wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 09:04 PM EST

PDB ID	:	4WQU
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with elongation factor G trapped by the antibiotic dityromycin
Authors	:	Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on	:	2014-10-22
Resolution	:	2.80 Å(reported)

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

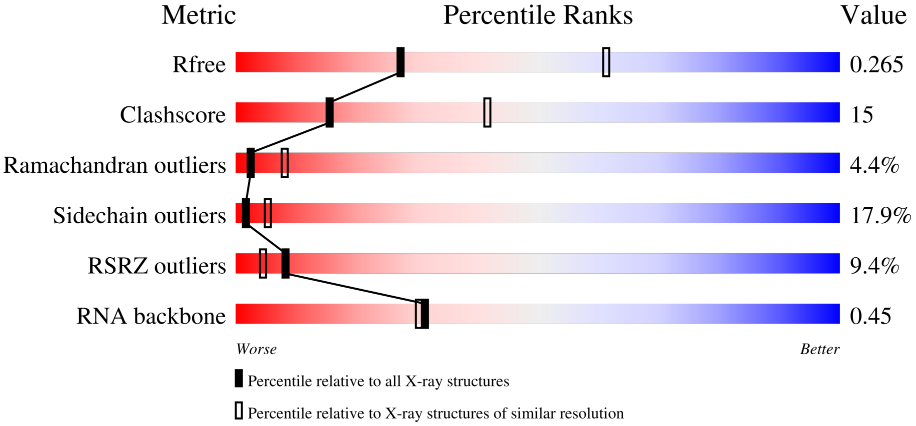
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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

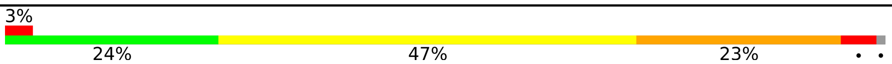
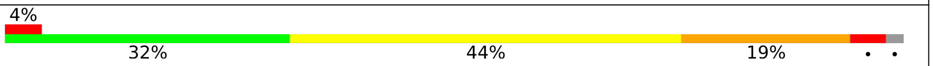
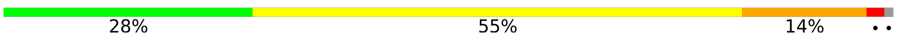
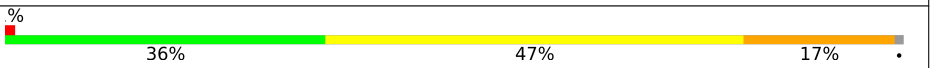
The reported resolution of this entry is 2.80 Å.

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	2915	
1	CA	2915	
2	AB	121	
2	CB	121	

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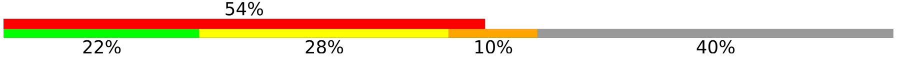
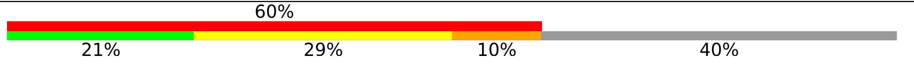
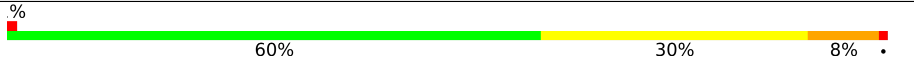
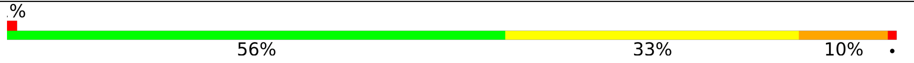
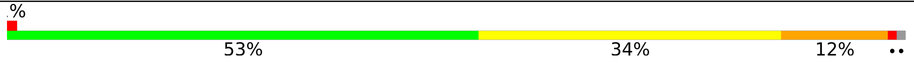
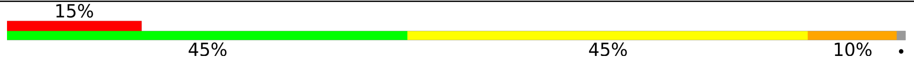
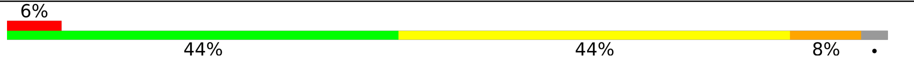
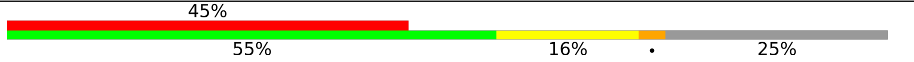
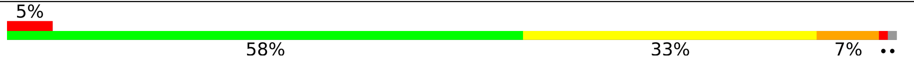
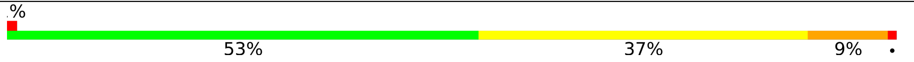
Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150	
13	CP	150	
14	AQ	141	
14	CQ	141	
15	AR	118	

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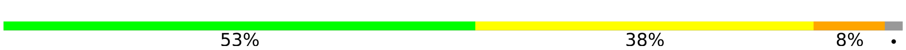
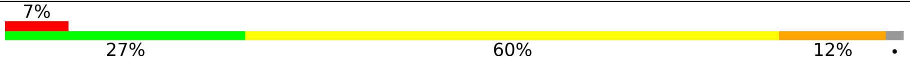
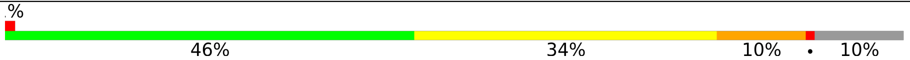
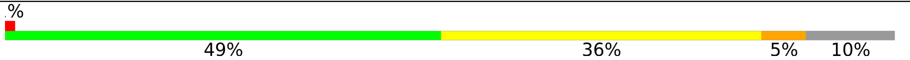
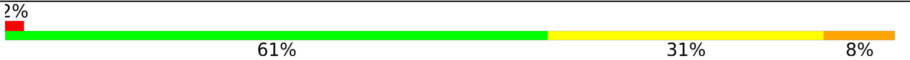
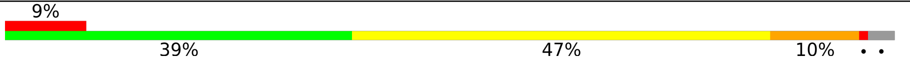
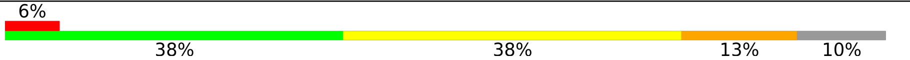
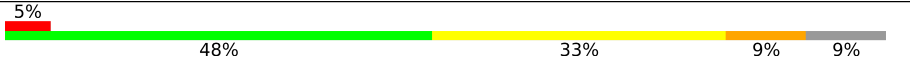
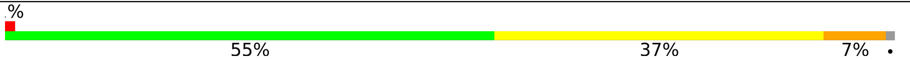
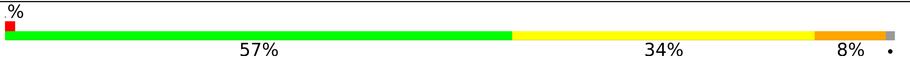
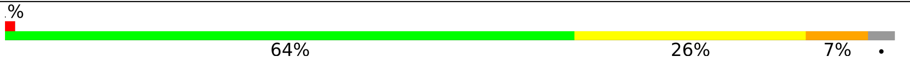
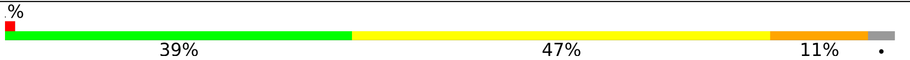
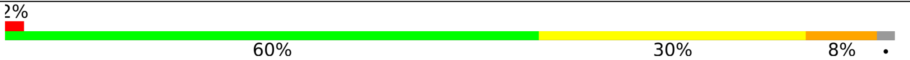
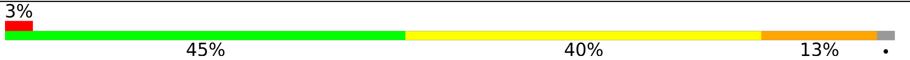
Mol	Chain	Length	Quality of chain
15	CR	118	 58% 31% 9% •
16	AS	112	 53% 38% 8% •
16	CS	112	 7% 27% 60% 12% •
17	AT	146	 % 46% 34% 10% • 10%
17	CT	146	 % 49% 36% 5% 10%
18	AU	118	 62% 31% • • •
18	CU	118	 58% 31% 9% •
19	AV	101	 72% 24% •
19	CV	101	 2% 61% 31% 8%
20	AW	113	 61% 31% 5% • •
20	CW	113	 60% 32% 7% •
21	AX	96	 68% 27% • •
21	CX	96	 4% 51% 43% • • •
22	AY	110	 % 51% 35% 12% •
22	CY	110	 9% 39% 47% 10% • •
23	AZ	206	 46% 32% 9% • 10%
23	CZ	206	 6% 38% 38% 13% 10%
24	A0	85	 65% 19% 6% • 9%
24	C0	85	 5% 48% 33% 9% 9%
25	A1	98	 % 55% 37% 7% •
25	C1	98	 % 57% 34% 8% •
26	A2	72	 % 64% 26% 7% •
26	C2	72	 % 39% 47% 11% •
27	A3	60	 2% 60% 30% 8% •
27	C3	60	 3% 45% 40% 13% •

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Mol	Chain	Length	Quality of chain
28	A4	71	17% 35% 52% 10% •
28	C4	71	30% 39% 42% 15% •
29	A5	60	67% 28% • •
29	C5	60	2% 57% 38% • •
30	A6	54	44% 44% 9% •
30	C6	54	50% 35% 13% •
31	A7	49	2% 61% 29% 6% • •
31	C7	49	63% 24% 10% •
32	A8	65	48% 43% 6% • •
32	C8	65	51% 45% • •
33	A9	37	57% 38% 5%
33	C9	37	46% 49% 5%
34	BA	1521	3% 31% 48% 17% • •
34	DA	1521	6% 34% 48% 16% • •
35	BB	256	9% 46% 34% 8% • 10%
35	DB	256	21% 39% 39% 12% 10%
36	BC	239	9% 48% 33% 5% 14%
36	DC	239	28% 44% 39% • 14%
37	BD	209	5% 52% 38% 8% •
37	DD	209	% 47% 42% 10%
38	BE	162	46% 35% 10% • 9%
38	DE	162	4% 38% 38% 15% • 9%
39	BF	101	52% 37% 10% •
39	DF	101	2% 54% 38% 7% •
40	BG	156	12% 54% 37% 8% • •

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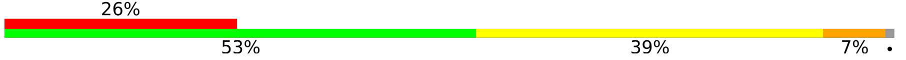
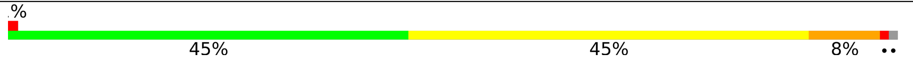
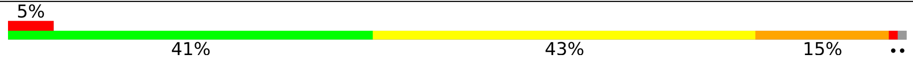
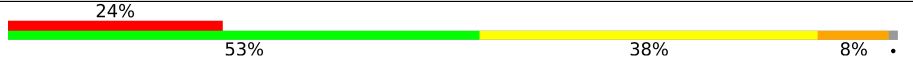
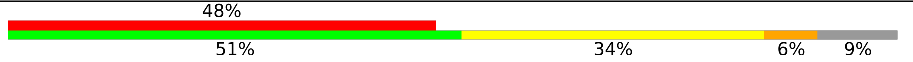
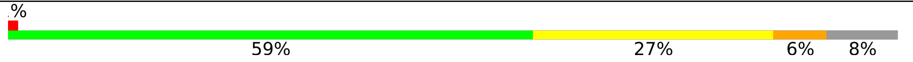
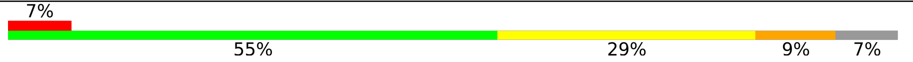
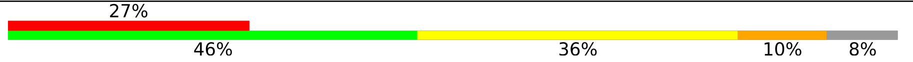
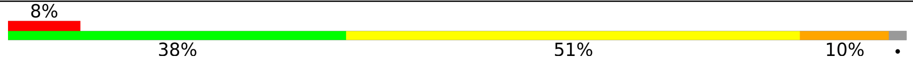
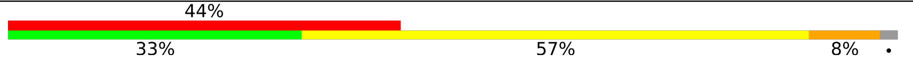
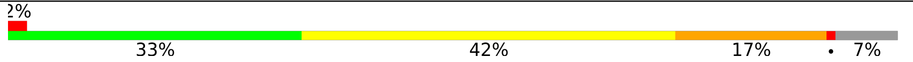
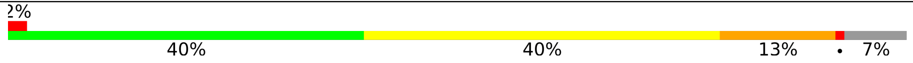
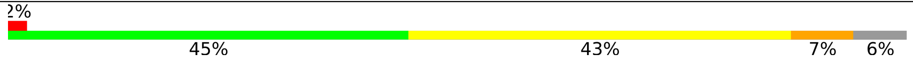
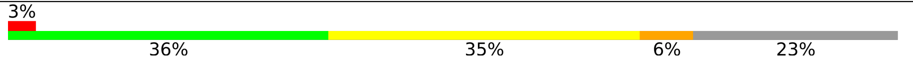
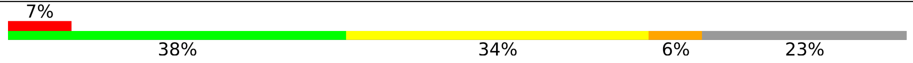
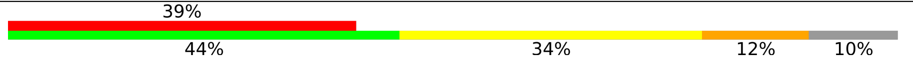
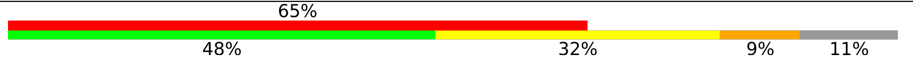
Mol	Chain	Length	Quality of chain
40	DG	156	
41	BH	138	
41	DH	138	
42	BI	128	
42	DI	128	
43	BJ	105	
43	DJ	105	
44	BK	129	
44	DK	129	
45	BL	132	
45	DL	132	
46	BM	126	
46	DM	126	
47	BN	61	
47	DN	61	
48	BO	89	
48	DO	89	
49	BP	88	
49	DP	88	
50	BQ	105	
50	DQ	105	
51	BR	88	
51	DR	88	
52	BS	93	
52	DS	93	

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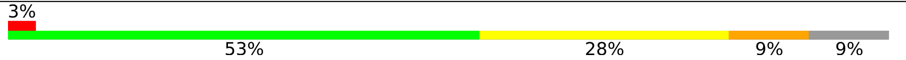
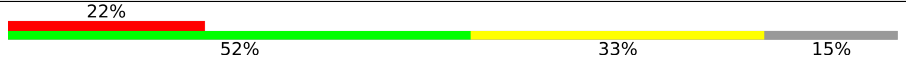
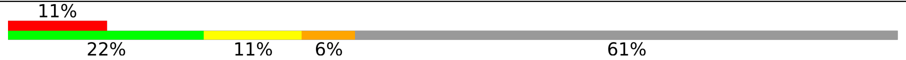
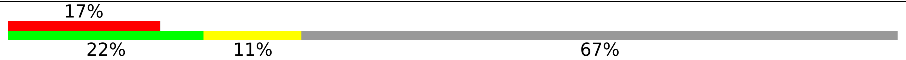
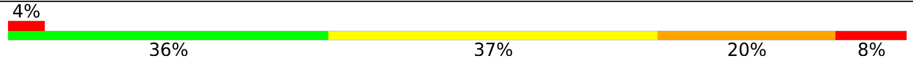
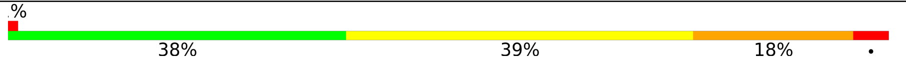
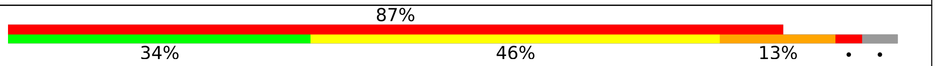
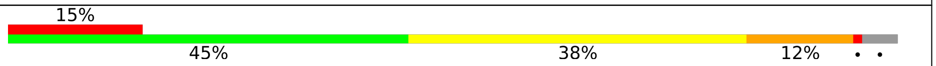
Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	18	
55	DV	18	
56	BW	76	
56	BY	76	
56	DW	76	
56	DY	76	
57	BZ	758	
57	DZ	758	
58	BX	10	
58	DX	10	

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	PSU	BY	32	-	-	-	X
56	MIA	BY	37	-	-	-	X
56	PSU	BY	39	-	-	-	X
56	5MU	BY	54	-	-	-	X
56	PSU	BY	55	-	-	-	X
56	PSU	DY	32	-	-	-	X
56	MIA	DY	37	-	-	-	X
56	PSU	DY	39	-	-	-	X
56	7MG	DY	46	-	-	-	X
56	5MU	DY	54	-	-	-	X
56	PSU	DY	55	-	-	-	X
56	4SU	DY	8	-	-	-	X
58	2QY	DX	10	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3016	-	-	-	X
59	MG	AA	3067	-	-	-	X
59	MG	AA	3108	-	-	-	X
59	MG	AA	3122	-	-	-	X
59	MG	AA	3140	-	-	-	X
59	MG	AA	3212	-	-	-	X
59	MG	AA	3238	-	-	-	X
59	MG	AA	3266	-	-	-	X
59	MG	AA	3273	-	-	-	X
59	MG	AA	3277	-	-	-	X
59	MG	AA	3582	-	-	-	X
59	MG	AA	3712	-	-	-	X
59	MG	AA	3717	-	-	-	X
59	MG	AA	3773	-	-	-	X
59	MG	AA	3814	-	-	-	X
59	MG	AA	3816	-	-	-	X
59	MG	AA	3820	-	-	-	X
59	MG	AD	305	-	-	-	X
59	MG	AE	301	-	-	-	X
59	MG	AF	305	-	-	-	X
59	MG	BA	1665	-	-	-	X
59	MG	BA	1691	-	-	-	X
59	MG	BA	1697	-	-	-	X
59	MG	BA	1698	-	-	-	X
59	MG	BA	1767	-	-	-	X
59	MG	CA	3030	-	-	-	X
59	MG	CA	3037	-	-	-	X
59	MG	CA	3040	-	-	-	X
59	MG	CA	3041	-	-	-	X
59	MG	CA	3075	-	-	-	X
59	MG	CA	3082	-	-	-	X
59	MG	CA	3084	-	-	-	X
59	MG	CA	3089	-	-	-	X
59	MG	CA	3092	-	-	-	X
59	MG	CA	3093	-	-	-	X
59	MG	CA	3101	-	-	-	X
59	MG	CA	3127	-	-	-	X
59	MG	CA	3139	-	-	-	X
59	MG	CA	3146	-	-	-	X
59	MG	CA	3186	-	-	-	X
59	MG	CA	3205	-	-	-	X
59	MG	CA	3208	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	3216	-	-	-	X
59	MG	CA	3236	-	-	-	X
59	MG	CA	3237	-	-	-	X
59	MG	CA	3240	-	-	-	X
59	MG	CA	3460	-	-	-	X
59	MG	CA	3499	-	-	-	X
59	MG	CA	3501	-	-	-	X
59	MG	CA	3502	-	-	-	X
59	MG	CA	3514	-	-	-	X
59	MG	CA	3542	-	-	-	X
59	MG	CA	3600	-	-	-	X
59	MG	CA	3620	-	-	-	X
59	MG	CV	201	-	-	-	X
59	MG	DA	1639	-	-	-	X
59	MG	DA	1724	-	-	-	X
59	MG	DA	1738	-	-	-	X
59	MG	DA	1754	-	-	-	X
59	MG	DA	1756	-	-	-	X
59	MG	DA	1757	-	-	-	X
59	MG	DA	1769	-	-	-	X
59	MG	DT	3001	-	-	-	X
61	SF4	DD	501	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 310038 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2872	Total 61861	C 27532	N 11574	O 19884	P 2871	0	0	0
1	CA	2868	Total 61771	C 27492	N 11554	O 19858	P 2867	0	0	0

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0
2	CB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	137	Total 1063	C 669	N 201	O 192	S 1	0	0	0
3	CC	137	Total 1063	C 669	N 201	O 192	S 1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	275	Total 2136	C 1349	N 423	O 361	S 3	0	0	0
4	CD	275	Total 2142	C 1352	N 426	O 361	S 3	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	AE	204	Total C N O S 1559 985 298 270 6	0	0	0
5	CE	204	Total C N O S 1559 985 298 270 6	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	AF	203	Total C N O S 1584 1009 298 275 2	0	0	1
6	CF	203	Total C N O S 1580 1007 297 274 2	0	0	1

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	AG	181	Total C N O S 1425 914 256 251 4	0	0	0
7	CG	181	Total C N O S 1424 911 258 251 4	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	AH	174	Total C N O S 1330 845 248 236 1	0	0	0
8	CH	174	Total C N O S 1330 845 248 236 1	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	AK	130	Total C N O 641 381 130 130	0	0	0
9	CK	130	Total C N O 641 381 130 130	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	AL	66	Total C N O S 498 310 93 92 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	CL	66	498	310	93	92	3	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AN	140	1117	719	207	187	4	0	0	0
11	CN	140	1117	719	207	187	4	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AP	149	1139	709	231	196	3	0	0	0
13	CP	149	1135	706	230	196	3	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AQ	141	1122	715	212	188	7	0	0	0
14	CQ	141	1122	715	212	188	7	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AR	118	968	604	203	160	1	0	0	0
15	CR	118	968	604	203	160	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AS	110	Total 877	C 553	N 175	O 149	0	0	0
16	CS	110	Total 870	C 549	N 173	O 148	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	131	Total 1091	C 680	N 225	O 185	S 1	0	0	0
17	CT	131	Total 1083	C 675	N 224	O 183	S 1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AU	116	Total 959	C 608	N 201	O 149	S 1	0	0	0
18	CU	116	Total 959	C 608	N 201	O 149	S 1	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	101	Total 771	C 495	N 140	O 135	S 1	0	0	0
19	CV	101	Total 771	C 495	N 140	O 135	S 1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	112	Total 886	C 557	N 174	O 153	S 2	0	0	0
20	CW	112	Total 886	C 557	N 174	O 153	S 2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	AX	95	Total C N O S 750 488 135 126 1	0	0	0
21	CX	95	Total C N O S 750 488 135 126 1	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	AY	107	Total C N O S 806 517 152 131 6	0	0	0
22	CY	107	Total C N O S 806 517 152 131 6	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	AZ	185	Total C N O S 1451 927 258 264 2	0	0	0
23	CZ	185	Total C N O S 1451 927 258 264 2	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	A0	77	Total C N O S 608 375 129 103 1	0	0	0
24	C0	77	Total C N O S 608 375 129 103 1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	A1	97	Total C N O S 755 475 148 131 1	0	0	0
25	C1	97	Total C N O S 755 475 148 131 1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	A2	70	Total C N O S 588 365 118 103 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C2	70	Total 588	C 365	N 118	O 103	S 2	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	A3	59	Total 469	C 298	N 90	O 81	0	0	0
27	C3	59	Total 464	C 296	N 90	O 78	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	69	Total 558	C 352	N 102	O 99	S 5	0	0	0
28	C4	69	Total 532	C 339	N 97	O 91	S 5	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	59	Total 455	C 285	N 89	O 76	S 5	0	0	0
29	C5	59	Total 455	C 285	N 89	O 76	S 5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total 453	C 281	N 91	O 77	S 4	0	0	0
30	C6	53	Total 449	C 279	N 91	O 75	S 4	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	48	Total 418	C 257	N 104	O 55	S 2	0	0	0
31	C7	48	Total 418	C 257	N 104	O 55	S 2	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	A8	64	Total C N O S 517 331 102 82 2	0	0	0
32	C8	64	Total C N O S 517 331 102 82 2	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	A9	37	Total C N O S 307 188 68 47 4	0	0	0
33	C9	37	Total C N O S 307 188 68 47 4	0	0	0

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	BA	1495	Total C N O P 32141 14304 5958 10384 1495	0	0	0
34	DA	1501	Total C N O P 32268 14361 5980 10426 1501	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	BB	231	Total C N O S 1846 1179 331 331 5	0	0	0
35	DB	231	Total C N O S 1825 1167 326 327 5	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BC	206	Total C N O S 1552 976 302 273 1	0	0	0
36	DC	206	Total C N O S 1544 970 300 273 1	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	208	Total 1659	C 1040	N 326	O 286	S 7	0	0	0
37	DD	208	Total 1678	C 1052	N 333	O 286	S 7	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	148	Total 1129	C 714	N 213	O 198	S 4	0	0	0
38	DE	148	Total 1133	C 716	N 214	O 199	S 4	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	100	Total 812	C 514	N 146	O 149	S 3	0	0	0
39	DF	100	Total 820	C 518	N 147	O 152	S 3	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	155	Total 1231	C 766	N 243	O 216	S 6	0	0	0
40	DG	155	Total 1235	C 769	N 244	O 216	S 6	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	137	Total 1088	C 689	N 206	O 191	S 2	0	0	0
41	DH	137	Total 1088	C 689	N 206	O 191	S 2	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BI	127	Total 986	C 626	N 193	O 167	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	DI	127	978	619	190	169	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	BJ	97	709	440	138	131	0	0	0
			Total	C	N	O			
43	DJ	96	714	445	138	131	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BK	114	833	519	156	155	3	0	0	0
			Total	C	N	O	S			
44	DK	114	833	519	156	155	3	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BL	122	930	585	185	159	1	0	0	0
			Total	C	N	O	S			
45	DL	122	930	585	185	159	1	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BM	117	923	570	191	160	2	0	0	0
			Total	C	N	O	S			
46	DM	116	907	558	188	159	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	BN	60	492	312	104	72	4	0	0	0
			Total	C	N	O	S			
47	DN	60	492	312	104	72	4	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
48	DO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
49	DP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
50	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BR	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	DR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BS	84	Total	C	N	O	S	0	0	0
			661	423	122	114	2			
52	DS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
53	DT	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BU	23	Total	C	N	O	0	0	0
			199	122	48	29			
54	DU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			
55	DV	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

- Molecule 56 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	BW	76	Total	C	N	O	P	S	0	0	0
			1631	731	290	532	76	2			
56	BY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
56	DW	76	Total	C	N	O	P	S	0	0	0
			1631	731	290	532	76	2			
56	DY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 57 is a protein called 50S ribosomal protein L9,Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	728	Total	C	N	O	S	0	0	0
			5663	3599	973	1072	19			
57	DZ	730	Total	C	N	O	S	0	0	0
			5682	3611	978	1074	19			

- Molecule 58 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BX	10	Total 93	C 67	N 10	O 16	0	0	0
58	DX	10	Total 93	C 67	N 10	O 16	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	832	Total 832	Mg 832	0	0
59	AB	23	Total 23	Mg 23	0	0
59	AD	10	Total 10	Mg 10	0	0
59	AE	5	Total 5	Mg 5	0	0
59	AF	6	Total 6	Mg 6	0	0
59	AG	2	Total 2	Mg 2	0	0
59	AH	1	Total 1	Mg 1	0	0
59	AN	3	Total 3	Mg 3	0	0
59	AO	1	Total 1	Mg 1	0	0
59	AP	3	Total 3	Mg 3	0	0
59	AQ	4	Total 4	Mg 4	0	0
59	AR	1	Total 1	Mg 1	0	0
59	AU	5	Total 5	Mg 5	0	0
59	AV	2	Total 2	Mg 2	0	0
59	AW	3	Total 3	Mg 3	0	0
59	AX	1	Total 1	Mg 1	0	0
59	AY	1	Total 1	Mg 1	0	0
59	AZ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	A0	5	Total 5	Mg 5	0	0
59	A2	1	Total 1	Mg 1	0	0
59	A5	1	Total 1	Mg 1	0	0
59	A6	2	Total 2	Mg 2	0	0
59	A7	1	Total 1	Mg 1	0	0
59	A8	1	Total 1	Mg 1	0	0
59	A9	1	Total 1	Mg 1	0	0
59	BA	215	Total 215	Mg 215	0	0
59	BB	1	Total 1	Mg 1	0	0
59	BD	1	Total 1	Mg 1	0	0
59	BE	1	Total 1	Mg 1	0	0
59	BF	1	Total 1	Mg 1	0	0
59	BK	1	Total 1	Mg 1	0	0
59	BL	2	Total 2	Mg 2	0	0
59	BM	1	Total 1	Mg 1	0	0
59	BN	2	Total 2	Mg 2	0	0
59	BS	1	Total 1	Mg 1	0	0
59	BT	1	Total 1	Mg 1	0	0
59	BW	3	Total 3	Mg 3	0	0
59	BZ	1	Total 1	Mg 1	0	0
59	CA	664	Total 664	Mg 664	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	CB	13	Total Mg 13 13	0	0
59	CD	4	Total Mg 4 4	0	0
59	CE	5	Total Mg 5 5	0	0
59	CF	4	Total Mg 4 4	0	0
59	CG	1	Total Mg 1 1	0	0
59	CN	1	Total Mg 1 1	0	0
59	CO	1	Total Mg 1 1	0	0
59	CP	1	Total Mg 1 1	0	0
59	CQ	4	Total Mg 4 4	0	0
59	CR	1	Total Mg 1 1	0	0
59	CU	1	Total Mg 1 1	0	0
59	CV	2	Total Mg 2 2	0	0
59	CW	1	Total Mg 1 1	0	0
59	CX	1	Total Mg 1 1	0	0
59	C0	1	Total Mg 1 1	0	0
59	C1	1	Total Mg 1 1	0	0
59	C3	1	Total Mg 1 1	0	0
59	C5	1	Total Mg 1 1	0	0
59	C7	1	Total Mg 1 1	0	0
59	C8	1	Total Mg 1 1	0	0
59	DA	171	Total Mg 171 171	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	DD	1	Total Mg 1 1	0	0
59	DE	2	Total Mg 2 2	0	0
59	DF	1	Total Mg 1 1	0	0
59	DJ	1	Total Mg 1 1	0	0
59	DK	1	Total Mg 1 1	0	0
59	DT	1	Total Mg 1 1	0	0
59	DW	3	Total Mg 3 3	0	0
59	DZ	2	Total Mg 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AY	1	Total Zn 1 1	0	0
60	A4	1	Total Zn 1 1	0	0
60	A5	1	Total Zn 1 1	0	0
60	A6	1	Total Zn 1 1	0	0
60	A9	1	Total Zn 1 1	0	0
60	BN	1	Total Zn 1 1	0	0
60	CY	1	Total Zn 1 1	0	0
60	C4	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0
60	C6	1	Total Zn 1 1	0	0
60	C9	1	Total Zn 1 1	0	0

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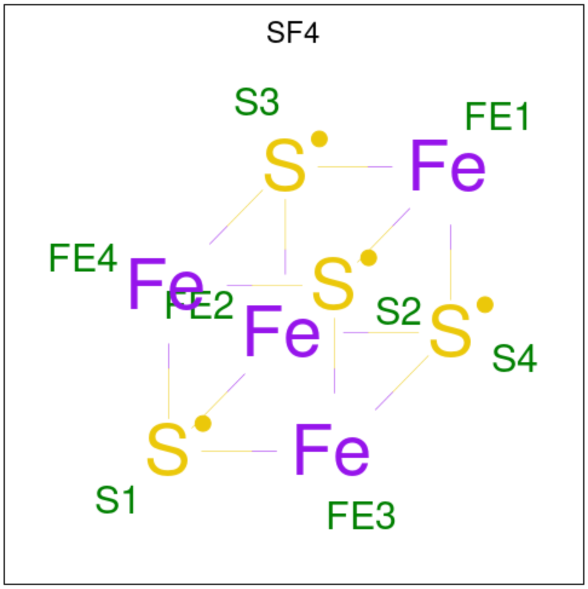
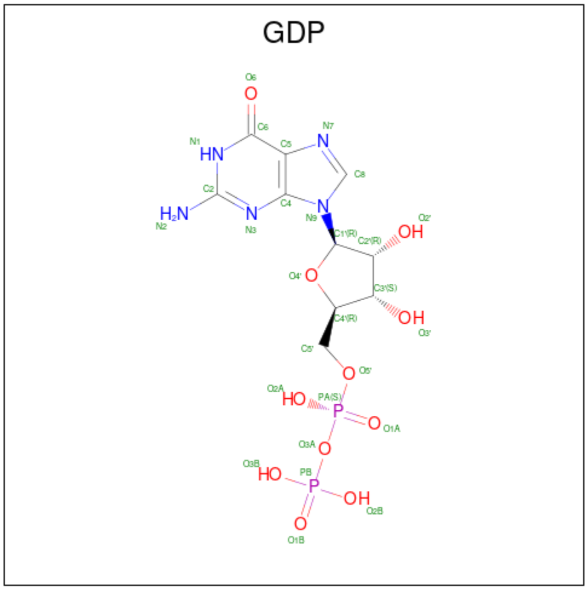
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	DN	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BD	1	Total Fe S 8 4 4	0	0
61	DD	1	Total Fe S 8 4 4	0	0

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	BZ	1	Total C N O P 28 10 5 11 2	0	0
62	DZ	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	AA	1413	Total O 1413 1413	0	0
63	AB	38	Total O 38 38	0	0
63	AD	10	Total O 10 10	0	0
63	AE	17	Total O 17 17	0	0
63	AF	11	Total O 11 11	0	0
63	AG	3	Total O 3 3	0	0
63	AH	1	Total O 1 1	0	0
63	AN	1	Total O 1 1	0	0
63	AO	3	Total O 3 3	0	0
63	AP	16	Total O 16 16	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	AQ	4	Total O 4 4	0	0
63	AR	2	Total O 2 2	0	0
63	AS	1	Total O 1 1	0	0
63	AT	1	Total O 1 1	0	0
63	AU	4	Total O 4 4	0	0
63	AV	1	Total O 1 1	0	0
63	AW	1	Total O 1 1	0	0
63	AX	3	Total O 3 3	0	0
63	AZ	1	Total O 1 1	0	0
63	A0	6	Total O 6 6	0	0
63	A1	2	Total O 2 2	0	0
63	A3	2	Total O 2 2	0	0
63	A5	3	Total O 3 3	0	0
63	A6	1	Total O 1 1	0	0
63	A7	2	Total O 2 2	0	0
63	A8	10	Total O 10 10	0	0
63	A9	1	Total O 1 1	0	0
63	BA	213	Total O 213 213	0	0
63	BD	1	Total O 1 1	0	0
63	BM	1	Total O 1 1	0	0
63	BO	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	BP	1	Total O 1 1	0	0
63	BV	1	Total O 1 1	0	0
63	BW	1	Total O 1 1	0	0
63	BZ	2	Total O 2 2	0	0
63	CA	983	Total O 983 983	0	0
63	CB	9	Total O 9 9	0	0
63	CD	15	Total O 15 15	0	0
63	CE	9	Total O 9 9	0	0
63	CF	6	Total O 6 6	0	0
63	CN	1	Total O 1 1	0	0
63	CO	1	Total O 1 1	0	0
63	CP	11	Total O 11 11	0	0
63	CQ	2	Total O 2 2	0	0
63	CT	3	Total O 3 3	0	0
63	CU	2	Total O 2 2	0	0
63	CV	1	Total O 1 1	0	0
63	CW	1	Total O 1 1	0	0
63	CX	1	Total O 1 1	0	0
63	CY	2	Total O 2 2	0	0
63	C0	4	Total O 4 4	0	0
63	C3	2	Total O 2 2	0	0

