	-0.28	0	100	100	26, 76, 186, 196	0
24	AX	11/24 (45%)	-0.11	1 (9%)	9	5	12, 33, 170, 190	0
24	CX	11/24 (45%)	0.28	2 (18%)	1	1	14, 39, 167, 197	0
25	B0	85/85 (100%)	0.44	7 (8%)	11	6	8, 43, 138, 196	0
25	D0	85/85 (100%)	0.54	9 (10%)	6	3	18, 57, 137, 179	0
26	B1	89/98 (90%)	0.05	4 (4%)	33	23	1, 35, 143, 157	0
26	D1	89/98 (90%)	-0.06	2 (2%)	62	52	1, 44, 145, 200	0
27	B2	51/72 (70%)	0.03	5 (9%)	7	4	5, 66, 145, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
27	D2	51/72 (70%)	0.53	7 (13%)	3	1	13, 79, 154, 200	0
28	B3	60/60 (100%)	0.24	4 (6%)	17	10	5, 57, 140, 190	0
28	D3	60/60 (100%)	0.28	2 (3%)	46	36	5, 58, 146, 198	0
29	B4	50/71 (70%)	-0.49	1 (2%)	65	56	38, 90, 158, 173	0
29	D4	50/71 (70%)	0.07	5 (10%)	7	4	54, 117, 160, 198	0
30	B5	59/60 (98%)	0.59	10 (16%)	1	1	5, 51, 192, 200	0
30	D5	59/60 (98%)	0.38	7 (11%)	4	2	1, 65, 179, 200	0
31	B6	45/54 (83%)	1.92	21 (46%)	0	0	54, 103, 171, 180	0
31	D6	45/54 (83%)	2.77	26 (57%)	0	0	64, 139, 171, 189	0
32	B7	49/49 (100%)	-0.15	3 (6%)	21	13	1, 19, 115, 165	0
32	D7	49/49 (100%)	-0.16	4 (8%)	11	6	1, 19, 88, 174	0
33	B8	64/65 (98%)	0.37	5 (7%)	13	7	4, 44, 140, 195	0
33	D8	64/65 (98%)	0.28	4 (6%)	20	12	5, 52, 155, 192	0
34	BA	2772/2787 (99%)	-0.52	33 (1%)	79	73	1, 29, 145, 200	0
34	DA	2772/2787 (99%)	-0.49	25 (0%)	84	80	1, 30, 152, 200	0
35	BB	119/122 (97%)	-0.54	0	100	100	22, 64, 108, 197	0
35	DB	119/122 (97%)	-0.38	0	100	100	34, 76, 127, 188	0
36	BC	191/229 (83%)	1.99	73 (38%)	0	0	51, 144, 186, 200	0
36	DC	191/229 (83%)	2.54	97 (50%)	0	0	61, 146, 186, 200	0
37	BD	272/276 (98%)	-0.52	2 (0%)	87	84	1, 19, 89, 196	0
37	DD	272/276 (98%)	-0.49	2 (0%)	87	84	1, 21, 89, 200	0
38	BE	205/206 (99%)	0.04	7 (3%)	45	35	1, 46, 141, 193	0
38	DE	205/206 (99%)	-0.15	7 (3%)	45	35	1, 43, 144, 199	0
39	BF	208/210 (99%)	-0.26	9 (4%)	35	25	1, 44, 155, 200	0
39	DF	208/210 (99%)	0.07	13 (6%)	20	12	1, 44, 160, 200	0
40	BG	181/182 (99%)	-0.09	8 (4%)	34	24	8, 65, 142, 188	0
40	DG	181/182 (99%)	0.15	13 (7%)	15	8	10, 82, 149, 195	0
41	BH	160/180 (88%)	1.07	35 (21%)	0	0	51, 124, 174, 200	0
41	DH	160/180 (88%)	0.80	28 (17%)	1	1	10, 102, 174, 194	0
42	BI	146/148 (98%)	0.25	13 (8%)	9	5	5, 78, 148, 187	0
42	DI	146/148 (98%)	2.60	56 (38%)	0	0	9, 124, 184, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB($Å^2$)	Q<0.9
43	BN	139/140 (99%)	-0.04	5 (3%) 42 32	10, 68, 144, 163	0
43	DN	139/140 (99%)	0.11	9 (6%) 18 11	15, 63, 141, 165	0
44	BO	122/122 (100%)	-0.44	0 100 100	3, 32, 103, 177	0
44	DO	122/122 (100%)	-0.49	0 100 100	1, 33, 102, 126	0
45	BP	146/150 (97%)	0.12	3 (2%) 63 54	1, 61, 159, 193	0
45	DP	146/150 (97%)	0.25	10 (6%) 17 10	2, 71, 165, 198	0
46	BQ	136/141 (96%)	0.46	9 (6%) 18 11	7, 58, 171, 200	0
46	DQ	136/141 (96%)	0.16	11 (8%) 12 6	7, 54, 164, 200	0
47	BR	117/118 (99%)	-0.20	1 (0%) 84 80	3, 32, 132, 146	0
47	DR	117/118 (99%)	-0.11	0 100 100	3, 42, 126, 166	0
48	BS	99/112 (88%)	0.33	8 (8%) 12 6	21, 76, 134, 173	0
48	DS	99/112 (88%)	0.81	15 (15%) 2 1	24, 89, 143, 170	0
49	BT	138/146 (94%)	0.02	9 (6%) 18 11	3, 67, 169, 190	0
49	DT	138/146 (94%)	-0.00	7 (5%) 28 19	7, 65, 171, 200	0
50	BU	117/118 (99%)	-0.04	4 (3%) 45 35	5, 50, 142, 200	0
50	DU	117/118 (99%)	-0.14	2 (1%) 70 63	1, 46, 145, 190	0
51	BV	101/101 (100%)	0.25	5 (4%) 28 19	14, 96, 174, 192	0
51	DV	101/101 (100%)	0.16	4 (3%) 38 28	11, 93, 172, 193	0
52	BW	113/113 (100%)	-0.46	0 100 100	1, 26, 121, 161	0
52	DW	113/113 (100%)	-0.37	0 100 100	3, 28, 126, 200	0
53	BX	93/96 (96%)	-0.22	4 (4%) 35 25	1, 46, 137, 168	0
53	DX	93/96 (96%)	-0.02	4 (4%) 35 25	8, 54, 138, 157	0
54	BY	101/110 (91%)	0.95	15 (14%) 2 1	1, 79, 170, 195	0
54	DY	101/110 (91%)	1.38	25 (24%) 0 0	1, 79, 177, 196	0
55	BZ	177/206 (85%)	0.20	11 (6%) 20 13	19, 96, 177, 200	0
55	DZ	177/206 (85%)	0.26	14 (7%) 12 7	18, 98, 178, 198	0
All	All	20972/21886 (95%)	-0.08	1115 (5%) 26 17	1, 51, 163, 200	0

The worst 5 of 1115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DI	84	GLY	32.2
46	BQ	140	ALA	23.1

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Mol	Chain	Res	Type	RSRZ
42	DI	120	ILE	21.9
42	DI	88	ILE	21.5
17	CQ	101	ARG	20.9

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, 95^{th} 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
22	5MU	AV	54	21/22	0.92	0.14	75,83,108,108	0
22	5MU	CV	54	21/22	0.93	0.12	64,75,79,79	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	DA	3261	1/1	0.23	0.80	94,94,94,94	0
56	MG	BB	213	1/1	0.27	0.60	71,71,71,71	0
56	MG	DA	3187	1/1	0.41	0.41	86,86,86,86	0
56	MG	CV	103	1/1	0.46	0.18	56,56,56,56	0
56	MG	CA	1637	1/1	0.51	0.46	81,81,81,81	0
56	MG	CW	111	1/1	0.54	0.22	77,77,77,77	0
56	MG	BA	3233	1/1	0.55	0.33	77,77,77,77	0
56	MG	CA	1685	1/1	0.56	0.47	82,82,82,82	0
56	MG	DA	3255	1/1	0.57	0.47	92,92,92,92	0
56	MG	CA	1719	1/1	0.58	1.11	99,99,99,99	0
56	MG	AA	1633	1/1	0.58	0.44	90,90,90,90	0
56	MG	CA	1622	1/1	0.60	0.81	123,123,123,123	0
56	MG	BA	3043	1/1	0.61	0.33	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1725	1/1	0.62	0.26	56,56,56,56	0
56	MG	BA	3403	1/1	0.62	0.48	78,78,78,78	0
56	MG	DA	3168	1/1	0.65	0.38	56,56,56,56	0
56	MG	BA	3004	1/1	0.67	0.41	77,77,77,77	0
56	MG	BA	3408	1/1	0.67	0.17	46,46,46,46	0
56	MG	CA	1646	1/1	0.68	0.42	62,62,62,62	0
56	MG	DA	3208	1/1	0.69	0.21	40,40,40,40	0
56	MG	DA	3213	1/1	0.69	0.35	84,84,84,84	0
56	MG	BB	201	1/1	0.69	0.42	54,54,54,54	1
56	MG	BA	3413	1/1	0.69	0.47	63,63,63,63	0
56	MG	BA	3433	1/1	0.70	0.17	74,74,74,74	0
56	MG	CA	1729	1/1	0.70	0.51	71,71,71,71	0
56	MG	CA	1673	1/1	0.71	0.21	80,80,80,80	1
56	MG	DA	3219	1/1	0.72	0.56	75,75,75,75	0
56	MG	DA	3231	1/1	0.72	0.40	72,72,72,72	0
56	MG	AA	1697	1/1	0.72	0.45	88,88,88,88	0
56	MG	BA	3353	1/1	0.72	0.39	42,42,42,42	1
56	MG	CA	1706	1/1	0.73	0.19	54,54,54,54	0
56	MG	DA	3217	1/1	0.73	0.14	62,62,62,62	0
56	MG	CW	107	1/1	0.73	0.27	63,63,63,63	1
56	MG	DA	3275	1/1	0.73	0.36	75,75,75,75	0
56	MG	CA	1752	1/1	0.74	0.51	83,83,83,83	0
56	MG	DA	3273	1/1	0.74	0.60	59,59,59,59	0
56	MG	BA	3278	1/1	0.74	0.37	90,90,90,90	0
56	MG	DA	3155	1/1	0.75	0.09	50,50,50,50	0
56	MG	BA	3323	1/1	0.75	0.13	79,79,79,79	0
56	MG	DA	3169	1/1	0.75	0.23	27,27,27,27	0
56	MG	DA	3238	1/1	0.75	0.26	54,54,54,54	0
56	MG	DA	3002	1/1	0.76	0.28	38,38,38,38	0
56	MG	AA	1618	1/1	0.76	0.41	66,66,66,66	0
56	MG	CA	1751	1/1	0.76	0.18	81,81,81,81	0
56	MG	DA	3320	1/1	0.76	0.17	70,70,70,70	0
56	MG	AA	1748	1/1	0.77	0.26	59,59,59,59	0
56	MG	CA	1675	1/1	0.77	0.24	57,57,57,57	0
56	MG	BA	3296	1/1	0.78	0.34	75,75,75,75	0
56	MG	DA	3004	1/1	0.78	0.41	90,90,90,90	0
56	MG	DA	3268	1/1	0.78	0.21	51,51,51,51	0
56	MG	CA	1739	1/1	0.79	0.15	66,66,66,66	0
56	MG	AA	1651	1/1	0.79	0.22	35,35,35,35	0
56	MG	CA	1722	1/1	0.79	0.31	70,70,70,70	0
56	MG	DA	3358	1/1	0.79	0.36	54,54,54,54	0
56	MG	DA	3380	1/1	0.79	0.33	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	DH	201	1/1	0.79	0.19	36,36,36,36	0
56	MG	AA	1647	1/1	0.80	0.18	71,71,71,71	0
56	MG	CA	1695	1/1	0.80	0.14	70,70,70,70	0
56	MG	AA	1698	1/1	0.80	0.15	38,38,38,38	0
56	MG	AA	1733	1/1	0.80	0.40	63,63,63,63	0
56	MG	DA	3250	1/1	0.80	0.08	57,57,57,57	0
56	MG	BA	3212	1/1	0.80	0.17	47,47,47,47	0
56	MG	DA	3138	1/1	0.80	0.27	40,40,40,40	0
56	MG	AY	101	1/1	0.81	0.18	56,56,56,56	0
56	MG	BA	3376	1/1	0.81	0.20	47,47,47,47	0
56	MG	AA	1661	1/1	0.81	0.30	60,60,60,60	0
56	MG	BA	3285	1/1	0.81	0.51	74,74,74,74	0
56	MG	DA	3310	1/1	0.81	0.30	50,50,50,50	0
56	MG	CA	1716	1/1	0.81	0.31	67,67,67,67	0
56	MG	DA	3342	1/1	0.81	0.27	49,49,49,49	0
56	MG	AA	1714	1/1	0.81	0.25	28,28,28,28	0
56	MG	AA	1782	1/1	0.81	0.28	68,68,68,68	0
56	MG	CW	109	1/1	0.81	0.11	81,81,81,81	0
56	MG	DA	3258	1/1	0.82	0.49	80,80,80,80	0
56	MG	BA	3227	1/1	0.82	0.27	49,49,49,49	0
56	MG	DA	3262	1/1	0.82	0.33	72,72,72,72	0
56	MG	AW	116	1/1	0.82	0.12	58,58,58,58	0
56	MG	CA	1691	1/1	0.82	0.23	56,56,56,56	0
56	MG	DA	3274	1/1	0.82	0.10	53,53,53,53	0
56	MG	AA	1660	1/1	0.82	0.30	61,61,61,61	0
56	MG	DA	3277	1/1	0.82	0.20	55,55,55,55	0
56	MG	CA	1745	1/1	0.82	0.42	77,77,77,77	0
56	MG	CA	1750	1/1	0.82	0.10	50,50,50,50	0
56	MG	AA	1750	1/1	0.82	0.12	57,57,57,57	0
56	MG	DA	3248	1/1	0.82	0.94	82,82,82,82	0
56	MG	AA	1677	1/1	0.82	0.12	41,41,41,41	0
56	MG	DB	204	1/1	0.82	0.16	48,48,48,48	0
56	MG	AW	110	1/1	0.82	0.26	46,46,46,46	0
56	MG	CA	1696	1/1	0.83	0.25	51,51,51,51	0
56	MG	AA	1694	1/1	0.83	0.35	58,58,58,58	0
56	MG	DA	3036	1/1	0.83	0.19	43,43,43,43	0
56	MG	DA	3067	1/1	0.83	0.13	26,26,26,26	0
56	MG	CA	1647	1/1	0.83	0.39	57,57,57,57	0
56	MG	DA	3312	1/1	0.83	0.20	44,44,44,44	0
56	MG	AW	113	1/1	0.83	0.26	46,46,46,46	1
56	MG	BA	3257	1/1	0.83	0.15	55,55,55,55	0
56	MG	AA	1794	1/1	0.83	0.28	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3279	1/1	0.83	0.21	55,55,55,55	0
56	MG	DA	3391	1/1	0.83	0.21	62,62,62,62	1
56	MG	DA	3394	1/1	0.83	0.32	66,66,66,66	0
56	MG	AX	102	1/1	0.83	0.09	32,32,32,32	0
56	MG	CW	112	1/1	0.83	0.08	53,53,53,53	0
56	MG	DA	3319	1/1	0.84	0.24	52,52,52,52	0
56	MG	AA	1693	1/1	0.84	0.42	43,43,43,43	0
56	MG	BA	3109	1/1	0.84	0.28	34,34,34,34	0
56	MG	BA	3147	1/1	0.84	0.20	20,20,20,20	0
56	MG	BA	3152	1/1	0.84	0.21	45,45,45,45	0
56	MG	DA	3381	1/1	0.84	0.23	77,77,77,77	0
56	MG	AA	1658	1/1	0.84	0.21	37,37,37,37	0
56	MG	DA	3016	1/1	0.84	0.12	52,52,52,52	0
56	MG	BA	3216	1/1	0.84	0.23	50,50,50,50	0
56	MG	CA	1645	1/1	0.84	0.14	74,74,74,74	0
56	MG	BA	3393	1/1	0.85	0.60	60,60,60,60	0
56	MG	BA	3261	1/1	0.85	0.11	24,24,24,24	0
56	MG	CA	1688	1/1	0.85	0.07	46,46,46,46	0
56	MG	D5	102	1/1	0.85	0.11	6,6,6,6	1
56	MG	BA	3275	1/1	0.85	0.17	19,19,19,19	0
56	MG	AW	103	1/1	0.85	0.18	51,51,51,51	0
56	MG	BA	3422	1/1	0.85	0.22	39,39,39,39	0
56	MG	DA	3024	1/1	0.85	0.16	20,20,20,20	0
56	MG	BA	3178	1/1	0.85	0.12	54,54,54,54	0
56	MG	BA	3451	1/1	0.85	0.09	43,43,43,43	0
56	MG	AA	1727	1/1	0.85	0.16	40,40,40,40	0
56	MG	BB	205	1/1	0.85	0.36	35,35,35,35	1
56	MG	AA	1670	1/1	0.85	0.17	52,52,52,52	0
56	MG	CA	1615	1/1	0.85	0.34	61,61,61,61	0
56	MG	DA	3330	1/1	0.85	0.49	81,81,81,81	0
56	MG	DA	3334	1/1	0.85	0.09	34,34,34,34	1
56	MG	BA	3103	1/1	0.85	0.18	55,55,55,55	0
56	MG	DA	3357	1/1	0.85	0.17	26,26,26,26	0
56	MG	BA	3346	1/1	0.85	0.22	60,60,60,60	0
56	MG	CA	1642	1/1	0.85	0.15	56,56,56,56	0
56	MG	AA	1716	1/1	0.85	0.39	73,73,73,73	0
56	MG	BA	3375	1/1	0.85	0.26	42,42,42,42	1
56	MG	CA	1767	1/1	0.85	0.27	67,67,67,67	0
56	MG	AA	1799	1/1	0.85	0.09	71,71,71,71	0
56	MG	BA	3377	1/1	0.85	0.21	43,43,43,43	0
56	MG	DA	3048	1/1	0.86	0.27	53,53,53,53	0
56	MG	BA	3329	1/1	0.86	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3332	1/1	0.86	0.20	53,53,53,53	1
56	MG	DA	3149	1/1	0.86	0.48	84,84,84,84	0
56	MG	DA	3276	1/1	0.86	0.37	45,45,45,45	0
56	MG	BA	3412	1/1	0.86	0.21	48,48,48,48	0
56	MG	CA	1753	1/1	0.86	0.23	33,33,33,33	0
56	MG	BA	3143	1/1	0.86	0.26	21,21,21,21	0
56	MG	AA	1626	1/1	0.86	0.25	50,50,50,50	0
56	MG	CA	1644	1/1	0.86	0.22	59,59,59,59	0
56	MG	BA	3425	1/1	0.86	0.22	61,61,61,61	0
56	MG	AE	201	1/1	0.86	0.09	47,47,47,47	0
56	MG	BA	3237	1/1	0.86	0.32	35,35,35,35	0
56	MG	DA	3353	1/1	0.86	0.35	42,42,42,42	0
56	MG	CX	102	1/1	0.86	0.40	75,75,75,75	0
56	MG	AA	1747	1/1	0.86	0.14	37,37,37,37	0
56	MG	CA	1730	1/1	0.86	0.18	56,56,56,56	0
56	MG	BB	203	1/1	0.86	0.15	52,52,52,52	0
56	MG	CA	1742	1/1	0.86	0.15	76,76,76,76	0
56	MG	DA	3022	1/1	0.86	0.19	37,37,37,37	0
56	MG	CA	1744	1/1	0.86	0.16	64,64,64,64	0
56	MG	AA	1730	1/1	0.86	0.36	82,82,82,82	0
56	MG	DO	201	1/1	0.86	0.13	67,67,67,67	0
56	MG	DA	3283	1/1	0.87	0.20	35,35,35,35	0
56	MG	BA	3342	1/1	0.87	0.35	52,52,52,52	1
56	MG	AW	120	1/1	0.87	0.10	52,52,52,52	0
56	MG	BA	3107	1/1	0.87	0.17	53,53,53,53	0
56	MG	CA	1763	1/1	0.87	0.18	32,32,32,32	0
56	MG	DA	3329	1/1	0.87	0.17	45,45,45,45	0
56	MG	BA	3372	1/1	0.87	0.11	43,43,43,43	1
56	MG	AA	1795	1/1	0.87	0.25	30,30,30,30	0
56	MG	CW	104	1/1	0.87	0.08	46,46,46,46	0
56	MG	AA	1657	1/1	0.87	0.16	50,50,50,50	0
56	MG	BA	3293	1/1	0.87	0.19	51,51,51,51	0
56	MG	BA	3383	1/1	0.87	0.09	37,37,37,37	0
56	MG	DA	3160	1/1	0.87	0.17	37,37,37,37	0
56	MG	B3	101	1/1	0.87	0.24	48,48,48,48	1
56	MG	BA	3247	1/1	0.87	0.14	0,0,0,0	0
56	MG	AA	1802	1/1	0.87	0.13	44,44,44,44	0
56	MG	DB	202	1/1	0.87	0.18	57,57,57,57	0
56	MG	DA	3193	1/1	0.87	0.22	35,35,35,35	0
56	MG	AA	1663	1/1	0.87	0.13	24,24,24,24	0
56	MG	DA	3212	1/1	0.87	0.24	61,61,61,61	0
56	MG	AA	1734	1/1	0.88	0.20	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	CA	1618	1/1	0.88	0.12	25,25,25,25	0
56	MG	CA	1697	1/1	0.88	0.14	49,49,49,49	0
56	MG	CV	102	1/1	0.88	0.08	56,56,56,56	0
56	MG	CA	1619	1/1	0.88	0.17	55,55,55,55	0
56	MG	CA	1714	1/1	0.88	0.16	81,81,81,81	0
56	MG	DA	3171	1/1	0.88	0.20	37,37,37,37	0
56	MG	BA	3374	1/1	0.88	0.26	48,48,48,48	0
56	MG	BA	3414	1/1	0.88	0.32	44,44,44,44	0
56	MG	BA	3419	1/1	0.88	0.24	39,39,39,39	0
56	MG	BA	3258	1/1	0.88	0.11	70,70,70,70	0
56	MG	CA	1726	1/1	0.88	0.12	29,29,29,29	0
56	MG	CX	103	1/1	0.88	0.23	40,40,40,40	0
56	MG	BA	3222	1/1	0.88	0.21	41,41,41,41	0
56	MG	BA	3265	1/1	0.88	0.23	37,37,37,37	0
56	MG	AA	1688	1/1	0.88	0.29	39,39,39,39	0
56	MG	DA	3246	1/1	0.88	0.15	38,38,38,38	0
56	MG	BA	3064	1/1	0.88	0.20	30,30,30,30	0
56	MG	DA	3249	1/1	0.88	0.47	57,57,57,57	0
56	MG	BA	3400	1/1	0.88	0.14	46,46,46,46	0
56	MG	CA	1680	1/1	0.88	0.19	51,51,51,51	0
56	MG	BA	3181	1/1	0.88	0.07	36,36,36,36	0
56	MG	BB	209	1/1	0.88	0.12	49,49,49,49	0
56	MG	DB	209	1/1	0.88	0.16	20,20,20,20	0
56	MG	BA	3070	1/1	0.88	0.21	24,24,24,24	0
56	MG	DA	3137	1/1	0.88	0.15	62,62,62,62	0
56	MG	CA	1759	1/1	0.89	0.20	68,68,68,68	0
56	MG	CA	1761	1/1	0.89	0.26	26,26,26,26	0
56	MG	DA	3111	1/1	0.89	0.24	1,1,1,1	0
56	MG	DA	3272	1/1	0.89	0.41	47,47,47,47	0
56	MG	BA	3009	1/1	0.89	0.23	20,20,20,20	0
56	MG	BA	3333	1/1	0.89	0.17	41,41,41,41	0
56	MG	CA	1786	1/1	0.89	0.23	29,29,29,29	0
56	MG	DA	3153	1/1	0.89	0.31	40,40,40,40	0
56	MG	CA	1789	1/1	0.89	0.18	33,33,33,33	0
56	MG	DA	3278	1/1	0.89	0.17	38,38,38,38	0
56	MG	DA	3159	1/1	0.89	0.23	57,57,57,57	0
56	MG	CJ	201	1/1	0.89	0.10	44,44,44,44	0
56	MG	BA	3206	1/1	0.89	0.19	25,25,25,25	0
56	MG	BA	3018	1/1	0.89	0.24	22,22,22,22	0
56	MG	CV	104	1/1	0.89	0.21	36,36,36,36	0
56	MG	DA	3173	1/1	0.89	0.13	41,41,41,41	0
56	MG	BA	3415	1/1	0.89	0.32	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	BA	3124	1/1	0.89	0.19	17,17,17,17	0
56	MG	BA	3142	1/1	0.89	0.26	66,66,66,66	0
56	MG	B2	102	1/1	0.89	0.20	44,44,44,44	0
56	MG	BA	3282	1/1	0.89	0.31	49,49,49,49	0
56	MG	CA	1663	1/1	0.89	0.16	32,32,32,32	0
56	MG	AA	1665	1/1	0.89	0.21	27,27,27,27	0
56	MG	BA	3001	1/1	0.89	0.18	38,38,38,38	0
56	MG	BA	3379	1/1	0.89	0.11	39,39,39,39	0
56	MG	BA	3166	1/1	0.89	0.06	39,39,39,39	0
56	MG	DA	3008	1/1	0.89	0.17	23,23,23,23	0
56	MG	BA	3300	1/1	0.89	0.10	6,6,6,6	0
56	MG	BA	3254	1/1	0.89	0.11	48,48,48,48	0
56	MG	BN	201	1/1	0.89	0.31	25,25,25,25	0
56	MG	DN	201	1/1	0.89	0.09	16,16,16,16	0
56	MG	AA	1643	1/1	0.89	0.17	22,22,22,22	0
56	MG	CA	1723	1/1	0.90	0.34	65,65,65,65	0
56	MG	CX	106	1/1	0.90	0.37	47,47,47,47	0
56	MG	AA	1763	1/1	0.90	0.43	58,58,58,58	1
56	MG	AA	1810	1/1	0.90	0.26	47,47,47,47	0
56	MG	BA	3286	1/1	0.90	0.19	38,38,38,38	0
56	MG	B2	103	1/1	0.90	0.29	46,46,46,46	0
56	MG	DA	3009	1/1	0.90	0.18	3,3,3,3	0
56	MG	CA	1732	1/1	0.90	0.23	43,43,43,43	0
56	MG	CA	1734	1/1	0.90	0.14	59,59,59,59	0
56	MG	BA	3230	1/1	0.90	0.16	36,36,36,36	0
56	MG	CA	1627	1/1	0.90	0.14	34,34,34,34	0
56	MG	BA	3140	1/1	0.90	0.11	10,10,10,10	0
56	MG	DA	3057	1/1	0.90	0.30	35,35,35,35	0
56	MG	AA	1768	1/1	0.90	0.15	14,14,14,14	1
56	MG	CA	1643	1/1	0.90	0.42	48,48,48,48	0
56	MG	DA	3132	1/1	0.90	0.09	13,13,13,13	0
56	MG	BA	3409	1/1	0.90	0.13	53,53,53,53	0
56	MG	BA	3241	1/1	0.90	0.19	43,43,43,43	0
56	MG	BA	3330	1/1	0.90	0.06	33,33,33,33	0
56	MG	BA	3331	1/1	0.90	0.08	45,45,45,45	0
56	MG	AA	1772	1/1	0.90	0.23	73,73,73,73	0
56	MG	AA	1776	1/1	0.90	0.10	30,30,30,30	0
56	MG	AA	1620	1/1	0.90	0.14	28,28,28,28	0
56	MG	DA	3165	1/1	0.90	0.17	38,38,38,38	0
56	MG	BA	3345	1/1	0.90	0.18	59,59,59,59	0
56	MG	BA	3429	1/1	0.90	0.16	41,41,41,41	0