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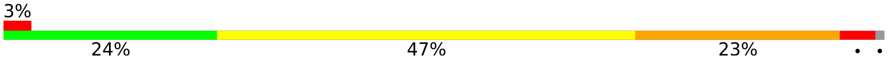
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	C5	1	Total O 1 1	0	0
63	C7	2	Total O 2 2	0	0
63	C8	4	Total O 4 4	0	0
63	DA	157	Total O 157 157	0	0
63	DD	1	Total O 1 1	0	0
63	DE	2	Total O 2 2	0	0
63	DH	1	Total O 1 1	0	0
63	DJ	1	Total O 1 1	0	0
63	DK	2	Total O 2 2	0	0
63	DL	1	Total O 1 1	0	0
63	DT	1	Total O 1 1	0	0

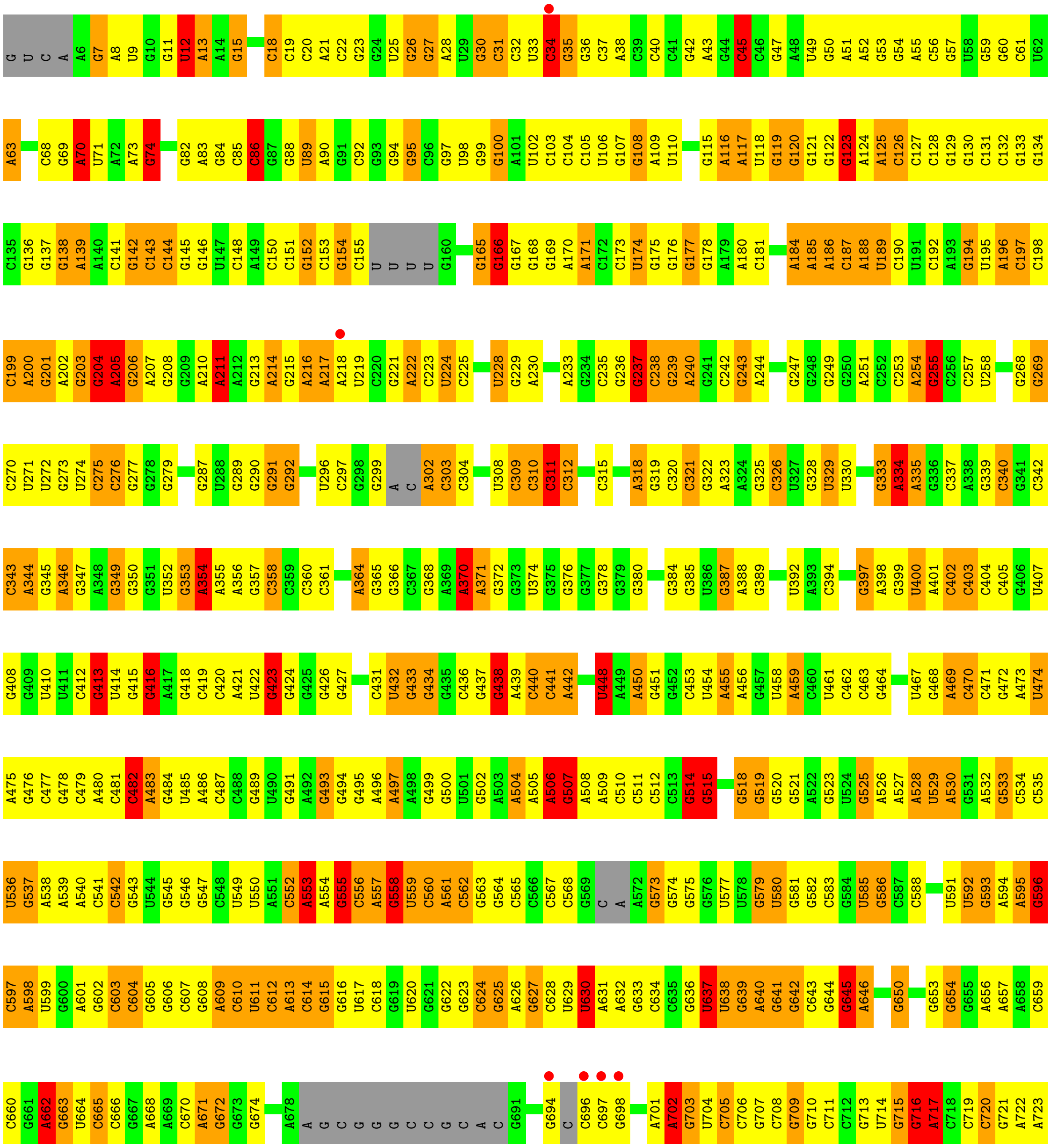
3 Residue-property plots ⓘ

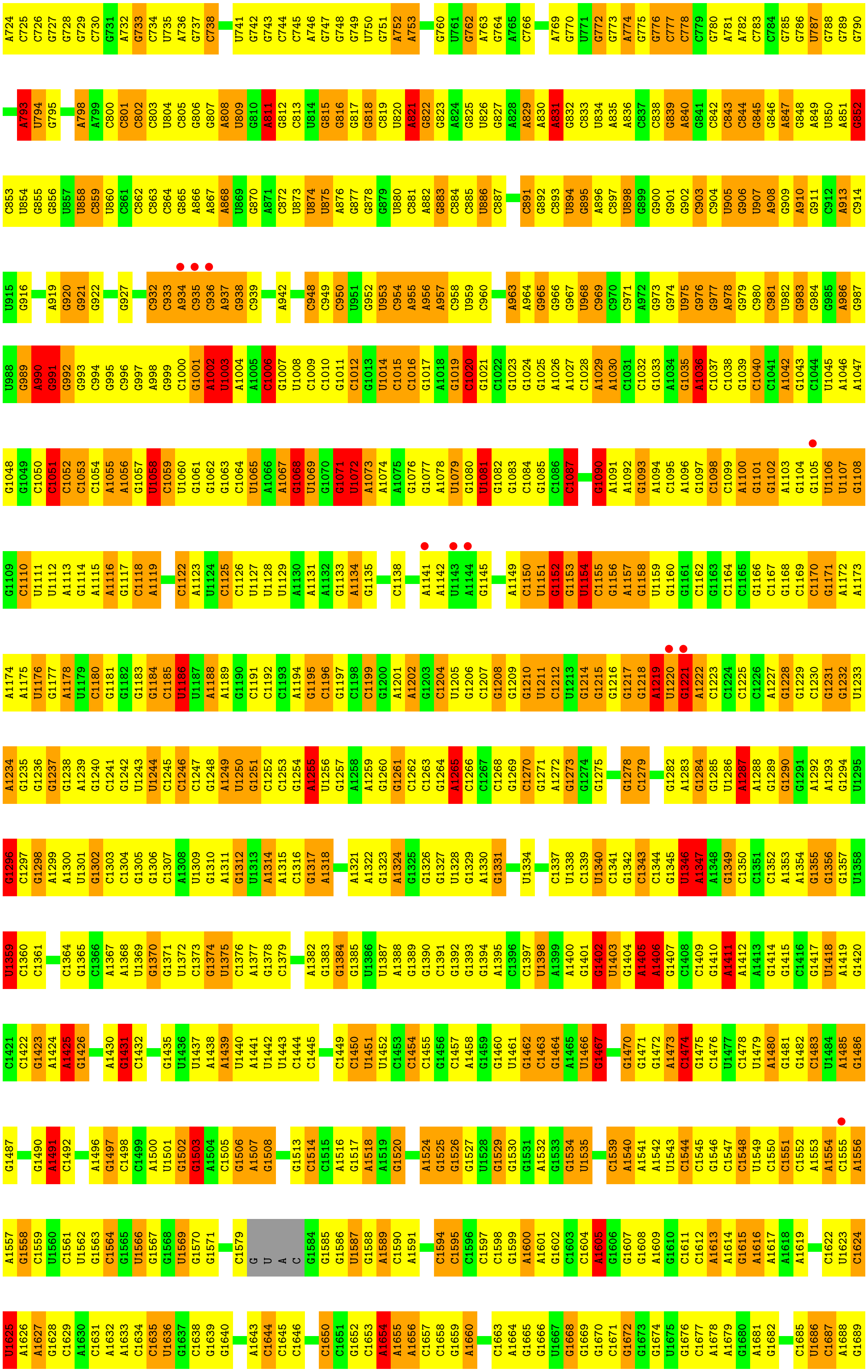
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S Ribosomal RNA

Chain AA:



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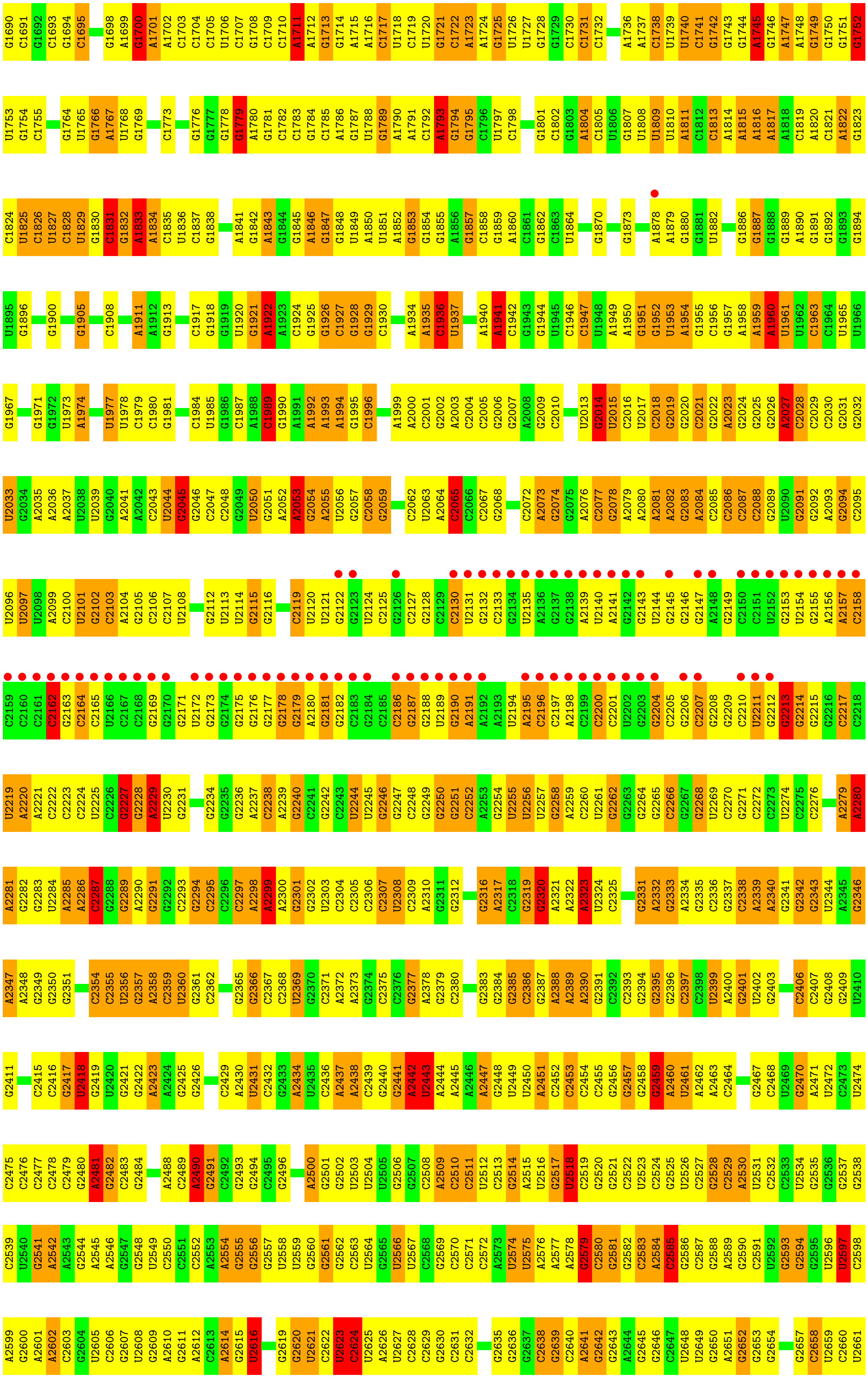
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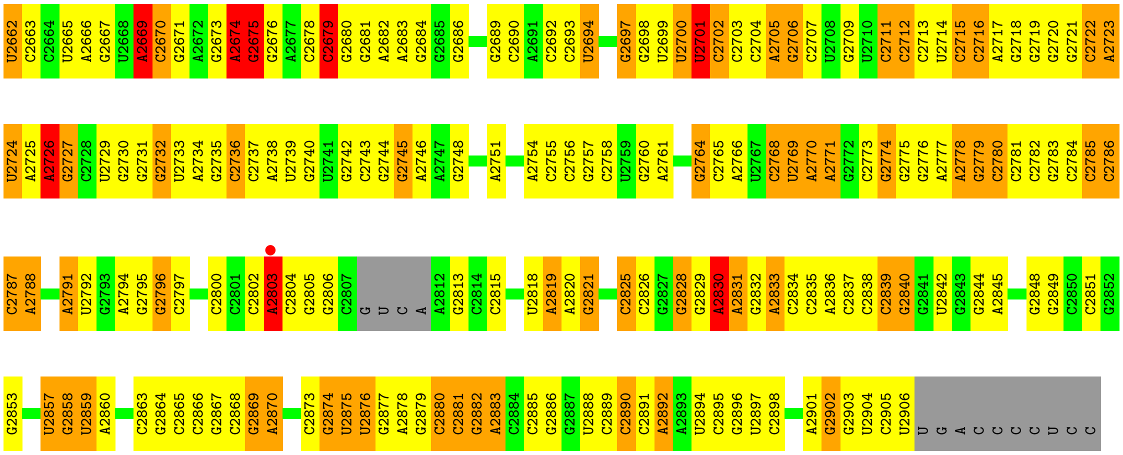

- Molecule 1: 23S Ribosomal RNA

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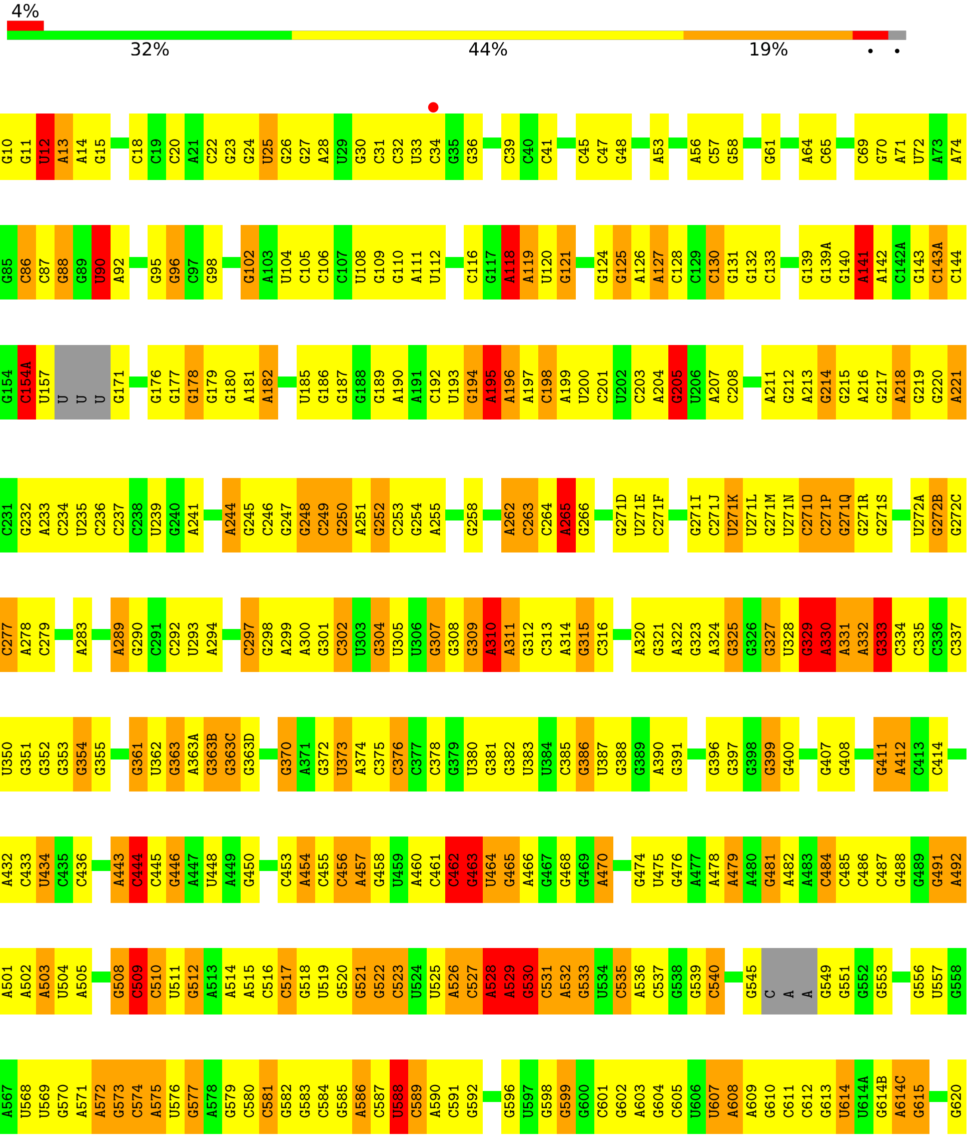

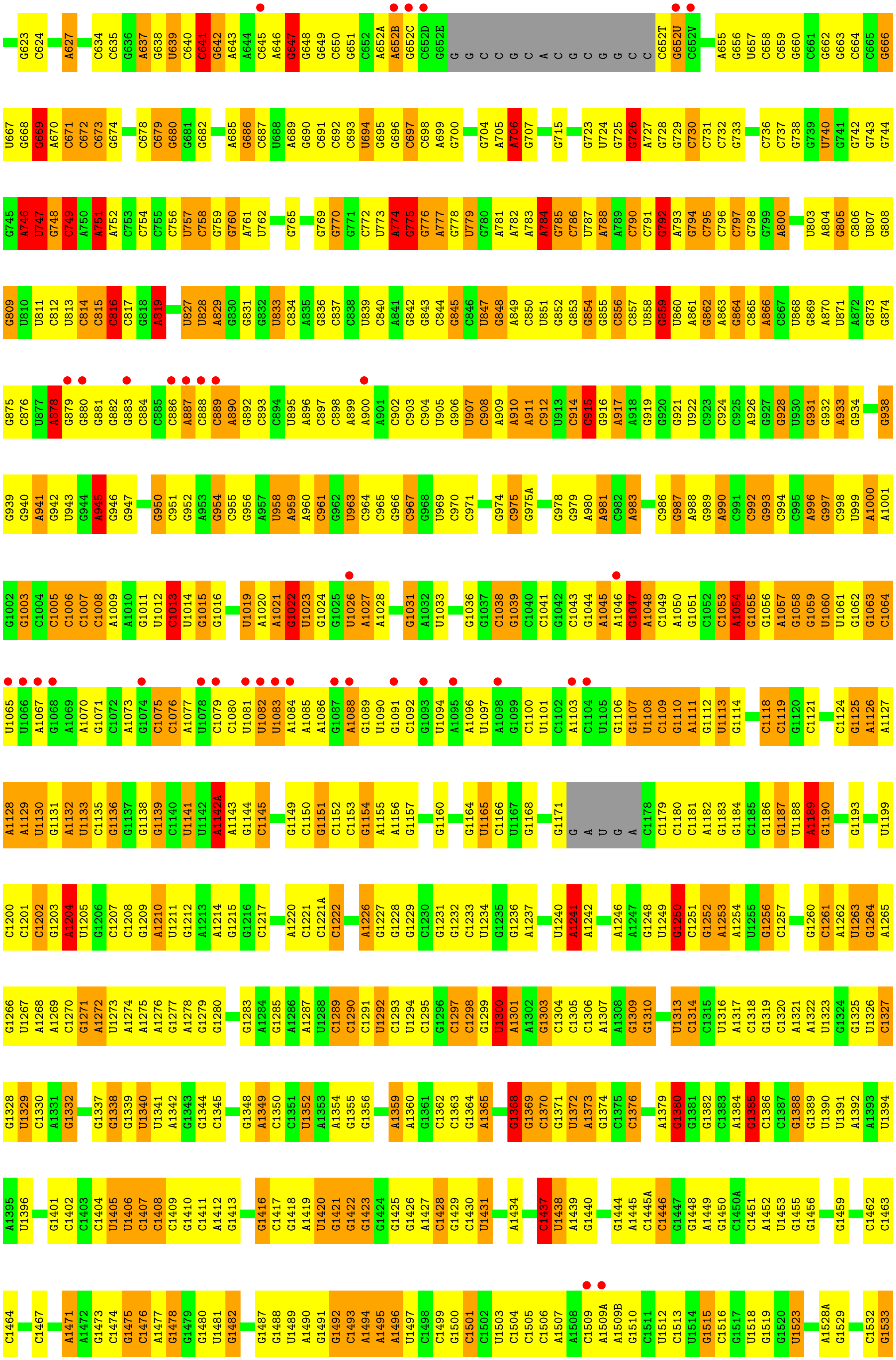
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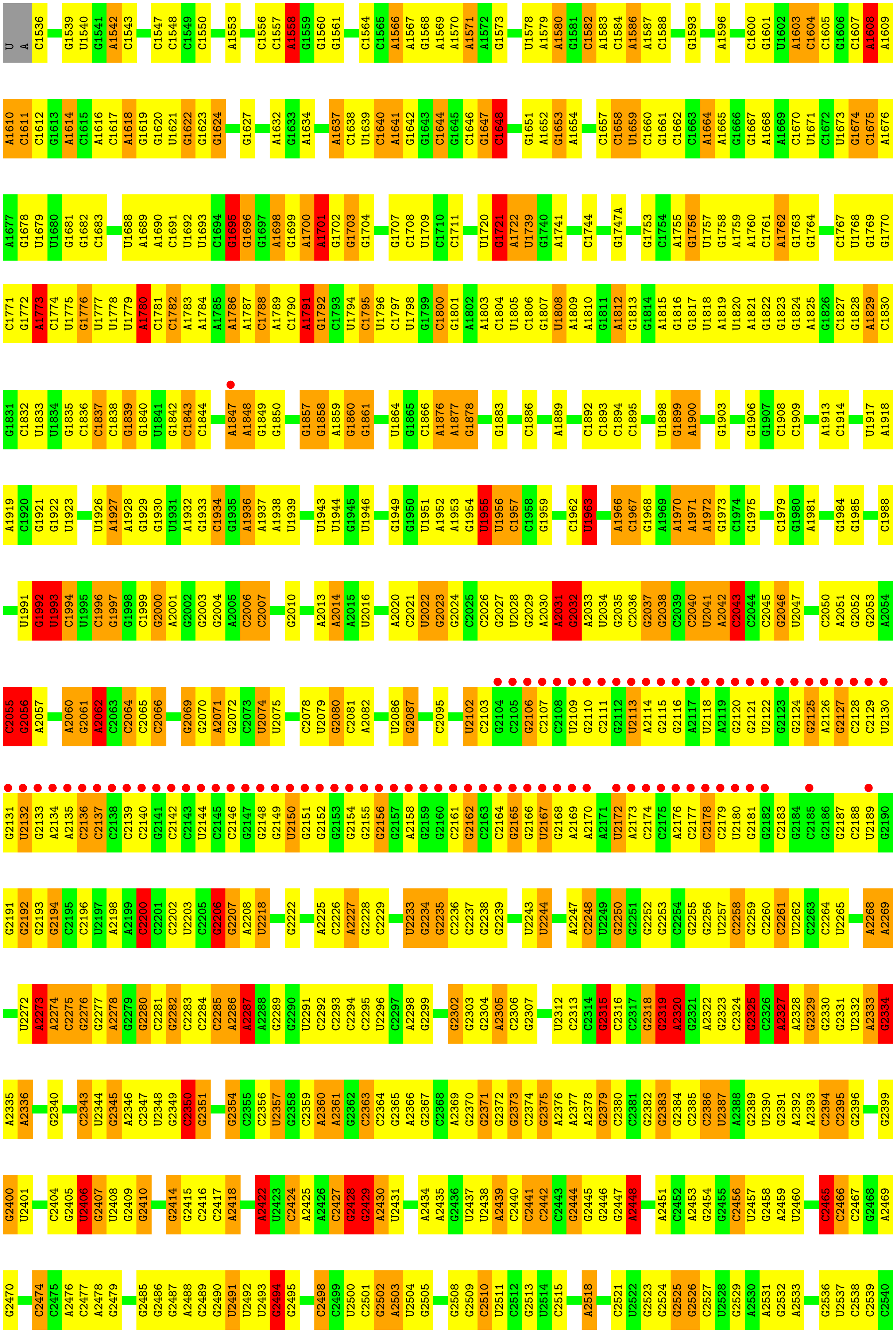

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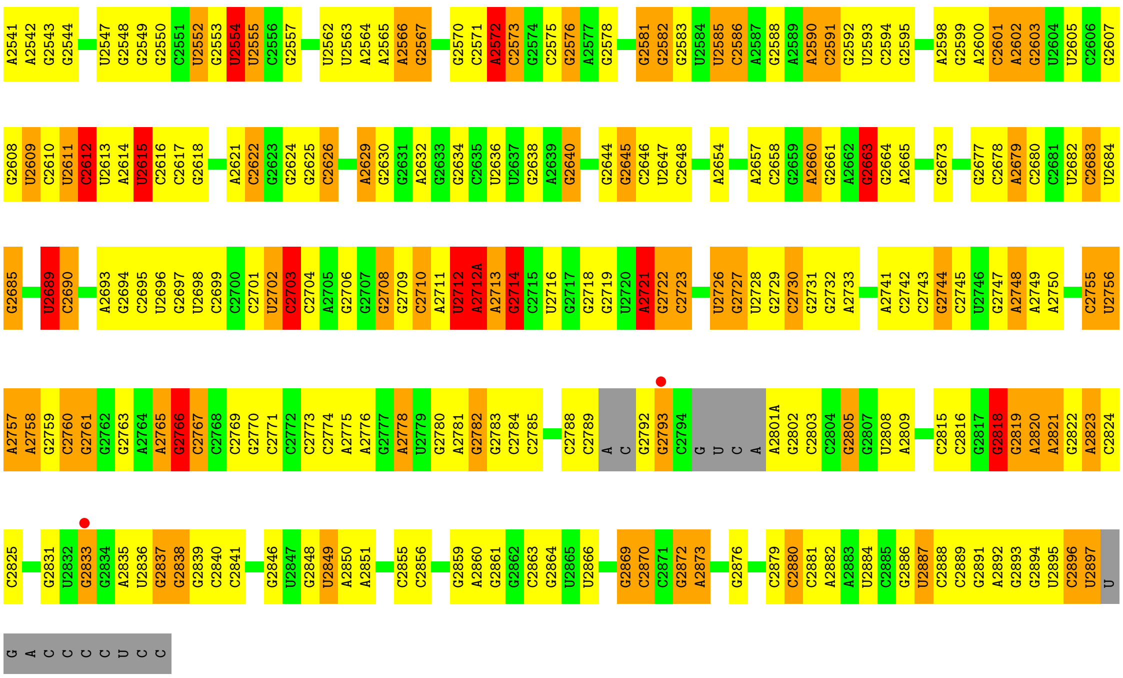

- Molecule 2: 5S Ribosomal RNA

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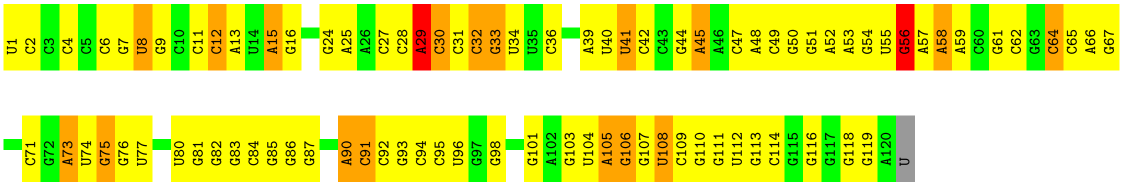

- Molecule 2: 5S Ribosomal RNA

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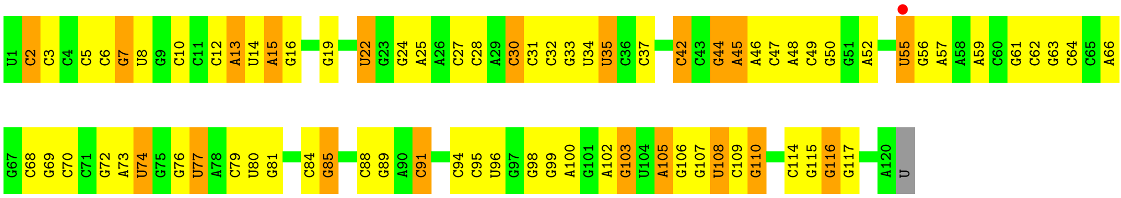

- Molecule 3: 50S ribosomal protein L1

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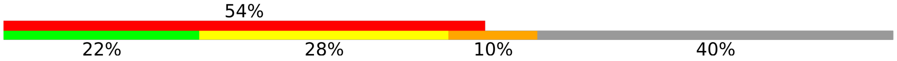

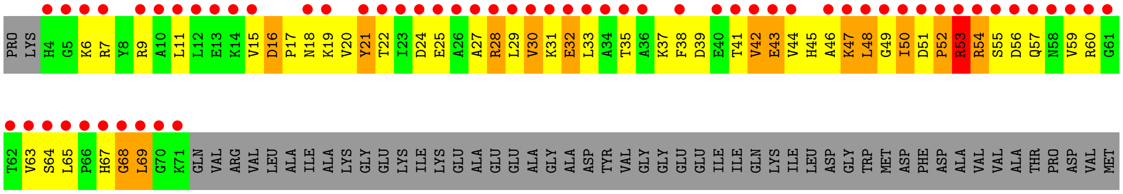

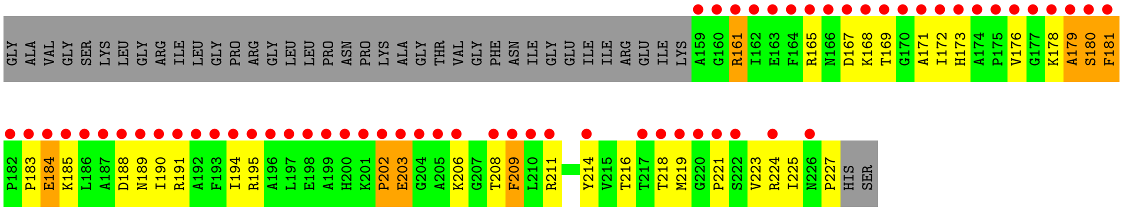

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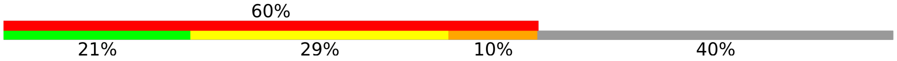

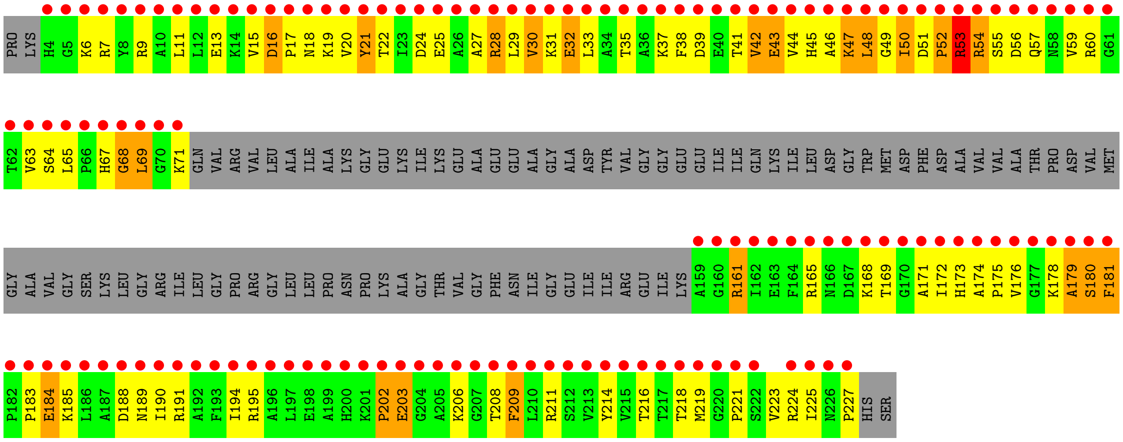

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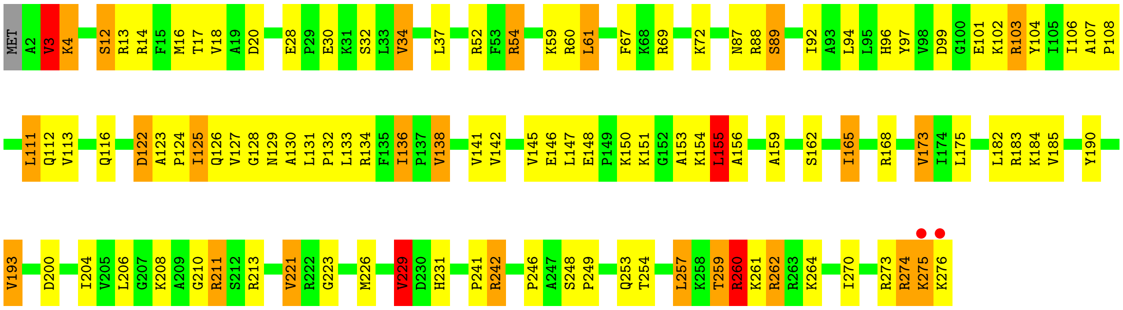

- Molecule 4: 50S ribosomal protein L2

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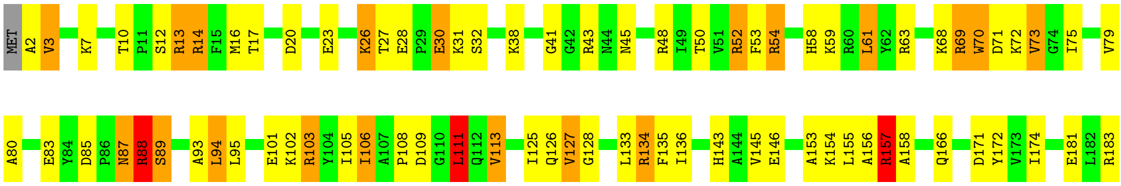

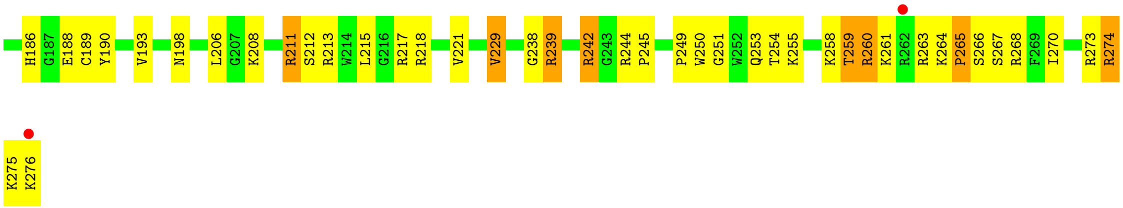

- Molecule 5: 50S ribosomal protein L3

Chain AE:

- Molecule 5: 50S ribosomal protein L3

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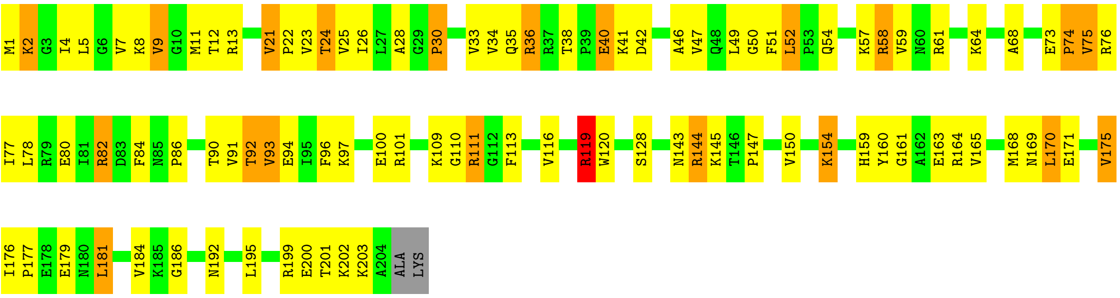