56	MG	BA	3154	1/1	0.90	0.14	28,28,28,28	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	BA	3435	1/1	0.90	0.09	52,52,52,52	1
56	MG	DA	3368	1/1	0.90	0.67	71,71,71,71	0
56	MG	DA	3369	1/1	0.90	0.15	46,46,46,46	0
56	MG	DA	3371	1/1	0.90	0.12	40,40,40,40	0
56	MG	BA	3446	1/1	0.90	0.13	43,43,43,43	0
56	MG	AA	1708	1/1	0.90	0.20	41,41,41,41	0
56	MG	DA	3387	1/1	0.90	0.11	11,11,11,11	0
56	MG	BA	3367	1/1	0.90	0.26	50,50,50,50	0
56	MG	AW	118	1/1	0.90	0.16	46,46,46,46	0
56	MG	AA	1749	1/1	0.90	0.15	38,38,38,38	0
56	MG	CW	110	1/1	0.90	0.12	38,38,38,38	0
56	MG	AW	121	1/1	0.90	0.09	36,36,36,36	0
56	MG	BB	212	1/1	0.90	0.11	18,18,18,18	1
56	MG	AA	1745	1/1	0.90	0.17	56,56,56,56	0
56	MG	DA	3240	1/1	0.90	0.11	43,43,43,43	0
56	MG	CA	1711	1/1	0.91	0.29	63,63,63,63	0
56	MG	BA	3358	1/1	0.91	0.19	42,42,42,42	0
56	MG	DA	3245	1/1	0.91	0.15	38,38,38,38	0
56	MG	BB	204	1/1	0.91	0.14	42,42,42,42	0
56	MG	CX	104	1/1	0.91	0.17	31,31,31,31	1
56	MG	BA	3002	1/1	0.91	0.17	21,21,21,21	0
56	MG	BB	206	1/1	0.91	0.38	78,78,78,78	0
56	MG	AA	1780	1/1	0.91	0.13	60,60,60,60	0
56	MG	AA	1627	1/1	0.91	0.45	39,39,39,39	0
56	MG	BA	3160	1/1	0.91	0.12	17,17,17,17	0
56	MG	BB	214	1/1	0.91	0.20	46,46,46,46	0
56	MG	BB	218	1/1	0.91	0.12	36,36,36,36	1
56	MG	BA	3016	1/1	0.91	0.21	37,37,37,37	0
56	MG	BA	3167	1/1	0.91	0.14	33,33,33,33	0
56	MG	CA	1737	1/1	0.91	0.15	35,35,35,35	0
56	MG	AA	1792	1/1	0.91	0.19	74,74,74,74	0
56	MG	AA	1738	1/1	0.91	0.20	49,49,49,49	0
56	MG	BA	3051	1/1	0.91	0.12	56,56,56,56	0
56	MG	DA	3069	1/1	0.91	0.21	45,45,45,45	0
56	MG	AA	1743	1/1	0.91	0.10	44,44,44,44	0
56	MG	DA	3298	1/1	0.91	0.14	5,5,5,5	0
56	MG	CA	1633	1/1	0.91	0.27	19,19,19,19	0
56	MG	DA	3133	1/1	0.91	0.11	39,39,39,39	0
56	MG	BA	3294	1/1	0.91	0.10	6,6,6,6	0
56	MG	AA	1796	1/1	0.91	0.10	10,10,10,10	1
56	MG	BA	3219	1/1	0.91	0.06	45,45,45,45	0
56	MG	BA	3410	1/1	0.91	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	CA	1760	1/1	0.91	0.15	33,33,33,33	0
56	MG	BA	3322	1/1	0.91	0.14	35,35,35,35	0
56	MG	DA	3344	1/1	0.91	0.31	32,32,32,32	0
56	MG	AA	1767	1/1	0.91	0.22	48,48,48,48	0
56	MG	AA	1729	1/1	0.91	0.09	45,45,45,45	0
56	MG	CA	1772	1/1	0.91	0.18	37,37,37,37	0
56	MG	AA	1808	1/1	0.91	0.08	33,33,33,33	0
56	MG	BA	3231	1/1	0.91	0.42	45,45,45,45	0
56	MG	BA	3111	1/1	0.91	0.16	27,27,27,27	0
56	MG	AA	1638	1/1	0.91	0.24	24,24,24,24	0
56	MG	BA	3129	1/1	0.91	0.14	21,21,21,21	0
56	MG	DA	3197	1/1	0.91	0.16	13,13,13,13	0
56	MG	DA	3389	1/1	0.91	0.11	22,22,22,22	0
56	MG	DA	3201	1/1	0.91	0.18	7,7,7,7	0
56	MG	DA	3393	1/1	0.91	0.13	80,80,80,80	0
56	MG	BA	3343	1/1	0.91	0.30	34,34,34,34	0
56	MG	AA	1629	1/1	0.91	0.13	29,29,29,29	0
56	MG	AV	106	1/1	0.91	0.07	40,40,40,40	0
56	MG	BA	3448	1/1	0.91	0.07	35,35,35,35	0
56	MG	DF	301	1/1	0.91	0.13	29,29,29,29	0
56	MG	BA	3349	1/1	0.91	0.16	28,28,28,28	1
56	MG	AV	107	1/1	0.91	0.10	25,25,25,25	0
56	MG	DA	3233	1/1	0.91	0.12	0,0,0,0	0
56	MG	DU	201	1/1	0.91	0.13	45,45,45,45	0
56	MG	DZ	301	1/1	0.91	0.12	27,27,27,27	0
56	MG	AA	1809	1/1	0.92	0.17	40,40,40,40	1
56	MG	BA	3180	1/1	0.92	0.10	33,33,33,33	0
56	MG	BA	3071	1/1	0.92	0.24	20,20,20,20	0
56	MG	BA	3190	1/1	0.92	0.21	49,49,49,49	0
56	MG	B2	101	1/1	0.92	0.12	36,36,36,36	0
56	MG	AA	1601	1/1	0.92	0.11	35,35,35,35	0
56	MG	DA	3257	1/1	0.92	0.19	27,27,27,27	0
56	MG	BA	3388	1/1	0.92	0.22	22,22,22,22	0
56	MG	BA	3214	1/1	0.92	0.39	44,44,44,44	0
56	MG	BV	201	1/1	0.92	0.12	23,23,23,23	0
56	MG	DA	3267	1/1	0.92	0.13	13,13,13,13	0
56	MG	AA	1640	1/1	0.92	0.29	18,18,18,18	0
56	MG	DA	3270	1/1	0.92	0.09	47,47,47,47	0
56	MG	AA	1632	1/1	0.92	0.10	24,24,24,24	0
56	MG	BA	3308	1/1	0.92	0.20	25,25,25,25	0
56	MG	BA	3316	1/1	0.92	0.27	49,49,49,49	0
56	MG	DA	3040	1/1	0.92	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3318	1/1	0.92	0.18	30,30,30,30	0
56	MG	AA	1783	1/1	0.92	0.37	46,46,46,46	0
56	MG	AA	1731	1/1	0.92	0.14	56,56,56,56	0
56	MG	DA	3279	1/1	0.92	0.19	15,15,15,15	0
56	MG	CA	1639	1/1	0.92	0.23	71,71,71,71	0
56	MG	DA	3296	1/1	0.92	0.10	59,59,59,59	0
56	MG	AA	1686	1/1	0.92	0.18	52,52,52,52	0
56	MG	DA	3116	1/1	0.92	0.11	10,10,10,10	0
56	MG	AA	1755	1/1	0.92	0.26	47,47,47,47	0
56	MG	AA	1615	1/1	0.92	0.12	33,33,33,33	0
56	MG	AA	1737	1/1	0.92	0.13	60,60,60,60	0
56	MG	CA	1758	1/1	0.92	0.15	44,44,44,44	0
56	MG	BA	3150	1/1	0.92	0.12	35,35,35,35	0
56	MG	DA	3333	1/1	0.92	0.23	67,67,67,67	0
56	MG	AA	1715	1/1	0.92	0.09	24,24,24,24	0
56	MG	CA	1661	1/1	0.92	0.17	13,13,13,13	0
56	MG	BA	3431	1/1	0.92	0.09	51,51,51,51	0
56	MG	DA	3350	1/1	0.92	0.19	37,37,37,37	0
56	MG	CA	1665	1/1	0.92	0.43	71,71,71,71	0
56	MG	CA	1769	1/1	0.92	0.11	18,18,18,18	0
56	MG	BA	3250	1/1	0.92	0.19	22,22,22,22	1
56	MG	CA	1775	1/1	0.92	0.22	35,35,35,35	0
56	MG	CA	1776	1/1	0.92	0.18	44,44,44,44	0
56	MG	DA	3172	1/1	0.92	0.22	25,25,25,25	0
56	MG	DA	3379	1/1	0.92	0.22	31,31,31,31	0
56	MG	AA	1807	1/1	0.92	0.12	19,19,19,19	1
56	MG	CA	1788	1/1	0.92	0.21	42,42,42,42	1
56	MG	DA	3383	1/1	0.92	0.09	32,32,32,32	0
56	MG	DA	3188	1/1	0.92	0.32	42,42,42,42	0
56	MG	BA	3439	1/1	0.92	0.23	31,31,31,31	0
56	MG	CA	1682	1/1	0.92	0.12	32,32,32,32	0
56	MG	DA	3392	1/1	0.92	0.15	47,47,47,47	0
56	MG	CV	101	1/1	0.92	0.13	32,32,32,32	0
56	MG	BA	3157	1/1	0.92	0.28	39,39,39,39	0
56	MG	BA	3158	1/1	0.92	0.26	44,44,44,44	0
56	MG	BA	3450	1/1	0.92	0.09	55,55,55,55	0
56	MG	CA	1694	1/1	0.92	0.17	33,33,33,33	0
56	MG	BA	3052	1/1	0.92	0.24	0,0,0,0	0
56	MG	DA	3228	1/1	0.92	0.15	19,19,19,19	0
56	MG	BA	3061	1/1	0.92	0.16	0,0,0,0	0
56	MG	AA	1635	1/1	0.92	0.09	16,16,16,16	0
56	MG	CA	1700	1/1	0.92	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	BA	3277	1/1	0.92	0.19	38,38,38,38	0
56	MG	CA	1612	1/1	0.93	0.09	17,17,17,17	0
56	MG	BA	3155	1/1	0.93	0.44	66,66,66,66	0
56	MG	BA	3263	1/1	0.93	0.07	4,4,4,4	0
56	MG	AW	101	1/1	0.93	0.35	35,35,35,35	0
56	MG	BA	3268	1/1	0.93	0.14	24,24,24,24	0
56	MG	BA	3269	1/1	0.93	0.32	43,43,43,43	0
56	MG	CA	1762	1/1	0.93	0.25	39,39,39,39	0
56	MG	DA	3214	1/1	0.93	0.10	32,32,32,32	0
56	MG	DA	3216	1/1	0.93	0.12	34,34,34,34	0
56	MG	AA	1786	1/1	0.93	0.14	31,31,31,31	0
56	MG	DA	3218	1/1	0.93	0.07	27,27,27,27	0
56	MG	BA	3276	1/1	0.93	0.09	6,6,6,6	0
56	MG	BA	3390	1/1	0.93	0.11	20,20,20,20	1
56	MG	DA	3230	1/1	0.93	0.17	20,20,20,20	0
56	MG	AA	1791	1/1	0.93	0.45	22,22,22,22	1
56	MG	AW	111	1/1	0.93	0.25	32,32,32,32	1
56	MG	AA	1674	1/1	0.93	0.24	33,33,33,33	0
56	MG	BA	3407	1/1	0.93	0.11	40,40,40,40	0
56	MG	CA	1787	1/1	0.93	0.29	39,39,39,39	1
56	MG	BA	3168	1/1	0.93	0.10	22,22,22,22	0
56	MG	AA	1764	1/1	0.93	0.10	6,6,6,6	0
56	MG	AA	1765	1/1	0.93	0.05	43,43,43,43	0
56	MG	BA	3288	1/1	0.93	0.23	32,32,32,32	1
56	MG	AA	1654	1/1	0.93	0.20	50,50,50,50	0
56	MG	CA	1670	1/1	0.93	0.13	23,23,23,23	0
56	MG	CA	1671	1/1	0.93	0.26	42,42,42,42	0
56	MG	CW	102	1/1	0.93	0.07	52,52,52,52	0
56	MG	CA	1672	1/1	0.93	0.15	32,32,32,32	0
56	MG	AA	1678	1/1	0.93	0.10	43,43,43,43	0
56	MG	CA	1674	1/1	0.93	0.09	58,58,58,58	0
56	MG	AA	1769	1/1	0.93	0.20	61,61,61,61	0
56	MG	BA	3299	1/1	0.93	0.19	22,22,22,22	0
56	MG	AA	1803	1/1	0.93	0.17	48,48,48,48	0
56	MG	AA	1695	1/1	0.93	0.18	13,13,13,13	1
56	MG	BA	3428	1/1	0.93	0.49	72,72,72,72	1
56	MG	BA	3215	1/1	0.93	0.14	30,30,30,30	0
56	MG	BA	3119	1/1	0.93	0.25	16,16,16,16	0
56	MG	BA	3320	1/1	0.93	0.09	37,37,37,37	0
56	MG	AA	1735	1/1	0.93	0.18	84,84,84,84	0
56	MG	BA	3126	1/1	0.93	0.09	1,1,1,1	0
56	MG	DA	3006	1/1	0.93	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	CA	1698	1/1	0.93	0.37	42,42,42,42	0
56	MG	DA	3309	1/1	0.93	0.13	6,6,6,6	0
56	MG	BA	3442	1/1	0.93	0.09	29,29,29,29	0
56	MG	CA	1702	1/1	0.93	0.14	36,36,36,36	0
56	MG	DA	3313	1/1	0.93	0.12	35,35,35,35	1
56	MG	DA	3318	1/1	0.93	0.28	45,45,45,45	0
56	MG	AA	1681	1/1	0.93	0.13	21,21,21,21	0
56	MG	CA	1708	1/1	0.93	0.30	43,43,43,43	0
56	MG	DA	3321	1/1	0.93	0.11	45,45,45,45	1
56	MG	DA	3324	1/1	0.93	0.21	56,56,56,56	0
56	MG	DA	3325	1/1	0.93	0.11	35,35,35,35	0
56	MG	DA	3027	1/1	0.93	0.28	39,39,39,39	0
56	MG	BA	3447	1/1	0.93	0.09	37,37,37,37	0
56	MG	CA	1713	1/1	0.93	0.19	93,93,93,93	0
56	MG	BA	3228	1/1	0.93	0.13	46,46,46,46	0
56	MG	DA	3339	1/1	0.93	0.07	17,17,17,17	0
56	MG	DA	3341	1/1	0.93	0.11	26,26,26,26	0
56	MG	DA	3053	1/1	0.93	0.17	24,24,24,24	0
56	MG	AA	1648	1/1	0.93	0.19	86,86,86,86	0
56	MG	DA	3348	1/1	0.93	0.14	46,46,46,46	0
56	MG	DA	3058	1/1	0.93	0.20	6,6,6,6	0
56	MG	DA	3351	1/1	0.93	0.18	16,16,16,16	0
56	MG	CA	1718	1/1	0.93	0.22	47,47,47,47	0
56	MG	AA	1811	1/1	0.93	0.12	16,16,16,16	0
56	MG	DA	3096	1/1	0.93	0.24	21,21,21,21	0
56	MG	DA	3360	1/1	0.93	0.34	39,39,39,39	0
56	MG	DA	3367	1/1	0.93	0.11	19,19,19,19	0
56	MG	DA	3106	1/1	0.93	0.15	15,15,15,15	0
56	MG	CA	1721	1/1	0.93	0.27	57,57,57,57	0
56	MG	BA	3454	1/1	0.93	0.13	44,44,44,44	0
56	MG	DA	3375	1/1	0.93	0.10	42,42,42,42	1
56	MG	DA	3120	1/1	0.93	0.13	25,25,25,25	0
56	MG	AA	1758	1/1	0.93	0.13	62,62,62,62	0
56	MG	BA	3144	1/1	0.93	0.16	8,8,8,8	0
56	MG	BA	3146	1/1	0.93	0.24	0,0,0,0	0
56	MG	BA	3003	1/1	0.93	0.20	28,28,28,28	0
56	MG	DA	3140	1/1	0.93	0.14	22,22,22,22	0
56	MG	DA	3148	1/1	0.93	0.14	5,5,5,5	0
56	MG	AV	103	1/1	0.93	0.08	28,28,28,28	0
56	MG	BA	3253	1/1	0.93	0.11	38,38,38,38	0
56	MG	BB	210	1/1	0.93	0.10	33,33,33,33	1
56	MG	AA	1784	1/1	0.93	0.29	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	CA	1738	1/1	0.93	0.11	23,23,23,23	0
56	MG	DB	205	1/1	0.93	0.20	51,51,51,51	0
56	MG	DB	207	1/1	0.93	0.21	52,52,52,52	1
56	MG	BA	3153	1/1	0.93	0.12	37,37,37,37	0
56	MG	CA	1741	1/1	0.93	0.31	40,40,40,40	0
56	MG	BA	3362	1/1	0.93	0.18	58,58,58,58	0
56	MG	AA	1785	1/1	0.93	0.15	32,32,32,32	0
56	MG	BA	3370	1/1	0.93	0.28	28,28,28,28	1
56	MG	BA	3259	1/1	0.93	0.10	32,32,32,32	0
56	MG	CA	1611	1/1	0.93	0.27	67,67,67,67	0
57	PAR	AA	1816	42/42	0.93	0.16	15,20,38,42	0
57	PAR	CA	1790	42/42	0.93	0.17	7,11,29,33	0
56	MG	BA	3174	1/1	0.94	0.11	0,0,0,0	0
56	MG	CA	1638	1/1	0.94	0.13	42,42,42,42	0
56	MG	BA	3384	1/1	0.94	0.13	36,36,36,36	0
56	MG	DA	3203	1/1	0.94	0.10	58,58,58,58	0
56	MG	DA	3204	1/1	0.94	0.12	8,8,8,8	0
56	MG	BA	3272	1/1	0.94	0.40	49,49,49,49	0
56	MG	AA	1655	1/1	0.94	0.17	32,32,32,32	0
56	MG	AA	1709	1/1	0.94	0.15	33,33,33,33	0
56	MG	CA	1768	1/1	0.94	0.14	37,37,37,37	0
56	MG	BA	3395	1/1	0.94	0.20	54,54,54,54	1
56	MG	AA	1604	1/1	0.94	0.17	52,52,52,52	0
56	MG	AA	1616	1/1	0.94	0.14	18,18,18,18	0
56	MG	CA	1649	1/1	0.94	0.12	37,37,37,37	0
56	MG	CA	1779	1/1	0.94	0.20	31,31,31,31	0
56	MG	CA	1650	1/1	0.94	0.24	68,68,68,68	0
56	MG	CA	1652	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3232	1/1	0.94	0.12	13,13,13,13	0
56	MG	CA	1654	1/1	0.94	0.08	41,41,41,41	0
56	MG	DA	3235	1/1	0.94	0.08	39,39,39,39	0
56	MG	CA	1657	1/1	0.94	0.15	24,24,24,24	0
56	MG	CF	201	1/1	0.94	0.10	44,44,44,44	0
56	MG	BA	3199	1/1	0.94	0.14	9,9,9,9	0
56	MG	BA	3204	1/1	0.94	0.11	0,0,0,0	0
56	MG	BA	3117	1/1	0.94	0.24	3,3,3,3	0
56	MG	B2	104	1/1	0.94	0.09	34,34,34,34	0
56	MG	AA	1683	1/1	0.94	0.13	17,17,17,17	0
56	MG	B7	102	1/1	0.94	0.10	11,11,11,11	1
56	MG	AA	1717	1/1	0.94	0.08	21,21,21,21	0
56	MG	BA	3217	1/1	0.94	0.16	37,37,37,37	0
56	MG	BA	3218	1/1	0.94	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1676	1/1	0.94	0.36	46,46,46,46	0
56	MG	BA	3135	1/1	0.94	0.13	18,18,18,18	0
56	MG	BA	3301	1/1	0.94	0.20	19,19,19,19	0
56	MG	CA	1684	1/1	0.94	0.23	30,30,30,30	0
56	MG	BA	3221	1/1	0.94	0.13	49,49,49,49	0
56	MG	BA	3314	1/1	0.94	0.45	47,47,47,47	1
56	MG	AA	1790	1/1	0.94	0.08	65,65,65,65	0
56	MG	BA	3223	1/1	0.94	0.13	8,8,8,8	0
56	MG	BA	3226	1/1	0.94	0.10	20,20,20,20	0
56	MG	BA	3436	1/1	0.94	0.11	39,39,39,39	1
56	MG	BA	3141	1/1	0.94	0.10	20,20,20,20	0
56	MG	AA	1606	1/1	0.94	0.36	53,53,53,53	0
56	MG	DA	3282	1/1	0.94	0.15	41,41,41,41	0
56	MG	BA	3229	1/1	0.94	0.15	36,36,36,36	0
56	MG	DA	3010	1/1	0.94	0.14	44,44,44,44	0
56	MG	DA	3297	1/1	0.94	0.15	23,23,23,23	0
56	MG	DA	3012	1/1	0.94	0.16	27,27,27,27	0
56	MG	DA	3304	1/1	0.94	0.06	9,9,9,9	0
56	MG	DA	3307	1/1	0.94	0.11	34,34,34,34	1
56	MG	AW	102	1/1	0.94	0.26	51,51,51,51	0
56	MG	AA	1630	1/1	0.94	0.10	13,13,13,13	0
56	MG	AA	1690	1/1	0.94	0.12	48,48,48,48	0
56	MG	AA	1619	1/1	0.94	0.33	41,41,41,41	0
56	MG	BA	3452	1/1	0.94	0.11	39,39,39,39	0
56	MG	BA	3335	1/1	0.94	0.13	45,45,45,45	0
56	MG	BA	3149	1/1	0.94	0.10	10,10,10,10	0
56	MG	CA	1717	1/1	0.94	0.07	16,16,16,16	0
56	MG	DA	3056	1/1	0.94	0.16	9,9,9,9	0
56	MG	BA	3243	1/1	0.94	0.13	18,18,18,18	0
56	MG	BA	3344	1/1	0.94	0.15	17,17,17,17	0
56	MG	CA	1720	1/1	0.94	0.15	69,69,69,69	0
56	MG	DA	3331	1/1	0.94	0.26	42,42,42,42	0
56	MG	DA	3068	1/1	0.94	0.14	14,14,14,14	0
56	MG	BA	3028	1/1	0.94	0.30	36,36,36,36	0
56	MG	DA	3074	1/1	0.94	0.22	11,11,11,11	0
56	MG	DA	3086	1/1	0.94	0.21	0,0,0,0	0
56	MG	DA	3088	1/1	0.94	0.20	4,4,4,4	0
56	MG	BA	3030	1/1	0.94	0.11	0,0,0,0	0
56	MG	DA	3347	1/1	0.94	0.08	34,34,34,34	0
56	MG	AA	1609	1/1	0.94	0.15	44,44,44,44	0
56	MG	CA	1724	1/1	0.94	0.08	38,38,38,38	0
56	MG	AW	115	1/1	0.94	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	BA	3354	1/1	0.94	0.09	35,35,35,35	0
56	MG	DA	3122	1/1	0.94	0.18	43,43,43,43	0
56	MG	DA	3130	1/1	0.94	0.15	14,14,14,14	0
56	MG	BA	3255	1/1	0.94	0.14	28,28,28,28	0
56	MG	DA	3363	1/1	0.94	0.12	30,30,30,30	0
56	MG	BA	3361	1/1	0.94	0.24	53,53,53,53	0
56	MG	CA	1731	1/1	0.94	0.10	32,32,32,32	0
56	MG	BA	3256	1/1	0.94	0.09	22,22,22,22	0
56	MG	BA	3366	1/1	0.94	0.14	27,27,27,27	0
56	MG	DA	3143	1/1	0.94	0.22	36,36,36,36	0
56	MG	DA	3144	1/1	0.94	0.14	31,31,31,31	0
56	MG	CA	1736	1/1	0.94	0.14	30,30,30,30	0
56	MG	AA	1653	1/1	0.94	0.12	39,39,39,39	0
56	MG	DA	3151	1/1	0.94	0.21	46,46,46,46	0
56	MG	DA	3152	1/1	0.94	0.10	17,17,17,17	0
56	MG	CA	1601	1/1	0.94	0.17	26,26,26,26	0
56	MG	CA	1609	1/1	0.94	0.10	33,33,33,33	0
56	MG	AA	1622	1/1	0.94	0.10	8,8,8,8	0
56	MG	AA	1736	1/1	0.94	0.10	19,19,19,19	0
56	MG	DA	3161	1/1	0.94	0.13	39,39,39,39	0
56	MG	DA	3396	1/1	0.94	0.16	27,27,27,27	1
56	MG	BA	3373	1/1	0.94	0.04	39,39,39,39	0
56	MG	CA	1617	1/1	0.94	0.09	25,25,25,25	0
56	MG	AA	1676	1/1	0.94	0.07	7,7,7,7	0
56	MG	DA	3170	1/1	0.94	0.09	54,54,54,54	0
56	MG	DB	208	1/1	0.94	0.17	9,9,9,9	0
56	MG	AA	1701	1/1	0.94	0.12	18,18,18,18	0
56	MG	DB	210	1/1	0.94	0.05	15,15,15,15	0
56	MG	DD	302	1/1	0.94	0.09	7,7,7,7	0
56	MG	BA	3088	1/1	0.94	0.30	35,35,35,35	0
56	MG	BA	3266	1/1	0.94	0.28	28,28,28,28	0
56	MG	DA	3175	1/1	0.94	0.19	30,30,30,30	0
56	MG	DA	3180	1/1	0.94	0.26	0,0,0,0	0
56	MG	DA	3185	1/1	0.94	0.12	8,8,8,8	1
56	MG	CA	1757	1/1	0.94	0.12	56,56,56,56	0
56	MG	BA	3102	1/1	0.94	0.11	15,15,15,15	0
56	MG	DA	3189	1/1	0.94	0.23	34,34,34,34	0
56	MG	BA	3114	1/1	0.95	0.21	0,0,0,0	0
56	MG	AA	1684	1/1	0.95	0.13	17,17,17,17	0
56	MG	BA	3336	1/1	0.95	0.11	45,45,45,45	0
56	MG	AA	1804	1/1	0.95	0.12	31,31,31,31	0
56	MG	DA	3177	1/1	0.95	0.18	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3122	1/1	0.95	0.13	8,8,8,8	0
56	MG	BB	215	1/1	0.95	0.10	40,40,40,40	0
56	MG	DA	3186	1/1	0.95	0.24	24,24,24,24	0
56	MG	CA	1746	1/1	0.95	0.26	18,18,18,18	0
56	MG	AA	1770	1/1	0.95	0.12	16,16,16,16	0
56	MG	BB	219	1/1	0.95	0.08	24,24,24,24	0
56	MG	DA	3191	1/1	0.95	0.16	25,25,25,25	0
56	MG	BF	302	1/1	0.95	0.24	46,46,46,46	0
56	MG	AA	1685	1/1	0.95	0.07	38,38,38,38	0
56	MG	AA	1773	1/1	0.95	0.09	41,41,41,41	0
56	MG	BX	101	1/1	0.95	0.13	26,26,26,26	0
56	MG	BA	3347	1/1	0.95	0.17	22,22,22,22	1
56	MG	DA	3207	1/1	0.95	0.11	8,8,8,8	0
56	MG	CA	1602	1/1	0.95	0.12	14,14,14,14	0
56	MG	DA	3211	1/1	0.95	0.10	1,1,1,1	0
56	MG	AA	1668	1/1	0.95	0.07	23,23,23,23	0
56	MG	CA	1610	1/1	0.95	0.22	15,15,15,15	0
56	MG	BA	3351	1/1	0.95	0.28	78,78,78,78	0
56	MG	CA	1764	1/1	0.95	0.11	15,15,15,15	0
56	MG	CA	1765	1/1	0.95	0.08	38,38,38,38	0
56	MG	BA	3234	1/1	0.95	0.26	29,29,29,29	0
56	MG	BA	3139	1/1	0.95	0.11	9,9,9,9	0
56	MG	CA	1616	1/1	0.95	0.24	24,24,24,24	0
56	MG	DA	3229	1/1	0.95	0.21	1,1,1,1	0
56	MG	BA	3240	1/1	0.95	0.23	15,15,15,15	0
56	MG	AA	1777	1/1	0.95	0.11	55,55,55,55	0
56	MG	AA	1812	1/1	0.95	0.12	50,50,50,50	0
56	MG	CA	1620	1/1	0.95	0.16	32,32,32,32	0
56	MG	CA	1781	1/1	0.95	0.17	29,29,29,29	0
56	MG	DA	3236	1/1	0.95	0.13	54,54,54,54	0
56	MG	CA	1785	1/1	0.95	0.14	44,44,44,44	0