- Molecule 6: 50S ribosomal protein L4

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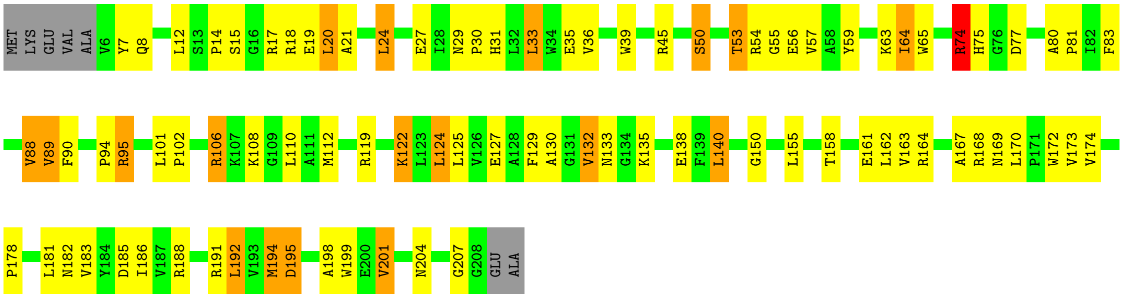

- Molecule 6: 50S ribosomal protein L4

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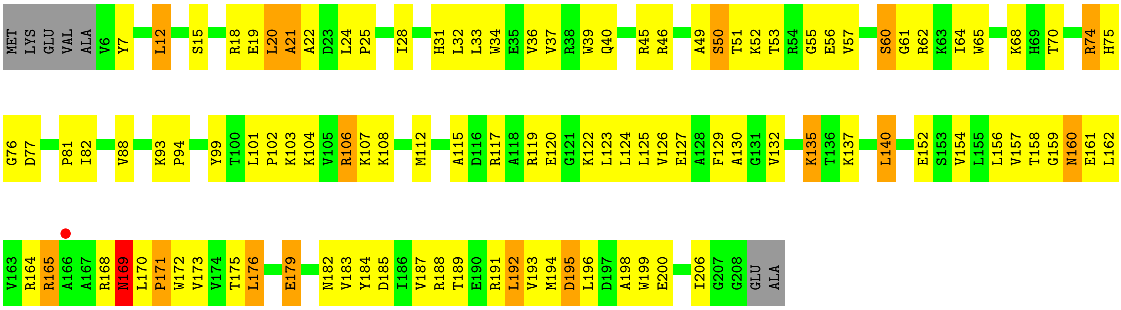

- Molecule 7: 50S ribosomal protein L5

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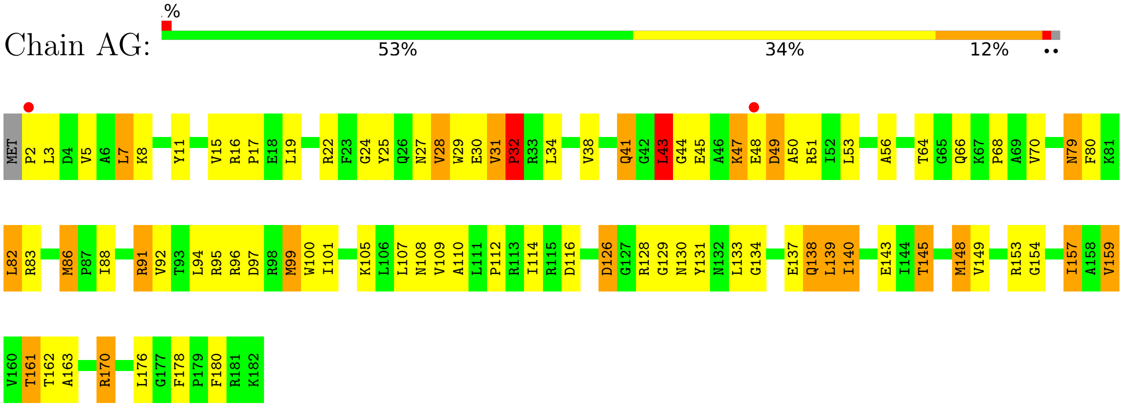

- Molecule 7: 50S ribosomal protein L5

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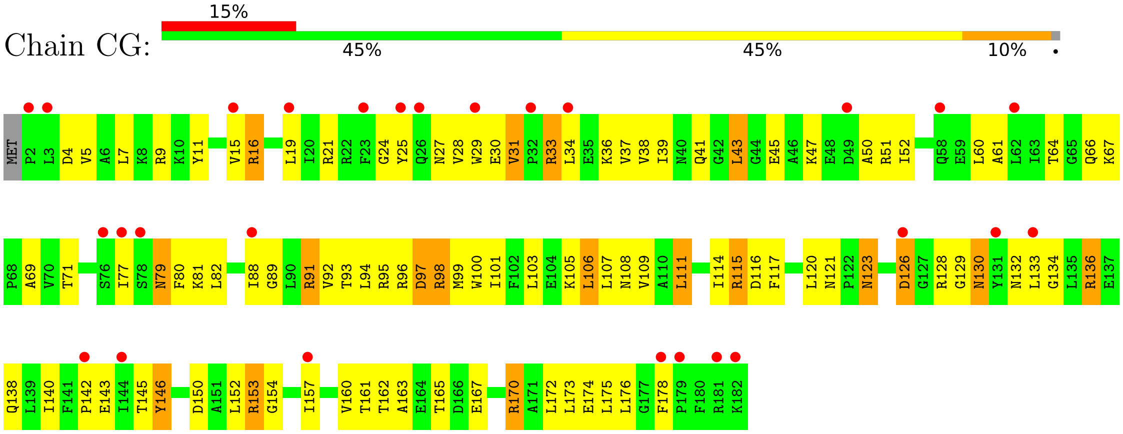

- Molecule 8: 50S ribosomal protein L6

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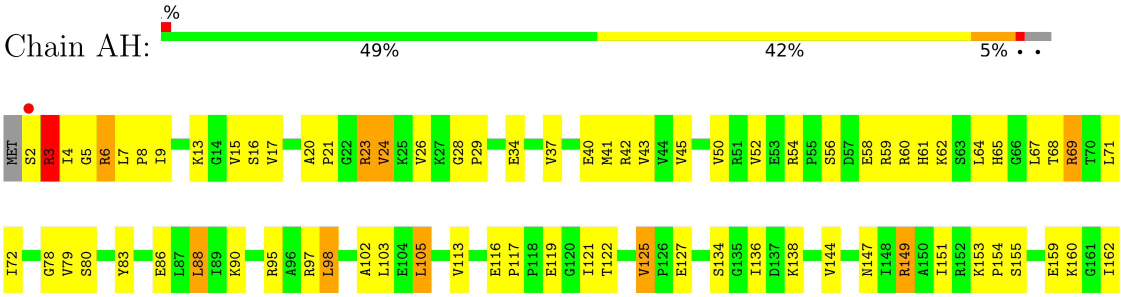
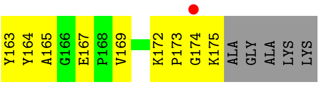
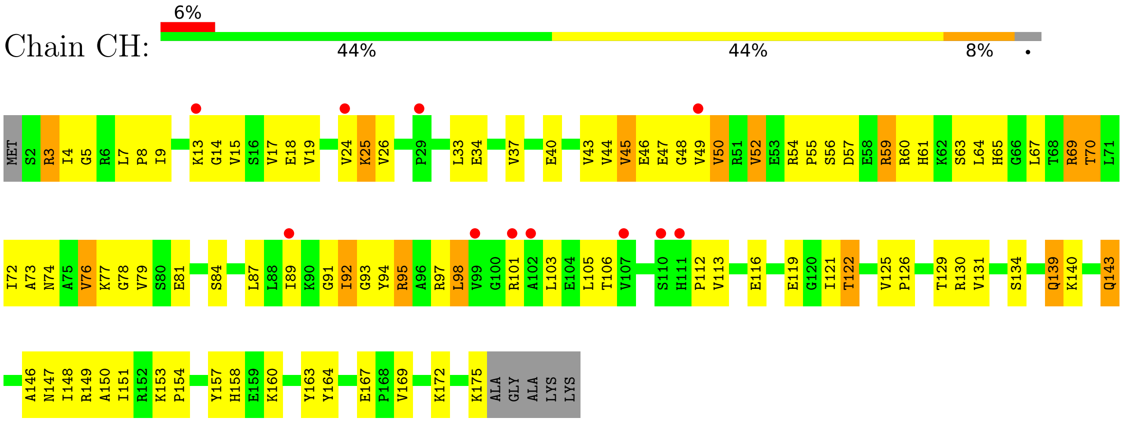




- Molecule 8: 50S ribosomal protein L6



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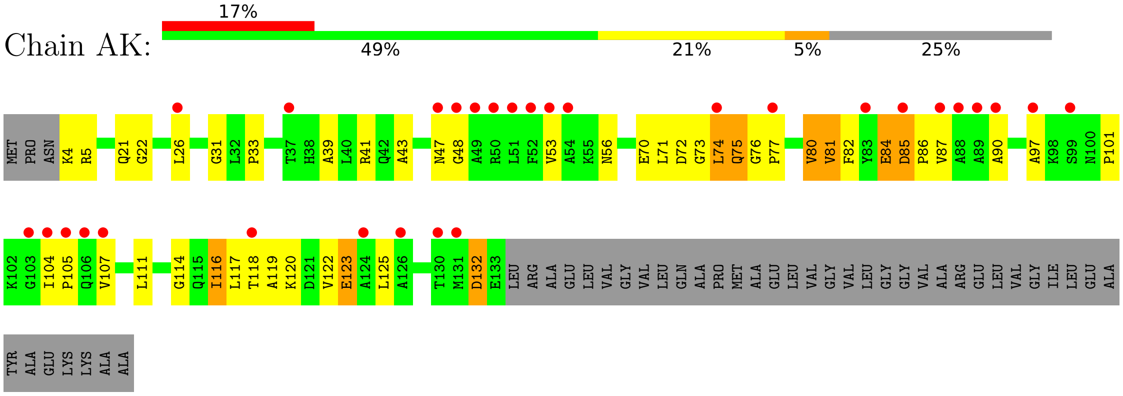

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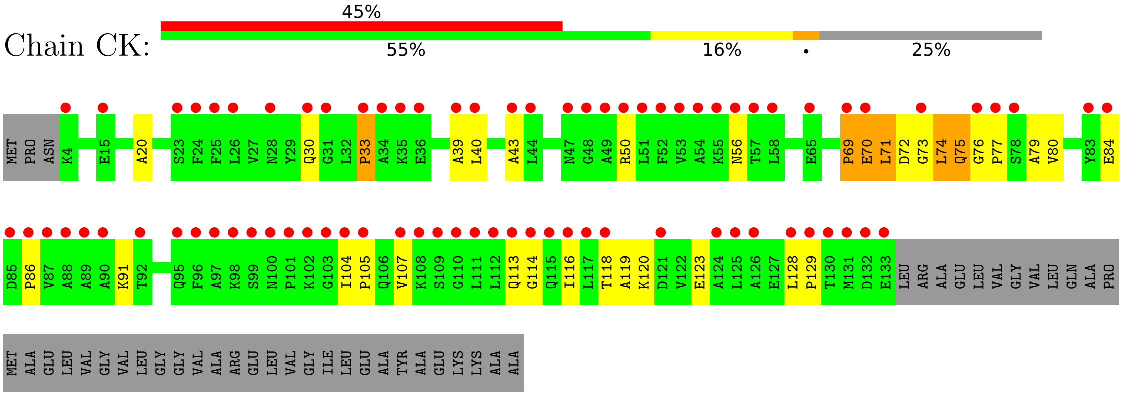
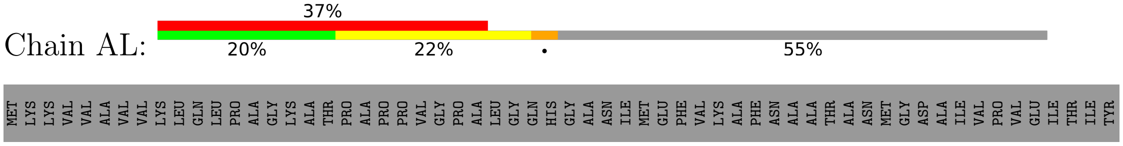
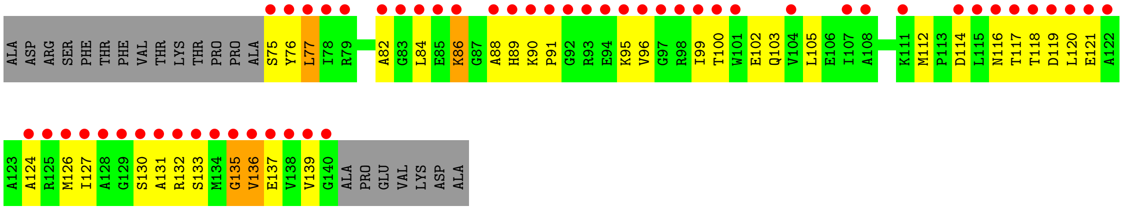
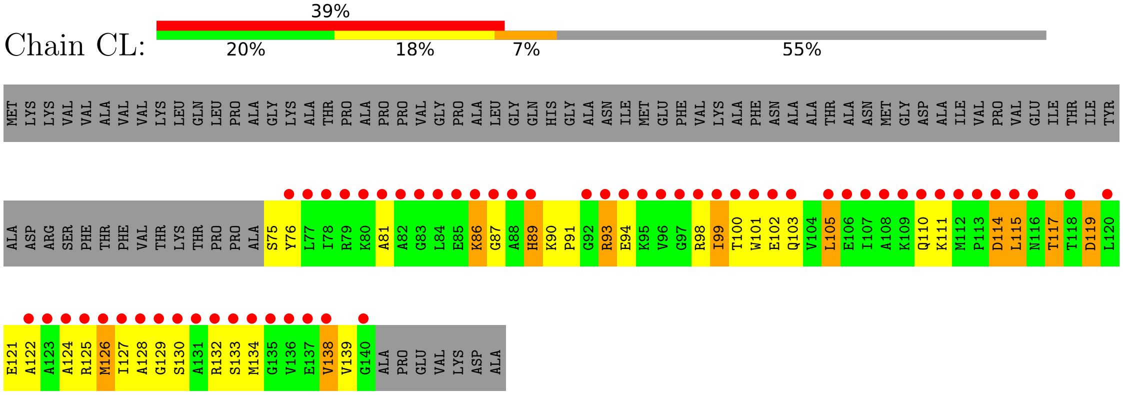


- Molecule 10: 50S ribosomal protein L11





- Molecule 10: 50S ribosomal protein L11



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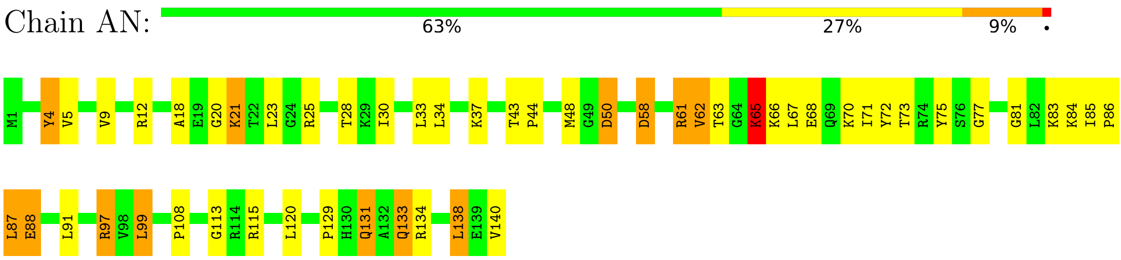

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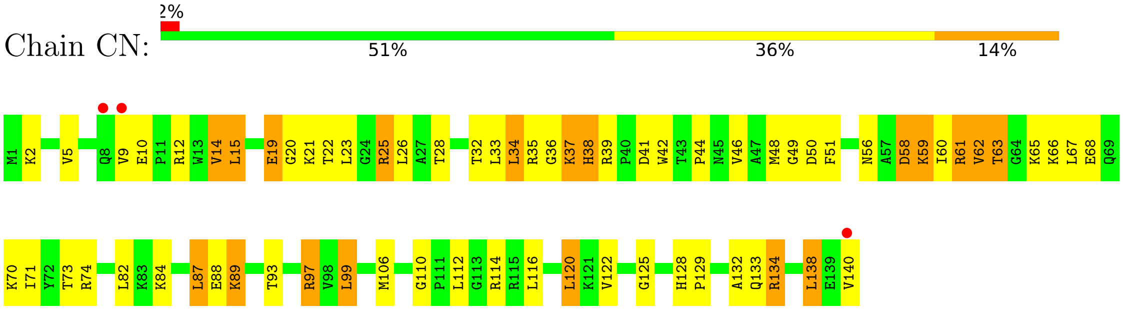

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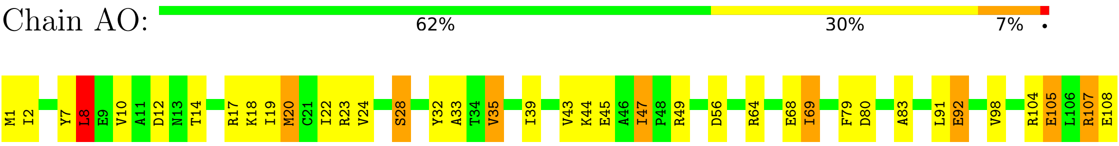

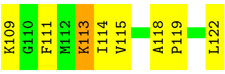

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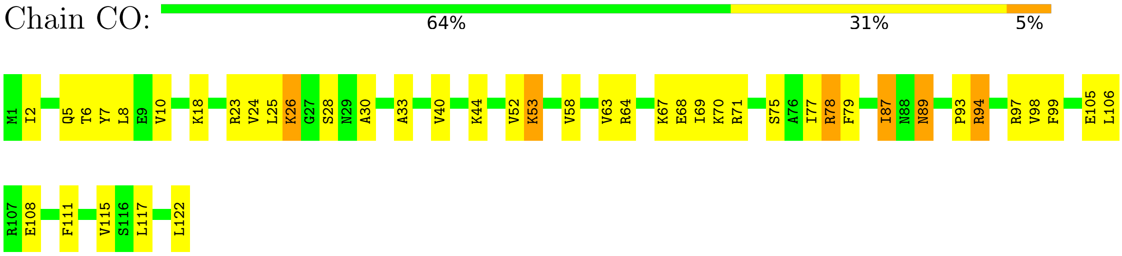
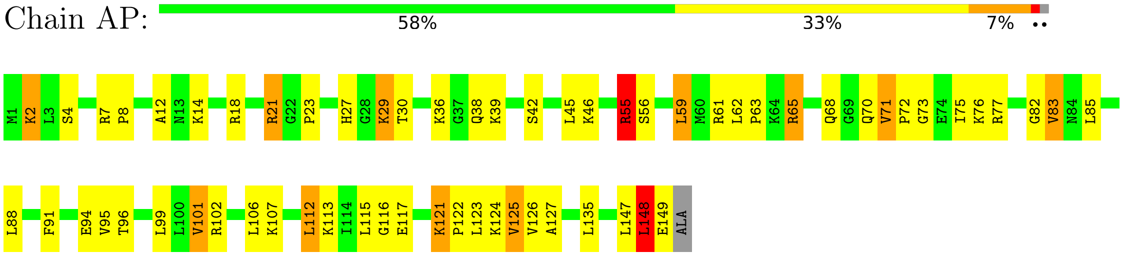


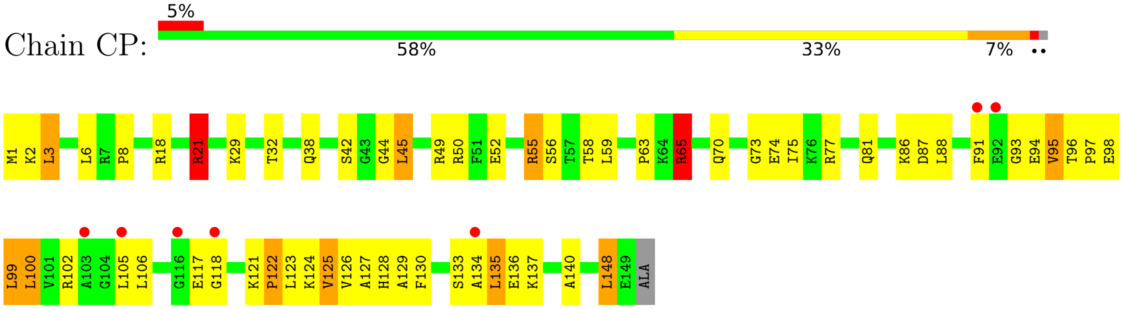
- Molecule 13: 50S ribosomal protein L15

Chain AP:



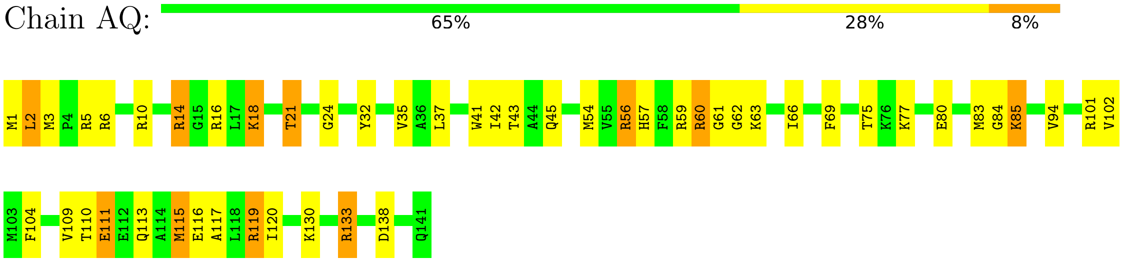
- Molecule 13: 50S ribosomal protein L15

Chain CP:



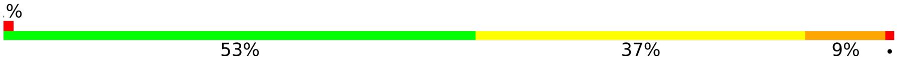
- Molecule 14: 50S ribosomal protein L16

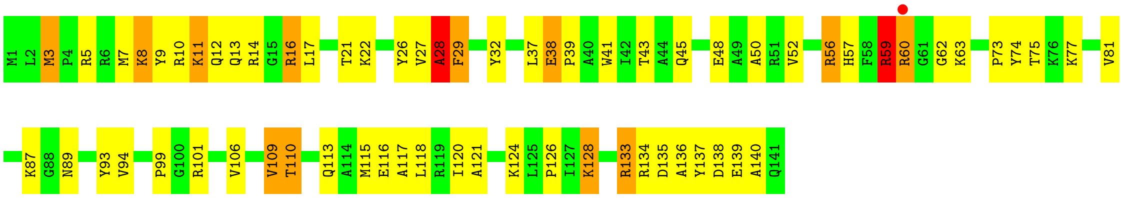
Chain AQ:



- Molecule 14: 50S ribosomal protein L16

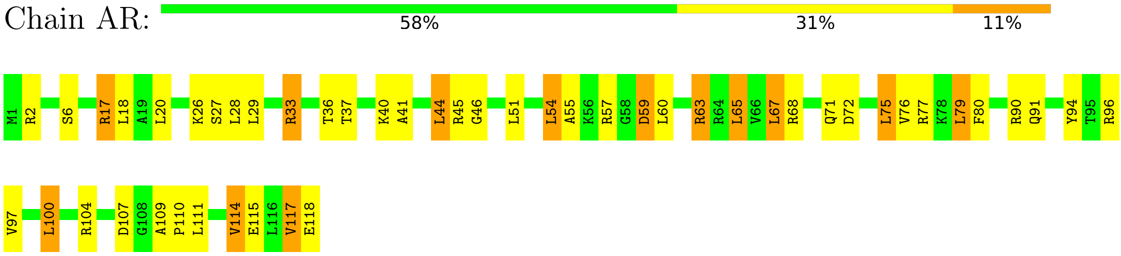
Chain CQ:





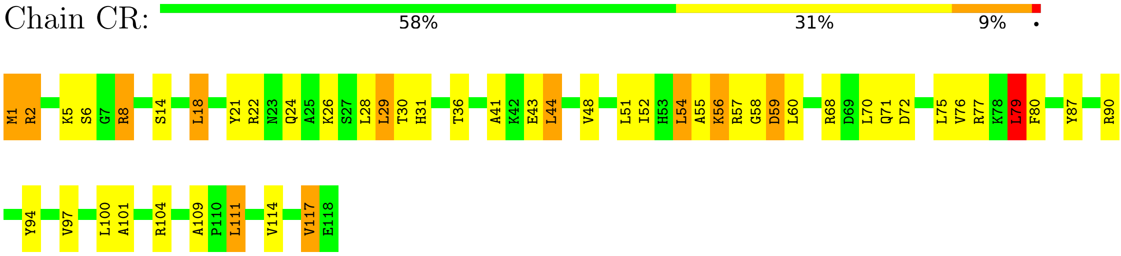
- Molecule 15: 50S ribosomal protein L17

Chain AR:



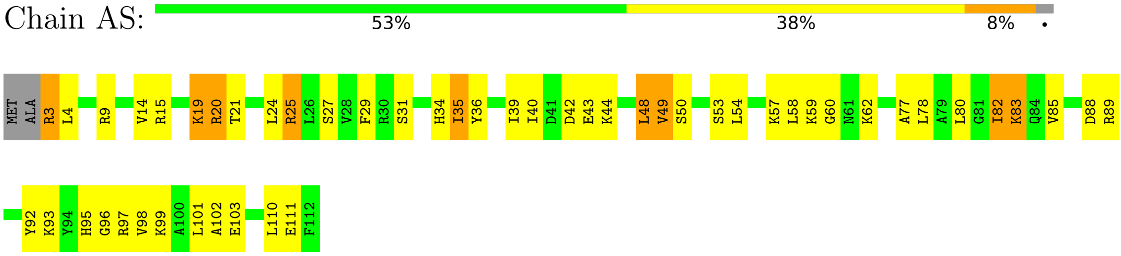
- Molecule 15: 50S ribosomal protein L17

Chain CR:



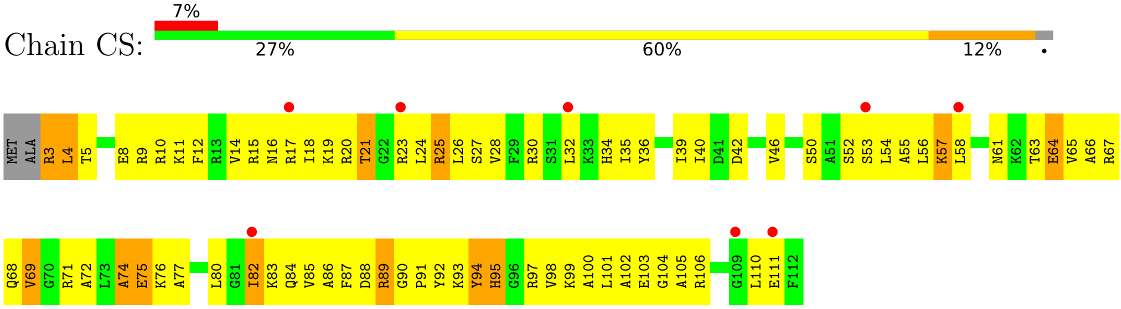
- Molecule 16: 50S ribosomal protein L18

Chain AS:



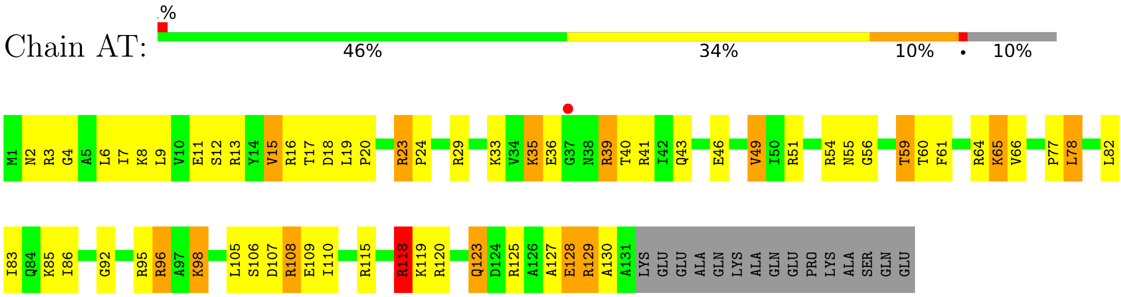
- Molecule 16: 50S ribosomal protein L18

Chain CS:



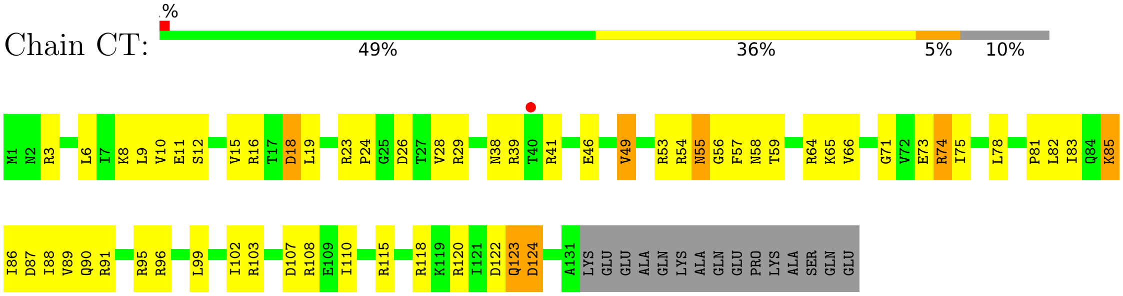
- Molecule 17: 50S ribosomal protein L19

Chain AT:



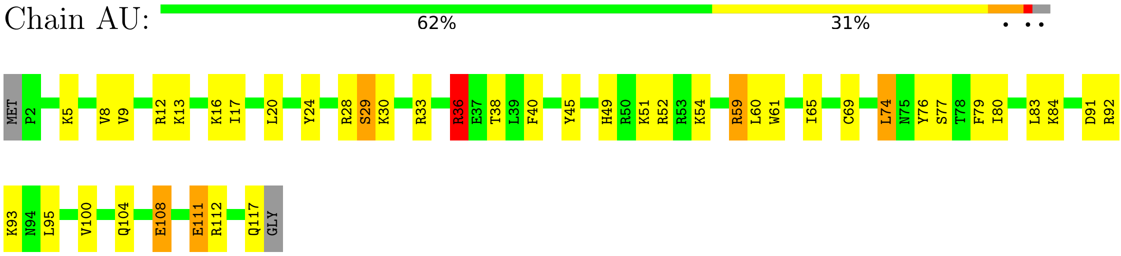
- Molecule 17: 50S ribosomal protein L19

Chain CT:



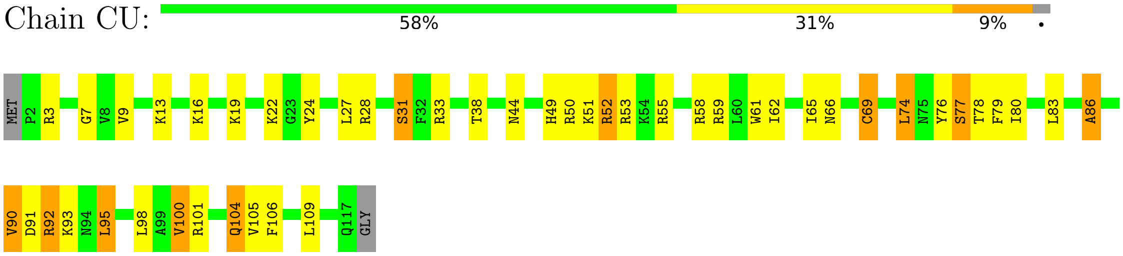
- Molecule 18: 50S ribosomal protein L20

Chain AU:



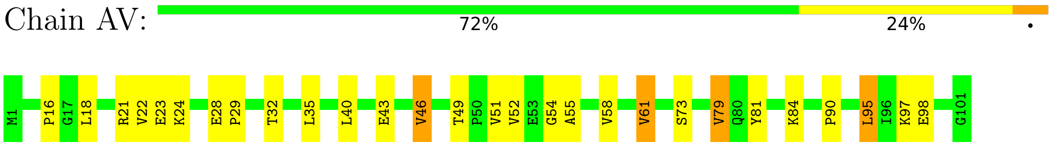
- Molecule 18: 50S ribosomal protein L20

Chain CU:



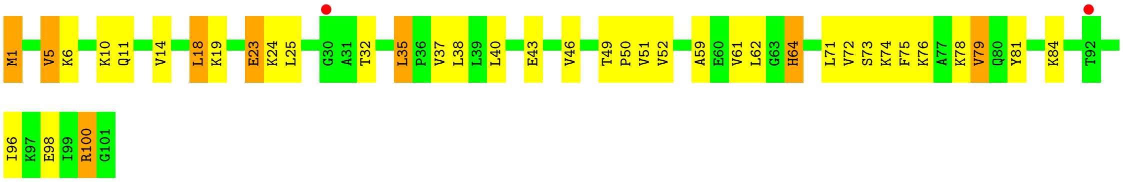
- Molecule 19: 50S ribosomal protein L21

Chain AV:



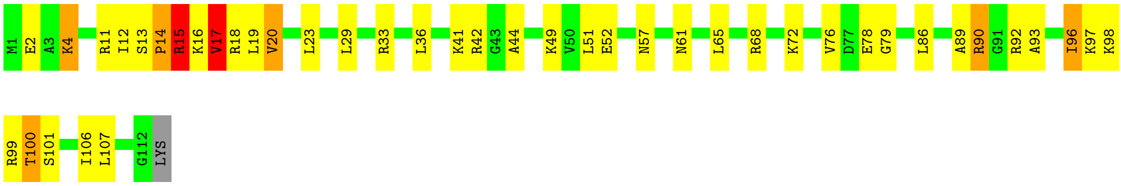
- Molecule 19: 50S ribosomal protein L21

Chain CV:



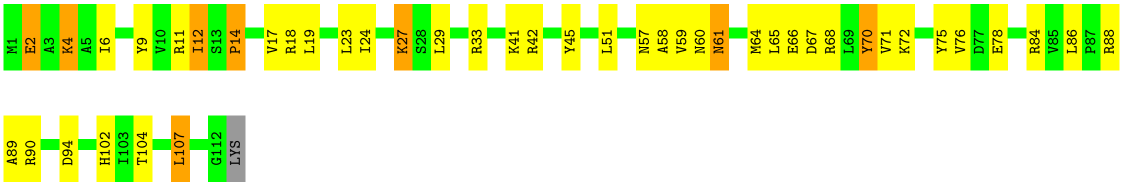
- Molecule 20: 50S ribosomal protein L22

Chain AW:



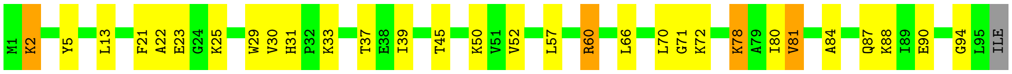
- Molecule 20: 50S ribosomal protein L22

Chain CW:



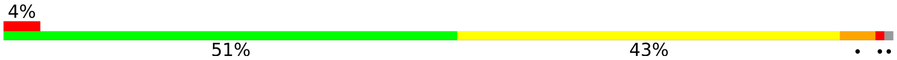
- Molecule 21: 50S ribosomal protein L23

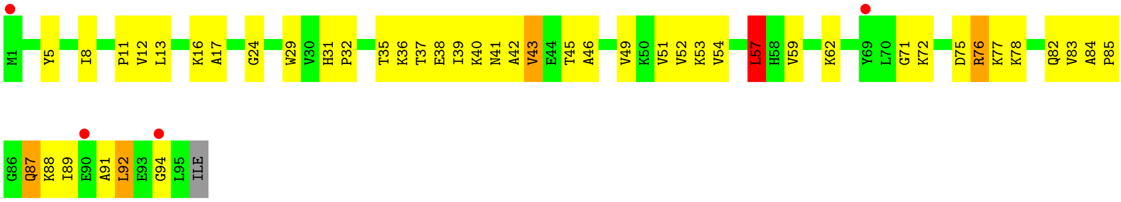
Chain AX:



- Molecule 21: 50S ribosomal protein L23

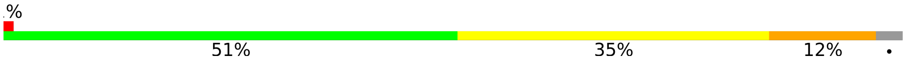
Chain CX:





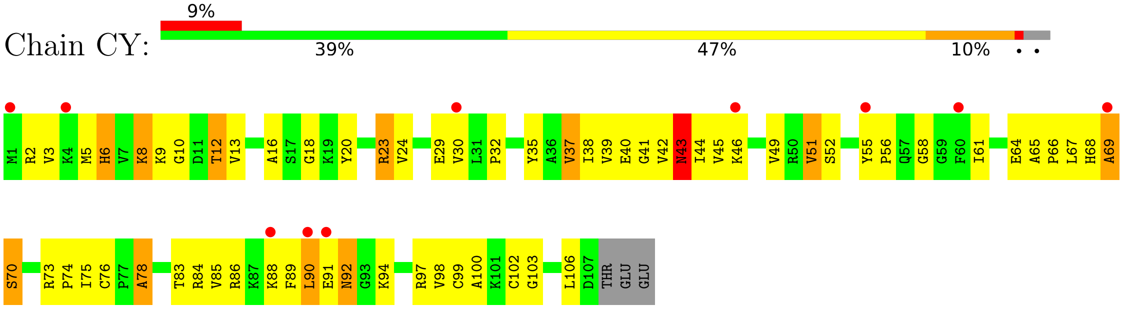
- Molecule 22: 50S ribosomal protein L24

Chain AY:



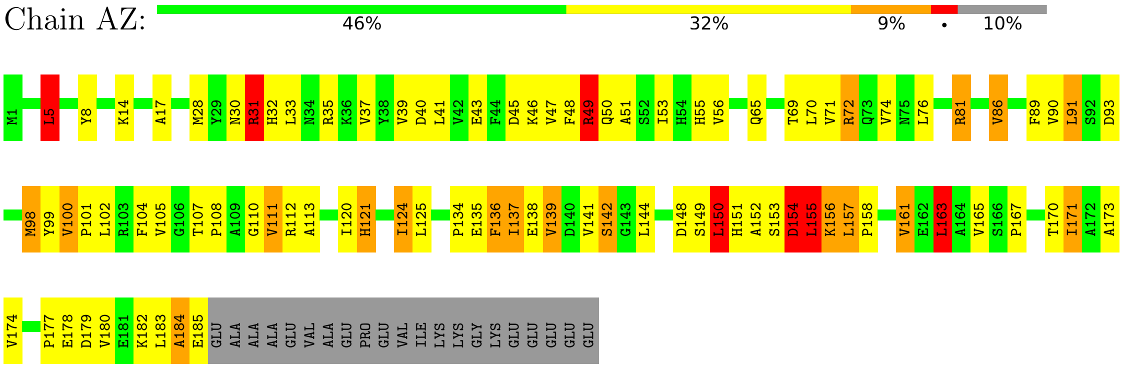
- Molecule 22: 50S ribosomal protein L24

Chain CY:



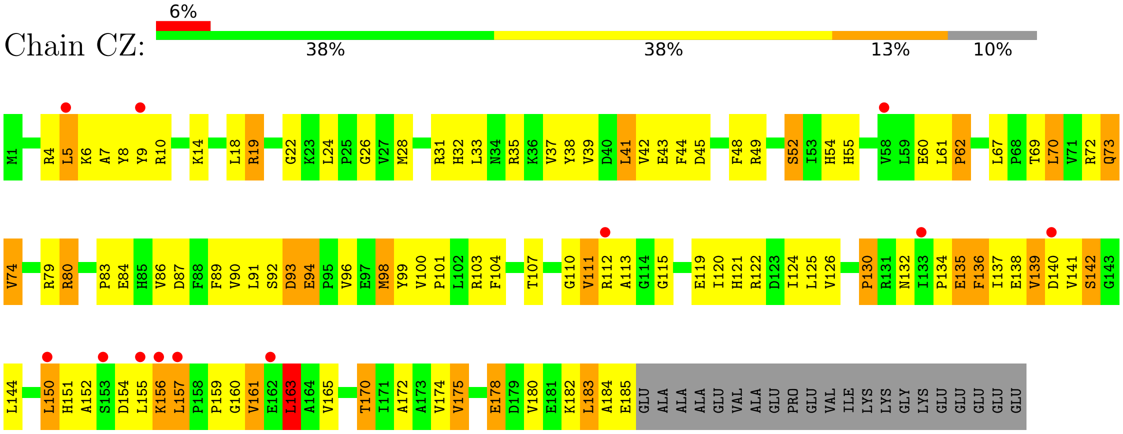
- Molecule 23: 50S ribosomal protein L25

Chain AZ:



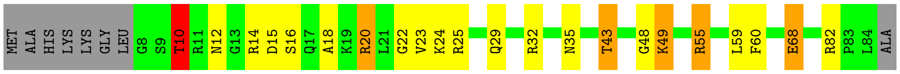
- Molecule 23: 50S ribosomal protein L25

Chain CZ:



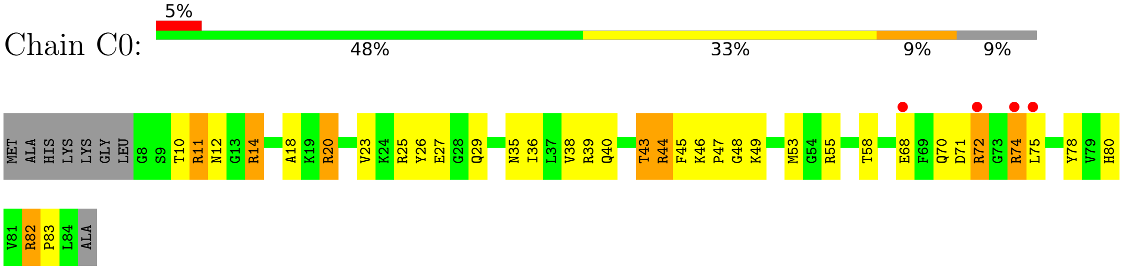
- Molecule 24: 50S ribosomal protein L27

Chain A0:



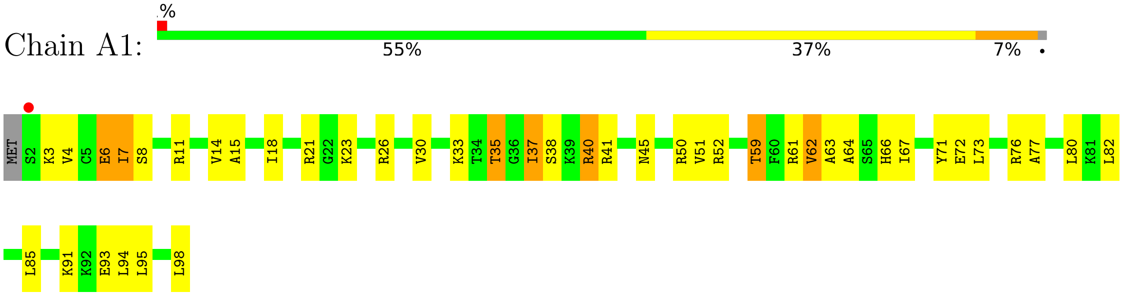
- Molecule 24: 50S ribosomal protein L27

Chain C0:



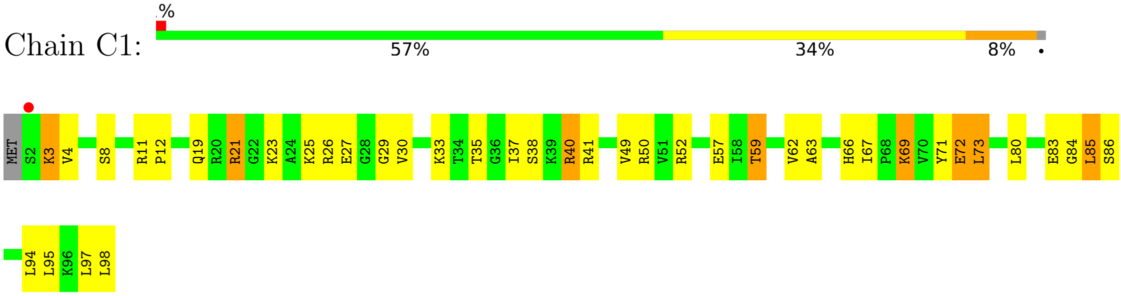
- Molecule 25: 50S ribosomal protein L28

Chain A1:



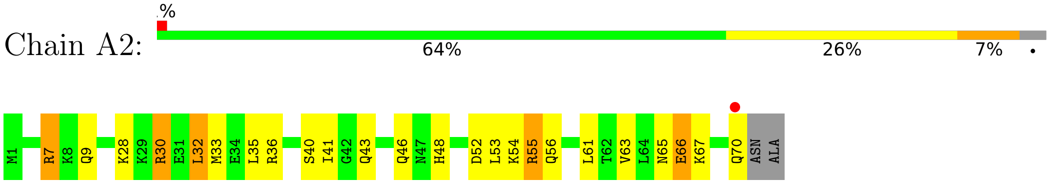
- Molecule 25: 50S ribosomal protein L28

Chain C1:



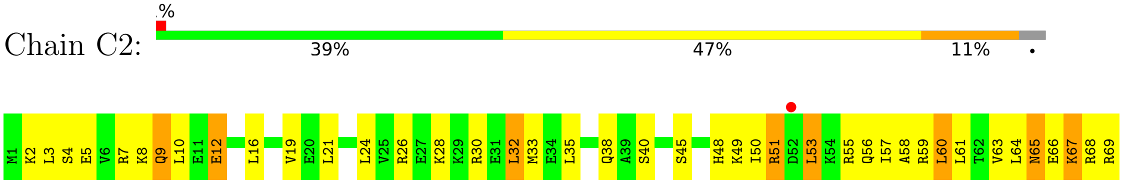
- Molecule 26: 50S ribosomal protein L29

Chain A2:



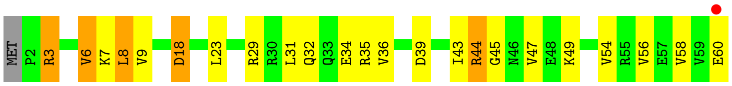
- Molecule 26: 50S ribosomal protein L29

Chain C2:



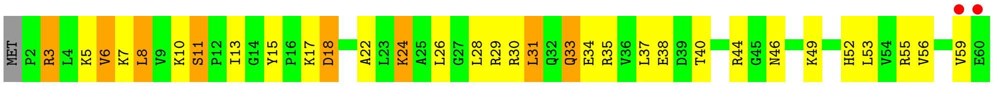
- Molecule 27: 50S ribosomal protein L30

Chain A3:



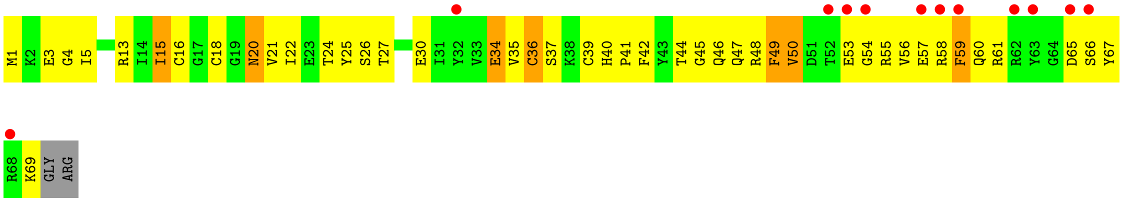
- Molecule 27: 50S ribosomal protein L30

Chain C3:



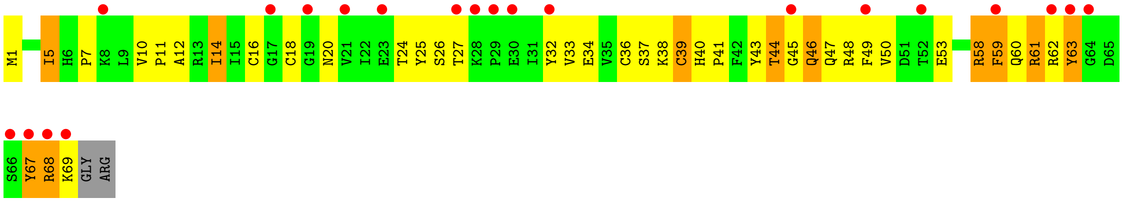
- Molecule 28: 50S ribosomal protein L31

Chain A4:



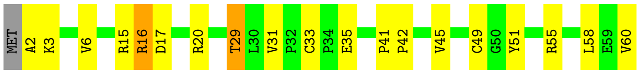
- Molecule 28: 50S ribosomal protein L31

Chain C4:



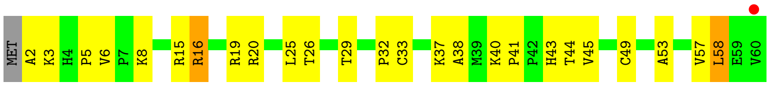
- Molecule 29: 50S ribosomal protein L32

Chain A5:



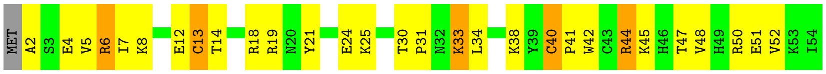
- Molecule 29: 50S ribosomal protein L32

Chain C5:



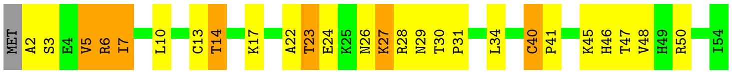
- Molecule 30: 50S ribosomal protein L33

Chain A6:



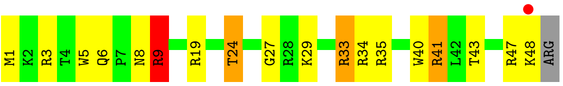
- Molecule 30: 50S ribosomal protein L33

Chain C6:



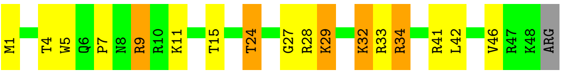
- Molecule 31: 50S ribosomal protein L34

Chain A7:



- Molecule 31: 50S ribosomal protein L34

Chain C7:

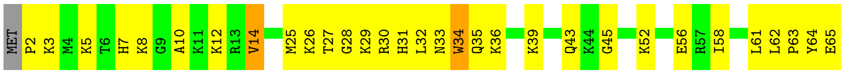


- Molecule 32: 50S ribosomal protein L35

Chain A8:

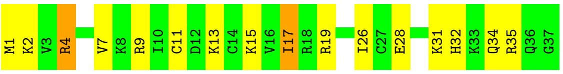
- Molecule 32: 50S ribosomal protein L35

Chain C8:



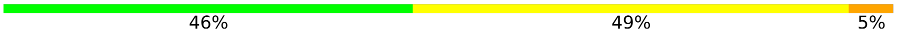
- Molecule 33: 50S ribosomal protein L36

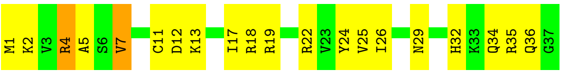
Chain A9:



- Molecule 33: 50S ribosomal protein L36

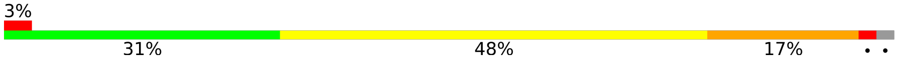
Chain C9:

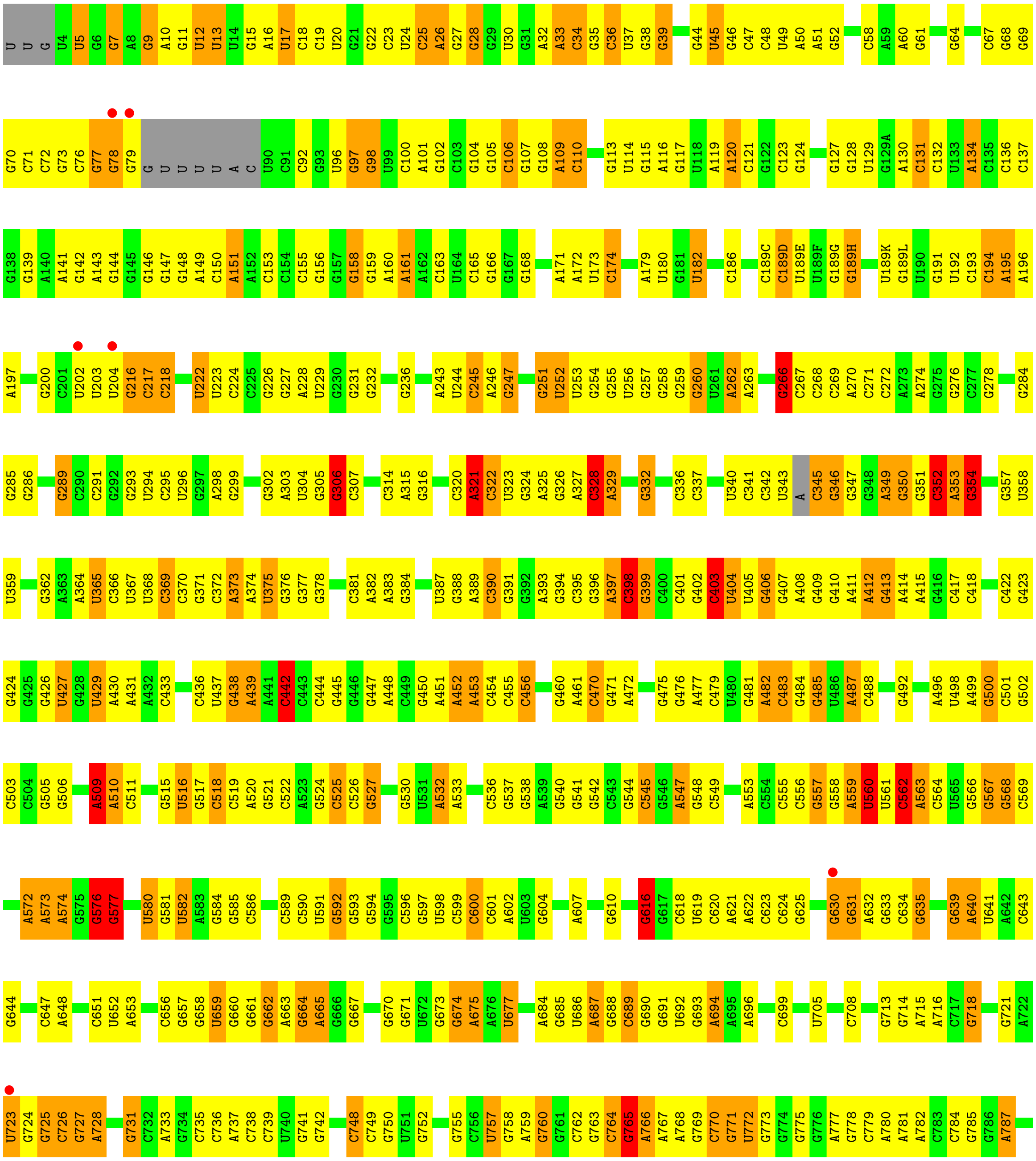


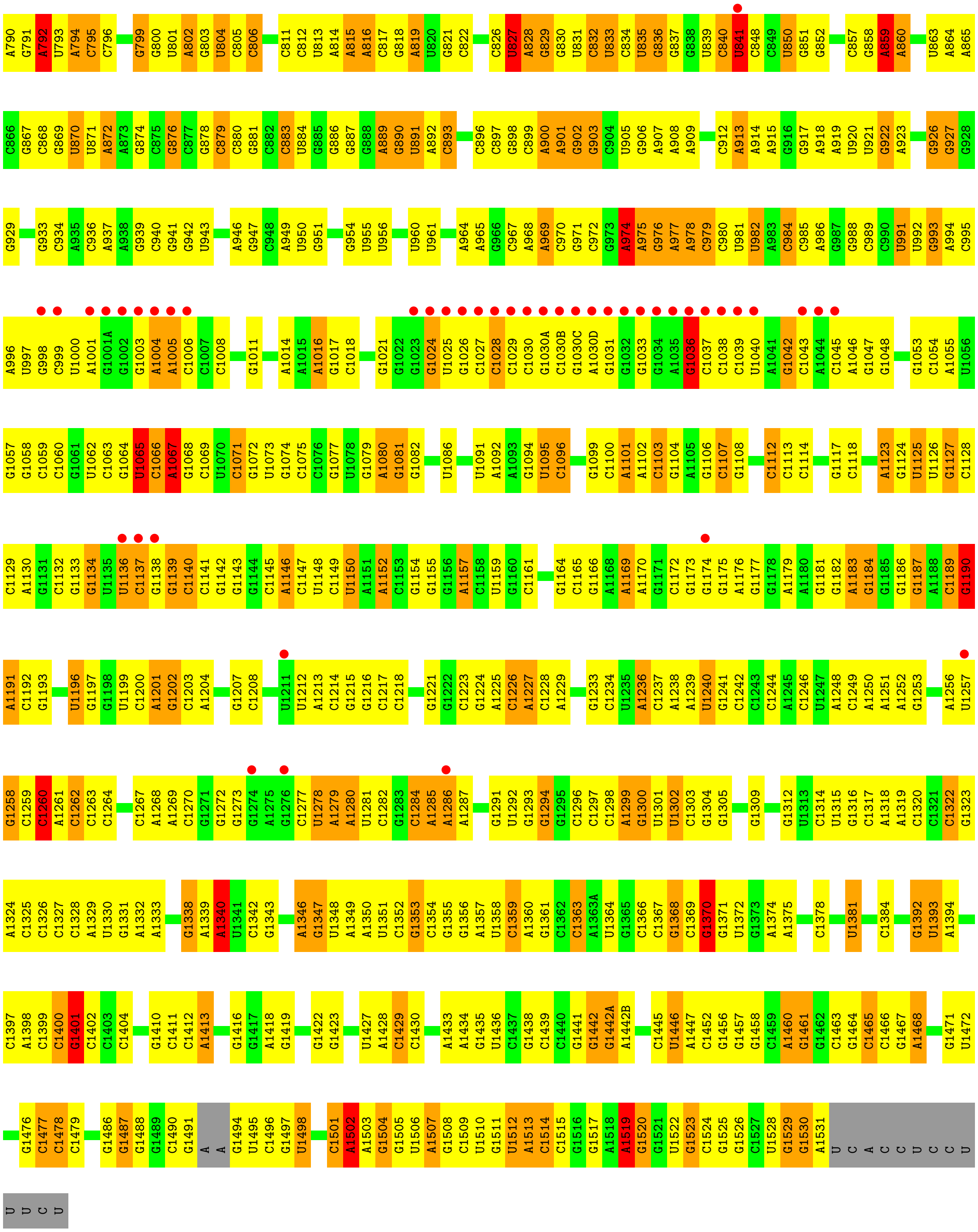


- Molecule 34: 16S Ribosomal RNA

Chain BA:

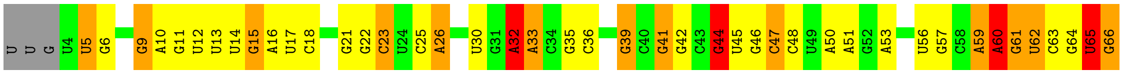


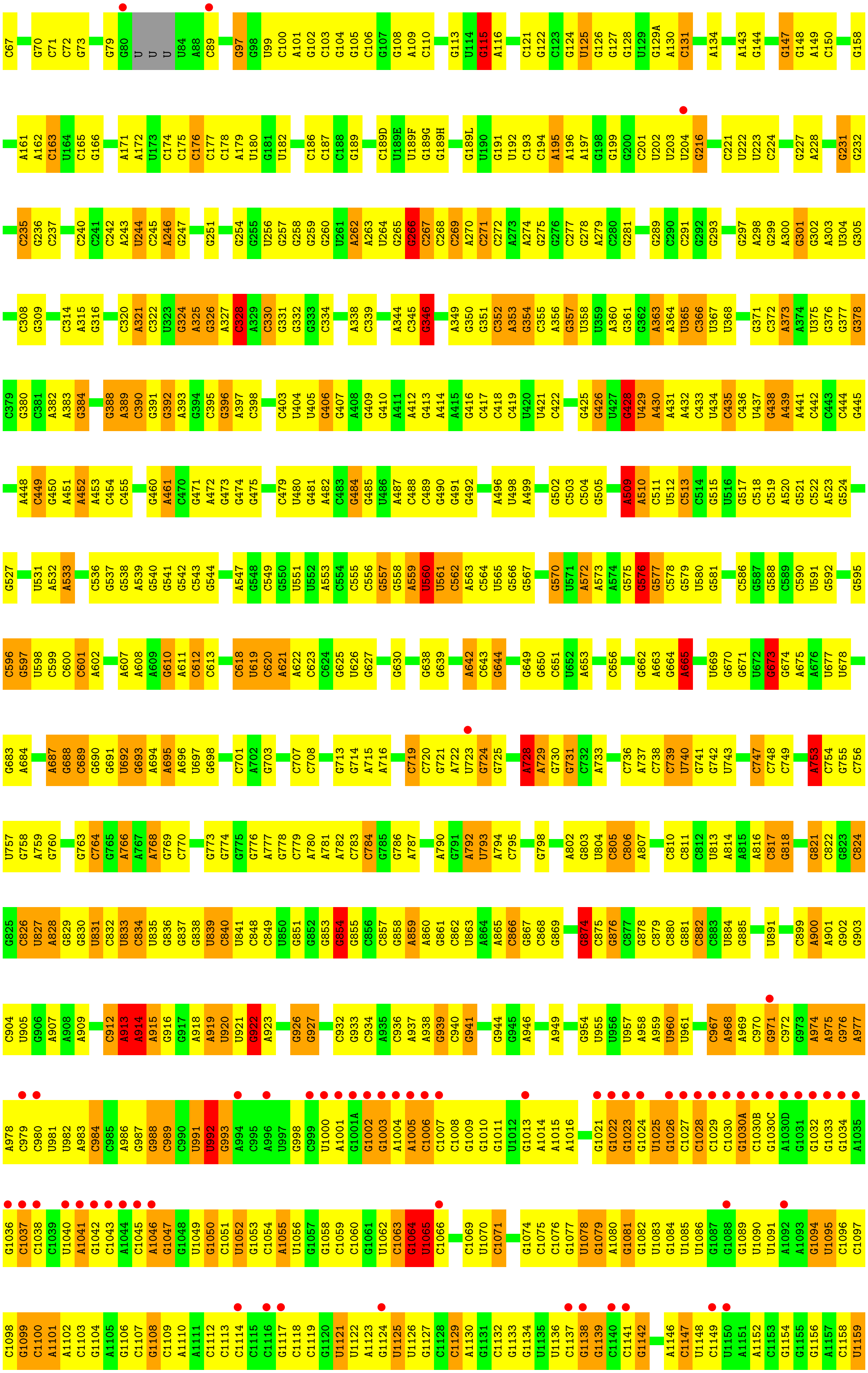




- Molecule 34: 16S Ribosomal RNA

Chain DA:

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A161 A162 C163 U164 C165 G166 A171 A172 U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 C186 C187 C188 G189 C189D U189E U189F G189G G189H G189L U190 G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 C201 U202 U203 U204 G216 C221 U222 U223 C224 G227 A228 G231 G232
C235 G236 C237 C240 C241 C242 A243 U244 C245 A246 G247 G251 G254 G255 U256 G257 G258 G259 G260 U261 A262 A263 U264 G265 G266 C267 C268 C269 A270 C271 C272 A273 A274 G275 G276 C277 G278 A279 C280 G281 G289 C290 C291 G292 G293 G297 A298 G299 A300 G301 G302 A303 U304 G305
C308 G309 C314 A315 G316 C320 A321 C322 U323 G324 A325 G326 A327 C328 A329 C330 G331 C332 G333 C334 A338 C339 A344 C345 G346 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 U359 A360 G361 G362 A363 A364 U365 C366 U367 U368 G371 C372 A373 A374 U375 G376 G377 G378
C379 G380 C381 A382 A383 G384 G388 A389 C390 G391 G392 A393 G394 C395 G396 A397 C398 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 C417 C418 C419 U420 U421 C422 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445
A448 C449 G450 A451 A452 A453 C454 C455 G460 A461 C470 G471 A472 G473 G474 G475 C479 U480 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490 G491 G492 A496 U498 A499 G502 C503 C504 G505 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G524
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C596 G597 U598 C599 C600 C601 A602 A607 A608 A609 G610 A611 C612 C613 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G630 G638 G639 A642 C643 G644 G649 G650 C651 U652 A653 C656 G662 A663 G664 A665 U669 G670 C671 U672 G673 G674 A675 A676 U677 U678
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G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 C849 U850 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 G874 C875 G876 C877 G878 C879 C880 G881 C882 C883 U884 G885 U891 C899 A900 A901 G902 G903
C904 U905 G906 A907 A908 A909 C912 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 A923 G926 G927 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G944 G945 A946 A949 G954 U955 U956 U957 A958 A959 U960 U961 C967 A968 C970 G971 C972 G973 A974 A975 G976 A977
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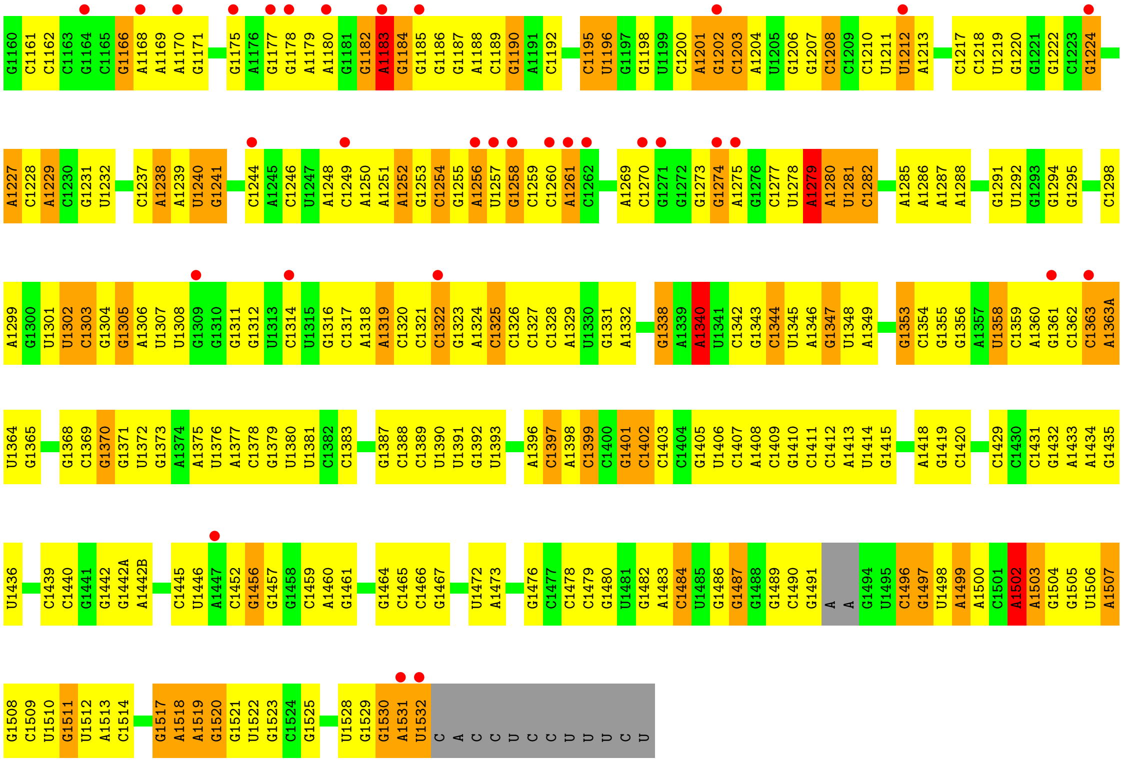
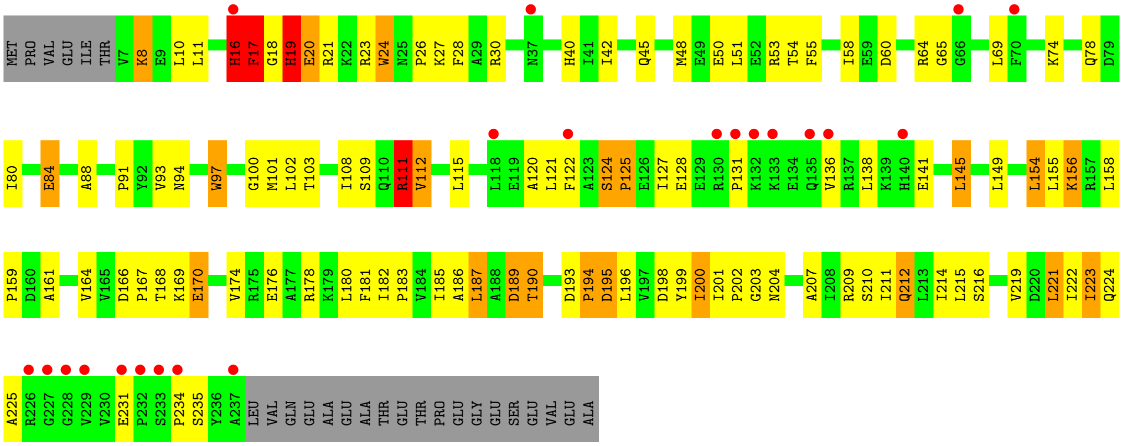
C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 C1154 G1155 G1156 A1157 C1158 U1159



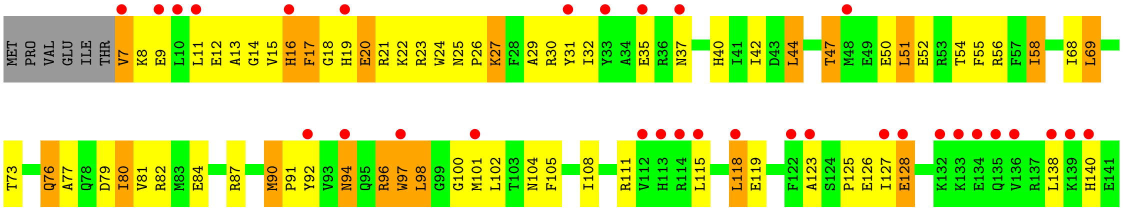
- Molecule 35: 30S ribosomal protein S2

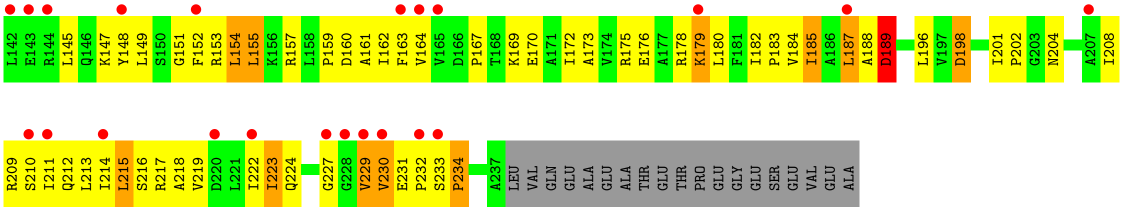
Chain BB:



- Molecule 35: 30S ribosomal protein S2

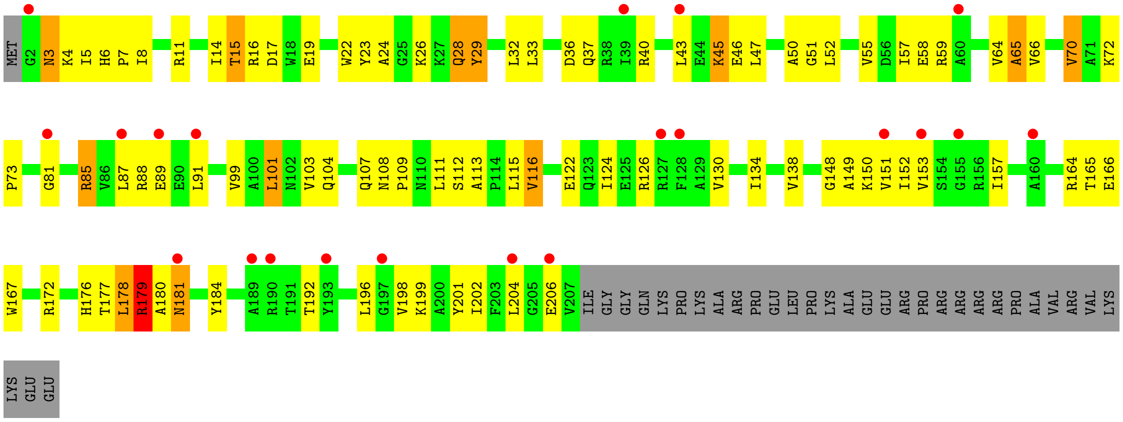
Chain DB:





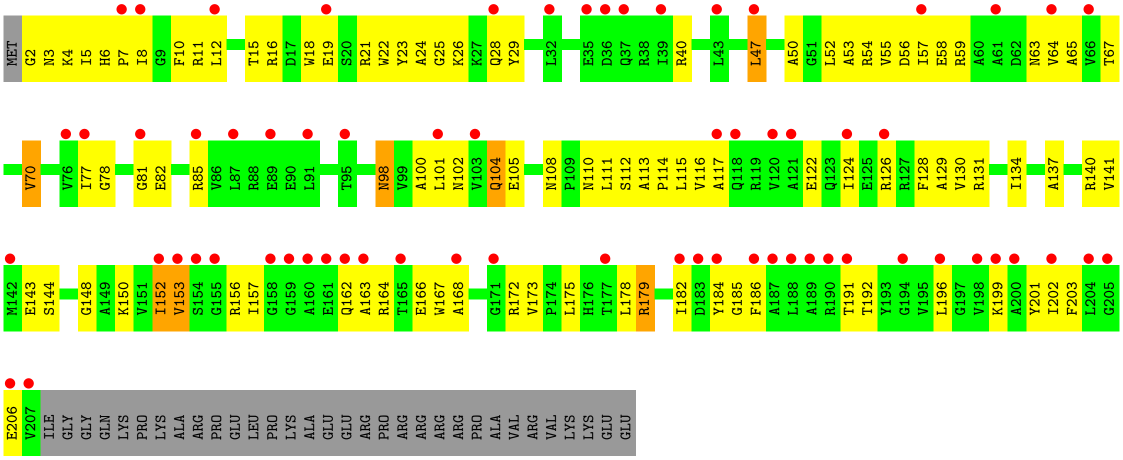
- Molecule 36: 30S ribosomal protein S3

Chain BC:



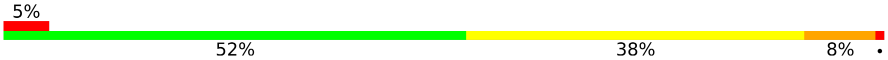
- Molecule 36: 30S ribosomal protein S3

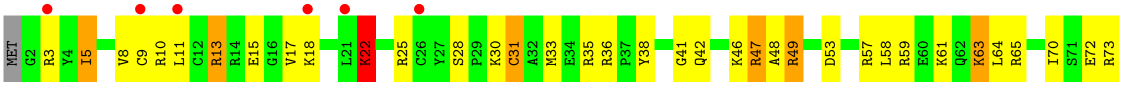
Chain DC:

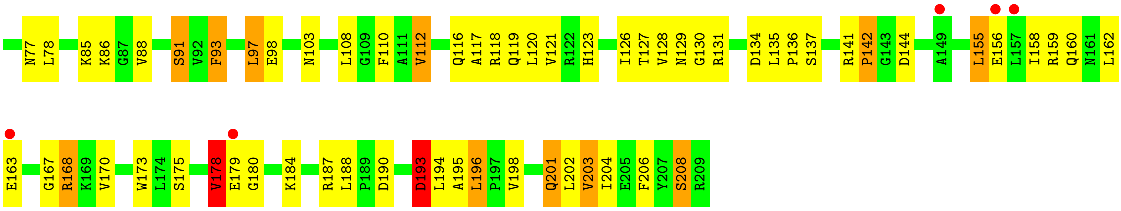


- Molecule 37: 30S ribosomal protein S4

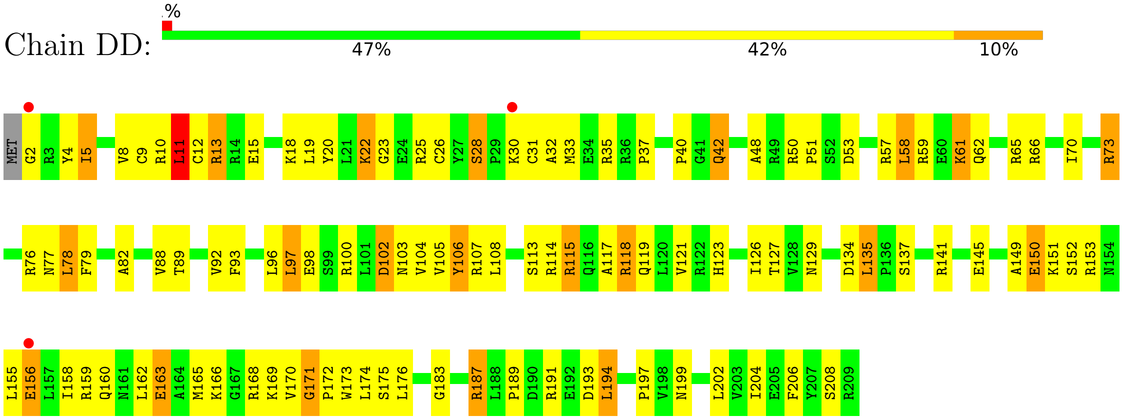
Chain BD:



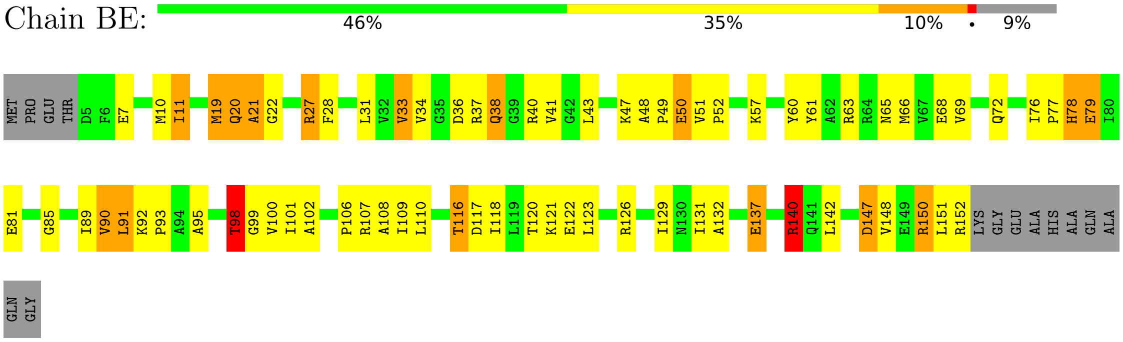




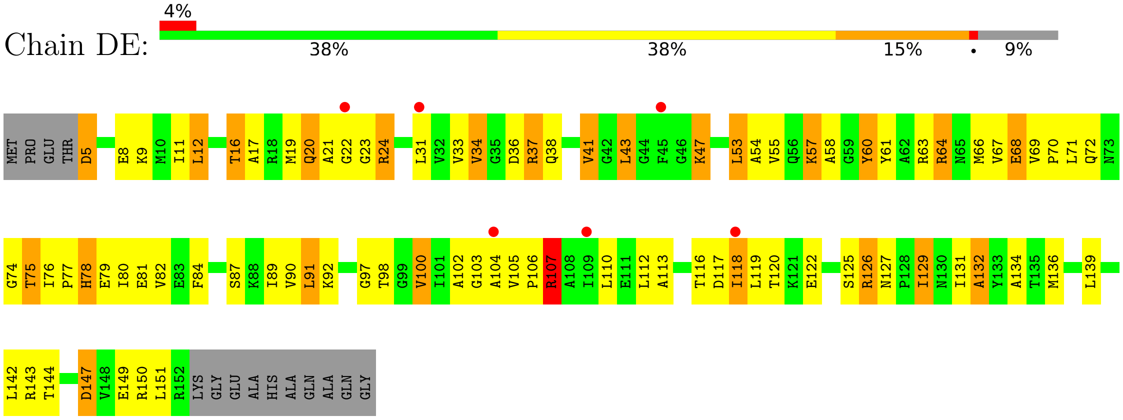
- Molecule 37: 30S ribosomal protein S4



- Molecule 38: 30S ribosomal protein S5

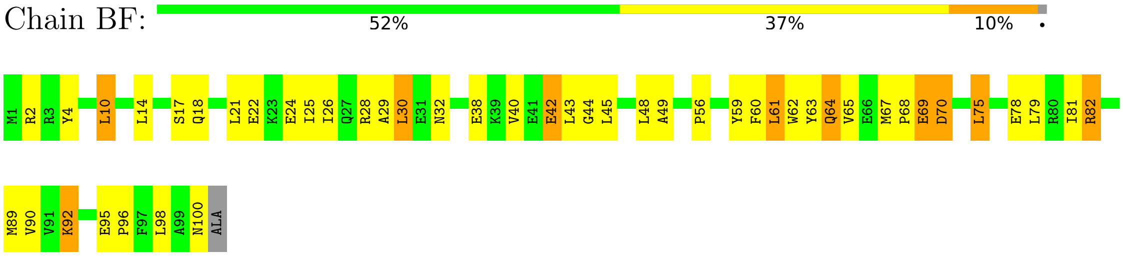


- Molecule 38: 30S ribosomal protein S5



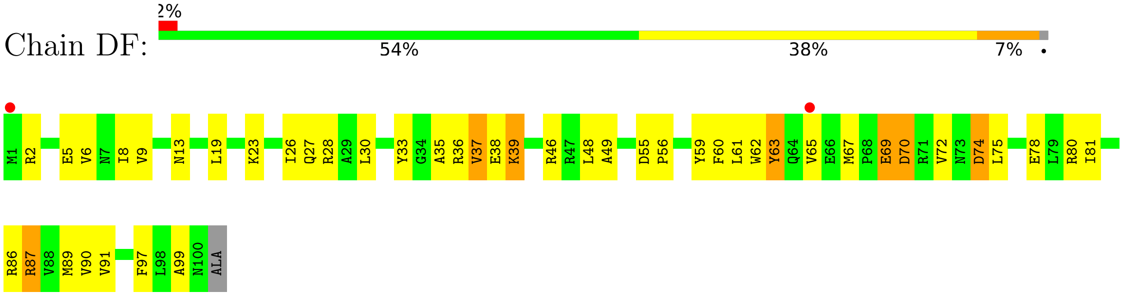
- Molecule 39: 30S ribosomal protein S6

Chain BF:



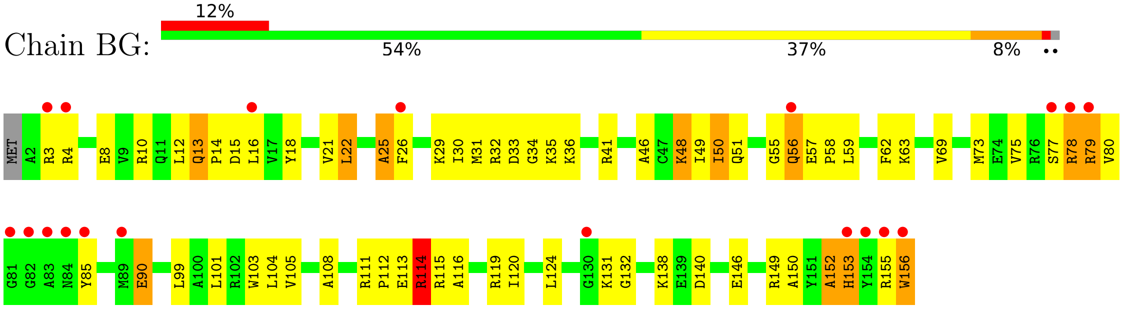
- Molecule 39: 30S ribosomal protein S6

Chain DF:



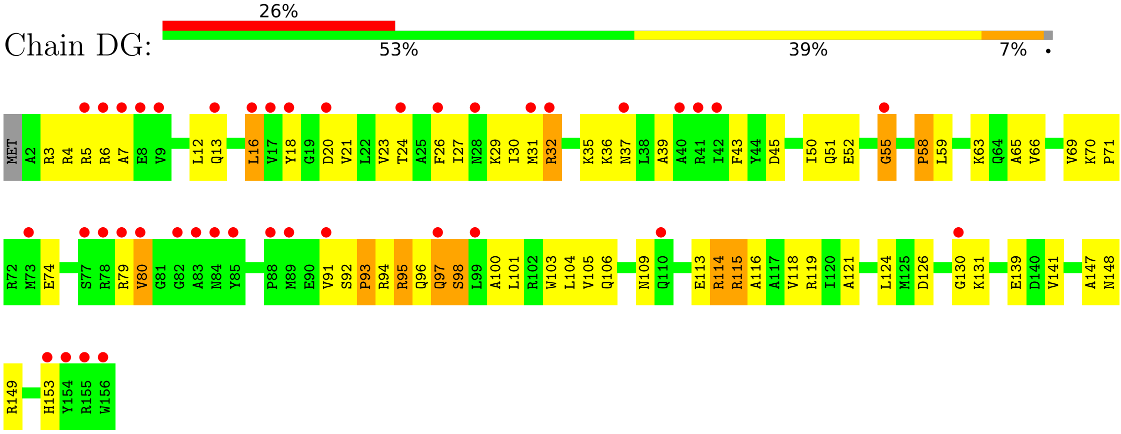
- Molecule 40: 30S ribosomal protein S7

Chain BG:



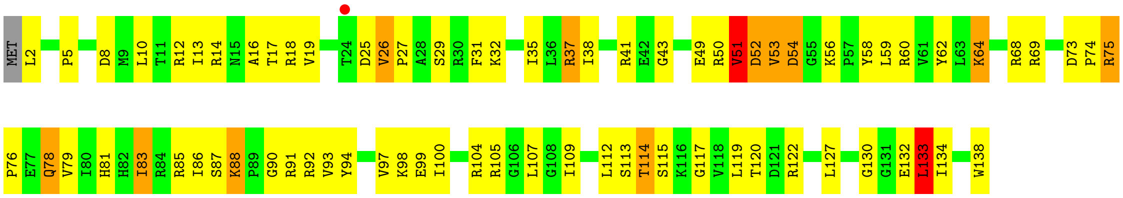
- Molecule 40: 30S ribosomal protein S7

Chain DG:



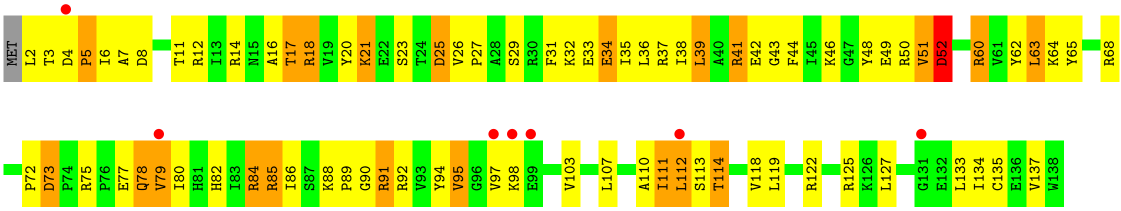
- Molecule 41: 30S ribosomal protein S8

Chain BH:



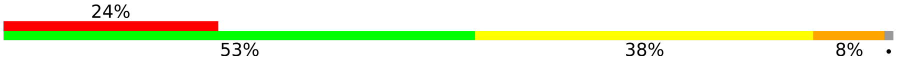
- Molecule 41: 30S ribosomal protein S8

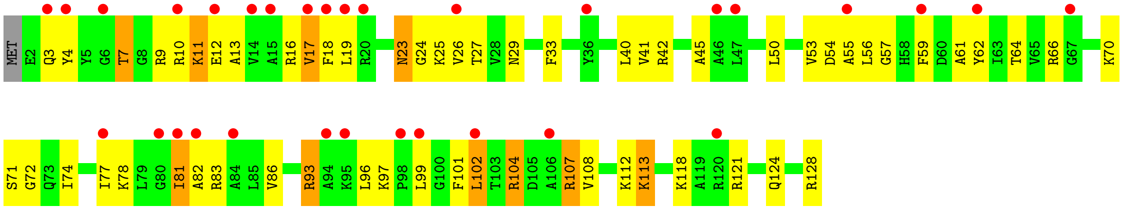
Chain DH:



- Molecule 42: 30S ribosomal protein S9

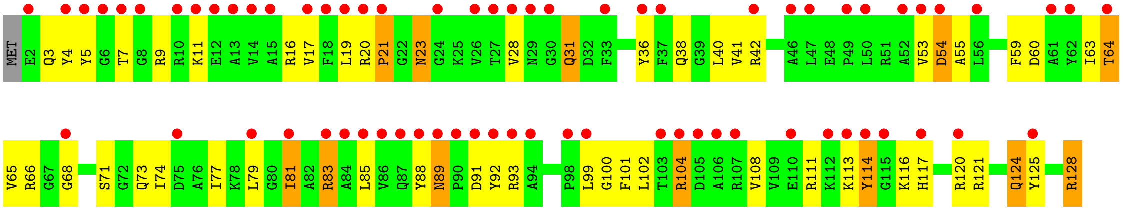
Chain BI:





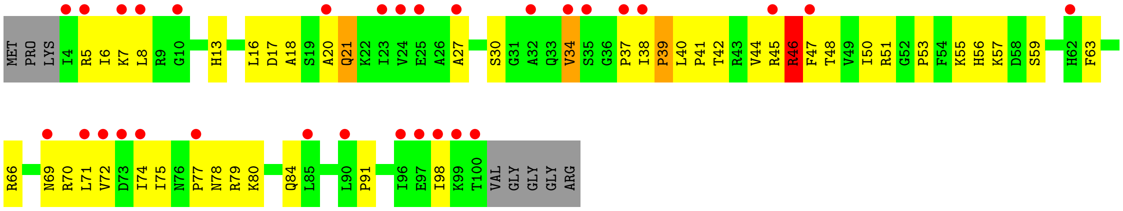
- Molecule 42: 30S ribosomal protein S9

Chain DI:

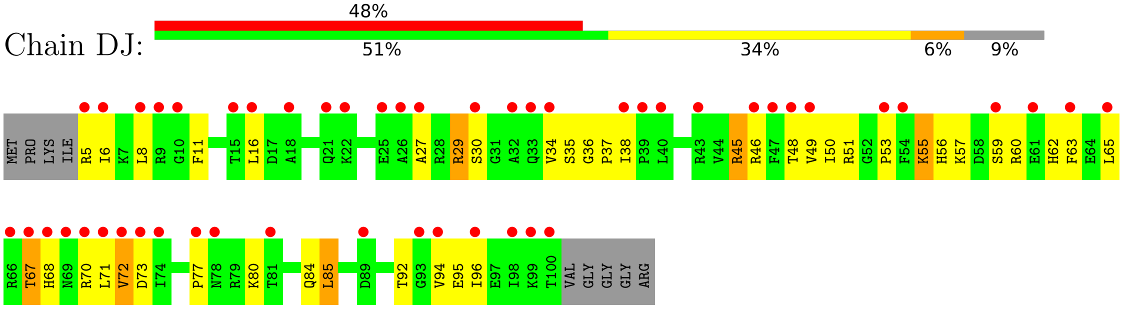


- Molecule 43: 30S ribosomal protein S10

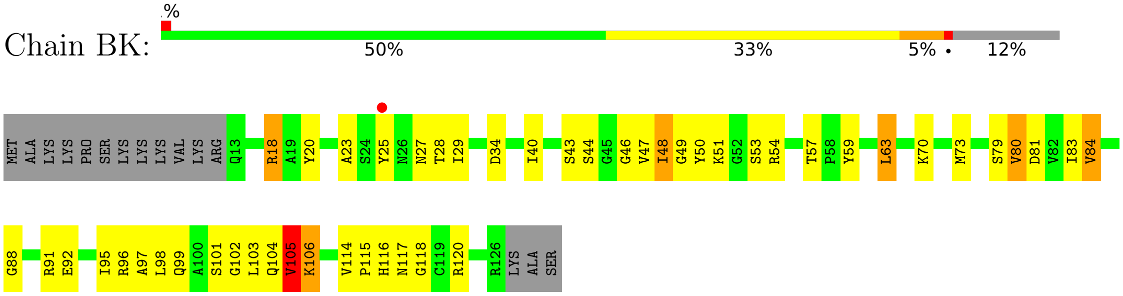
Chain BJ:



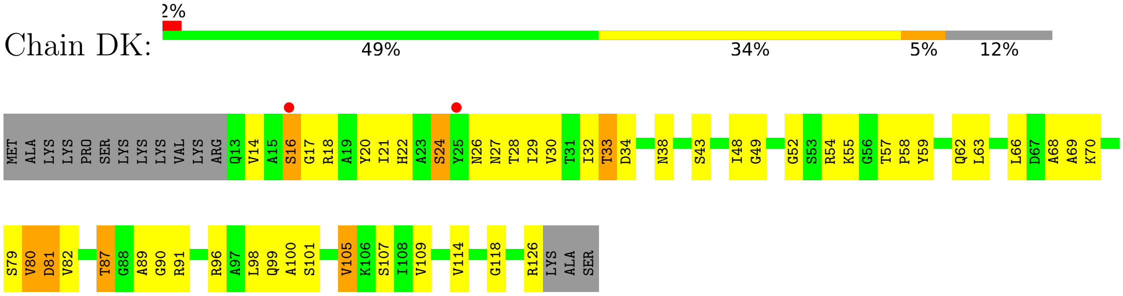
- Molecule 43: 30S ribosomal protein S10



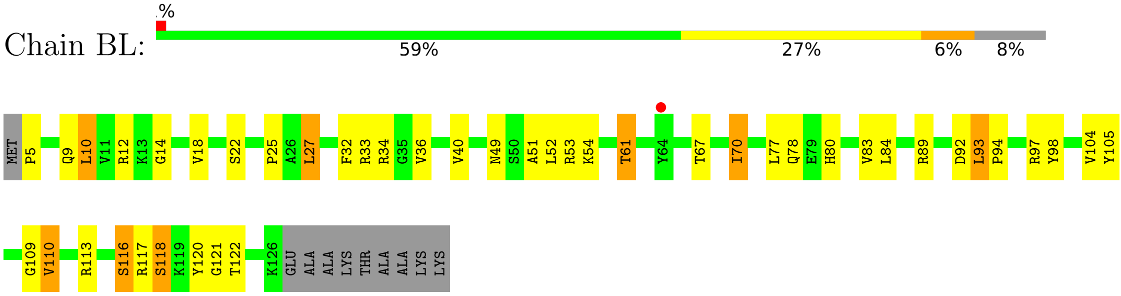
- Molecule 44: 30S ribosomal protein S11



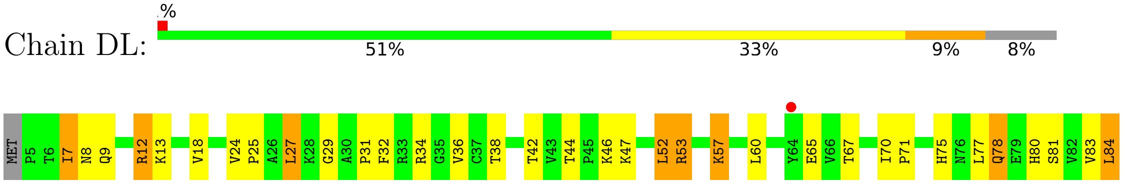
- Molecule 44: 30S ribosomal protein S11

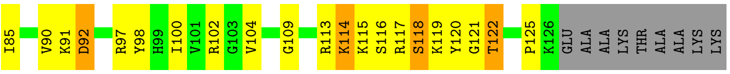


- Molecule 45: 30S ribosomal protein S12

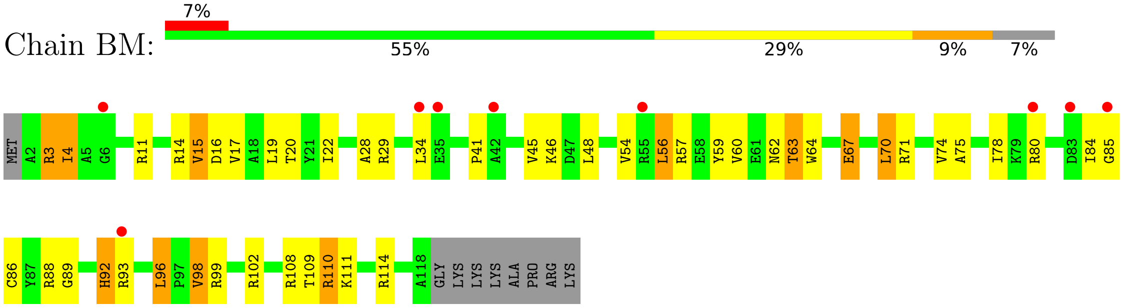


- Molecule 45: 30S ribosomal protein S12

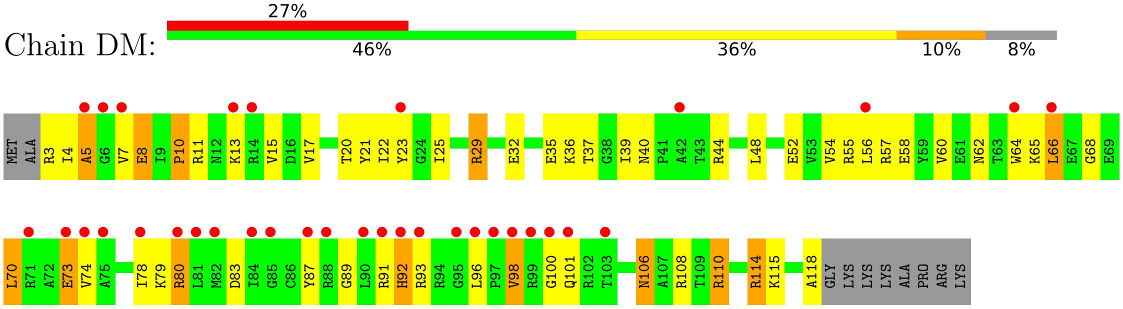




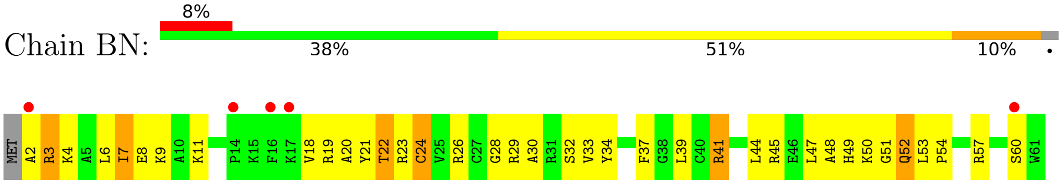
- Molecule 46: 30S ribosomal protein S13



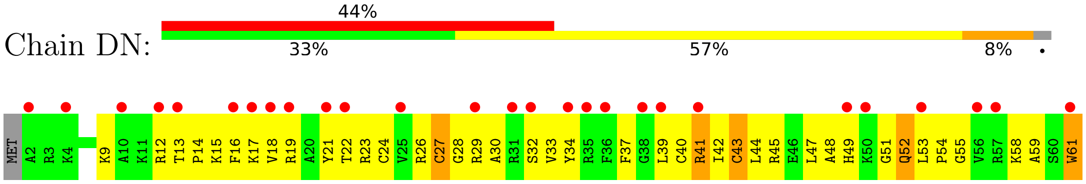
- Molecule 46: 30S ribosomal protein S13



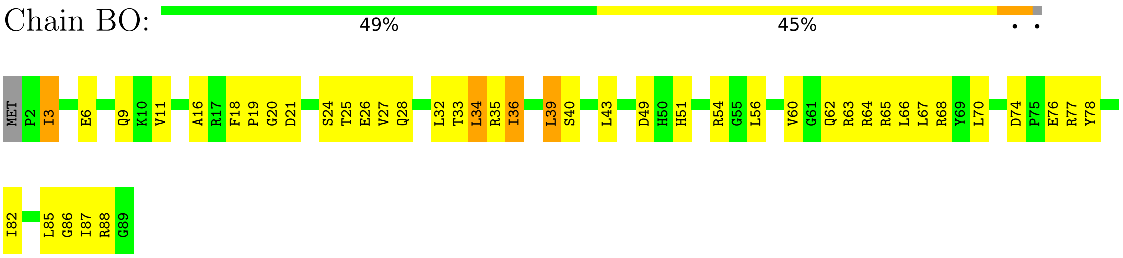
- Molecule 47: 30S ribosomal protein S14 type Z



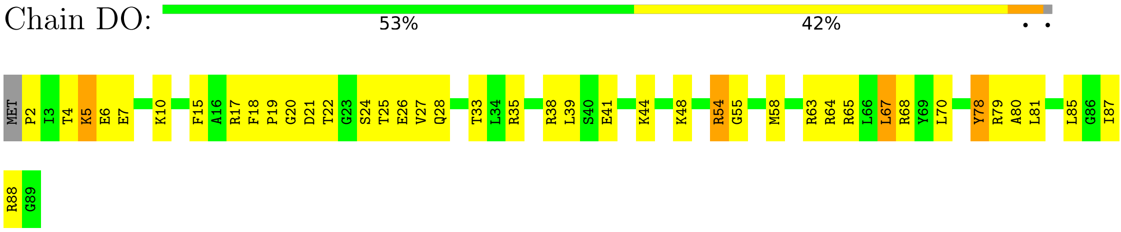
- Molecule 47: 30S ribosomal protein S14 type Z



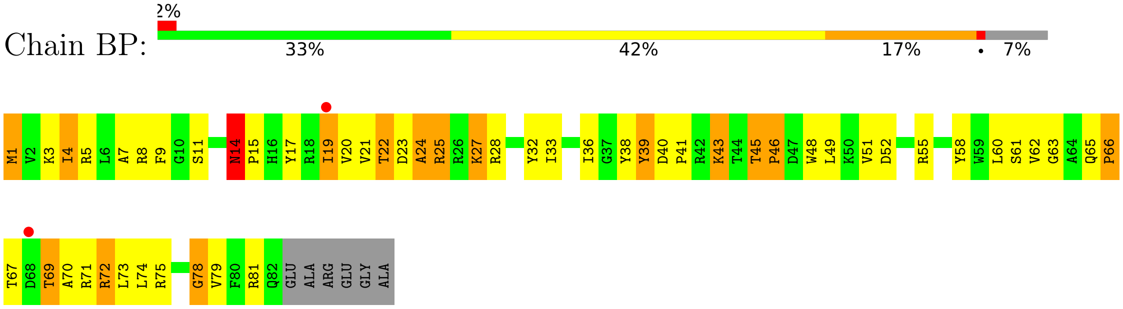
- Molecule 48: 30S ribosomal protein S15



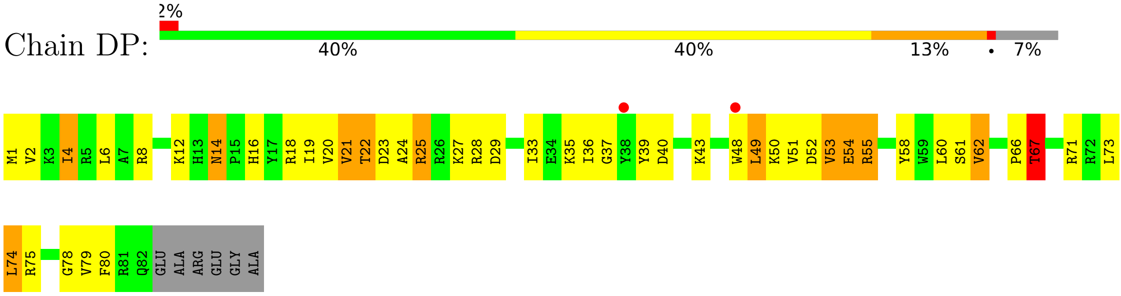
- Molecule 48: 30S ribosomal protein S15



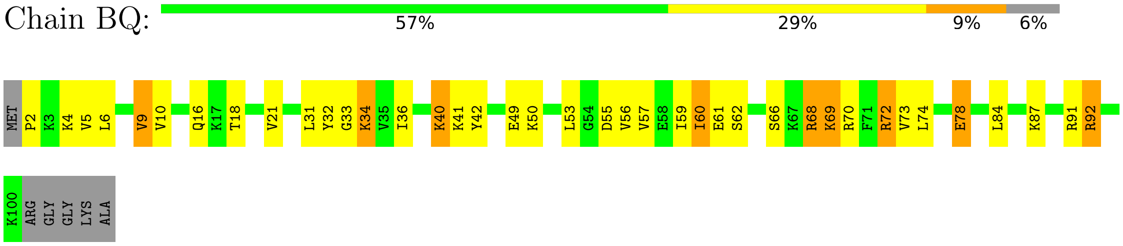
- Molecule 49: 30S ribosomal protein S16



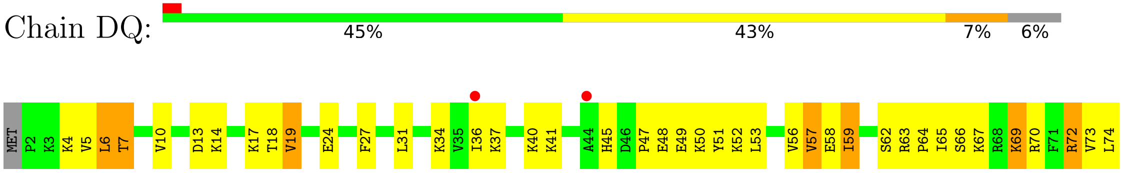
- Molecule 49: 30S ribosomal protein S16

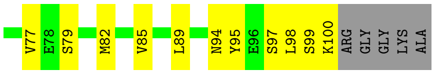


- Molecule 50: 30S ribosomal protein S17



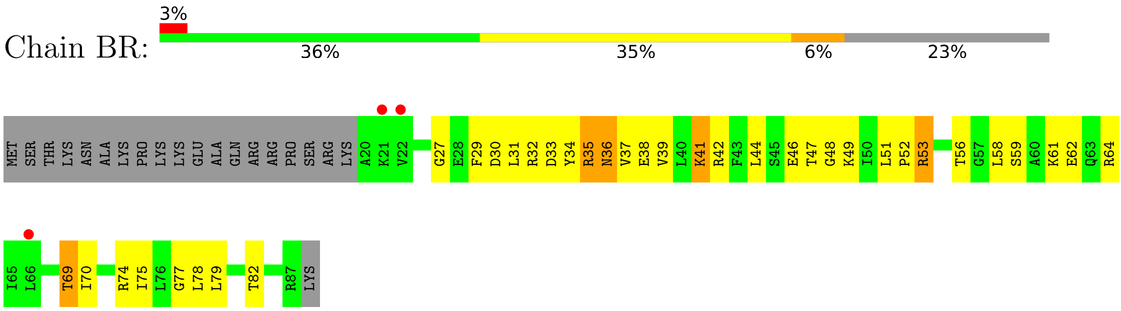
- Molecule 50: 30S ribosomal protein S17





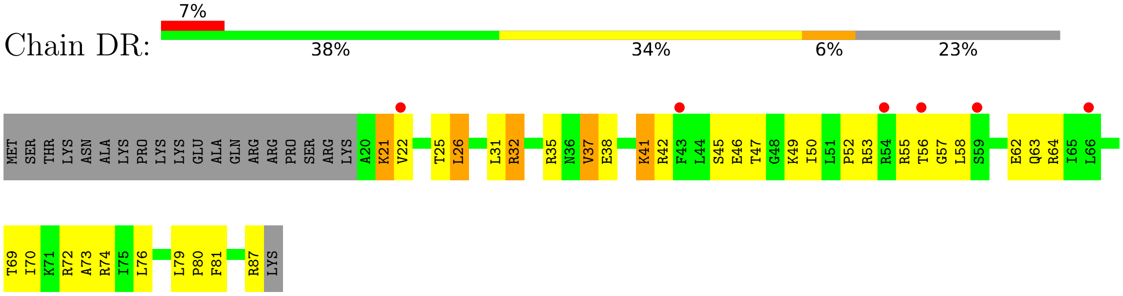
- Molecule 51: 30S ribosomal protein S18

Chain BR:



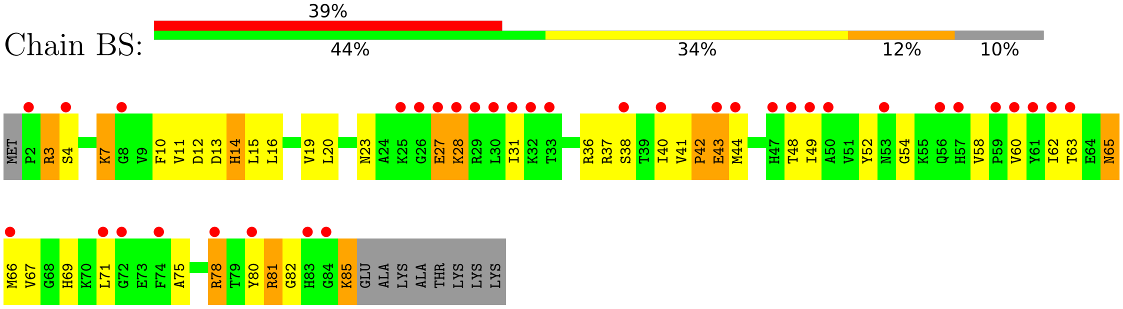
- Molecule 51: 30S ribosomal protein S18

Chain DR:



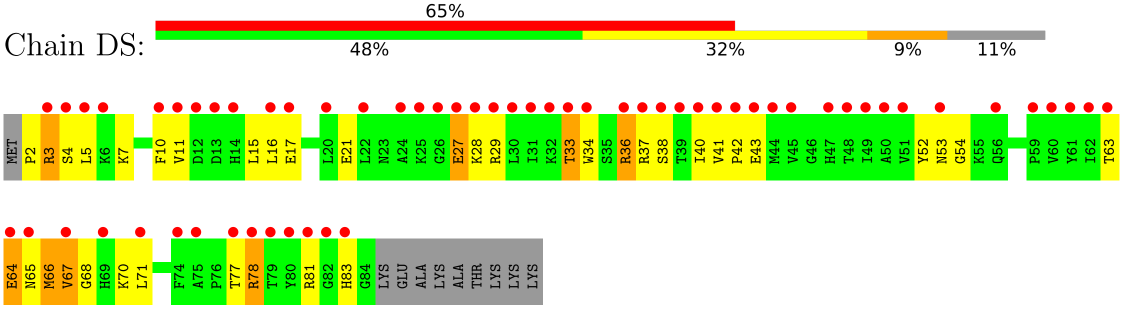
- Molecule 52: 30S ribosomal protein S19

Chain BS:



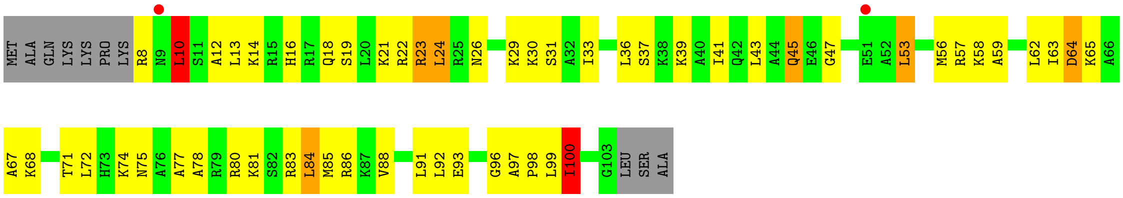
- Molecule 52: 30S ribosomal protein S19

Chain DS:



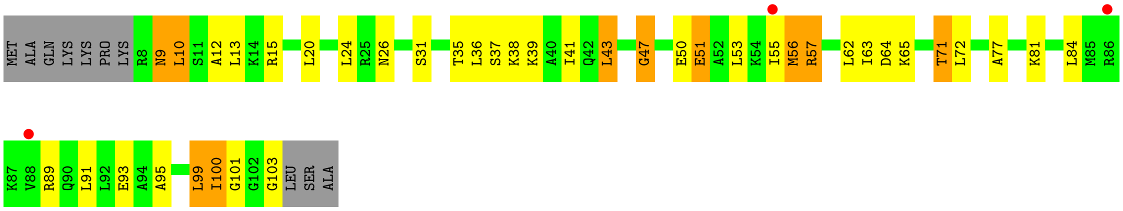
- Molecule 53: 30S ribosomal protein S20

Chain BT:



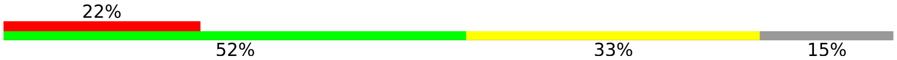
- Molecule 53: 30S ribosomal protein S20

Chain DT:



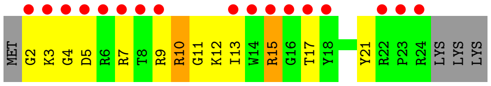
- Molecule 54: 30S ribosomal protein Thx

Chain BU:



- Molecule 54: 30S ribosomal protein Thx

Chain DU:



- Molecule 55: mRNA

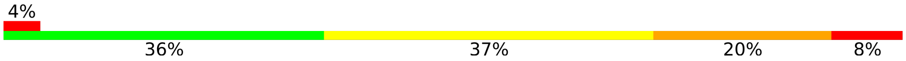
Chain BV:

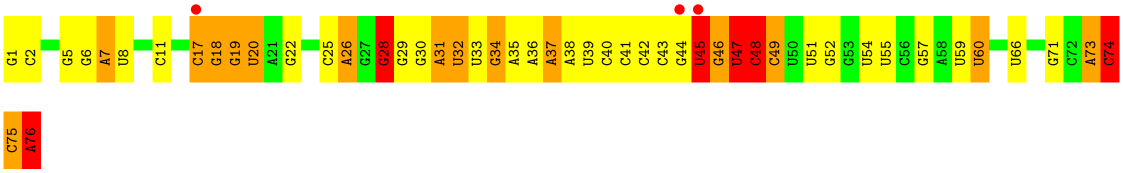
- Molecule 55: mRNA

Chain DV:

- Molecule 56: P-site tRNA

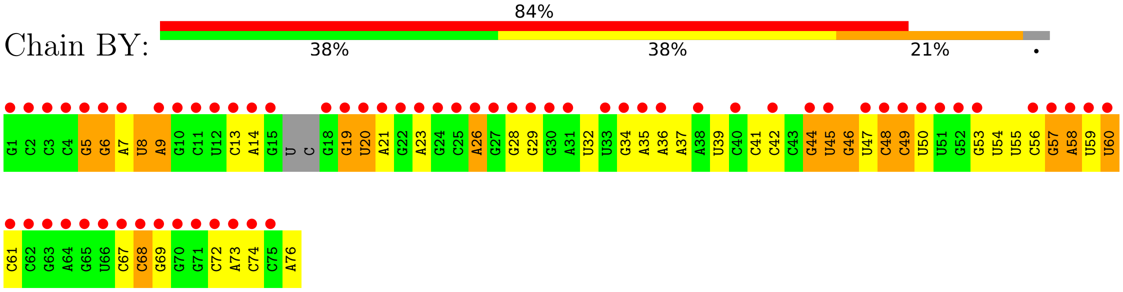
Chain BW:





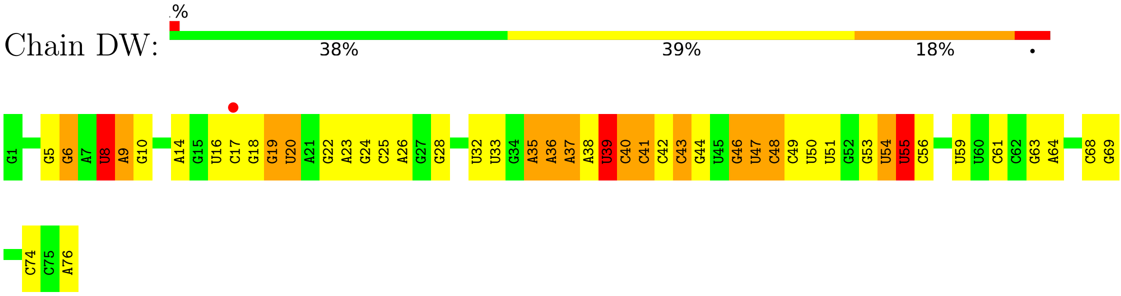
- Molecule 56: P-site tRNA

Chain BY:



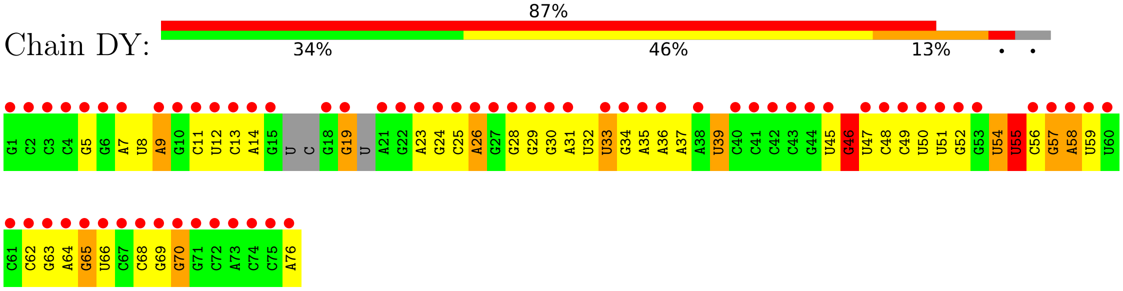
- Molecule 56: P-site tRNA

Chain DW:



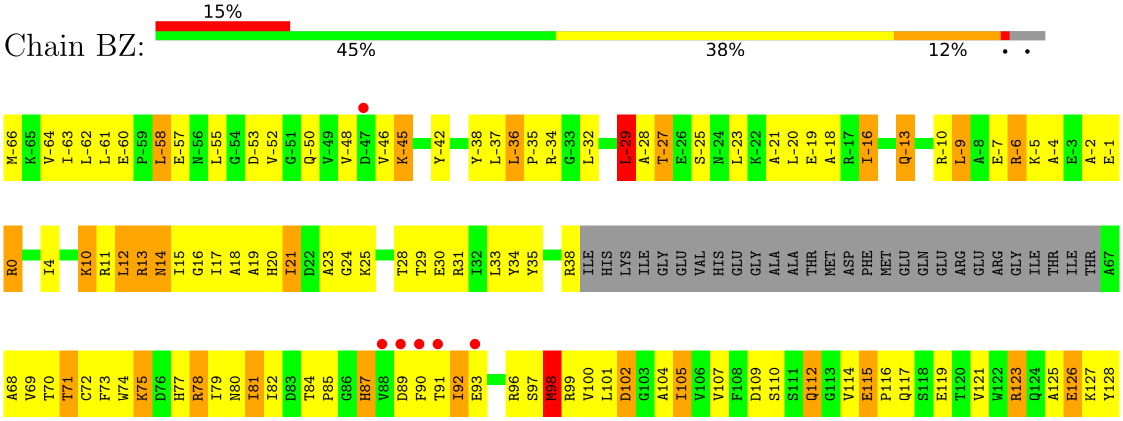
- Molecule 56: P-site tRNA

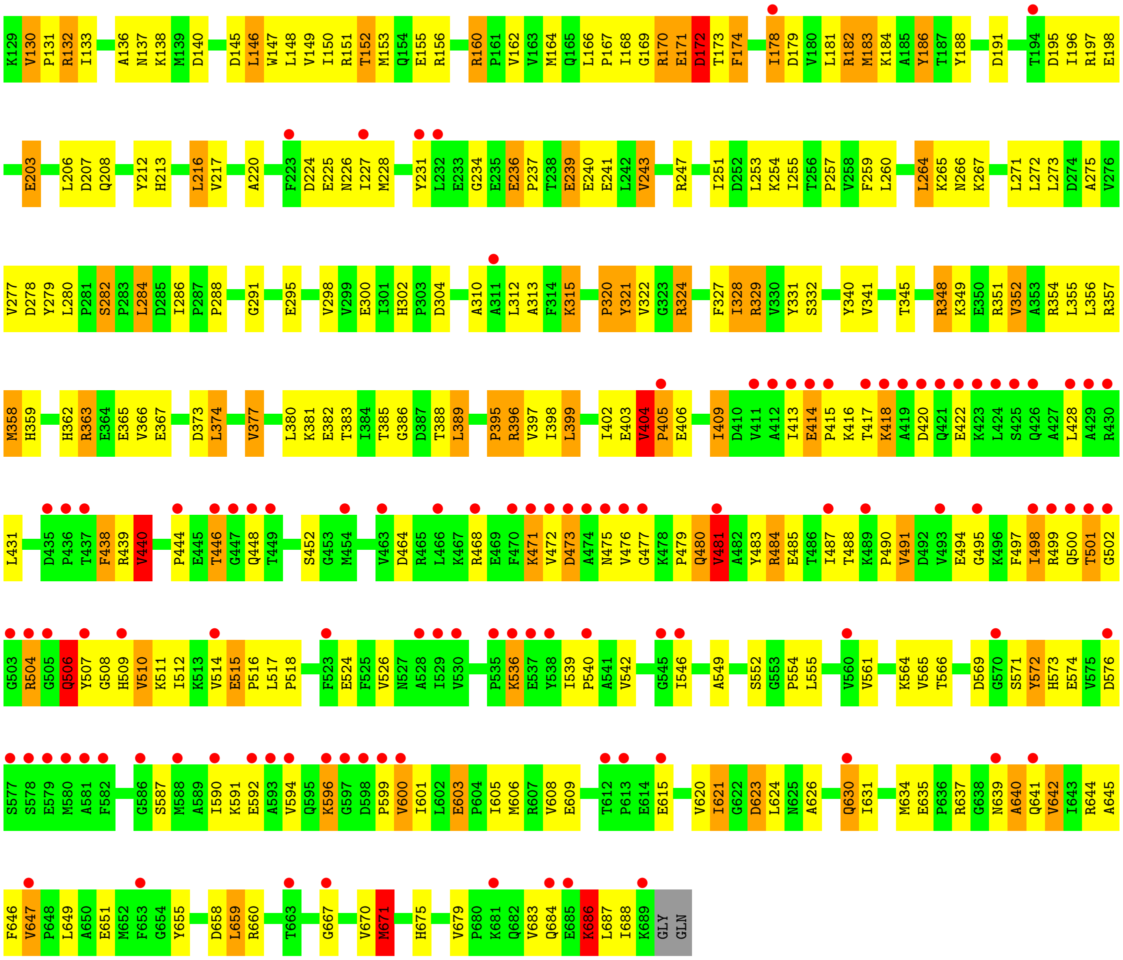
Chain DY:



- Molecule 57: 50S ribosomal protein L9,Elongation factor G

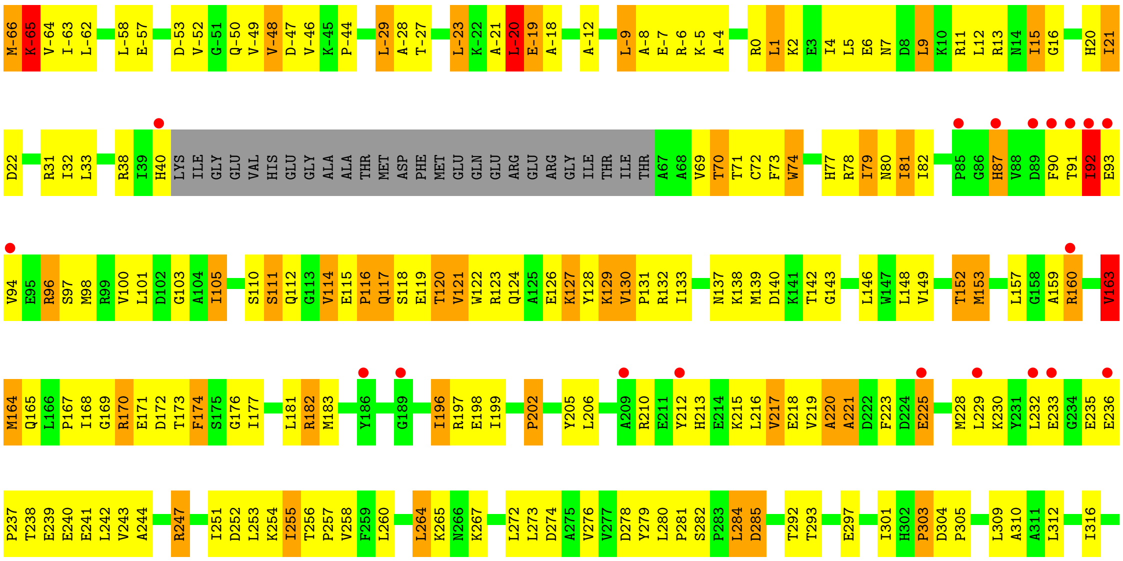
Chain BZ:

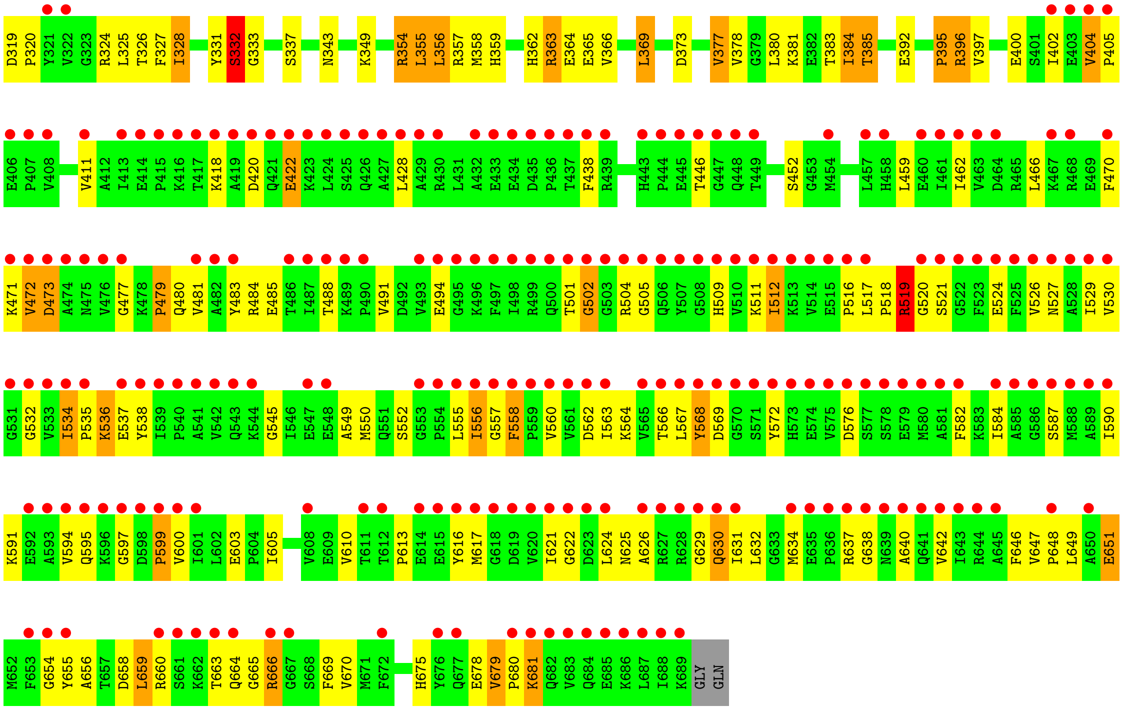




- Molecule 57: 50S ribosomal protein L9,Elongation factor G

Chain DZ:





- Molecule 58: Dityromycin

Chain BX:

- Molecule 58: Dityromycin

Chain DX:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.84Å 450.58Å 623.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.81-2.80) 94.5 (49.80-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.264 0.210 , 0.265	Depositor DCC
R_{free} test set	67916 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	310038	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: 2QZ, 2QY, 5MU, ZN, MVA, 4SU, MG, GDP, 2R3, SF4, 2R1, MIA, 004, PSU, 7MG

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	1.41	444/69281 (0.6%)	2.07	3848/108144 (3.6%)
1	CA	1.00	75/69179 (0.1%)	1.66	1653/107984 (1.5%)
2	AB	1.17	7/2878 (0.2%)	1.92	120/4490 (2.7%)
2	CB	0.66	0/2878	1.33	24/4490 (0.5%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.94	2/2186 (0.1%)	1.04	5/2944 (0.2%)
4	CD	0.74	0/2192	0.95	6/2951 (0.2%)
5	AE	0.93	0/1592	1.08	2/2149 (0.1%)
5	CE	0.72	0/1592	0.91	1/2149 (0.0%)
6	AF	0.91	2/1619 (0.1%)	1.01	4/2193 (0.2%)
6	CF	0.63	0/1615	0.83	1/2188 (0.0%)
7	AG	0.60	0/1450	0.83	2/1959 (0.1%)
7	CG	0.36	0/1449	0.62	0/1958
8	AH	0.84	0/1356	0.96	1/1834 (0.1%)
8	CH	0.49	0/1356	0.67	0/1834
9	AK	0.34	0/640	0.67	0/889
9	CK	0.28	0/640	0.61	0/889
10	AL	0.31	0/503	0.54	0/673
10	CL	0.34	0/503	0.60	0/673
11	AN	0.95	0/1144	1.01	3/1543 (0.2%)
11	CN	0.61	0/1144	0.81	0/1543
12	AO	0.91	1/943 (0.1%)	1.02	3/1269 (0.2%)
12	CO	0.77	0/943	0.87	0/1269
13	AP	0.85	0/1156	1.03	4/1537 (0.3%)
13	CP	0.57	0/1152	0.87	2/1533 (0.1%)
14	AQ	0.91	0/1143	0.97	2/1527 (0.1%)
14	CQ	0.64	0/1143	0.82	1/1527 (0.1%)
15	AR	0.90	0/982	1.07	4/1312 (0.3%)
15	CR	0.65	0/982	0.88	1/1312 (0.1%)
16	AS	0.76	0/887	0.95	1/1180 (0.1%)
16	CS	0.49	0/880	0.74	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AT	0.89	0/1105	1.02	3/1477 (0.2%)
17	CT	0.65	0/1097	0.89	1/1468 (0.1%)
18	AU	1.11	3/977 (0.3%)	1.05	1/1301 (0.1%)
18	CU	0.69	1/977 (0.1%)	0.79	0/1301
19	AV	0.98	0/782	1.08	2/1049 (0.2%)
19	CV	0.58	0/782	0.79	0/1049
20	AW	1.10	2/897 (0.2%)	1.09	7/1205 (0.6%)
20	CW	0.80	0/897	0.92	0/1205
21	AX	0.96	0/764	0.99	0/1025
21	CX	0.67	0/764	0.83	1/1025 (0.1%)
22	AY	0.88	0/819	0.97	0/1095
22	CY	0.56	0/819	0.72	0/1095
23	AZ	0.72	1/1483 (0.1%)	0.93	4/2017 (0.2%)
23	CZ	0.45	0/1483	0.73	0/2017
24	A0	0.87	0/616	1.05	1/821 (0.1%)
24	C0	0.60	0/616	0.76	0/821
25	A1	0.87	0/762	0.92	0/1014
25	C1	0.67	0/762	0.89	1/1014 (0.1%)
26	A2	0.79	0/590	0.93	1/781 (0.1%)
26	C2	0.59	0/590	0.73	0/781
27	A3	1.01	0/474	1.06	0/635
27	C3	0.57	0/469	0.81	0/630
28	A4	0.50	0/571	0.72	0/768
28	C4	0.35	0/545	0.59	0/737
29	A5	0.99	0/469	1.05	0/635
29	C5	0.76	1/469 (0.2%)	0.86	0/635
30	A6	0.95	0/460	1.03	1/613 (0.2%)
30	C6	0.71	0/456	0.81	1/608 (0.2%)
31	A7	0.99	0/426	1.11	3/561 (0.5%)
31	C7	0.77	0/426	0.99	1/561 (0.2%)
32	A8	0.95	0/525	0.94	0/691
32	C8	0.63	0/525	0.82	0/691
33	A9	0.98	0/310	1.05	0/407
33	C9	0.64	0/310	0.80	0/407
34	BA	0.77	3/35976 (0.0%)	1.42	439/56145 (0.8%)
34	DA	0.68	1/36119 (0.0%)	1.30	238/56370 (0.4%)
35	BB	0.45	0/1881	0.69	1/2542 (0.0%)
35	DB	0.38	0/1860	0.66	0/2518
36	BC	0.40	0/1576	0.61	0/2130
36	DC	0.35	0/1568	0.55	0/2122
37	BD	0.49	0/1689	0.71	0/2267
37	DD	0.51	0/1708	0.73	1/2289 (0.0%)
38	BE	0.60	0/1145	0.79	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DE	0.51	0/1149	0.77	0/1548
39	BF	0.50	0/825	0.77	0/1118
39	DF	0.51	0/833	0.72	0/1128
40	BG	0.43	0/1250	0.60	0/1679
40	DG	0.35	0/1254	0.58	0/1683
41	BH	0.55	0/1108	0.76	0/1494
41	DH	0.45	0/1108	0.75	1/1494 (0.1%)
42	BI	0.44	0/1005	0.64	0/1350
42	DI	0.34	0/997	0.56	0/1343
43	BJ	0.39	0/722	0.71	2/982 (0.2%)
43	DJ	0.34	0/727	0.59	0/988
44	BK	0.56	0/848	0.72	0/1149
44	DK	0.48	0/848	0.63	0/1149
45	BL	0.65	0/946	0.79	0/1274
45	DL	0.64	0/946	0.84	1/1274 (0.1%)
46	BM	0.42	0/933	0.67	0/1253
46	DM	0.30	0/917	0.52	0/1234
47	BN	0.45	0/501	0.67	0/664
47	DN	0.33	0/501	0.60	0/664
48	BO	0.57	0/739	0.74	0/985
48	DO	0.50	0/739	0.70	0/985
49	BP	0.55	0/697	0.81	1/939 (0.1%)
49	DP	0.49	0/693	0.72	0/935
50	BQ	0.58	0/836	0.78	0/1117
50	DQ	0.51	0/836	0.72	0/1117
51	BR	0.55	0/560	0.83	0/746
51	DR	0.48	0/560	0.70	0/746
52	BS	0.34	0/676	0.59	0/911
52	DS	0.31	0/661	0.66	0/893
53	BT	0.50	0/730	0.81	0/965
53	DT	0.46	0/733	0.72	0/969
54	BU	0.42	0/203	0.69	0/266
54	DU	0.38	0/203	0.59	0/266
55	BV	0.64	0/165	1.06	0/254
55	DV	0.54	0/137	1.11	0/211
56	BW	0.86	0/1650	1.64	45/2569 (1.8%)
56	BY	0.42	0/1602	0.95	1/2493 (0.0%)
56	DW	0.65	0/1650	1.29	7/2569 (0.3%)
56	DY	0.35	0/1579	0.86	0/2455
57	BZ	0.49	0/5763	0.72	1/7804 (0.0%)
57	DZ	0.45	0/5784	0.69	1/7835 (0.0%)
58	BX	0.67	0/20	0.66	0/23
58	DX	0.70	0/20	1.43	0/23

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
All	All	0.95	543/329767 (0.2%)	1.50	6455/491645 (1.3%)

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
5	AE	0	1
6	AF	0	1
19	AV	0	1
35	BB	0	1
57	DZ	0	1
58	BX	0	1
All	All	0	6

The worst 5 of 543 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1067	A	N9-C4	-15.28	1.28	1.37
1	AA	354	A	N9-C4	-13.92	1.29	1.37
1	AA	2299	A	N9-C4	-13.50	1.29	1.37
1	AA	1188	A	N9-C4	-13.32	1.29	1.37
1	AA	990	A	N9-C4	-11.81	1.30	1.37

The worst 5 of 6455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	553	A	N1-C6-N6	26.84	134.71	118.60
1	AA	990	A	N1-C2-N3	21.55	140.07	129.30
1	AA	990	A	C6-C5-N7	-21.18	117.48	132.30
1	AA	354	A	C2-N3-C4	-21.03	100.09	110.60
1	AA	553	A	C6-C5-N7	-20.90	117.67	132.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	74	PRO	Peptide
6	AF	194	MET	Peptide
19	AV	54	GLY	Peptide

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Mol	Chain	Res	Type	Group
35	BB	93	VAL	Peptide
58	BX	3	004	Peptide

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	61861	0	31172	850	0
1	CA	61771	0	31146	1166	0
2	AB	2573	0	1306	27	0
2	CB	2573	0	1306	57	0
3	AC	1063	0	1091	153	4
3	CC	1063	0	1090	186	17
4	AD	2136	0	2218	84	0
4	CD	2142	0	2229	85	0
5	AE	1559	0	1618	58	0
5	CE	1559	0	1618	76	0
6	AF	1584	0	1625	62	0
6	CF	1580	0	1619	75	0
7	AG	1425	0	1443	64	0
7	CG	1424	0	1434	82	0
8	AH	1330	0	1407	53	0
8	CH	1330	0	1407	54	0
9	AK	641	0	309	15	0
9	CK	641	0	309	9	0
10	AL	498	0	521	20	0
10	CL	498	0	521	29	0
11	AN	1117	0	1184	31	0
11	CN	1117	0	1184	38	0
12	AO	933	0	996	30	0
12	CO	933	0	996	26	0
13	AP	1139	0	1223	44	0
13	CP	1135	0	1212	57	0
14	AQ	1122	0	1179	37	0
14	CQ	1122	0	1179	54	0
15	AR	968	0	1033	32	0
15	CR	968	0	1033	37	0
16	AS	877	0	938	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CS	870	0	923	67	0
17	AT	1091	0	1151	48	0
17	CT	1083	0	1136	42	0
18	AU	959	0	1019	29	0
18	CU	959	0	1018	40	0
19	AV	771	0	830	11	0
19	CV	771	0	830	24	0
20	AW	886	0	940	23	0
20	CW	886	0	940	40	0
21	AX	750	0	814	24	0
21	CX	750	0	814	28	0
22	AY	806	0	881	37	0
22	CY	806	0	882	45	0
23	AZ	1451	0	1457	61	0
23	CZ	1451	0	1457	72	0
24	A0	608	0	622	20	0
24	C0	608	0	622	27	0
25	A1	755	0	826	29	0
25	C1	755	0	826	23	0
26	A2	588	0	643	16	0
26	C2	588	0	643	28	0
27	A3	469	0	518	12	0
27	C3	464	0	514	25	0
28	A4	558	0	545	31	0
28	C4	532	0	507	28	0
29	A5	455	0	465	15	0
29	C5	455	0	465	16	0
30	A6	453	0	473	17	0
30	C6	449	0	469	20	0
31	A7	418	0	467	16	0
31	C7	418	0	467	12	0
32	A8	517	0	582	25	0
32	C8	517	0	582	24	0
33	A9	307	0	335	11	0
33	C9	307	0	335	13	0
34	BA	32141	0	16224	681	0
34	DA	32268	0	16287	742	0
35	BB	1846	0	1867	78	0
35	DB	1825	0	1828	101	0
36	BC	1552	0	1546	65	0
36	DC	1544	0	1524	63	0
37	BD	1659	0	1679	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1719	86	0
38	BE	1129	0	1185	51	0
38	DE	1133	0	1191	69	0
39	BF	812	0	804	29	0
39	DF	820	0	814	37	0
40	BG	1231	0	1238	45	0
40	DG	1235	0	1249	52	0
41	BH	1088	0	1126	53	0
41	DH	1088	0	1126	74	0
42	BI	986	0	995	52	0
42	DI	978	0	966	56	0
43	BJ	709	0	650	32	0
43	DJ	714	0	672	32	0
44	BK	833	0	836	34	0
44	DK	833	0	836	26	0
45	BL	930	0	980	39	0
45	DL	930	0	980	45	0
46	BM	923	0	970	37	0
46	DM	907	0	934	39	0
47	BN	492	0	529	30	0
47	DN	492	0	531	46	0
48	BO	728	0	760	29	0
48	DO	728	0	760	29	0
49	BP	681	0	697	50	0
49	DP	677	0	686	36	0
50	BQ	823	0	891	32	0
50	DQ	823	0	891	35	0
51	BR	555	0	618	24	0
51	DR	555	0	618	30	0
52	BS	661	0	675	36	0
52	DS	646	0	644	34	0
53	BT	728	0	798	36	0
53	DT	731	0	807	27	0
54	BU	199	0	208	7	0
54	DU	199	0	208	9	0
55	BV	148	0	76	3	0
55	DV	123	0	66	1	0
56	BW	1631	0	839	25	0
56	BY	1581	0	805	24	0
56	DW	1631	0	839	33	0
56	DY	1561	0	796	34	0
57	BZ	5663	0	5747	265	17

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DZ	5682	0	5766	236	4
58	BX	93	0	85	14	0
58	DX	93	0	85	15	0
59	A0	5	0	0	0	0
59	A2	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	2	0	0	0	0
59	A7	1	0	0	0	0
59	A8	1	0	0	0	0
59	A9	1	0	0	0	0
59	AA	832	0	0	0	0
59	AB	23	0	0	0	0
59	AD	10	0	0	0	0
59	AE	5	0	0	0	0
59	AF	6	0	0	0	0
59	AG	2	0	0	0	0
59	AH	1	0	0	0	0
59	AN	3	0	0	0	0
59	AO	1	0	0	0	0
59	AP	3	0	0	0	0
59	AQ	4	0	0	0	0
59	AR	1	0	0	0	0
59	AU	5	0	0	0	0
59	AV	2	0	0	0	0
59	AW	3	0	0	0	0
59	AX	1	0	0	0	0
59	AY	1	0	0	0	0
59	AZ	1	0	0	0	0
59	BA	215	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
59	BK	1	0	0	0	0
59	BL	2	0	0	0	0
59	BM	1	0	0	0	0
59	BN	2	0	0	0	0
59	BS	1	0	0	0	0
59	BT	1	0	0	0	0
59	BW	3	0	0	0	0
59	BZ	1	0	0	0	0
59	C0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	C1	1	0	0	0	0
59	C3	1	0	0	0	0
59	C5	1	0	0	0	0
59	C7	1	0	0	0	0
59	C8	1	0	0	0	0
59	CA	664	0	0	0	0
59	CB	13	0	0	0	0
59	CD	4	0	0	0	0
59	CE	5	0	0	0	0
59	CF	4	0	0	0	0
59	CG	1	0	0	0	0
59	CN	1	0	0	0	0
59	CO	1	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	4	0	0	0	0
59	CR	1	0	0	0	0
59	CU	1	0	0	0	0
59	CV	2	0	0	0	0
59	CW	1	0	0	0	0
59	CX	1	0	0	0	0
59	DA	171	0	0	0	0
59	DD	1	0	0	0	0
59	DE	2	0	0	0	0
59	DF	1	0	0	0	0
59	DJ	1	0	0	0	0
59	DK	1	0	0	0	0
59	DT	1	0	0	0	0
59	DW	3	0	0	0	0
59	DZ	2	0	0	0	0
60	A4	1	0	0	0	0
60	A5	1	0	0	0	0
60	A6	1	0	0	0	0
60	A9	1	0	0	0	0
60	AY	1	0	0	0	0
60	BN	1	0	0	0	0
60	C4	1	0	0	0	0
60	C5	1	0	0	0	0
60	C6	1	0	0	0	0
60	C9	1	0	0	0	0
60	CY	1	0	0	0	0
60	DN	1	0	0	0	0
61	BD	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DD	8	0	0	2	0
62	BZ	28	0	12	5	0
62	DZ	28	0	12	7	0
63	A0	6	0	0	0	0
63	A1	2	0	0	0	0
63	A3	2	0	0	0	0
63	A5	3	0	0	0	0
63	A6	1	0	0	0	0
63	A7	2	0	0	1	0
63	A8	10	0	0	1	0
63	A9	1	0	0	0	0
63	AA	1413	0	0	66	0
63	AB	38	0	0	3	0
63	AD	10	0	0	2	0
63	AE	17	0	0	4	0
63	AF	11	0	0	1	0
63	AG	3	0	0	1	0
63	AH	1	0	0	0	0
63	AN	1	0	0	0	0
63	AO	3	0	0	0	0
63	AP	16	0	0	1	0
63	AQ	4	0	0	1	0
63	AR	2	0	0	0	0
63	AS	1	0	0	1	0
63	AT	1	0	0	0	0
63	AU	4	0	0	0	0
63	AV	1	0	0	0	0
63	AW	1	0	0	0	0
63	AX	3	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	213	0	0	19	0
63	BD	1	0	0	0	0
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BP	1	0	0	0	0
63	BV	1	0	0	0	0
63	BW	1	0	0	0	0
63	BZ	2	0	0	0	0
63	C0	4	0	0	0	0
63	C3	2	0	0	0	0
63	C5	1	0	0	0	0
63	C7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C8	4	0	0	0	0
63	CA	983	0	0	79	0
63	CB	9	0	0	1	0
63	CD	15	0	0	1	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CN	1	0	0	0	0
63	CO	1	0	0	0	0
63	CP	11	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	0	0
63	CV	1	0	0	1	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	2	0	0	1	0
63	DA	157	0	0	13	0
63	DD	1	0	0	0	0
63	DE	2	0	0	2	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DT	1	0	0	0	0
All	All	310038	0	209219	7358	21

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 15.