56	MG	BA	3364	1/1	0.95	0.13	35,35,35,35	0
56	MG	DA	3241	1/1	0.95	0.10	12,12,12,12	0
56	MG	CA	1625	1/1	0.95	0.20	19,19,19,19	0
56	MG	CA	1626	1/1	0.95	0.14	11,11,11,11	0
56	MG	AA	1814	1/1	0.95	0.12	25,25,25,25	0
56	MG	BA	3248	1/1	0.95	0.21	33,33,33,33	0
56	MG	CA	1636	1/1	0.95	0.13	36,36,36,36	0
56	MG	DA	3253	1/1	0.95	0.15	71,71,71,71	0
56	MG	AA	1687	1/1	0.95	0.12	10,10,10,10	0
56	MG	BA	3252	1/1	0.95	0.14	25,25,25,25	0
56	MG	AA	1781	1/1	0.95	0.23	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3005	1/1	0.95	0.11	26,26,26,26	0
56	MG	AA	1607	1/1	0.95	0.07	12,12,12,12	0
56	MG	BA	3148	1/1	0.95	0.17	37,37,37,37	0
56	MG	BA	3012	1/1	0.95	0.13	20,20,20,20	0
56	MG	AA	1673	1/1	0.95	0.10	26,26,26,26	0
56	MG	BA	3380	1/1	0.95	0.33	77,77,77,77	0
56	MG	AA	1721	1/1	0.95	0.10	28,28,28,28	0
56	MG	BA	3019	1/1	0.95	0.32	0,0,0,0	0
56	MG	BA	3026	1/1	0.95	0.22	0,0,0,0	0
56	MG	AA	1725	1/1	0.95	0.15	53,53,53,53	0
56	MG	BA	3392	1/1	0.95	0.11	8,8,8,8	0
56	MG	CA	1658	1/1	0.95	0.10	40,40,40,40	0
56	MG	AA	1726	1/1	0.95	0.11	12,12,12,12	0
56	MG	DA	3001	1/1	0.95	0.15	20,20,20,20	0
56	MG	BA	3033	1/1	0.95	0.20	30,30,30,30	0
56	MG	DA	3285	1/1	0.95	0.20	15,15,15,15	0
56	MG	BA	3399	1/1	0.95	0.19	27,27,27,27	0
56	MG	CA	1667	1/1	0.95	0.20	41,41,41,41	0
56	MG	DA	3007	1/1	0.95	0.31	39,39,39,39	0
56	MG	BA	3034	1/1	0.95	0.09	0,0,0,0	0
56	MG	BA	3401	1/1	0.95	0.22	48,48,48,48	0
56	MG	BA	3402	1/1	0.95	0.18	19,19,19,19	0
56	MG	BA	3035	1/1	0.95	0.28	10,10,10,10	0
56	MG	DA	3014	1/1	0.95	0.18	4,4,4,4	0
56	MG	BA	3405	1/1	0.95	0.09	11,11,11,11	0
56	MG	DA	3314	1/1	0.95	0.10	16,16,16,16	0
56	MG	DA	3019	1/1	0.95	0.24	0,0,0,0	0
56	MG	BA	3406	1/1	0.95	0.16	18,18,18,18	0
56	MG	AW	105	1/1	0.95	0.09	64,64,64,64	0
56	MG	AW	106	1/1	0.95	0.06	26,26,26,26	0
56	MG	AA	1789	1/1	0.95	0.13	18,18,18,18	0
56	MG	DA	3037	1/1	0.95	0.12	4,4,4,4	0
56	MG	DA	3328	1/1	0.95	0.10	27,27,27,27	0
56	MG	CA	1683	1/1	0.95	0.10	2,2,2,2	0
56	MG	AA	1650	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3179	1/1	0.95	0.09	28,28,28,28	0
56	MG	AW	112	1/1	0.95	0.16	29,29,29,29	0
56	MG	CA	1690	1/1	0.95	0.09	19,19,19,19	0
56	MG	BA	3069	1/1	0.95	0.15	36,36,36,36	0
56	MG	DA	3061	1/1	0.95	0.25	0,0,0,0	0
56	MG	CA	1692	1/1	0.95	0.09	19,19,19,19	0
56	MG	BA	3183	1/1	0.95	0.07	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	DA	3346	1/1	0.95	0.08	29,29,29,29	0
56	MG	BA	3416	1/1	0.95	0.15	16,16,16,16	0
56	MG	BA	3287	1/1	0.95	0.21	46,46,46,46	0
56	MG	DA	3082	1/1	0.95	0.18	10,10,10,10	0
56	MG	DA	3084	1/1	0.95	0.10	29,29,29,29	0
56	MG	AA	1756	1/1	0.95	0.22	15,15,15,15	0
56	MG	DA	3354	1/1	0.95	0.06	2,2,2,2	0
56	MG	BA	3292	1/1	0.95	0.12	14,14,14,14	0
56	MG	DA	3093	1/1	0.95	0.08	16,16,16,16	0
56	MG	BA	3426	1/1	0.95	0.09	3,3,3,3	0
56	MG	DA	3361	1/1	0.95	0.27	5,5,5,5	0
56	MG	BA	3195	1/1	0.95	0.19	16,16,16,16	0
56	MG	DA	3364	1/1	0.95	0.11	57,57,57,57	0
56	MG	CA	1705	1/1	0.95	0.15	22,22,22,22	0
56	MG	DA	3115	1/1	0.95	0.11	16,16,16,16	0
56	MG	BA	3197	1/1	0.95	0.12	18,18,18,18	0
56	MG	BA	3430	1/1	0.95	0.21	30,30,30,30	0
56	MG	DA	3373	1/1	0.95	0.11	28,28,28,28	0
56	MG	DA	3374	1/1	0.95	0.17	50,50,50,50	0
56	MG	AA	1631	1/1	0.95	0.28	21,21,21,21	0
56	MG	BA	3201	1/1	0.95	0.20	21,21,21,21	0
56	MG	BA	3072	1/1	0.95	0.20	13,13,13,13	0
56	MG	BA	3205	1/1	0.95	0.11	0,0,0,0	0
56	MG	BA	3438	1/1	0.95	0.10	25,25,25,25	0
56	MG	DA	3384	1/1	0.95	0.08	25,25,25,25	0
56	MG	BA	3075	1/1	0.95	0.19	0,0,0,0	0
56	MG	BA	3441	1/1	0.95	0.10	33,33,33,33	0
56	MG	DA	3142	1/1	0.95	0.08	52,52,52,52	0
56	MG	BA	3309	1/1	0.95	0.15	14,14,14,14	0
56	MG	BA	3311	1/1	0.95	0.08	2,2,2,2	0
56	MG	DA	3145	1/1	0.95	0.11	27,27,27,27	0
56	MG	DA	3146	1/1	0.95	0.15	22,22,22,22	0
56	MG	DA	3147	1/1	0.95	0.12	19,19,19,19	0
56	MG	DB	203	1/1	0.95	0.14	33,33,33,33	0
56	MG	BA	3207	1/1	0.95	0.14	0,0,0,0	0
56	MG	AA	1602	1/1	0.95	0.12	39,39,39,39	0
56	MG	DA	3150	1/1	0.95	0.18	40,40,40,40	0
56	MG	BA	3449	1/1	0.95	0.14	27,27,27,27	0
56	MG	BA	3317	1/1	0.95	0.16	50,50,50,50	0
56	MG	BA	3091	1/1	0.95	0.15	20,20,20,20	0
56	MG	DB	211	1/1	0.95	0.07	45,45,45,45	0
56	MG	CA	1727	1/1	0.95	0.23	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DE	301	1/1	0.95	0.23	18,18,18,18	0
56	MG	BA	3093	1/1	0.95	0.13	15,15,15,15	0
56	MG	AA	1612	1/1	0.95	0.12	31,31,31,31	0
56	MG	AA	1634	1/1	0.95	0.22	34,34,34,34	0
56	MG	DA	3162	1/1	0.95	0.21	35,35,35,35	0
56	MG	AA	1666	1/1	0.95	0.18	1,1,1,1	0
56	MG	AA	1706	1/1	0.95	0.09	10,10,10,10	0
56	MG	AX	104	1/1	0.95	0.16	44,44,44,44	0
56	MG	BA	3112	1/1	0.95	0.13	31,31,31,31	0
56	MG	BA	3017	1/1	0.96	0.09	19,19,19,19	0
56	MG	DA	3192	1/1	0.96	0.13	17,17,17,17	0
56	MG	CA	1780	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3116	1/1	0.96	0.30	12,12,12,12	0
56	MG	DA	3199	1/1	0.96	0.09	26,26,26,26	0
56	MG	DA	3200	1/1	0.96	0.17	26,26,26,26	0
56	MG	CA	1782	1/1	0.96	0.10	29,29,29,29	0
56	MG	DA	3202	1/1	0.96	0.20	37,37,37,37	0
56	MG	AA	1779	1/1	0.96	0.16	46,46,46,46	0
56	MG	AA	1667	1/1	0.96	0.23	50,50,50,50	0
56	MG	DA	3205	1/1	0.96	0.09	19,19,19,19	0
56	MG	DA	3206	1/1	0.96	0.09	47,47,47,47	0
56	MG	BA	3120	1/1	0.96	0.08	23,23,23,23	0
56	MG	CA	1648	1/1	0.96	0.13	34,34,34,34	0
56	MG	BA	3021	1/1	0.96	0.23	17,17,17,17	0
56	MG	BA	3304	1/1	0.96	0.10	35,35,35,35	0
56	MG	BA	3411	1/1	0.96	0.18	62,62,62,62	0
56	MG	CU	101	1/1	0.96	0.11	38,38,38,38	0
56	MG	DA	3215	1/1	0.96	0.05	31,31,31,31	0
56	MG	BA	3305	1/1	0.96	0.20	30,30,30,30	0
56	MG	CA	1656	1/1	0.96	0.08	14,14,14,14	0
56	MG	BA	3022	1/1	0.96	0.14	25,25,25,25	0
56	MG	BA	3125	1/1	0.96	0.31	18,18,18,18	0
56	MG	DA	3222	1/1	0.96	0.23	24,24,24,24	0
56	MG	AA	1623	1/1	0.96	0.11	32,32,32,32	0
56	MG	BA	3128	1/1	0.96	0.16	18,18,18,18	0
56	MG	CW	106	1/1	0.96	0.06	50,50,50,50	1
56	MG	BA	3417	1/1	0.96	0.30	29,29,29,29	0
56	MG	BA	3315	1/1	0.96	0.13	43,43,43,43	0
56	MG	CA	1668	1/1	0.96	0.09	42,42,42,42	0
56	MG	DA	3234	1/1	0.96	0.10	33,33,33,33	0
56	MG	BA	3420	1/1	0.96	0.25	59,59,59,59	1
56	MG	BA	3421	1/1	0.96	0.05	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3220	1/1	0.96	0.14	29,29,29,29	0
56	MG	BA	3423	1/1	0.96	0.16	21,21,21,21	0
56	MG	AA	1760	1/1	0.96	0.08	48,48,48,48	0
56	MG	DA	3243	1/1	0.96	0.08	3,3,3,3	0
56	MG	BA	3029	1/1	0.96	0.22	30,30,30,30	0
56	MG	AA	1703	1/1	0.96	0.22	23,23,23,23	0
56	MG	DA	3247	1/1	0.96	0.21	18,18,18,18	0
56	MG	CA	1677	1/1	0.96	0.10	28,28,28,28	0
56	MG	BA	3032	1/1	0.96	0.07	17,17,17,17	0
56	MG	CA	1681	1/1	0.96	0.07	40,40,40,40	0
56	MG	DA	3251	1/1	0.96	0.16	20,20,20,20	0
56	MG	AA	1741	1/1	0.96	0.06	38,38,38,38	0
56	MG	BA	3324	1/1	0.96	0.15	18,18,18,18	1
56	MG	BA	3326	1/1	0.96	0.11	49,49,49,49	0
56	MG	BA	3327	1/1	0.96	0.09	30,30,30,30	0
56	MG	AA	1742	1/1	0.96	0.40	45,45,45,45	0
56	MG	DA	3011	1/1	0.96	0.20	11,11,11,11	0
56	MG	DA	3264	1/1	0.96	0.10	11,11,11,11	0
56	MG	AA	1669	1/1	0.96	0.40	38,38,38,38	0
56	MG	BA	3038	1/1	0.96	0.22	10,10,10,10	0
56	MG	DA	3269	1/1	0.96	0.35	33,33,33,33	0
56	MG	BA	3040	1/1	0.96	0.05	22,22,22,22	0
56	MG	DA	3271	1/1	0.96	0.32	7,7,7,7	0
56	MG	DA	3018	1/1	0.96	0.09	3,3,3,3	0
56	MG	CA	1693	1/1	0.96	0.15	18,18,18,18	1
56	MG	AA	1787	1/1	0.96	0.09	15,15,15,15	0
56	MG	BA	3049	1/1	0.96	0.28	36,36,36,36	0
56	MG	BA	3236	1/1	0.96	0.10	3,3,3,3	0
56	MG	BA	3337	1/1	0.96	0.05	57,57,57,57	0
56	MG	BA	3339	1/1	0.96	0.10	0,0,0,0	1
56	MG	AA	1815	1/1	0.96	0.13	36,36,36,36	0
56	MG	DA	3280	1/1	0.96	0.06	16,16,16,16	0
56	MG	DA	3044	1/1	0.96	0.14	15,15,15,15	0
56	MG	AA	1788	1/1	0.96	0.09	16,16,16,16	0
56	MG	DA	3052	1/1	0.96	0.16	0,0,0,0	0
56	MG	DA	3288	1/1	0.96	0.08	25,25,25,25	1
56	MG	DA	3289	1/1	0.96	0.09	18,18,18,18	0
56	MG	DA	3291	1/1	0.96	0.10	0,0,0,0	0
56	MG	DA	3293	1/1	0.96	0.10	2,2,2,2	0
56	MG	CA	1704	1/1	0.96	0.10	5,5,5,5	0
56	MG	DA	3054	1/1	0.96	0.13	5,5,5,5	0
56	MG	BA	3151	1/1	0.96	0.07	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3300	1/1	0.96	0.14	13,13,13,13	0
56	MG	BA	3453	1/1	0.96	0.15	49,49,49,49	0
56	MG	DA	3305	1/1	0.96	0.12	28,28,28,28	0
56	MG	BA	3242	1/1	0.96	0.08	4,4,4,4	0
56	MG	DA	3308	1/1	0.96	0.07	20,20,20,20	0
56	MG	BA	3055	1/1	0.96	0.12	0,0,0,0	0
56	MG	DA	3063	1/1	0.96	0.13	0,0,0,0	0
56	MG	DA	3311	1/1	0.96	0.16	53,53,53,53	0
56	MG	DA	3066	1/1	0.96	0.23	0,0,0,0	0
56	MG	BA	3057	1/1	0.96	0.27	17,17,17,17	0
56	MG	BA	3348	1/1	0.96	0.18	26,26,26,26	0
56	MG	DA	3316	1/1	0.96	0.12	7,7,7,7	0
56	MG	CA	1715	1/1	0.96	0.09	55,55,55,55	0
56	MG	DA	3071	1/1	0.96	0.10	18,18,18,18	0
56	MG	AV	101	1/1	0.96	0.06	5,5,5,5	0
56	MG	DA	3081	1/1	0.96	0.20	4,4,4,4	0
56	MG	BA	3350	1/1	0.96	0.16	32,32,32,32	0
56	MG	AA	1689	1/1	0.96	0.06	50,50,50,50	0
56	MG	BA	3156	1/1	0.96	0.06	28,28,28,28	0
56	MG	BB	211	1/1	0.96	0.10	40,40,40,40	1
56	MG	BA	3065	1/1	0.96	0.09	1,1,1,1	0
56	MG	DA	3094	1/1	0.96	0.09	10,10,10,10	0
56	MG	AA	1680	1/1	0.96	0.18	30,30,30,30	0
56	MG	DA	3098	1/1	0.96	0.09	19,19,19,19	0
56	MG	DA	3337	1/1	0.96	0.06	4,4,4,4	0
56	MG	DA	3338	1/1	0.96	0.08	53,53,53,53	0
56	MG	DA	3100	1/1	0.96	0.22	21,21,21,21	0
56	MG	DA	3340	1/1	0.96	0.10	30,30,30,30	0
56	MG	DA	3101	1/1	0.96	0.13	38,38,38,38	0
56	MG	DA	3102	1/1	0.96	0.11	0,0,0,0	0
56	MG	DA	3105	1/1	0.96	0.18	6,6,6,6	0
56	MG	AA	1611	1/1	0.96	0.15	18,18,18,18	0
56	MG	DA	3109	1/1	0.96	0.15	0,0,0,0	0
56	MG	BA	3162	1/1	0.96	0.19	12,12,12,12	0
56	MG	DA	3349	1/1	0.96	0.12	27,27,27,27	0
56	MG	DA	3112	1/1	0.96	0.07	0,0,0,0	0
56	MG	DA	3113	1/1	0.96	0.09	11,11,11,11	0
56	MG	DA	3352	1/1	0.96	0.11	9,9,9,9	0
56	MG	BA	3163	1/1	0.96	0.13	17,17,17,17	0
56	MG	BA	3165	1/1	0.96	0.17	0,0,0,0	0
56	MG	B5	102	1/1	0.96	0.29	24,24,24,24	0
56	MG	CA	1728	1/1	0.96	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	DA	3126	1/1	0.96	0.08	29,29,29,29	0
56	MG	AA	1671	1/1	0.96	0.12	19,19,19,19	0
56	MG	BO	201	1/1	0.96	0.18	13,13,13,13	0
56	MG	BA	3371	1/1	0.96	0.09	15,15,15,15	0
56	MG	DA	3365	1/1	0.96	0.09	29,29,29,29	0
56	MG	AA	1793	1/1	0.96	0.13	71,71,71,71	0
56	MG	AA	1617	1/1	0.96	0.28	24,24,24,24	0
56	MG	CA	1735	1/1	0.96	0.16	17,17,17,17	0
56	MG	DA	3370	1/1	0.96	0.10	22,22,22,22	0
56	MG	BA	3090	1/1	0.96	0.15	0,0,0,0	0
56	MG	CA	1603	1/1	0.96	0.09	25,25,25,25	0
56	MG	CA	1605	1/1	0.96	0.07	10,10,10,10	0
56	MG	CA	1607	1/1	0.96	0.19	15,15,15,15	0
56	MG	DA	3376	1/1	0.96	0.09	25,25,25,25	0
56	MG	DA	3377	1/1	0.96	0.10	6,6,6,6	1
56	MG	CA	1608	1/1	0.96	0.12	0,0,0,0	0
56	MG	BA	3267	1/1	0.96	0.11	43,43,43,43	0
56	MG	AA	1775	1/1	0.96	0.10	29,29,29,29	0
56	MG	AA	1752	1/1	0.96	0.22	25,25,25,25	0
56	MG	BA	3101	1/1	0.96	0.12	3,3,3,3	0
56	MG	CA	1747	1/1	0.96	0.09	28,28,28,28	0
56	MG	CA	1748	1/1	0.96	0.07	7,7,7,7	0
56	MG	AW	108	1/1	0.96	0.12	35,35,35,35	0
56	MG	BA	3381	1/1	0.96	0.10	21,21,21,21	0
56	MG	BA	3184	1/1	0.96	0.16	1,1,1,1	0
56	MG	BA	3186	1/1	0.96	0.16	25,25,25,25	0
56	MG	CA	1756	1/1	0.96	0.14	41,41,41,41	0
56	MG	DA	3398	1/1	0.96	0.13	7,7,7,7	0
56	MG	BA	3006	1/1	0.96	0.26	24,24,24,24	0
56	MG	BA	3389	1/1	0.96	0.09	0,0,0,0	0
56	MG	DA	3167	1/1	0.96	0.11	101,101,101,101	0
56	MG	BA	3191	1/1	0.96	0.23	23,23,23,23	0
56	MG	BA	3280	1/1	0.96	0.12	10,10,10,10	0
56	MG	BA	3193	1/1	0.96	0.22	8,8,8,8	0
56	MG	BA	3394	1/1	0.96	0.10	26,26,26,26	0
56	MG	CA	1632	1/1	0.96	0.06	11,11,11,11	0
56	MG	BA	3104	1/1	0.96	0.18	12,12,12,12	0
56	MG	DB	212	1/1	0.96	0.08	27,27,27,27	0
56	MG	CA	1635	1/1	0.96	0.21	19,19,19,19	0
56	MG	CA	1766	1/1	0.96	0.23	18,18,18,18	0
56	MG	BA	3396	1/1	0.96	0.18	15,15,15,15	0
56	MG	DA	3183	1/1	0.96	0.06	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	DA	3184	1/1	0.96	0.09	10,10,10,10	0
56	MG	AW	109	1/1	0.96	0.06	34,34,34,34	1
56	MG	AA	1628	1/1	0.96	0.14	2,2,2,2	0
56	MG	BA	3015	1/1	0.96	0.15	0,0,0,0	0
56	MG	CA	1641	1/1	0.96	0.16	13,13,13,13	0
56	MG	AA	1778	1/1	0.96	0.14	0,0,0,0	0
56	MG	CW	101	1/1	0.97	0.08	36,36,36,36	0
56	MG	AV	104	1/1	0.97	0.17	27,27,27,27	0
56	MG	CW	103	1/1	0.97	0.05	45,45,45,45	0
56	MG	BA	3194	1/1	0.97	0.13	30,30,30,30	0
56	MG	CW	105	1/1	0.97	0.08	30,30,30,30	0
56	MG	CA	1660	1/1	0.97	0.23	22,22,22,22	0
56	MG	BA	3297	1/1	0.97	0.24	7,7,7,7	0
56	MG	DA	3209	1/1	0.97	0.31	31,31,31,31	0
56	MG	DA	3210	1/1	0.97	0.11	0,0,0,0	0
56	MG	CW	108	1/1	0.97	0.04	10,10,10,10	1
56	MG	CA	1662	1/1	0.97	0.09	18,18,18,18	0
56	MG	BA	3298	1/1	0.97	0.31	25,25,25,25	0
56	MG	BA	3105	1/1	0.97	0.19	13,13,13,13	0
56	MG	BA	3008	1/1	0.97	0.38	22,22,22,22	0
56	MG	CW	113	1/1	0.97	0.05	24,24,24,24	0
56	MG	BA	3418	1/1	0.97	0.11	64,64,64,64	0
56	MG	CA	1669	1/1	0.97	0.06	0,0,0,0	0
56	MG	BA	3108	1/1	0.97	0.11	0,0,0,0	0
56	MG	DA	3220	1/1	0.97	0.10	3,3,3,3	0
56	MG	BA	3302	1/1	0.97	0.18	14,14,14,14	0
56	MG	DA	3223	1/1	0.97	0.31	11,11,11,11	0
56	MG	DA	3225	1/1	0.97	0.25	22,22,22,22	0
56	MG	DA	3226	1/1	0.97	0.08	5,5,5,5	0
56	MG	D5	101	1/1	0.97	0.07	7,7,7,7	0
56	MG	BA	3303	1/1	0.97	0.17	15,15,15,15	0
56	MG	BA	3200	1/1	0.97	0.07	5,5,5,5	1
56	MG	AV	105	1/1	0.97	0.13	12,12,12,12	0
56	MG	BA	3424	1/1	0.97	0.15	38,38,38,38	0
56	MG	BA	3306	1/1	0.97	0.20	20,20,20,20	0
56	MG	BA	3203	1/1	0.97	0.21	14,14,14,14	0
56	MG	BA	3110	1/1	0.97	0.11	0,0,0,0	0
56	MG	BA	3010	1/1	0.97	0.06	30,30,30,30	0
56	MG	BA	3313	1/1	0.97	0.11	21,21,21,21	0
56	MG	BA	3011	1/1	0.97	0.20	0,0,0,0	0
56	MG	BA	3432	1/1	0.97	0.07	15,15,15,15	0
56	MG	AA	1614	1/1	0.97	0.07	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3244	1/1	0.97	0.29	0,0,0,0	0
56	MG	CA	1686	1/1	0.97	0.11	57,57,57,57	0
56	MG	BA	3434	1/1	0.97	0.07	28,28,28,28	0
56	MG	BA	3208	1/1	0.97	0.11	8,8,8,8	0
56	MG	DA	3020	1/1	0.97	0.30	1,1,1,1	0
56	MG	BA	3209	1/1	0.97	0.15	15,15,15,15	0
56	MG	BA	3211	1/1	0.97	0.16	42,42,42,42	0
56	MG	DA	3026	1/1	0.97	0.26	0,0,0,0	0
56	MG	BA	3319	1/1	0.97	0.06	0,0,0,0	0
56	MG	DA	3254	1/1	0.97	0.10	1,1,1,1	0
56	MG	DA	3029	1/1	0.97	0.15	36,36,36,36	0
56	MG	DA	3256	1/1	0.97	0.09	22,22,22,22	0
56	MG	DA	3031	1/1	0.97	0.08	0,0,0,0	0
56	MG	DA	3033	1/1	0.97	0.20	17,17,17,17	1
56	MG	DA	3260	1/1	0.97	0.37	44,44,44,44	0
56	MG	DA	3034	1/1	0.97	0.07	7,7,7,7	0
56	MG	BA	3440	1/1	0.97	0.19	33,33,33,33	0
56	MG	BA	3115	1/1	0.97	0.09	0,0,0,0	0
56	MG	DA	3266	1/1	0.97	0.07	11,11,11,11	0
56	MG	AA	1722	1/1	0.97	0.14	20,20,20,20	0
56	MG	DA	3041	1/1	0.97	0.19	8,8,8,8	0
56	MG	DA	3042	1/1	0.97	0.56	58,58,58,58	0
56	MG	AA	1723	1/1	0.97	0.07	9,9,9,9	0
56	MG	DA	3045	1/1	0.97	0.14	1,1,1,1	0
56	MG	DA	3046	1/1	0.97	0.26	0,0,0,0	0
56	MG	BA	3118	1/1	0.97	0.11	0,0,0,0	0
56	MG	BA	3325	1/1	0.97	0.07	28,28,28,28	0
56	MG	AA	1753	1/1	0.97	0.11	26,26,26,26	0
56	MG	AA	1754	1/1	0.97	0.12	16,16,16,16	0
56	MG	AA	1724	1/1	0.97	0.07	0,0,0,0	0
56	MG	AA	1664	1/1	0.97	0.11	0,0,0,0	0
56	MG	AA	1636	1/1	0.97	0.20	27,27,27,27	1
56	MG	DA	3060	1/1	0.97	0.31	0,0,0,0	0
56	MG	DA	3281	1/1	0.97	0.20	14,14,14,14	1
56	MG	CA	1709	1/1	0.97	0.07	9,9,9,9	0
56	MG	CA	1710	1/1	0.97	0.09	22,22,22,22	0
56	MG	DA	3284	1/1	0.97	0.13	12,12,12,12	0
56	MG	BA	3023	1/1	0.97	0.28	0,0,0,0	0
56	MG	DA	3287	1/1	0.97	0.25	17,17,17,17	0
56	MG	CA	1712	1/1	0.97	0.16	19,19,19,19	0
56	MG	BA	3024	1/1	0.97	0.13	0,0,0,0	0
56	MG	DA	3290	1/1	0.97	0.07	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1603	1/1	0.97	0.13	47,47,47,47	0
56	MG	DA	3070	1/1	0.97	0.18	0,0,0,0	0
56	MG	AA	1762	1/1	0.97	0.14	18,18,18,18	0
56	MG	BA	3136	1/1	0.97	0.21	8,8,8,8	0
56	MG	DA	3076	1/1	0.97	0.13	0,0,0,0	0
56	MG	DA	3080	1/1	0.97	0.17	0,0,0,0	0
56	MG	DA	3301	1/1	0.97	0.08	18,18,18,18	0
56	MG	DA	3302	1/1	0.97	0.09	11,11,11,11	0
56	MG	BA	3138	1/1	0.97	0.17	12,12,12,12	0
56	MG	BB	207	1/1	0.97	0.08	23,23,23,23	0
56	MG	DA	3083	1/1	0.97	0.24	13,13,13,13	0
56	MG	BB	208	1/1	0.97	0.08	27,27,27,27	0
56	MG	AA	1682	1/1	0.97	0.19	17,17,17,17	0
56	MG	AA	1700	1/1	0.97	0.16	31,31,31,31	0
56	MG	AA	1605	1/1	0.97	0.09	16,16,16,16	0
56	MG	AW	114	1/1	0.97	0.10	25,25,25,25	1
56	MG	BA	3235	1/1	0.97	0.06	7,7,7,7	0
56	MG	AA	1766	1/1	0.97	0.11	23,23,23,23	0
56	MG	DA	3099	1/1	0.97	0.12	10,10,10,10	0
56	MG	DA	3317	1/1	0.97	0.06	11,11,11,11	1
56	MG	AA	1798	1/1	0.97	0.14	36,36,36,36	0
56	MG	BB	217	1/1	0.97	0.11	34,34,34,34	0
56	MG	BA	3239	1/1	0.97	0.25	12,12,12,12	0
56	MG	DA	3103	1/1	0.97	0.13	9,9,9,9	0
56	MG	DA	3322	1/1	0.97	0.08	27,27,27,27	0