The worst 5 of 7358 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)
1:AA:1891:G:H5”	3:AC:206:LYS:CG	1.32	1.59
1:AA:1891:G:C5’	3:AC:206:LYS:HD2	1.36	1.52
1:CA:2128:C:H5”	3:CC:219:MET:CE	1.36	1.51
1:CA:2132:U:C4	3:CC:6:LYS:HE3	1.51	1.41
1:AA:1891:G:C5’	3:AC:206:LYS:CD	2.01	1.37

The worst 5 of 21 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BZ:502:GLY:CA	3:CC:9:ARG:CD[2_655]	1.16	1.04
3:AC:9:ARG:NH2	57:DZ:504:ARG:NH1[3_654]	1.36	0.84
57:BZ:502:GLY:N	3:CC:9:ARG:CB[2_655]	1.54	0.66
57:BZ:502:GLY:N	3:CC:9:ARG:CD[2_655]	1.69	0.51
57:BZ:573:HIS:CE1	3:CC:13:GLU:OE1[2_655]	1.71	0.49

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	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	249 (91%)	19 (7%)	5 (2%)	8	28
4	CD	273/276 (99%)	234 (86%)	26 (10%)	13 (5%)	2	7
5	AE	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	15	44
5	CE	202/206 (98%)	179 (89%)	20 (10%)	3 (2%)	10	33
6	AF	201/210 (96%)	182 (90%)	18 (9%)	1 (0%)	29	61
6	CF	201/210 (96%)	177 (88%)	17 (8%)	7 (4%)	3	12
7	AG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	13
7	CG	179/182 (98%)	141 (79%)	31 (17%)	7 (4%)	3	10
8	AH	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	9	29
8	CH	172/180 (96%)	144 (84%)	17 (10%)	11 (6%)	1	3
9	AK	128/173 (74%)	66 (52%)	36 (28%)	26 (20%)	0	0
9	CK	128/173 (74%)	76 (59%)	27 (21%)	25 (20%)	0	0
10	AL	64/147 (44%)	43 (67%)	17 (27%)	4 (6%)	1	3
10	CL	64/147 (44%)	42 (66%)	19 (30%)	3 (5%)	2	7
11	AN	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	53
11	CN	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
12	CO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	5	19
13	AP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	11	34
13	CP	147/150 (98%)	119 (81%)	25 (17%)	3 (2%)	7	24
14	AQ	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	22	53
14	CQ	139/141 (99%)	123 (88%)	14 (10%)	2 (1%)	11	34
15	AR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
15	CR	116/118 (98%)	102 (88%)	11 (10%)	3 (3%)	5	18
16	AS	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	3	11
16	CS	108/112 (96%)	83 (77%)	20 (18%)	5 (5%)	2	7
17	AT	129/146 (88%)	114 (88%)	13 (10%)	2 (2%)	9	31
17	CT	129/146 (88%)	116 (90%)	11 (8%)	2 (2%)	9	31
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	100 (88%)	11 (10%)	3 (3%)	5	18
19	AV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44
19	CV	99/101 (98%)	86 (87%)	10 (10%)	3 (3%)	4	15
20	AW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
20	CW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	AX	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	6	22
21	CX	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	2	5
22	AY	105/110 (96%)	93 (89%)	9 (9%)	3 (3%)	4	15
22	CY	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	7
23	AZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	3
23	CZ	183/206 (89%)	134 (73%)	33 (18%)	16 (9%)	1	1
24	A0	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
24	C0	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	12	36
25	A1	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
25	C1	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	4	13
26	A2	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	10	33
27	A3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	12
28	A4	67/71 (94%)	46 (69%)	12 (18%)	9 (13%)	0	0
28	C4	67/71 (94%)	43 (64%)	15 (22%)	9 (13%)	0	0
29	A5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
29	C5	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	28
30	A6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	C6	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	7	24
31	A7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	C7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	6	22
32	A8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	9	31
32	C8	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	9	31
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	182 (80%)	33 (14%)	14 (6%)	1	4
35	DB	229/256 (90%)	170 (74%)	41 (18%)	18 (8%)	1	2
36	BC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	2	5
36	DC	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	4	15
37	BD	206/209 (99%)	166 (81%)	28 (14%)	12 (6%)	1	4
37	DD	206/209 (99%)	171 (83%)	27 (13%)	8 (4%)	3	10
38	BE	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	2	5
38	DE	146/162 (90%)	117 (80%)	22 (15%)	7 (5%)	2	7
39	BF	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	4	14
39	DF	98/101 (97%)	90 (92%)	5 (5%)	3 (3%)	4	14
40	BG	153/156 (98%)	128 (84%)	13 (8%)	12 (8%)	1	2
40	DG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	4	13
41	BH	135/138 (98%)	110 (82%)	22 (16%)	3 (2%)	6	22
41	DH	135/138 (98%)	114 (84%)	14 (10%)	7 (5%)	2	6
42	BI	125/128 (98%)	103 (82%)	15 (12%)	7 (6%)	2	5
42	DI	125/128 (98%)	100 (80%)	21 (17%)	4 (3%)	4	13
43	BJ	95/105 (90%)	76 (80%)	12 (13%)	7 (7%)	1	2
43	DJ	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	8	28
44	DK	112/129 (87%)	92 (82%)	16 (14%)	4 (4%)	3	11
45	BL	120/132 (91%)	108 (90%)	11 (9%)	1 (1%)	19	49
45	DL	120/132 (91%)	100 (83%)	16 (13%)	4 (3%)	4	13
46	BM	115/126 (91%)	93 (81%)	18 (16%)	4 (4%)	3	12
46	DM	114/126 (90%)	88 (77%)	17 (15%)	9 (8%)	1	2
47	BN	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	6
47	DN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	13
48	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	12
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	7
49	BP	80/88 (91%)	54 (68%)	17 (21%)	9 (11%)	0	1
49	DP	80/88 (91%)	58 (72%)	18 (22%)	4 (5%)	2	6
50	BQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	4	14
50	DQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	4	15
51	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	BS	82/93 (88%)	64 (78%)	14 (17%)	4 (5%)	2	7
52	DS	81/93 (87%)	63 (78%)	15 (18%)	3 (4%)	3	11
53	BT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2	8
53	DT	94/106 (89%)	75 (80%)	13 (14%)	6 (6%)	1	3
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	0	1
57	BZ	722/758 (95%)	563 (78%)	107 (15%)	52 (7%)	1	2
57	DZ	726/758 (96%)	537 (74%)	132 (18%)	57 (8%)	1	2
58	BX	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
58	DX	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
All	All	13227/14464 (91%)	10975 (83%)	1666 (13%)	586 (4%)	2	8

5 of 586 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS

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Mol	Chain	Res	Type
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE

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	
3	AC	111/180 (62%)	103 (93%)	8 (7%)	14	38
3	CC	111/180 (62%)	103 (93%)	8 (7%)	14	38
4	AD	215/218 (99%)	173 (80%)	42 (20%)	1	4
4	CD	216/218 (99%)	178 (82%)	38 (18%)	2	5
5	AE	164/166 (99%)	138 (84%)	26 (16%)	2	7
5	CE	164/166 (99%)	137 (84%)	27 (16%)	2	7
6	AF	160/166 (96%)	132 (82%)	28 (18%)	2	6
6	CF	159/166 (96%)	126 (79%)	33 (21%)	1	3
7	AG	143/156 (92%)	115 (80%)	28 (20%)	1	4
7	CG	142/156 (91%)	114 (80%)	28 (20%)	1	4
8	AH	144/148 (97%)	120 (83%)	24 (17%)	2	6
8	CH	144/148 (97%)	118 (82%)	26 (18%)	1	5
10	AL	50/111 (45%)	39 (78%)	11 (22%)	1	2
10	CL	50/111 (45%)	35 (70%)	15 (30%)	0	1
11	AN	118/119 (99%)	93 (79%)	25 (21%)	1	3
11	CN	118/119 (99%)	85 (72%)	33 (28%)	0	1
12	AO	100/100 (100%)	87 (87%)	13 (13%)	4	13
12	CO	100/100 (100%)	86 (86%)	14 (14%)	3	11
13	AP	116/116 (100%)	97 (84%)	19 (16%)	2	7
13	CP	115/116 (99%)	95 (83%)	20 (17%)	2	6
14	AQ	111/111 (100%)	94 (85%)	17 (15%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	111/111 (100%)	83 (75%)	28 (25%)	0	1
15	AR	101/101 (100%)	80 (79%)	21 (21%)	1	3
15	CR	101/101 (100%)	87 (86%)	14 (14%)	3	11
16	AS	87/88 (99%)	71 (82%)	16 (18%)	1	5
16	CS	85/88 (97%)	68 (80%)	17 (20%)	1	4
17	AT	115/127 (91%)	96 (84%)	19 (16%)	2	7
17	CT	113/127 (89%)	98 (87%)	15 (13%)	4	12
18	AU	93/94 (99%)	77 (83%)	16 (17%)	2	6
18	CU	93/94 (99%)	81 (87%)	12 (13%)	4	13
19	AV	80/82 (98%)	67 (84%)	13 (16%)	2	7
19	CV	80/82 (98%)	65 (81%)	15 (19%)	1	5
20	AW	90/92 (98%)	76 (84%)	14 (16%)	2	8
20	CW	90/92 (98%)	75 (83%)	15 (17%)	2	6
21	AX	77/78 (99%)	67 (87%)	10 (13%)	4	13
21	CX	77/78 (99%)	66 (86%)	11 (14%)	3	10
22	AY	85/91 (93%)	66 (78%)	19 (22%)	1	2
22	CY	85/91 (93%)	66 (78%)	19 (22%)	1	2
23	AZ	156/179 (87%)	120 (77%)	36 (23%)	1	2
23	CZ	156/179 (87%)	125 (80%)	31 (20%)	1	4
24	A0	61/67 (91%)	55 (90%)	6 (10%)	8	24
24	C0	61/67 (91%)	50 (82%)	11 (18%)	1	5
25	A1	80/83 (96%)	66 (82%)	14 (18%)	2	6
25	C1	80/83 (96%)	66 (82%)	14 (18%)	2	6
26	A2	65/67 (97%)	56 (86%)	9 (14%)	3	11
26	C2	65/67 (97%)	51 (78%)	14 (22%)	1	3
27	A3	51/52 (98%)	41 (80%)	10 (20%)	1	4
27	C3	50/52 (96%)	38 (76%)	12 (24%)	0	2
28	A4	60/63 (95%)	52 (87%)	8 (13%)	4	12
28	C4	53/63 (84%)	39 (74%)	14 (26%)	0	1
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	11
29	C5	50/52 (96%)	42 (84%)	8 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	A6	51/52 (98%)	37 (72%)	14 (28%)	0 1
30	C6	50/52 (96%)	43 (86%)	7 (14%)	3 11
31	A7	41/42 (98%)	35 (85%)	6 (15%)	3 9
31	C7	41/42 (98%)	35 (85%)	6 (15%)	3 9
32	A8	54/55 (98%)	43 (80%)	11 (20%)	1 4
32	C8	54/55 (98%)	48 (89%)	6 (11%)	6 19
33	A9	34/34 (100%)	30 (88%)	4 (12%)	5 16
33	C9	34/34 (100%)	30 (88%)	4 (12%)	5 16
35	BB	192/220 (87%)	157 (82%)	35 (18%)	1 5
35	DB	187/220 (85%)	148 (79%)	39 (21%)	1 3
36	BC	143/188 (76%)	127 (89%)	16 (11%)	6 18
36	DC	141/188 (75%)	113 (80%)	28 (20%)	1 4
37	BD	170/181 (94%)	136 (80%)	34 (20%)	1 4
37	DD	174/181 (96%)	143 (82%)	31 (18%)	2 5
38	BE	113/123 (92%)	86 (76%)	27 (24%)	0 2
38	DE	114/123 (93%)	82 (72%)	32 (28%)	0 1
39	BF	84/90 (93%)	70 (83%)	14 (17%)	2 6
39	DF	86/90 (96%)	74 (86%)	12 (14%)	3 11
40	BG	119/127 (94%)	99 (83%)	20 (17%)	2 6
40	DG	120/127 (94%)	104 (87%)	16 (13%)	4 12
41	BH	114/119 (96%)	90 (79%)	24 (21%)	1 3
41	DH	114/119 (96%)	86 (75%)	28 (25%)	0 2
42	BI	91/99 (92%)	78 (86%)	13 (14%)	3 10
42	DI	89/99 (90%)	73 (82%)	16 (18%)	1 5
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	5 15
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	2 7
44	BK	83/99 (84%)	65 (78%)	18 (22%)	1 3
44	DK	83/99 (84%)	64 (77%)	19 (23%)	1 2
45	BL	97/109 (89%)	83 (86%)	14 (14%)	3 10
45	DL	97/109 (89%)	74 (76%)	23 (24%)	1 2
46	BM	91/101 (90%)	80 (88%)	11 (12%)	5 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	88/101 (87%)	75 (85%)	13 (15%)	3	9
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	2
47	DN	49/50 (98%)	42 (86%)	7 (14%)	3	10
48	BO	78/80 (98%)	70 (90%)	8 (10%)	7	21
48	DO	78/80 (98%)	66 (85%)	12 (15%)	2	8
49	BP	69/74 (93%)	54 (78%)	15 (22%)	1	3
49	DP	68/74 (92%)	51 (75%)	17 (25%)	0	2
50	BQ	94/97 (97%)	82 (87%)	12 (13%)	4	13
50	DQ	94/97 (97%)	80 (85%)	14 (15%)	3	9
51	BR	59/77 (77%)	49 (83%)	10 (17%)	2	6
51	DR	59/77 (77%)	52 (88%)	7 (12%)	5	16
52	BS	70/80 (88%)	59 (84%)	11 (16%)	2	8
52	DS	67/80 (84%)	55 (82%)	12 (18%)	2	5
53	BT	70/82 (85%)	53 (76%)	17 (24%)	0	2
53	DT	71/82 (87%)	59 (83%)	12 (17%)	2	6
54	BU	18/22 (82%)	17 (94%)	1 (6%)	21	51
54	DU	18/22 (82%)	16 (89%)	2 (11%)	6	19
57	BZ	604/636 (95%)	477 (79%)	127 (21%)	1	3
57	DZ	607/636 (95%)	509 (84%)	98 (16%)	2	7
58	BX	3/3 (100%)	3 (100%)	0	100	100
58	DX	3/3 (100%)	3 (100%)	0	100	100
All	All	10664/11678 (91%)	8760 (82%)	1904 (18%)	2	5

5 of 1904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BZ	623	ASP
51	DR	21	LYS
11	CN	138	LEU
49	DP	60	LEU
57	DZ	624	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 172 such sidechains are listed below:

Mol	Chain	Res	Type
24	C0	70	GLN
42	DI	89	ASN
35	DB	40	HIS
37	DD	160	GLN
44	DK	93	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2865/2915 (98%)	526 (18%)	51 (1%)
1	CA	2860/2915 (98%)	611 (21%)	39 (1%)
2	AB	119/121 (98%)	15 (12%)	0
2	CB	119/121 (98%)	27 (22%)	0
34	BA	1491/1521 (98%)	331 (22%)	20 (1%)
34	DA	1498/1521 (98%)	350 (23%)	22 (1%)
55	BV	6/18 (33%)	2 (33%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	74/76 (97%)	16 (21%)	1 (1%)
56	BY	71/76 (93%)	23 (32%)	2 (2%)
56	DW	74/76 (97%)	23 (31%)	2 (2%)
56	DY	69/76 (90%)	21 (30%)	1 (1%)
All	All	9251/9454 (97%)	1946 (21%)	138 (1%)

5 of 1946 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

5 of 138 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	DA	115	G
34	DA	428	G
34	DA	1065	U
1	AA	2769	U
1	AA	2739	U

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

42 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	$\#\|Z\| > 2$
58	2QZ	BX	1	58	7,8,9	0.76	0	8,10,12	4.49	5 (62%)
56	4SU	DW	8	56	18,21,22	1.73	5 (27%)	26,30,33	2.24	4 (15%)
56	MIA	BY	37	56	18,24,32	1.19	2 (11%)	18,35,47	1.37	3 (16%)
56	7MG	BY	46	56	22,26,27	1.30	3 (13%)	29,39,42	2.59	7 (24%)
56	PSU	BY	32	56	18,21,22	1.37	2 (11%)	22,30,33	1.80	3 (13%)
58	004	DX	3	58	9,10,11	1.30	1 (11%)	9,12,14	1.10	0
56	4SU	BW	8	56	18,21,22	1.41	2 (11%)	26,30,33	2.09	5 (19%)
58	2R3	BX	8	58	12,14,15	0.67	0	16,18,20	2.12	7 (43%)
58	MVA	DX	9	58	6,7,8	1.13	1 (16%)	7,8,10	1.45	1 (14%)
56	PSU	BW	39	56	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
58	004	BX	3	58	9,10,11	1.28	1 (11%)	9,12,14	2.45	2 (22%)
56	MIA	DY	37	56	18,24,32	1.10	2 (11%)	18,35,47	1.31	2 (11%)
56	7MG	DY	46	56	22,26,27	1.24	3 (13%)	29,39,42	2.65	8 (27%)
56	PSU	DW	39	56	18,21,22	1.35	2 (11%)	22,30,33	1.94	4 (18%)
56	5MU	BY	54	56	19,22,23	1.53	5 (26%)	28,32,35	2.18	8 (28%)
56	PSU	DY	32	56	18,21,22	1.33	2 (11%)	22,30,33	1.82	4 (18%)
56	5MU	DY	54	56	19,22,23	1.44	6 (31%)	28,32,35	2.05	5 (17%)
58	2QZ	DX	1	58	7,8,9	0.51	0	8,10,12	4.28	3 (37%)
58	MVA	BX	9	58	6,7,8	0.76	0	7,8,10	1.41	0
56	MIA	BW	37	56	24,31,32	2.37	5 (20%)	26,44,47	2.38	9 (34%)
56	5MU	DW	54	56	19,22,23	1.49	4 (21%)	28,32,35	2.05	7 (25%)
58	2QY	BX	10	58	12,13,14	1.87	1 (8%)	13,16,18	3.61	5 (38%)
58	2R3	DX	8	58	12,14,15	0.58	0	16,18,20	1.76	5 (31%)
56	4SU	DY	8	56	18,21,22	1.75	4 (22%)	26,30,33	2.27	5 (19%)
58	2R1	DX	6	58	10,10,11	1.62	2 (20%)	6,13,15	2.53	3 (50%)
56	PSU	BY	55	56	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
56	7MG	DW	46	56	22,26,27	1.31	3 (13%)	29,39,42	2.60	8 (27%)
56	PSU	DW	32	56	18,21,22	1.40	3 (16%)	22,30,33	2.00	4 (18%)
58	MVA	BX	5	58	6,7,8	0.51	0	7,8,10	1.35	1 (14%)
56	PSU	DY	39	56	18,21,22	1.41	2 (11%)	22,30,33	1.82	3 (13%)
58	MVA	DX	5	58	6,7,8	1.04	0	7,8,10	1.44	1 (14%)
58	2R1	BX	6	58	10,10,11	1.99	3 (30%)	6,13,15	4.42	2 (33%)
58	2QY	DX	10	58	12,13,14	1.86	1 (8%)	13,16,18	3.06	5 (38%)
56	7MG	BW	46	56	22,26,27	1.31	4 (18%)	29,39,42	2.64	7 (24%)
56	5MU	BW	54	56	19,22,23	1.44	4 (21%)	28,32,35	1.94	8 (28%)
56	PSU	BW	32	56	18,21,22	1.32	3 (16%)	22,30,33	1.70	5 (22%)
56	PSU	DY	55	56	18,21,22	1.39	2 (11%)	22,30,33	1.87	3 (13%)
56	MIA	DW	37	56	24,31,32	2.19	4 (16%)	26,44,47	2.29	9 (34%)
56	4SU	BY	8	56	18,21,22	1.67	5 (27%)	26,30,33	2.07	6 (23%)
56	PSU	BY	39	56	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
56	PSU	BW	55	56	18,21,22	1.34	1 (5%)	22,30,33	1.80	3 (13%)
56	PSU	DW	55	56	18,21,22	1.37	2 (11%)	22,30,33	1.86	4 (18%)

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
58	2QZ	BX	1	58	-	2/6/10/12	-
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
56	MIA	BY	37	56	-	2/3/25/34	0/3/3/3
56	7MG	BY	46	56	-	4/7/37/38	0/3/3/3
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
58	004	DX	3	58	-	0/4/6/8	0/1/1/1
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2
58	2R3	BX	8	58	-	6/11/12/14	0/1/1/1
58	MVA	DX	9	58	-	4/6/8/10	-
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
58	004	BX	3	58	-	0/4/6/8	0/1/1/1
56	MIA	DY	37	56	-	3/3/25/34	0/3/3/3
56	7MG	DY	46	56	-	2/7/37/38	0/3/3/3
56	PSU	DW	39	56	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	BY	54	56	-	3/7/25/26	0/2/2/2
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
56	5MU	DY	54	56	-	2/7/25/26	0/2/2/2
58	2QZ	DX	1	58	-	2/6/10/12	-
58	MVA	BX	9	58	-	2/6/8/10	-
56	MIA	BW	37	56	-	5/11/33/34	0/3/3/3
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
58	2QY	BX	10	58	-	3/4/8/10	0/1/1/1
58	2R3	DX	8	58	-	6/11/12/14	0/1/1/1
56	4SU	DY	8	56	-	1/7/25/26	0/2/2/2
58	2R1	DX	6	58	-	2/2/14/16	0/1/1/1
56	PSU	BY	55	56	-	2/7/25/26	0/2/2/2
56	7MG	DW	46	56	-	4/7/37/38	0/3/3/3
56	PSU	DW	32	56	-	2/7/25/26	0/2/2/2
58	MVA	BX	5	58	-	4/6/8/10	-
56	PSU	DY	39	56	-	2/7/25/26	0/2/2/2
58	MVA	DX	5	58	-	4/6/8/10	-
58	2R1	BX	6	58	-	1/2/14/16	0/1/1/1
58	2QY	DX	10	58	-	3/4/8/10	0/1/1/1
56	7MG	BW	46	56	-	1/7/37/38	0/3/3/3
56	5MU	BW	54	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	56	-	3/7/25/26	0/2/2/2
56	PSU	DY	55	56	-	2/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	7/11/33/34	0/3/3/3
56	4SU	BY	8	56	-	1/7/25/26	0/2/2/2
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	55	56	-	2/7/25/26	0/2/2/2
56	PSU	DW	55	56	-	2/7/25/26	0/2/2/2

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C13-C14	7.83	1.54	1.32
56	DW	37	MIA	C13-C14	7.42	1.53	1.32
56	BW	37	MIA	C2-S10	-6.89	1.69	1.75
58	DX	10	2QY	C-CA	6.02	1.52	1.43
58	BX	10	2QY	C-CA	5.64	1.51	1.43

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	BX	1	2QZ	OG1-CB-CG2	11.55	143.95	109.74
58	DX	1	2QZ	OG1-CB-CG2	11.24	143.03	109.74
58	BX	10	2QY	CN-N-CA	-10.66	107.25	123.45
58	BX	6	2R1	OD2-CG2-CB	-9.89	94.26	112.24
56	BW	46	7MG	N9-C4-N3	9.46	139.62	125.47

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	32	PSU	C2'-C1'-C5-C4
56	BW	32	PSU	O4'-C1'-C5-C4
56	BW	32	PSU	O4'-C1'-C5-C6
56	BW	37	MIA	N6-C12-C13-C14
56	BW	37	MIA	C12-C13-C14-C15

There are no ring outliers.

23 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DW	8	4SU	1	0
58	DX	3	004	1	0
58	BX	8	2R3	2	0
58	DX	9	MVA	4	0
58	BX	3	004	4	0
56	DY	46	7MG	2	0
56	DW	39	PSU	6	0
58	DX	1	2QZ	2	0
58	BX	9	MVA	2	0
56	BW	37	MIA	2	0
56	DW	54	5MU	1	0
58	BX	10	2QY	1	0
58	DX	8	2R3	2	0
58	DX	6	2R1	2	0
58	BX	5	MVA	2	0
58	DX	5	MVA	2	0
58	BX	6	2R1	5	0
58	DX	10	2QY	9	0
56	BW	32	PSU	1	0
56	DY	55	PSU	3	0
56	DW	37	MIA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BY	8	4SU	1	0
56	DW	55	PSU	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2056 ligands modelled in this entry, 2052 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
62	GDP	DZ	703	59	24,30,30	1.02	1 (4%)	30,47,47	1.25	2 (6%)
61	SF4	DD	501	37	0,12,12	-	-	-		
61	SF4	BD	501	-	0,12,12	-	-	-		
62	GDP	BZ	702	59	24,30,30	0.95	0	30,47,47	1.42	4 (13%)

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
62	GDP	DZ	703	59	-	1/12/32/32	0/3/3/3
62	GDP	BZ	702	59	-	3/12/32/32	0/3/3/3
61	SF4	BD	501	-	-	-	0/6/5/5
61	SF4	DD	501	37	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	DZ	703	GDP	C6-N1	-2.02	1.34	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	BZ	702	GDP	PA-O3A-PB	-4.62	116.96	132.83
62	DZ	703	GDP	PA-O3A-PB	-3.88	119.51	132.83
62	BZ	702	GDP	C8-N7-C5	2.75	108.23	102.99
62	BZ	702	GDP	O3B-PB-O2B	2.25	116.22	107.64
62	BZ	702	GDP	O3'-C3'-C2'	-2.06	105.17	111.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	BZ	702	GDP	C5'-O5'-PA-O3A
62	BZ	702	GDP	C5'-O5'-PA-O1A
62	BZ	702	GDP	C5'-O5'-PA-O2A
62	DZ	703	GDP	C5'-O5'-PA-O1A

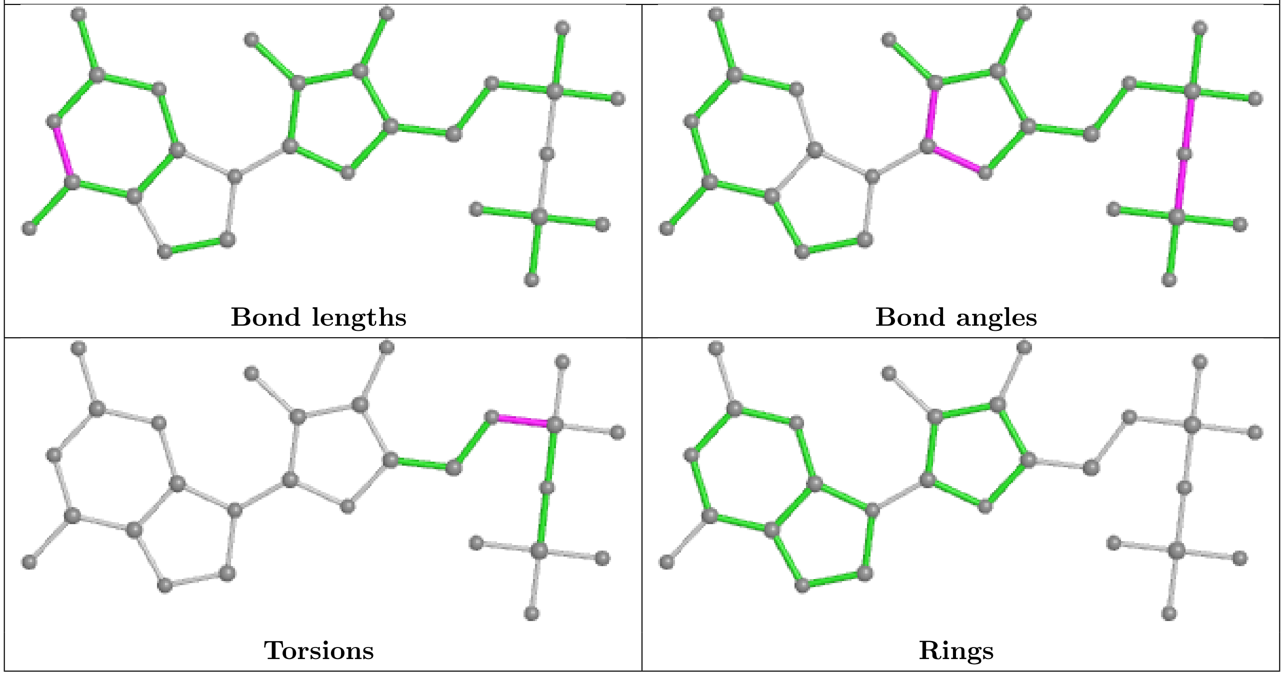
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	DZ	703	GDP	7	0
61	DD	501	SF4	2	0
61	BD	501	SF4	1	0
62	BZ	702	GDP	5	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 GDP DZ 703



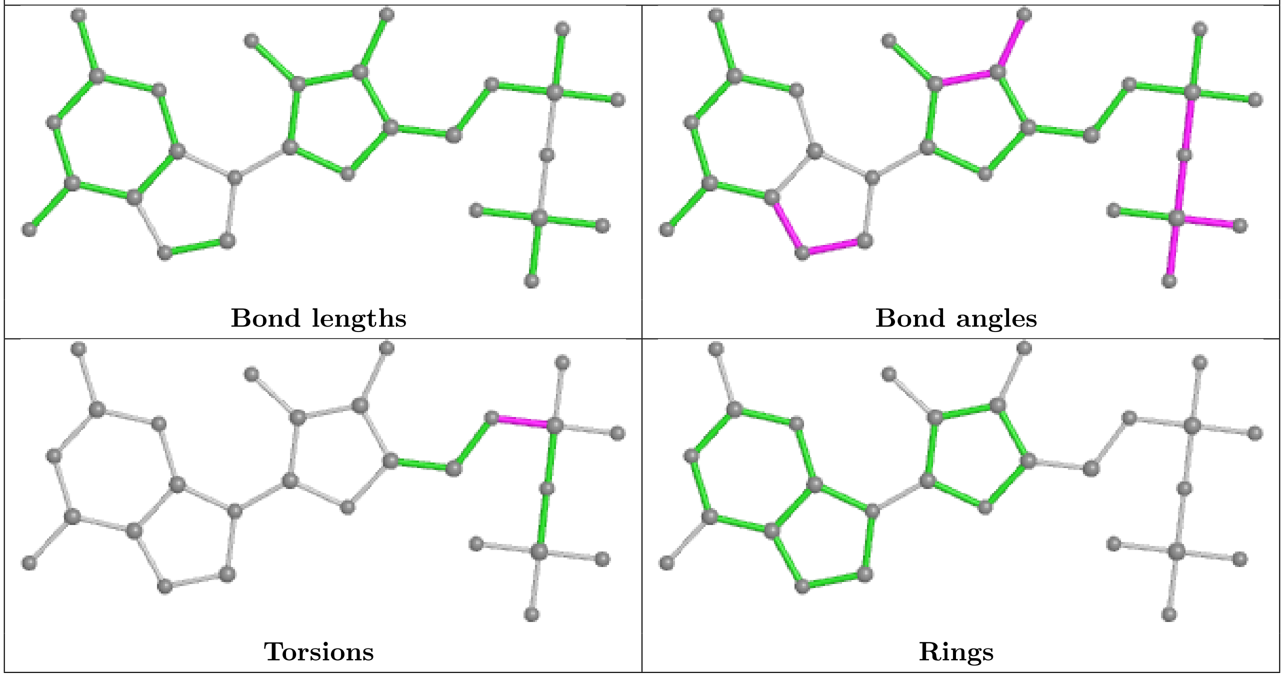
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP BZ 702