56	MG	DA	3323	1/1	0.97	0.20	31,31,31,31	0
56	MG	DA	3104	1/1	0.97	0.12	9,9,9,9	0
56	MG	AA	1702	1/1	0.97	0.21	23,23,23,23	0
56	MG	BF	301	1/1	0.97	0.16	17,17,17,17	0
56	MG	AW	119	1/1	0.97	0.06	19,19,19,19	0
56	MG	AA	1801	1/1	0.97	0.20	34,34,34,34	0
56	MG	CA	1733	1/1	0.97	0.14	31,31,31,31	0
56	MG	DA	3332	1/1	0.97	0.06	45,45,45,45	0
56	MG	AA	1641	1/1	0.97	0.06	0,0,0,0	0
56	MG	DA	3114	1/1	0.97	0.09	8,8,8,8	0
56	MG	DA	3336	1/1	0.97	0.17	3,3,3,3	1
56	MG	BA	3245	1/1	0.97	0.11	9,9,9,9	0
56	MG	BA	3246	1/1	0.97	0.14	15,15,15,15	0
56	MG	DA	3117	1/1	0.97	0.06	1,1,1,1	0
56	MG	DA	3118	1/1	0.97	0.09	6,6,6,6	0
56	MG	AW	122	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3363	1/1	0.97	0.09	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3123	1/1	0.97	0.10	20,20,20,20	0
56	MG	DA	3345	1/1	0.97	0.21	17,17,17,17	0
56	MG	AA	1642	1/1	0.97	0.14	8,8,8,8	0
56	MG	AX	103	1/1	0.97	0.08	29,29,29,29	0
56	MG	AA	1621	1/1	0.97	0.10	14,14,14,14	0
56	MG	BA	3368	1/1	0.97	0.07	32,32,32,32	0
56	MG	DA	3136	1/1	0.97	0.21	3,3,3,3	0
56	MG	AA	1806	1/1	0.97	0.23	24,24,24,24	0
56	MG	BA	3063	1/1	0.97	0.25	0,0,0,0	0
56	MG	DA	3139	1/1	0.97	0.09	28,28,28,28	0
56	MG	B1	101	1/1	0.97	0.17	0,0,0,0	0
56	MG	DA	3355	1/1	0.97	0.07	7,7,7,7	0
56	MG	AA	1644	1/1	0.97	0.16	17,17,17,17	0
56	MG	CA	1749	1/1	0.97	0.08	7,7,7,7	0
56	MG	DA	3359	1/1	0.97	0.25	15,15,15,15	0
56	MG	BA	3068	1/1	0.97	0.18	0,0,0,0	0
56	MG	AA	1710	1/1	0.97	0.19	29,29,29,29	0
56	MG	DA	3362	1/1	0.97	0.21	10,10,10,10	1
56	MG	AA	1774	1/1	0.97	0.08	9,9,9,9	0
56	MG	BA	3260	1/1	0.97	0.07	23,23,23,23	0
56	MG	CA	1754	1/1	0.97	0.14	6,6,6,6	0
56	MG	CA	1755	1/1	0.97	0.16	26,26,26,26	1
56	MG	AA	1739	1/1	0.97	0.11	23,23,23,23	0
56	MG	BA	3164	1/1	0.97	0.06	9,9,9,9	0
56	MG	BA	3264	1/1	0.97	0.24	0,0,0,0	0
56	MG	CA	1624	1/1	0.97	0.08	16,16,16,16	0
56	MG	B2	105	1/1	0.97	0.16	0,0,0,0	0
56	MG	DA	3157	1/1	0.97	0.25	34,34,34,34	0
56	MG	BA	3073	1/1	0.97	0.08	4,4,4,4	0
56	MG	BA	3387	1/1	0.97	0.10	38,38,38,38	0
56	MG	CA	1629	1/1	0.97	0.14	10,10,10,10	0
56	MG	CA	1631	1/1	0.97	0.37	48,48,48,48	0
56	MG	DA	3164	1/1	0.97	0.07	8,8,8,8	0
56	MG	AA	1740	1/1	0.97	0.14	40,40,40,40	0
56	MG	DA	3382	1/1	0.97	0.09	6,6,6,6	0
56	MG	DA	3166	1/1	0.97	0.08	0,0,0,0	0
56	MG	BA	3080	1/1	0.97	0.12	0,0,0,0	0
56	MG	CA	1634	1/1	0.97	0.11	17,17,17,17	0
56	MG	DA	3388	1/1	0.97	0.16	15,15,15,15	0
56	MG	BA	3171	1/1	0.97	0.10	0,0,0,0	1
56	MG	BA	3271	1/1	0.97	0.11	33,33,33,33	0
56	MG	CA	1771	1/1	0.97	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3172	1/1	0.97	0.16	22,22,22,22	0
56	MG	BA	3173	1/1	0.97	0.16	14,14,14,14	0
56	MG	BA	3085	1/1	0.97	0.16	0,0,0,0	0
56	MG	DA	3397	1/1	0.97	0.20	31,31,31,31	0
56	MG	CA	1640	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3086	1/1	0.97	0.13	2,2,2,2	0
56	MG	DA	3182	1/1	0.97	0.09	5,5,5,5	0
56	MG	BA	3087	1/1	0.97	0.20	16,16,16,16	0
56	MG	AA	1711	1/1	0.97	0.09	8,8,8,8	0
56	MG	DB	206	1/1	0.97	0.09	0,0,0,0	1
56	MG	AA	1645	1/1	0.97	0.18	25,25,25,25	0
56	MG	AA	1608	1/1	0.97	0.13	47,47,47,47	0
56	MG	BA	3283	1/1	0.97	0.05	36,36,36,36	0
56	MG	AA	1662	1/1	0.97	0.10	31,31,31,31	0
56	MG	BA	3185	1/1	0.97	0.04	9,9,9,9	0
56	MG	DA	3190	1/1	0.97	0.07	2,2,2,2	0
56	MG	AA	1691	1/1	0.97	0.07	11,11,11,11	0
56	MG	BA	3189	1/1	0.97	0.10	3,3,3,3	0
56	MG	CA	1651	1/1	0.97	0.20	31,31,31,31	0
56	MG	DA	3194	1/1	0.97	0.10	0,0,0,0	1
56	MG	DA	3195	1/1	0.97	0.14	0,0,0,0	1
56	MG	DA	3196	1/1	0.97	0.24	18,18,18,18	0
56	MG	DS	201	1/1	0.97	0.45	14,14,14,14	1
56	MG	BA	3291	1/1	0.97	0.05	12,12,12,12	0
56	MG	AV	102	1/1	0.97	0.05	28,28,28,28	0
56	MG	CA	1655	1/1	0.97	0.12	0,0,0,0	0
56	MG	AA	1720	1/1	0.97	0.19	29,29,29,29	0
58	ZN	AN	101	1/1	0.97	0.05	50,50,50,50	0
56	MG	DA	3021	1/1	0.98	0.19	0,0,0,0	0
56	MG	BA	3340	1/1	0.98	0.08	28,28,28,28	0
56	MG	CA	1699	1/1	0.98	0.12	0,0,0,0	0
56	MG	BA	3244	1/1	0.98	0.11	19,19,19,19	0
56	MG	CA	1701	1/1	0.98	0.10	16,16,16,16	0
56	MG	DA	3028	1/1	0.98	0.13	0,0,0,0	0
56	MG	BB	202	1/1	0.98	0.10	14,14,14,14	0
56	MG	DA	3030	1/1	0.98	0.10	0,0,0,0	0
56	MG	DA	3221	1/1	0.98	0.10	11,11,11,11	0
56	MG	CA	1703	1/1	0.98	0.06	19,19,19,19	0
56	MG	DA	3032	1/1	0.98	0.15	59,59,59,59	0
56	MG	DA	3224	1/1	0.98	0.29	2,2,2,2	0
56	MG	BA	3161	1/1	0.98	0.08	11,11,11,11	0
56	MG	AA	1707	1/1	0.98	0.08	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3227	1/1	0.98	0.06	8,8,8,8	0
56	MG	DA	3035	1/1	0.98	0.09	0,0,0,0	0
56	MG	AA	1649	1/1	0.98	0.20	0,0,0,0	0
56	MG	CA	1707	1/1	0.98	0.19	6,6,6,6	0
56	MG	DA	3038	1/1	0.98	0.13	17,17,17,17	0
56	MG	BA	3094	1/1	0.98	0.22	0,0,0,0	0
56	MG	BA	3249	1/1	0.98	0.08	11,11,11,11	0
56	MG	BA	3096	1/1	0.98	0.09	0,0,0,0	0
56	MG	DA	3043	1/1	0.98	0.16	2,2,2,2	0
56	MG	BA	3251	1/1	0.98	0.15	11,11,11,11	0
56	MG	DA	3237	1/1	0.98	0.06	15,15,15,15	0
56	MG	BA	3097	1/1	0.98	0.07	2,2,2,2	0
56	MG	DA	3239	1/1	0.98	0.13	39,39,39,39	0
56	MG	BA	3098	1/1	0.98	0.07	5,5,5,5	0
56	MG	BA	3100	1/1	0.98	0.21	3,3,3,3	0
56	MG	DA	3049	1/1	0.98	0.18	0,0,0,0	0
56	MG	DA	3050	1/1	0.98	0.31	0,0,0,0	0
56	MG	BA	3169	1/1	0.98	0.07	8,8,8,8	0
56	MG	BA	3355	1/1	0.98	0.12	20,20,20,20	0
56	MG	BA	3357	1/1	0.98	0.07	19,19,19,19	0
56	MG	BA	3170	1/1	0.98	0.14	0,0,0,0	0
56	MG	BA	3359	1/1	0.98	0.05	75,75,75,75	0
56	MG	BA	3360	1/1	0.98	0.07	25,25,25,25	0
56	MG	BE	301	1/1	0.98	0.15	8,8,8,8	0
56	MG	DA	3252	1/1	0.98	0.08	0,0,0,0	1
56	MG	B5	101	1/1	0.98	0.15	6,6,6,6	0
56	MG	BA	3031	1/1	0.98	0.20	11,11,11,11	0
56	MG	DA	3064	1/1	0.98	0.20	0,0,0,0	0
56	MG	DA	3065	1/1	0.98	0.25	0,0,0,0	0
56	MG	AA	1624	1/1	0.98	0.07	33,33,33,33	0
56	MG	AA	1679	1/1	0.98	0.07	5,5,5,5	1
56	MG	BA	3176	1/1	0.98	0.07	11,11,11,11	0
56	MG	BA	3262	1/1	0.98	0.06	20,20,20,20	0
56	MG	BA	3177	1/1	0.98	0.07	7,7,7,7	0
56	MG	DA	3263	1/1	0.98	0.16	30,30,30,30	0
56	MG	BA	3369	1/1	0.98	0.12	30,30,30,30	0
56	MG	DA	3265	1/1	0.98	0.08	0,0,0,0	0
56	MG	DA	3072	1/1	0.98	0.05	0,0,0,0	0
56	MG	DA	3073	1/1	0.98	0.10	0,0,0,0	0
56	MG	AA	1692	1/1	0.98	0.19	0,0,0,0	0
56	MG	DA	3075	1/1	0.98	0.22	0,0,0,0	0
56	MG	CA	1604	1/1	0.98	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3077	1/1	0.98	0.17	0,0,0,0	0
56	MG	DA	3079	1/1	0.98	0.14	13,13,13,13	0
56	MG	AA	1813	1/1	0.98	0.14	25,25,25,25	0
56	MG	CA	1606	1/1	0.98	0.18	16,16,16,16	0
56	MG	BA	3036	1/1	0.98	0.13	25,25,25,25	0
56	MG	BA	3037	1/1	0.98	0.17	0,0,0,0	0
56	MG	BA	3182	1/1	0.98	0.09	16,16,16,16	0
56	MG	AA	1713	1/1	0.98	0.13	7,7,7,7	0
56	MG	DA	3087	1/1	0.98	0.30	23,23,23,23	0
56	MG	BA	3270	1/1	0.98	0.07	0,0,0,0	0
56	MG	DA	3089	1/1	0.98	0.11	4,4,4,4	0
56	MG	DA	3090	1/1	0.98	0.11	0,0,0,0	0
56	MG	DA	3091	1/1	0.98	0.13	0,0,0,0	0
56	MG	DA	3092	1/1	0.98	0.10	4,4,4,4	0
56	MG	AA	1639	1/1	0.98	0.14	30,30,30,30	0
56	MG	DA	3286	1/1	0.98	0.10	0,0,0,0	0
56	MG	CA	1613	1/1	0.98	0.21	4,4,4,4	0
56	MG	DA	3095	1/1	0.98	0.22	0,0,0,0	0
56	MG	CA	1614	1/1	0.98	0.12	20,20,20,20	0
56	MG	DA	3097	1/1	0.98	0.12	12,12,12,12	0
56	MG	CA	1743	1/1	0.98	0.18	1,1,1,1	0
56	MG	DA	3292	1/1	0.98	0.08	5,5,5,5	0
56	MG	BA	3041	1/1	0.98	0.14	0,0,0,0	0
56	MG	BA	3273	1/1	0.98	0.14	20,20,20,20	0
56	MG	BA	3113	1/1	0.98	0.24	14,14,14,14	0
56	MG	BA	3042	1/1	0.98	0.08	13,13,13,13	0
56	MG	DA	3299	1/1	0.98	0.10	0,0,0,0	0
56	MG	AA	1757	1/1	0.98	0.06	0,0,0,0	0
56	MG	BA	3386	1/1	0.98	0.07	85,85,85,85	0
56	MG	CA	1621	1/1	0.98	0.18	0,0,0,0	0
56	MG	DA	3303	1/1	0.98	0.10	11,11,11,11	0
56	MG	BA	3044	1/1	0.98	0.18	5,5,5,5	0
56	MG	DA	3107	1/1	0.98	0.27	12,12,12,12	0
56	MG	DA	3306	1/1	0.98	0.22	6,6,6,6	0
56	MG	DA	3108	1/1	0.98	0.25	0,0,0,0	0
56	MG	CA	1623	1/1	0.98	0.09	9,9,9,9	0
56	MG	DA	3110	1/1	0.98	0.21	1,1,1,1	0
56	MG	BA	3045	1/1	0.98	0.12	0,0,0,0	0
56	MG	AW	117	1/1	0.98	0.21	24,24,24,24	0
56	MG	BA	3007	1/1	0.98	0.24	0,0,0,0	0
56	MG	BA	3391	1/1	0.98	0.05	26,26,26,26	0
56	MG	BA	3196	1/1	0.98	0.06	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	DA	3315	1/1	0.98	0.06	4,4,4,4	0
56	MG	CA	1630	1/1	0.98	0.10	0,0,0,0	0
56	MG	AA	1675	1/1	0.98	0.23	4,4,4,4	0
56	MG	BA	3198	1/1	0.98	0.08	0,0,0,0	0
56	MG	DA	3119	1/1	0.98	0.12	7,7,7,7	0
56	MG	BA	3054	1/1	0.98	0.12	0,0,0,0	0
56	MG	DA	3121	1/1	0.98	0.10	12,12,12,12	0
56	MG	BA	3123	1/1	0.98	0.12	6,6,6,6	0
56	MG	BA	3398	1/1	0.98	0.07	9,9,9,9	1
56	MG	DA	3124	1/1	0.98	0.17	0,0,0,0	0
56	MG	DA	3125	1/1	0.98	0.13	0,0,0,0	0
56	MG	DA	3326	1/1	0.98	0.34	25,25,25,25	0
56	MG	AA	1759	1/1	0.98	0.11	5,5,5,5	1
56	MG	DA	3127	1/1	0.98	0.11	0,0,0,0	0
56	MG	DA	3128	1/1	0.98	0.09	0,0,0,0	0
56	MG	BA	3202	1/1	0.98	0.07	0,0,0,0	0
56	MG	DA	3131	1/1	0.98	0.17	0,0,0,0	0
56	MG	AA	1797	1/1	0.98	0.08	26,26,26,26	0
56	MG	BA	3059	1/1	0.98	0.10	16,16,16,16	0
56	MG	DA	3335	1/1	0.98	0.06	10,10,10,10	0
56	MG	DA	3134	1/1	0.98	0.21	4,4,4,4	0
56	MG	DA	3135	1/1	0.98	0.19	7,7,7,7	0
56	MG	BA	3295	1/1	0.98	0.17	16,16,16,16	0
56	MG	BA	3127	1/1	0.98	0.11	8,8,8,8	0
56	MG	CA	1770	1/1	0.98	0.08	14,14,14,14	0
56	MG	AA	1705	1/1	0.98	0.06	21,21,21,21	0
56	MG	AA	1761	1/1	0.98	0.15	16,16,16,16	0
56	MG	DA	3343	1/1	0.98	0.11	4,4,4,4	0
56	MG	DA	3141	1/1	0.98	0.07	0,0,0,0	0
56	MG	CA	1773	1/1	0.98	0.09	13,13,13,13	0
56	MG	CA	1774	1/1	0.98	0.16	21,21,21,21	0
56	MG	BA	3130	1/1	0.98	0.05	4,4,4,4	0
56	MG	BA	3131	1/1	0.98	0.18	0,0,0,0	0
56	MG	BA	3210	1/1	0.98	0.15	11,11,11,11	0
56	MG	BA	3132	1/1	0.98	0.13	2,2,2,2	0
56	MG	BA	3133	1/1	0.98	0.07	11,11,11,11	0
56	MG	BA	3213	1/1	0.98	0.23	19,19,19,19	0
56	MG	CA	1783	1/1	0.98	0.17	13,13,13,13	0
56	MG	CA	1784	1/1	0.98	0.10	15,15,15,15	0
56	MG	BA	3013	1/1	0.98	0.15	0,0,0,0	0
56	MG	BA	3014	1/1	0.98	0.24	7,7,7,7	0
56	MG	DA	3154	1/1	0.98	0.19	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3307	1/1	0.98	0.04	7,7,7,7	0
56	MG	DA	3156	1/1	0.98	0.15	36,36,36,36	0
56	MG	CA	1653	1/1	0.98	0.05	60,60,60,60	0
56	MG	DA	3158	1/1	0.98	0.10	5,5,5,5	0
56	MG	BA	3137	1/1	0.98	0.17	6,6,6,6	0
56	MG	BA	3067	1/1	0.98	0.11	5,5,5,5	0
56	MG	BA	3310	1/1	0.98	0.17	22,22,22,22	0
56	MG	DA	3366	1/1	0.98	0.10	3,3,3,3	0
56	MG	CM	201	1/1	0.98	0.06	21,21,21,21	0
56	MG	DA	3163	1/1	0.98	0.13	51,51,51,51	0
56	MG	AX	101	1/1	0.98	0.05	0,0,0,0	0
56	MG	BA	3312	1/1	0.98	0.19	0,0,0,0	0
56	MG	AA	1800	1/1	0.98	0.06	36,36,36,36	0
56	MG	AA	1652	1/1	0.98	0.09	7,7,7,7	0
56	MG	AA	1744	1/1	0.98	0.30	18,18,18,18	0
56	MG	AA	1718	1/1	0.98	0.15	0,0,0,0	0
56	MG	CA	1664	1/1	0.98	0.14	28,28,28,28	0
56	MG	BA	3020	1/1	0.98	0.26	1,1,1,1	0
56	MG	CA	1666	1/1	0.98	0.06	41,41,41,41	0
56	MG	BA	3427	1/1	0.98	0.06	12,12,12,12	0
56	MG	BA	3145	1/1	0.98	0.15	0,0,0,0	0
56	MG	AA	1746	1/1	0.98	0.11	11,11,11,11	0
56	MG	DA	3178	1/1	0.98	0.10	19,19,19,19	0
56	MG	DA	3179	1/1	0.98	0.05	10,10,10,10	0
56	MG	DA	3385	1/1	0.98	0.07	29,29,29,29	0
56	MG	DA	3386	1/1	0.98	0.28	0,0,0,0	0
56	MG	BA	3076	1/1	0.98	0.15	4,4,4,4	0
56	MG	DA	3181	1/1	0.98	0.10	17,17,17,17	0
56	MG	BA	3321	1/1	0.98	0.20	4,4,4,4	0
56	MG	BA	3077	1/1	0.98	0.22	6,6,6,6	0
56	MG	BA	3078	1/1	0.98	0.20	11,11,11,11	0
56	MG	BA	3079	1/1	0.98	0.17	0,0,0,0	0
56	MG	BA	3232	1/1	0.98	0.10	23,23,23,23	0
56	MG	DA	3395	1/1	0.98	0.18	45,45,45,45	0
56	MG	AW	104	1/1	0.98	0.04	28,28,28,28	0
56	MG	BA	3437	1/1	0.98	0.06	4,4,4,4	0
56	MG	CA	1678	1/1	0.98	0.15	0,0,0,0	0
56	MG	CX	105	1/1	0.98	0.08	41,41,41,41	0
56	MG	BA	3082	1/1	0.98	0.09	22,22,22,22	0
56	MG	BA	3328	1/1	0.98	0.06	30,30,30,30	0
56	MG	BA	3083	1/1	0.98	0.13	20,20,20,20	0
56	MG	AA	1732	1/1	0.98	0.07	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	AA	1719	1/1	0.98	0.11	65,65,65,65	0
56	MG	DA	3003	1/1	0.98	0.07	26,26,26,26	0
56	MG	BA	3443	1/1	0.98	0.04	20,20,20,20	0
56	MG	DA	3198	1/1	0.98	0.09	10,10,10,10	0
56	MG	DA	3005	1/1	0.98	0.07	13,13,13,13	0
56	MG	BA	3444	1/1	0.98	0.09	7,7,7,7	0
56	MG	CA	1687	1/1	0.98	0.08	0,0,0,0	0
56	MG	BA	3445	1/1	0.98	0.14	52,52,52,52	0
56	MG	CA	1689	1/1	0.98	0.07	0,0,0,0	0
56	MG	BA	3238	1/1	0.98	0.20	0,0,0,0	0
56	MG	BA	3025	1/1	0.98	0.14	0,0,0,0	0
56	MG	BA	3334	1/1	0.98	0.17	40,40,40,40	0
56	MG	AW	107	1/1	0.98	0.07	28,28,28,28	0
56	MG	BA	3089	1/1	0.98	0.17	6,6,6,6	0
56	MG	DA	3017	1/1	0.98	0.13	6,6,6,6	0
56	MG	BA	3159	1/1	0.98	0.18	12,12,12,12	0
56	MG	BA	3338	1/1	0.98	0.06	22,22,22,22	1
58	ZN	AD	301	1/1	0.98	0.18	21,21,21,21	0
56	MG	BA	3027	1/1	0.98	0.07	8,8,8,8	0
58	ZN	CD	301	1/1	0.98	0.19	24,24,24,24	0
56	MG	BA	3047	1/1	0.99	0.27	0,0,0,0	0
56	MG	DA	3176	1/1	0.99	0.20	13,13,13,13	0
56	MG	DA	3023	1/1	0.99	0.26	0,0,0,0	0
56	MG	BA	3224	1/1	0.99	0.21	2,2,2,2	0
56	MG	DA	3025	1/1	0.99	0.15	6,6,6,6	0
56	MG	DA	3259	1/1	0.99	0.17	14,14,14,14	0
56	MG	BA	3225	1/1	0.99	0.17	0,0,0,0	0
56	MG	CA	1777	1/1	0.99	0.19	0,0,0,0	0
56	MG	CA	1778	1/1	0.99	0.11	3,3,3,3	0
56	MG	BA	3365	1/1	0.99	0.13	60,60,60,60	0
56	MG	AA	1625	1/1	0.99	0.09	3,3,3,3	0
56	MG	BA	3050	1/1	0.99	0.14	0,0,0,0	0
56	MG	CA	1659	1/1	0.99	0.06	9,9,9,9	0
56	MG	AA	1699	1/1	0.99	0.14	0,0,0,0	0
56	MG	BA	3187	1/1	0.99	0.15	2,2,2,2	0
56	MG	BA	3188	1/1	0.99	0.21	13,13,13,13	0
56	MG	AA	1659	1/1	0.99	0.10	14,14,14,14	1
56	MG	BA	3274	1/1	0.99	0.06	0,0,0,0	0
56	MG	BA	3081	1/1	0.99	0.13	10,10,10,10	0
56	MG	DA	3356	1/1	0.99	0.08	12,12,12,12	0
56	MG	BA	3053	1/1	0.99	0.16	0,0,0,0	0
56	MG	BA	3192	1/1	0.99	0.11	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	AA	1712	1/1	0.99	0.06	22,22,22,22	0
56	MG	BA	3084	1/1	0.99	0.19	0,0,0,0	0
56	MG	BA	3378	1/1	0.99	0.04	54,54,54,54	1
56	MG	AA	1751	1/1	0.99	0.08	19,19,19,19	0
56	MG	BA	3281	1/1	0.99	0.13	0,0,0,0	0
56	MG	DA	3047	1/1	0.99	0.20	0,0,0,0	0
56	MG	BA	3056	1/1	0.99	0.17	0,0,0,0	0
56	MG	BA	3382	1/1	0.99	0.10	63,63,63,63	0
56	MG	BA	3121	1/1	0.99	0.12	2,2,2,2	0
56	MG	DA	3051	1/1	0.99	0.17	0,0,0,0	0
56	MG	BA	3284	1/1	0.99	0.19	14,14,14,14	0
56	MG	BA	3385	1/1	0.99	0.06	12,12,12,12	0
56	MG	DA	3129	1/1	0.99	0.17	6,6,6,6	0
56	MG	DA	3372	1/1	0.99	0.09	12,12,12,12	0
56	MG	B7	101	1/1	0.99	0.07	7,7,7,7	0
56	MG	DA	3055	1/1	0.99	0.20	0,0,0,0	0
56	MG	CA	1679	1/1	0.99	0.05	4,4,4,4	0
56	MG	CA	1740	1/1	0.99	0.07	19,19,19,19	0
56	MG	BA	3058	1/1	0.99	0.20	0,0,0,0	0
56	MG	DA	3378	1/1	0.99	0.10	8,8,8,8	0
56	MG	DA	3059	1/1	0.99	0.21	0,0,0,0	0
56	MG	DA	3294	1/1	0.99	0.19	0,0,0,0	0
56	MG	DA	3295	1/1	0.99	0.06	6,6,6,6	0
56	MG	AA	1613	1/1	0.99	0.22	2,2,2,2	0
56	MG	BA	3060	1/1	0.99	0.22	0,0,0,0	0
56	MG	DA	3062	1/1	0.99	0.27	13,13,13,13	0
56	MG	BA	3289	1/1	0.99	0.17	41,41,41,41	0
56	MG	BA	3290	1/1	0.99	0.08	2,2,2,2	0
56	MG	AA	1610	1/1	0.99	0.15	0,0,0,0	0
56	MG	BA	3092	1/1	0.99	0.19	0,0,0,0	0
56	MG	CX	101	1/1	0.99	0.15	3,3,3,3	0
56	MG	DA	3390	1/1	0.99	0.08	73,73,73,73	0
56	MG	BA	3062	1/1	0.99	0.23	0,0,0,0	0
56	MG	CA	1628	1/1	0.99	0.11	35,35,35,35	0
56	MG	BA	3341	1/1	0.99	0.17	21,21,21,21	0
56	MG	AA	1637	1/1	0.99	0.15	0,0,0,0	0
56	MG	BA	3397	1/1	0.99	0.10	32,32,32,32	0
56	MG	BA	3095	1/1	0.99	0.12	0,0,0,0	0
56	MG	AA	1728	1/1	0.99	0.08	2,2,2,2	0
56	MG	AA	1704	1/1	0.99	0.07	0,0,0,0	0
56	MG	DB	201	1/1	0.99	0.06	19,19,19,19	0
56	MG	BA	3066	1/1	0.99	0.08	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	BA	3134	1/1	0.99	0.11	1,1,1,1	0
56	MG	DA	3078	1/1	0.99	0.20	2,2,2,2	0
56	MG	BA	3099	1/1	0.99	0.21	1,1,1,1	0
56	MG	BA	3404	1/1	0.99	0.29	17,17,17,17	0
56	MG	BA	3039	1/1	0.99	0.31	31,31,31,31	0
56	MG	AA	1771	1/1	0.99	0.07	6,6,6,6	0
56	MG	AA	1656	1/1	0.99	0.16	12,12,12,12	0
56	MG	BA	3352	1/1	0.99	0.10	30,30,30,30	1
56	MG	DA	3085	1/1	0.99	0.20	0,0,0,0	0
56	MG	BA	3175	1/1	0.99	0.07	0,0,0,0	0
56	MG	DD	301	1/1	0.99	0.14	1,1,1,1	0
56	MG	AA	1646	1/1	0.99	0.17	3,3,3,3	0
56	MG	DA	3242	1/1	0.99	0.14	9,9,9,9	0
56	MG	AA	1696	1/1	0.99	0.09	0,0,0,0	0
56	MG	DA	3013	1/1	0.99	0.12	1,1,1,1	0
56	MG	DA	3327	1/1	0.99	0.08	6,6,6,6	0
56	MG	BA	3356	1/1	0.99	0.08	37,37,37,37	0
56	MG	DA	3015	1/1	0.99	0.10	0,0,0,0	0
56	MG	AA	1805	1/1	0.99	0.23	0,0,0,0	0
56	MG	BB	216	1/1	0.99	0.27	11,11,11,11	1
56	MG	BA	3106	1/1	0.99	0.18	0,0,0,0	0
56	MG	AA	1672	1/1	0.99	0.14	0,0,0,0	0
56	MG	BA	3074	1/1	0.99	0.19	10,10,10,10	0
56	MG	BA	3046	1/1	0.99	0.25	0,0,0,0	0
56	MG	DA	3174	1/1	0.99	0.23	26,26,26,26	0
58	ZN	CN	101	1/1	0.99	0.10	53,53,53,53	0
56	MG	DA	3039	1/1	1.00	0.17	10,10,10,10	0
56	MG	BA	3048	1/1	1.00	0.19	0,0,0,0	0

6.5 Other polymers ⓘ

There are no such residues in this entry.