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	2872/2915 (98%)	-0.06	94 (3%) 46 36	13, 31, 166, 313	0
1	CA	2868/2915 (98%)	0.06	122 (4%) 35 25	24, 54, 177, 331	0
2	AB	120/121 (99%)	-0.41	0 100 100	24, 47, 66, 112	0
2	CB	120/121 (99%)	0.01	1 (0%) 86 81	56, 104, 146, 178	0
3	AC	137/228 (60%)	5.85	122 (89%) 0 0	89, 187, 231, 259	0
3	CC	137/228 (60%)	8.38	136 (99%) 0 0	142, 205, 249, 270	0
4	AD	275/276 (99%)	-0.46	2 (0%) 87 84	8, 30, 56, 122	0
4	CD	275/276 (99%)	-0.37	2 (0%) 87 84	13, 44, 77, 134	0
5	AE	204/206 (99%)	-0.47	0 100 100	7, 31, 60, 100	0
5	CE	204/206 (99%)	-0.31	0 100 100	16, 51, 87, 143	0
6	AF	203/210 (96%)	-0.41	0 100 100	6, 32, 76, 141	0
6	CF	203/210 (96%)	-0.19	1 (0%) 91 88	20, 66, 123, 158	0
7	AG	181/182 (99%)	-0.28	2 (1%) 80 75	34, 67, 114, 180	0
7	CG	181/182 (99%)	0.82	27 (14%) 2 1	75, 125, 183, 211	0
8	AH	174/180 (96%)	-0.46	2 (1%) 80 75	21, 46, 74, 199	0
8	CH	174/180 (96%)	0.66	11 (6%) 20 12	52, 92, 139, 174	0
9	AK	130/173 (75%)	1.27	30 (23%) 0 0	65, 131, 198, 223	0
9	CK	130/173 (75%)	2.85	78 (60%) 0 0	85, 163, 212, 233	0
10	AL	66/147 (44%)	4.23	54 (81%) 0 0	112, 182, 229, 247	0
10	CL	66/147 (44%)	5.46	58 (87%) 0 0	105, 183, 232, 263	0
11	AN	140/140 (100%)	-0.58	0 100 100	11, 28, 57, 97	0
11	CN	140/140 (100%)	-0.12	3 (2%) 63 54	35, 59, 92, 143	0
12	AO	122/122 (100%)	-0.43	0 100 100	16, 35, 66, 93	0
12	CO	122/122 (100%)	-0.32	0 100 100	30, 49, 80, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AP	149/150 (99%)	-0.35	0	100	100	8, 38, 78, 128	0
13	CP	149/150 (99%)	0.27	7 (4%)	31	22	26, 75, 123, 155	0
14	AQ	141/141 (100%)	-0.48	0	100	100	9, 32, 54, 99	0
14	CQ	141/141 (100%)	-0.27	1 (0%)	87	84	19, 63, 95, 146	0
15	AR	118/118 (100%)	-0.48	0	100	100	14, 27, 52, 76	0
15	CR	118/118 (100%)	-0.32	0	100	100	26, 49, 75, 106	0
16	AS	110/112 (98%)	-0.28	0	100	100	24, 47, 76, 86	0
16	CS	110/112 (98%)	0.66	8 (7%)	15	8	61, 96, 140, 166	0
17	AT	131/146 (89%)	-0.30	1 (0%)	86	81	20, 40, 95, 219	0
17	CT	131/146 (89%)	-0.22	1 (0%)	86	81	36, 56, 104, 152	0
18	AU	116/118 (98%)	-0.51	0	100	100	7, 22, 39, 87	0
18	CU	116/118 (98%)	-0.18	0	100	100	31, 55, 88, 107	0
19	AV	101/101 (100%)	-0.60	0	100	100	11, 27, 58, 77	0
19	CV	101/101 (100%)	-0.07	2 (1%)	65	56	29, 69, 102, 162	0
20	AW	112/113 (99%)	-0.47	0	100	100	10, 24, 49, 145	0
20	CW	112/113 (99%)	-0.21	0	100	100	26, 45, 76, 159	0
21	AX	95/96 (98%)	-0.48	0	100	100	12, 33, 64, 108	0
21	CX	95/96 (98%)	0.15	4 (4%)	36	26	37, 63, 100, 173	0
22	AY	107/110 (97%)	-0.40	1 (0%)	84	80	18, 43, 88, 120	0
22	CY	107/110 (97%)	0.57	10 (9%)	8	4	48, 81, 124, 171	0
23	AZ	185/206 (89%)	-0.44	0	100	100	28, 56, 94, 136	0
23	CZ	185/206 (89%)	0.39	12 (6%)	18	11	52, 98, 145, 175	0
24	A0	77/85 (90%)	-0.42	0	100	100	10, 31, 54, 82	0
24	C0	77/85 (90%)	0.28	4 (5%)	27	18	27, 69, 104, 127	0
25	A1	97/98 (98%)	-0.31	1 (1%)	82	77	15, 39, 80, 98	0
25	C1	97/98 (98%)	-0.16	1 (1%)	82	77	31, 56, 95, 144	0
26	A2	70/72 (97%)	-0.39	1 (1%)	75	70	15, 43, 65, 135	0
26	C2	70/72 (97%)	-0.03	1 (1%)	75	70	47, 79, 110, 151	0
27	A3	59/60 (98%)	-0.40	1 (1%)	70	63	11, 26, 53, 112	0
27	C3	59/60 (98%)	0.39	2 (3%)	45	35	31, 63, 103, 162	0
28	A4	69/71 (97%)	0.73	12 (17%)	1	1	47, 102, 188, 221	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	C4	69/71 (97%)	1.31	21 (30%) 0 0	88, 158, 196, 229	0
29	A5	59/60 (98%)	-0.51	0 100 100	11, 23, 50, 68	0
29	C5	59/60 (98%)	-0.26	1 (1%) 70 63	16, 47, 82, 121	0
30	A6	53/54 (98%)	-0.44	0 100 100	17, 36, 62, 77	0
30	C6	53/54 (98%)	-0.11	0 100 100	41, 63, 86, 104	0
31	A7	48/49 (97%)	-0.34	1 (2%) 63 54	11, 21, 54, 100	0
31	C7	48/49 (97%)	-0.22	0 100 100	23, 36, 96, 120	0
32	A8	64/65 (98%)	-0.43	0 100 100	14, 26, 39, 63	0
32	C8	64/65 (98%)	-0.20	0 100 100	27, 53, 71, 94	0
33	A9	37/37 (100%)	-0.29	0 100 100	20, 33, 64, 67	0
33	C9	37/37 (100%)	0.05	0 100 100	44, 62, 90, 101	0
34	BA	1495/1521 (98%)	0.14	50 (3%) 46 36	24, 82, 180, 330	0
34	DA	1501/1521 (98%)	0.33	93 (6%) 20 13	40, 94, 207, 307	0
35	BB	231/256 (90%)	0.50	22 (9%) 8 4	53, 104, 167, 195	0
35	DB	231/256 (90%)	1.21	54 (23%) 0 0	67, 135, 197, 228	0
36	BC	206/239 (86%)	0.73	21 (10%) 6 3	74, 114, 169, 187	0
36	DC	206/239 (86%)	1.71	66 (32%) 0 0	88, 151, 198, 221	0
37	BD	208/209 (99%)	0.27	11 (5%) 26 17	54, 91, 141, 182	0
37	DD	208/209 (99%)	0.13	3 (1%) 75 70	53, 88, 134, 199	0
38	BE	148/162 (91%)	-0.09	0 100 100	37, 72, 110, 150	0
38	DE	148/162 (91%)	0.35	6 (4%) 37 27	43, 90, 131, 177	0
39	BF	100/101 (99%)	-0.12	0 100 100	43, 81, 124, 145	0
39	DF	100/101 (99%)	0.02	2 (2%) 65 56	49, 90, 133, 146	0
40	BG	155/156 (99%)	0.62	19 (12%) 4 2	66, 100, 155, 194	0
40	DG	155/156 (99%)	1.52	40 (25%) 0 0	81, 131, 178, 214	0
41	BH	137/138 (99%)	0.11	1 (0%) 87 84	45, 73, 105, 121	0
41	DH	137/138 (99%)	0.35	7 (5%) 28 19	52, 92, 126, 160	0
42	BI	127/128 (99%)	1.37	31 (24%) 0 0	59, 115, 169, 192	0
42	DI	127/128 (99%)	2.47	69 (54%) 0 0	79, 154, 192, 248	0
43	BJ	97/105 (92%)	1.59	31 (31%) 0 0	75, 123, 173, 194	0
43	DJ	96/105 (91%)	2.40	50 (52%) 0 0	77, 160, 201, 221	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	BK	114/129 (88%)	-0.28	1 (0%)	84	80	30, 73, 117, 125	0
44	DK	114/129 (88%)	0.23	2 (1%)	68	61	61, 93, 139, 170	0
45	BL	122/132 (92%)	-0.21	1 (0%)	86	81	27, 61, 88, 110	0
45	DL	122/132 (92%)	0.04	1 (0%)	86	81	41, 70, 101, 142	0
46	BM	117/126 (92%)	0.53	9 (7%)	13	7	62, 108, 154, 187	0
46	DM	116/126 (92%)	1.46	34 (29%)	0	0	64, 156, 202, 235	0
47	BN	60/61 (98%)	0.80	5 (8%)	11	6	60, 110, 153, 173	0
47	DN	60/61 (98%)	1.97	27 (45%)	0	0	95, 142, 192, 210	0
48	BO	88/89 (98%)	-0.17	0	100	100	36, 69, 107, 139	0
48	DO	88/89 (98%)	0.09	0	100	100	50, 83, 115, 140	0
49	BP	82/88 (93%)	0.20	2 (2%)	59	49	46, 81, 126, 151	0
49	DP	82/88 (93%)	0.30	2 (2%)	59	49	50, 76, 108, 121	0
50	BQ	99/105 (94%)	-0.09	0	100	100	46, 72, 103, 119	0
50	DQ	99/105 (94%)	0.22	2 (2%)	65	56	47, 80, 116, 148	0
51	BR	68/88 (77%)	0.25	3 (4%)	34	24	45, 71, 115, 136	0
51	DR	68/88 (77%)	0.52	6 (8%)	10	5	58, 90, 129, 147	0
52	BS	84/93 (90%)	2.00	36 (42%)	0	0	68, 127, 168, 222	0
52	DS	83/93 (89%)	3.09	60 (72%)	0	0	98, 164, 213, 222	0
53	BT	96/106 (90%)	0.31	2 (2%)	63	54	49, 84, 117, 160	0
53	DT	96/106 (90%)	0.16	3 (3%)	49	39	48, 81, 126, 145	0
54	BU	23/27 (85%)	1.34	6 (26%)	0	0	60, 100, 114, 154	0
54	DU	23/27 (85%)	2.81	17 (73%)	0	0	78, 134, 159, 181	0
55	BV	7/18 (38%)	1.22	2 (28%)	0	0	61, 69, 175, 190	0
55	DV	6/18 (33%)	1.85	3 (50%)	0	0	89, 95, 181, 204	0
56	BW	69/76 (90%)	0.28	3 (4%)	35	25	38, 69, 118, 210	0
56	BY	67/76 (88%)	4.14	64 (95%)	0	0	76, 232, 280, 304	0
56	DW	69/76 (90%)	0.56	1 (1%)	75	70	48, 108, 151, 254	0
56	DY	66/76 (86%)	6.43	66 (100%)	0	0	145, 283, 315, 338	0
57	BZ	728/758 (96%)	0.71	113 (15%)	2	1	38, 97, 190, 248	0
57	DZ	730/758 (96%)	1.48	242 (33%)	0	0	27, 113, 212, 264	0
58	BX	3/10 (30%)	-0.18	0	100	100	83, 83, 83, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
58	DX	3/10 (30%)	0.19	0	100	100	81, 81, 81, 81	0
All	All	22705/23918 (94%)	0.37	2127 (9%)	8	4	6, 70, 189, 338	0

The worst 5 of 2127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CC	166	ASN	26.6
3	CC	167	ASP	25.1
3	CC	179	ALA	24.3
3	AC	171	ALA	21.6
3	CC	175	PRO	19.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	PSU	DY	32	20/21	0.14	1.13	275,275,275,275	0
56	PSU	DY	39	20/21	0.18	1.02	291,291,291,291	0
56	PSU	BY	55	20/21	0.27	0.51	243,243,243,243	0
56	PSU	DY	55	20/21	0.29	0.66	252,252,252,252	0
56	5MU	DY	54	21/22	0.38	0.84	303,303,303,303	0
56	4SU	DY	8	20/21	0.40	0.42	277,277,277,277	0
56	MIA	DY	37	22/30	0.46	0.85	271,271,271,271	0
56	5MU	BY	54	21/22	0.47	0.58	246,246,246,246	0
56	PSU	BY	32	20/21	0.47	0.55	226,226,226,226	0
56	7MG	BY	46	24/25	0.49	0.34	276,276,276,276	0
56	4SU	BY	8	20/21	0.52	0.34	239,239,239,239	0
56	7MG	DY	46	24/25	0.52	0.40	266,266,266,266	0
56	PSU	BY	39	20/21	0.68	0.54	197,197,197,197	0
56	MIA	BY	37	22/30	0.72	0.42	186,186,186,186	0
56	PSU	DW	32	20/21	0.82	0.31	126,126,126,126	0
58	004	DX	3	10/11	0.83	0.19	81,81,81,81	0
58	2R1	DX	6	10/11	0.83	0.15	81,81,81,81	0
56	PSU	DW	39	20/21	0.86	0.28	112,112,112,112	1
58	MVA	BX	5	8/9	0.87	0.15	82,82,82,82	0
56	7MG	DW	46	24/25	0.87	0.23	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	PSU	DW	55	20/21	0.88	0.19	92,92,92,92	0
56	5MU	DW	54	21/22	0.89	0.20	95,95,95,95	1
58	2R1	BX	6	10/11	0.89	0.16	82,82,82,82	1
56	7MG	BW	46	24/25	0.89	0.19	76,76,76,76	3
58	004	BX	3	10/11	0.90	0.12	82,82,82,82	0
58	MVA	BX	9	8/9	0.90	0.31	82,82,82,82	0
58	2QY	BX	10	13/14	0.90	0.19	82,82,82,82	0
56	4SU	DW	8	20/21	0.91	0.14	103,103,103,103	0
56	PSU	BW	55	20/21	0.91	0.17	79,79,79,79	0
56	MIA	DW	37	29/30	0.91	0.24	109,109,109,109	0
56	5MU	BW	54	21/22	0.92	0.18	80,80,80,80	0
58	2R3	BX	8	14/15	0.92	0.14	82,82,82,82	0
58	2QY	DX	10	13/14	0.92	0.17	81,81,81,81	0
58	2QZ	BX	1	9/10	0.93	0.25	82,82,82,82	0
56	MIA	BW	37	29/30	0.94	0.22	79,79,79,79	0
58	MVA	DX	9	8/9	0.94	0.24	81,81,81,81	0
56	PSU	BW	32	20/21	0.94	0.20	73,73,73,73	1
58	2QZ	DX	1	9/10	0.94	0.24	81,81,81,81	0
58	MVA	DX	5	8/9	0.95	0.36	81,81,81,81	0
56	4SU	BW	8	20/21	0.96	0.14	60,60,60,60	1
58	2R3	DX	8	14/15	0.96	0.13	81,81,81,81	0
56	PSU	BW	39	20/21	0.96	0.14	65,65,65,65	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	1660	1/1	0.10	0.39	82,82,82,82	0
59	MG	CA	3460	1/1	0.11	0.95	104,104,104,104	0
59	MG	DA	1757	1/1	0.26	1.14	111,111,111,111	0
59	MG	DA	1738	1/1	0.29	0.48	95,95,95,95	0
59	MG	CA	3155	1/1	0.31	0.23	112,112,112,112	0
59	MG	CA	3096	1/1	0.32	0.24	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3139	1/1	0.32	0.70	126,126,126,126	0
59	MG	CA	3646	1/1	0.36	0.16	91,91,91,91	0
59	MG	BA	1755	1/1	0.38	0.14	86,86,86,86	0
59	MG	AA	3108	1/1	0.40	0.64	101,101,101,101	0
59	MG	AA	3040	1/1	0.42	0.17	113,113,113,113	0
59	MG	BA	1767	1/1	0.44	0.42	96,96,96,96	0
59	MG	AA	3212	1/1	0.45	0.82	81,81,81,81	0
59	MG	DA	1626	1/1	0.47	0.30	71,71,71,71	0
59	MG	CA	3565	1/1	0.47	0.19	95,95,95,95	0
59	MG	BA	1657	1/1	0.47	0.25	78,78,78,78	0
59	MG	AA	3747	1/1	0.48	0.33	85,85,85,85	0
59	MG	CA	3620	1/1	0.48	0.64	96,96,96,96	0
59	MG	DA	1754	1/1	0.48	0.40	120,120,120,120	0
59	MG	BA	1812	1/1	0.48	0.20	79,79,79,79	0
59	MG	AA	3266	1/1	0.49	0.78	90,90,90,90	0
59	MG	CA	3100	1/1	0.49	0.25	81,81,81,81	0
59	MG	AA	3807	1/1	0.50	0.31	77,77,77,77	0
59	MG	AA	3617	1/1	0.53	0.15	77,77,77,77	0
59	MG	AA	3122	1/1	0.53	0.70	99,99,99,99	0
59	MG	BA	1616	1/1	0.54	0.27	122,122,122,122	0
59	MG	CA	3244	1/1	0.54	0.30	89,89,89,89	0
59	MG	DA	1639	1/1	0.55	0.55	69,69,69,69	0
59	MG	AA	3269	1/1	0.55	0.33	63,63,63,63	0
59	MG	DA	1733	1/1	0.56	0.34	92,92,92,92	0
59	MG	CA	3546	1/1	0.56	0.15	88,88,88,88	0
59	MG	CA	3127	1/1	0.56	0.41	94,94,94,94	0
59	MG	CA	3485	1/1	0.56	0.30	85,85,85,85	0
59	MG	BA	1775	1/1	0.57	0.34	90,90,90,90	0
59	MG	AF	305	1/1	0.57	0.53	76,76,76,76	0
59	MG	CA	3080	1/1	0.58	0.24	75,75,75,75	0
59	MG	BA	1786	1/1	0.58	0.22	82,82,82,82	0
59	MG	AA	3754	1/1	0.58	0.25	64,64,64,64	0
59	MG	CA	3101	1/1	0.58	1.12	84,84,84,84	0
59	MG	DA	1717	1/1	0.59	0.28	95,95,95,95	0
59	MG	CA	3149	1/1	0.59	0.17	100,100,100,100	0
59	MG	BA	1691	1/1	0.59	0.45	86,86,86,86	0
59	MG	CA	3186	1/1	0.59	0.61	77,77,77,77	0
59	MG	AB	3017	1/1	0.59	0.17	59,59,59,59	0
59	MG	BA	1764	1/1	0.60	0.09	71,71,71,71	0
59	MG	BA	1673	1/1	0.60	0.20	80,80,80,80	0
59	MG	CA	3040	1/1	0.61	0.47	79,79,79,79	0
59	MG	BA	1790	1/1	0.61	0.15	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	CB	3013	1/1	0.62	0.17	100,100,100,100	0
59	MG	CA	3075	1/1	0.62	0.65	90,90,90,90	0
59	MG	BA	1741	1/1	0.63	0.19	88,88,88,88	0
59	MG	CA	3146	1/1	0.63	0.95	82,82,82,82	0
59	MG	BA	1776	1/1	0.64	0.21	97,97,97,97	0
59	MG	AA	3242	1/1	0.64	0.29	85,85,85,85	0
59	MG	DA	1655	1/1	0.64	0.24	83,83,83,83	0
59	MG	CQ	202	1/1	0.64	0.29	74,74,74,74	0
59	MG	DT	3001	1/1	0.64	0.42	60,60,60,60	0
59	MG	AA	3240	1/1	0.65	0.16	69,69,69,69	0
59	MG	CA	3624	1/1	0.65	0.16	118,118,118,118	0
59	MG	AA	3241	1/1	0.65	0.21	65,65,65,65	0
59	MG	AA	3195	1/1	0.65	0.37	69,69,69,69	0
59	MG	CP	201	1/1	0.65	0.16	62,62,62,62	1
59	MG	CA	3108	1/1	0.65	0.27	78,78,78,78	0
59	MG	DA	1623	1/1	0.65	0.24	72,72,72,72	0
59	MG	DK	5001	1/1	0.65	0.16	76,76,76,76	0
59	MG	AA	3016	1/1	0.65	0.45	64,64,64,64	0
59	MG	BA	1638	1/1	0.66	0.21	66,66,66,66	0
59	MG	CA	3654	1/1	0.66	0.40	90,90,90,90	0
59	MG	AA	3541	1/1	0.66	0.12	74,74,74,74	0
59	MG	DA	1746	1/1	0.66	0.10	81,81,81,81	0
59	MG	BL	201	1/1	0.67	0.37	84,84,84,84	0
59	MG	CA	3587	1/1	0.67	0.34	70,70,70,70	0
59	MG	DA	1718	1/1	0.67	0.32	101,101,101,101	0
59	MG	BA	1654	1/1	0.67	0.23	76,76,76,76	0
59	MG	DA	1642	1/1	0.67	0.20	62,62,62,62	0
59	MG	DA	1634	1/1	0.68	0.29	66,66,66,66	0
59	MG	AA	3680	1/1	0.69	0.33	79,79,79,79	0
59	MG	CA	3061	1/1	0.69	0.35	68,68,68,68	0
59	MG	DA	1659	1/1	0.69	0.29	78,78,78,78	0
59	MG	CA	3237	1/1	0.69	0.49	94,94,94,94	0
59	MG	AA	3582	1/1	0.69	0.58	76,76,76,76	0
59	MG	BA	1643	1/1	0.69	0.34	66,66,66,66	0
59	MG	BA	1802	1/1	0.70	0.24	76,76,76,76	0
59	MG	CA	3579	1/1	0.70	0.22	65,65,65,65	0
59	MG	CA	3117	1/1	0.70	0.28	67,67,67,67	0
59	MG	AA	3717	1/1	0.70	0.56	68,68,68,68	0
59	MG	CA	3242	1/1	0.70	0.39	82,82,82,82	0
59	MG	AD	305	1/1	0.70	0.63	86,86,86,86	0
59	MG	CA	3304	1/1	0.70	0.12	67,67,67,67	0
59	MG	AE	302	1/1	0.70	0.24	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3238	1/1	0.70	0.44	76,76,76,76	0
59	MG	CA	3501	1/1	0.70	0.45	74,74,74,74	0
59	MG	CA	3538	1/1	0.70	0.15	72,72,72,72	0
59	MG	CA	3154	1/1	0.70	0.20	64,64,64,64	0
59	MG	CA	3548	1/1	0.70	0.10	90,90,90,90	0
59	MG	DA	1756	1/1	0.71	0.57	86,86,86,86	0
59	MG	DA	1654	1/1	0.71	0.35	63,63,63,63	0
59	MG	CA	3499	1/1	0.72	0.49	62,62,62,62	0
59	MG	BA	1602	1/1	0.72	0.18	79,79,79,79	0
59	MG	AB	3004	1/1	0.72	0.32	69,69,69,69	0
59	MG	CA	3152	1/1	0.72	0.35	64,64,64,64	0
59	MG	BA	1631	1/1	0.72	0.17	71,71,71,71	0
59	MG	BA	1697	1/1	0.72	1.08	99,99,99,99	0
59	MG	AA	3739	1/1	0.72	0.17	38,38,38,38	0
59	MG	AA	3296	1/1	0.72	0.25	67,67,67,67	0
59	MG	CA	3112	1/1	0.72	0.38	69,69,69,69	0
59	MG	BA	1758	1/1	0.72	0.36	76,76,76,76	0
59	MG	CA	3294	1/1	0.72	0.09	72,72,72,72	0
59	MG	AA	3140	1/1	0.72	0.58	62,62,62,62	0
59	MG	CA	3325	1/1	0.72	0.13	38,38,38,38	0
59	MG	CA	3378	1/1	0.72	0.24	97,97,97,97	0
59	MG	CA	3135	1/1	0.72	0.31	59,59,59,59	0
59	MG	DA	1611	1/1	0.72	0.39	89,89,89,89	0
59	MG	AA	3277	1/1	0.72	0.69	99,99,99,99	0
59	MG	CA	3536	1/1	0.73	0.26	84,84,84,84	0
59	MG	CA	3205	1/1	0.73	0.53	81,81,81,81	0
59	MG	AA	3571	1/1	0.73	0.34	94,94,94,94	0
59	MG	CA	3486	1/1	0.73	0.24	81,81,81,81	0
59	MG	AA	3769	1/1	0.73	0.17	63,63,63,63	0
59	MG	CB	3008	1/1	0.73	0.20	66,66,66,66	0
59	MG	BA	1601	1/1	0.73	0.34	95,95,95,95	0
59	MG	CA	3505	1/1	0.74	0.09	67,67,67,67	0
59	MG	DA	1724	1/1	0.74	0.41	70,70,70,70	0
59	MG	AA	3363	1/1	0.74	0.20	82,82,82,82	0
59	MG	CA	3420	1/1	0.74	0.33	69,69,69,69	0
59	MG	BA	1716	1/1	0.74	0.24	86,86,86,86	0
59	MG	CA	3093	1/1	0.74	0.71	75,75,75,75	0
59	MG	CA	3553	1/1	0.74	0.19	90,90,90,90	0
59	MG	AA	3536	1/1	0.74	0.24	66,66,66,66	0
59	MG	BA	1612	1/1	0.74	0.25	92,92,92,92	0
59	MG	CA	3350	1/1	0.74	0.09	82,82,82,82	0
59	MG	CA	3041	1/1	0.75	0.41	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3814	1/1	0.75	0.59	72,72,72,72	0
59	MG	AA	3767	1/1	0.75	0.35	67,67,67,67	0
59	MG	AA	3625	1/1	0.75	0.21	51,51,51,51	0
59	MG	CA	3082	1/1	0.75	0.75	76,76,76,76	0
59	MG	CA	3089	1/1	0.75	0.47	87,87,87,87	0
59	MG	CA	3602	1/1	0.75	0.10	84,84,84,84	0
59	MG	BA	1707	1/1	0.75	0.11	72,72,72,72	0
59	MG	BA	1714	1/1	0.75	0.28	74,74,74,74	0
59	MG	BA	1604	1/1	0.75	0.19	63,63,63,63	0
59	MG	BA	1721	1/1	0.75	0.20	66,66,66,66	0
59	MG	CA	3216	1/1	0.75	0.47	79,79,79,79	0
59	MG	DA	1742	1/1	0.75	0.21	72,72,72,72	0
59	MG	CA	3502	1/1	0.75	0.66	90,90,90,90	0
59	MG	AA	3773	1/1	0.75	0.45	35,35,35,35	1
59	MG	AA	3067	1/1	0.75	0.42	61,61,61,61	0
59	MG	CQ	204	1/1	0.75	0.33	74,74,74,74	0
59	MG	BA	1670	1/1	0.75	0.23	69,69,69,69	0
59	MG	CA	3542	1/1	0.75	0.41	87,87,87,87	0
59	MG	AA	3712	1/1	0.76	0.69	70,70,70,70	0
59	MG	DA	1631	1/1	0.76	0.09	74,74,74,74	0
59	MG	AE	301	1/1	0.76	0.57	69,69,69,69	0
59	MG	DA	1769	1/1	0.76	0.44	74,74,74,74	0
59	MG	CA	3517	1/1	0.76	0.16	62,62,62,62	0
59	MG	CA	3390	1/1	0.76	0.23	80,80,80,80	0
59	MG	DA	1622	1/1	0.77	0.35	60,60,60,60	0
59	MG	CA	3194	1/1	0.77	0.23	52,52,52,52	0
59	MG	CA	3097	1/1	0.77	0.29	66,66,66,66	0
59	MG	CA	3084	1/1	0.77	0.41	56,56,56,56	0
59	MG	CA	3348	1/1	0.77	0.28	44,44,44,44	0
59	MG	CA	3236	1/1	0.77	0.68	81,81,81,81	0
59	MG	BA	1665	1/1	0.77	0.45	73,73,73,73	0
59	MG	BA	1788	1/1	0.77	0.19	79,79,79,79	0
59	MG	AA	3323	1/1	0.77	0.21	64,64,64,64	0
59	MG	CV	201	1/1	0.77	0.81	117,117,117,117	0
59	MG	DA	1674	1/1	0.77	0.28	77,77,77,77	0
59	MG	CA	3279	1/1	0.77	0.17	26,26,26,26	0
59	MG	CA	3572	1/1	0.78	0.16	70,70,70,70	0
59	MG	AA	3066	1/1	0.78	0.14	51,51,51,51	0
59	MG	BA	1698	1/1	0.78	0.42	63,63,63,63	0
59	MG	CA	3240	1/1	0.78	0.48	71,71,71,71	0
59	MG	CA	3494	1/1	0.78	0.24	97,97,97,97	0
59	MG	BB	3001	1/1	0.78	0.16	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3630	1/1	0.78	0.10	65,65,65,65	0
59	MG	DA	1715	1/1	0.78	0.28	79,79,79,79	0
59	MG	CA	3092	1/1	0.78	0.78	79,79,79,79	0
59	MG	AA	3732	1/1	0.78	0.28	70,70,70,70	0
59	MG	CA	3007	1/1	0.78	0.40	92,92,92,92	0
59	MG	BA	1614	1/1	0.78	0.14	72,72,72,72	0
59	MG	AA	3225	1/1	0.78	0.15	73,73,73,73	0
59	MG	CA	3158	1/1	0.78	0.37	54,54,54,54	0
59	MG	CA	3541	1/1	0.78	0.28	63,63,63,63	0
59	MG	CA	3055	1/1	0.78	0.12	77,77,77,77	0
59	MG	AA	3644	1/1	0.78	0.33	56,56,56,56	0
59	MG	CA	3388	1/1	0.78	0.14	90,90,90,90	0
59	MG	CA	3550	1/1	0.78	0.09	62,62,62,62	1
59	MG	AA	3181	1/1	0.78	0.33	79,79,79,79	0
59	MG	AA	3002	1/1	0.78	0.21	57,57,57,57	0
59	MG	CA	3389	1/1	0.79	0.34	59,59,59,59	0
59	MG	AA	3827	1/1	0.79	0.37	38,38,38,38	0
59	MG	CA	3150	1/1	0.79	0.19	57,57,57,57	0
59	MG	BA	1811	1/1	0.79	0.20	77,77,77,77	0
59	MG	BA	1634	1/1	0.79	0.39	64,64,64,64	0
59	MG	AA	3780	1/1	0.79	0.40	72,72,72,72	0
59	MG	DA	1722	1/1	0.79	0.13	77,77,77,77	0
59	MG	CA	3490	1/1	0.79	0.13	50,50,50,50	0
59	MG	AA	3167	1/1	0.79	0.19	45,45,45,45	0
59	MG	CA	3180	1/1	0.79	0.36	62,62,62,62	0
59	MG	BA	1644	1/1	0.79	0.19	74,74,74,74	0
59	MG	CA	3037	1/1	0.79	0.72	57,57,57,57	0
59	MG	CA	3591	1/1	0.79	0.11	60,60,60,60	0
59	MG	CA	3600	1/1	0.79	0.52	86,86,86,86	0
59	MG	AX	3001	1/1	0.79	0.31	52,52,52,52	0
59	MG	CA	3514	1/1	0.79	0.42	64,64,64,64	0
59	MG	AA	3281	1/1	0.79	0.29	75,75,75,75	0
59	MG	CA	3044	1/1	0.79	0.21	89,89,89,89	0
59	MG	AA	3768	1/1	0.80	0.19	58,58,58,58	0
59	MG	BA	1619	1/1	0.80	0.21	59,59,59,59	0
59	MG	CA	3208	1/1	0.80	0.63	74,74,74,74	0
59	MG	BA	1628	1/1	0.80	0.30	87,87,87,87	0
59	MG	AA	3273	1/1	0.80	0.77	90,90,90,90	0
59	MG	BA	1704	1/1	0.80	0.31	71,71,71,71	0
59	MG	AA	3219	1/1	0.80	0.21	61,61,61,61	0
59	MG	AA	3352	1/1	0.80	0.36	47,47,47,47	0
59	MG	AA	3012	1/1	0.80	0.35	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	BS	101	1/1	0.80	0.16	79,79,79,79	0
59	MG	DA	1633	1/1	0.80	0.27	55,55,55,55	0
59	MG	CA	3289	1/1	0.80	0.28	65,65,65,65	0
59	MG	CA	3005	1/1	0.80	0.19	48,48,48,48	0
59	MG	AA	3708	1/1	0.80	0.30	61,61,61,61	0
59	MG	CA	3307	1/1	0.80	0.31	60,60,60,60	0
59	MG	CA	3555	1/1	0.80	0.14	71,71,71,71	0
59	MG	CA	3557	1/1	0.80	0.22	76,76,76,76	0
59	MG	CA	3563	1/1	0.80	0.09	75,75,75,75	0
59	MG	CA	3030	1/1	0.80	0.51	59,59,59,59	0
59	MG	CA	3034	1/1	0.80	0.29	77,77,77,77	0
59	MG	AA	3816	1/1	0.80	0.70	66,66,66,66	0
59	MG	CA	3583	1/1	0.80	0.16	80,80,80,80	0
59	MG	CA	3038	1/1	0.80	0.51	97,97,97,97	0
59	MG	BA	1655	1/1	0.80	0.15	59,59,59,59	0
59	MG	AA	3820	1/1	0.80	0.43	85,85,85,85	0
59	MG	AA	3761	1/1	0.80	0.38	92,92,92,92	0
59	MG	CA	3605	1/1	0.80	0.21	70,70,70,70	0
59	MG	AB	3003	1/1	0.80	0.23	60,60,60,60	0
59	MG	BA	1668	1/1	0.80	0.16	69,69,69,69	0
59	MG	CA	3072	1/1	0.80	0.38	66,66,66,66	0
59	MG	AA	3586	1/1	0.80	0.35	74,74,74,74	0
59	MG	CA	3077	1/1	0.80	0.24	42,42,42,42	0
59	MG	BA	1778	1/1	0.80	0.16	54,54,54,54	0
59	MG	BA	1693	1/1	0.81	0.47	76,76,76,76	0
59	MG	AA	3128	1/1	0.81	0.47	89,89,89,89	0
59	MG	AA	3109	1/1	0.81	0.34	56,56,56,56	0
59	MG	AW	3002	1/1	0.81	0.25	47,47,47,47	0
59	MG	AA	3227	1/1	0.81	0.18	22,22,22,22	0
59	MG	BA	1713	1/1	0.81	0.58	68,68,68,68	0
59	MG	CA	3122	1/1	0.81	0.70	58,58,58,58	0
59	MG	BA	1810	1/1	0.81	0.13	82,82,82,82	0
59	MG	CA	3513	1/1	0.81	0.16	70,70,70,70	0
59	MG	DA	1704	1/1	0.81	0.18	49,49,49,49	0
59	MG	CA	3068	1/1	0.81	0.43	66,66,66,66	0
59	MG	AA	3627	1/1	0.81	0.15	76,76,76,76	0
59	MG	CA	3631	1/1	0.81	0.11	65,65,65,65	0
59	MG	CA	3145	1/1	0.81	0.44	76,76,76,76	0
59	MG	AA	3817	1/1	0.81	0.18	75,75,75,75	0
59	MG	DA	1727	1/1	0.81	0.13	61,61,61,61	0
59	MG	AA	3629	1/1	0.81	0.17	77,77,77,77	0
59	MG	CA	3078	1/1	0.81	0.48	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3643	1/1	0.81	0.24	84,84,84,84	0
59	MG	AA	3556	1/1	0.81	0.32	66,66,66,66	0
59	MG	AA	3653	1/1	0.81	0.22	60,60,60,60	0
59	MG	AA	3675	1/1	0.81	0.14	64,64,64,64	0
59	MG	CA	3013	1/1	0.81	0.23	42,42,42,42	0
59	MG	AA	3206	1/1	0.81	0.54	106,106,106,106	0
59	MG	AA	3051	1/1	0.81	0.47	48,48,48,48	0
59	MG	CA	3202	1/1	0.81	0.71	73,73,73,73	0
59	MG	BA	1689	1/1	0.82	0.51	71,71,71,71	0
59	MG	BA	1690	1/1	0.82	0.40	71,71,71,71	0
59	MG	CA	3406	1/1	0.82	0.13	77,77,77,77	0
59	MG	CA	3413	1/1	0.82	0.22	39,39,39,39	0
59	MG	DA	1632	1/1	0.82	0.29	57,57,57,57	0
59	MG	AA	3601	1/1	0.82	0.11	61,61,61,61	0
59	MG	CA	3457	1/1	0.82	0.26	43,43,43,43	0
59	MG	CA	3575	1/1	0.82	0.21	71,71,71,71	0
59	MG	AA	3660	1/1	0.82	0.22	61,61,61,61	0
59	MG	BA	1635	1/1	0.82	0.51	65,65,65,65	0
59	MG	CA	3050	1/1	0.82	0.45	75,75,75,75	0
59	MG	AA	3315	1/1	0.82	0.22	65,65,65,65	0
59	MG	DA	1669	1/1	0.82	0.20	65,65,65,65	0
59	MG	CA	3060	1/1	0.82	0.39	72,72,72,72	0
59	MG	CA	3125	1/1	0.82	0.32	78,78,78,78	0
59	MG	A0	101	1/1	0.82	0.20	69,69,69,69	0
59	MG	A7	101	1/1	0.82	0.16	55,55,55,55	0
59	MG	BA	1648	1/1	0.82	0.11	74,74,74,74	0
59	MG	AA	3149	1/1	0.82	0.33	51,51,51,51	0
59	MG	AA	3693	1/1	0.82	0.14	69,69,69,69	0
59	MG	AA	3558	1/1	0.82	0.08	48,48,48,48	0
59	MG	CA	3528	1/1	0.82	0.10	38,38,38,38	0
59	MG	BA	1723	1/1	0.82	0.24	70,70,70,70	0
59	MG	AB	3008	1/1	0.82	0.38	52,52,52,52	0
59	MG	CA	3333	1/1	0.82	0.36	68,68,68,68	0
59	MG	AA	3258	1/1	0.82	0.44	68,68,68,68	0
59	MG	AA	3640	1/1	0.82	0.21	68,68,68,68	0
59	MG	AA	3087	1/1	0.82	0.48	55,55,55,55	0
59	MG	DA	1610	1/1	0.82	0.71	71,71,71,71	0
59	MG	AA	3018	1/1	0.82	1.43	67,67,67,67	0
59	MG	DA	1614	1/1	0.82	0.18	65,65,65,65	0
59	MG	DA	1605	1/1	0.83	0.33	105,105,105,105	0
59	MG	AA	3809	1/1	0.83	0.29	57,57,57,57	0
59	MG	CA	3193	1/1	0.83	0.44	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3058	1/1	0.83	0.33	67,67,67,67	0
59	MG	AA	3656	1/1	0.83	0.23	80,80,80,80	0
59	MG	CA	3559	1/1	0.83	0.12	75,75,75,75	0
59	MG	AA	3622	1/1	0.83	0.22	60,60,60,60	0
59	MG	BA	1633	1/1	0.83	0.25	63,63,63,63	0
59	MG	CA	3566	1/1	0.83	0.35	30,30,30,30	1
59	MG	CA	3001	1/1	0.83	0.25	64,64,64,64	0
59	MG	CA	3225	1/1	0.83	0.34	64,64,64,64	0
59	MG	AA	3450	1/1	0.83	0.10	58,58,58,58	0
59	MG	AA	3070	1/1	0.83	0.40	81,81,81,81	0
59	MG	A0	102	1/1	0.83	0.09	56,56,56,56	0
59	MG	CA	3023	1/1	0.83	0.42	68,68,68,68	0
59	MG	DA	1656	1/1	0.83	0.13	63,63,63,63	0
59	MG	CA	3598	1/1	0.83	0.15	65,65,65,65	0
59	MG	AA	3583	1/1	0.83	0.14	63,63,63,63	0
59	MG	AA	3019	1/1	0.83	0.29	70,70,70,70	0
59	MG	AA	3596	1/1	0.83	0.31	65,65,65,65	0
59	MG	CA	3608	1/1	0.83	0.32	50,50,50,50	1
59	MG	BA	1603	1/1	0.83	0.11	61,61,61,61	0
59	MG	AA	3714	1/1	0.83	0.24	70,70,70,70	0
59	MG	AA	3776	1/1	0.83	0.12	69,69,69,69	0
59	MG	CA	3323	1/1	0.83	0.40	87,87,87,87	0
59	MG	CA	3644	1/1	0.83	0.20	66,66,66,66	0
59	MG	CA	3518	1/1	0.83	0.11	65,65,65,65	0
59	MG	AA	3056	1/1	0.83	1.05	96,96,96,96	0
59	MG	CA	3159	1/1	0.83	0.59	69,69,69,69	0
59	MG	CA	3172	1/1	0.83	0.35	81,81,81,81	0
59	MG	CD	302	1/1	0.83	0.53	56,56,56,56	0
59	MG	CA	3176	1/1	0.83	0.42	60,60,60,60	0
59	MG	CA	3367	1/1	0.83	0.21	63,63,63,63	0
59	MG	CA	3377	1/1	0.83	0.10	52,52,52,52	0
59	MG	DA	1770	1/1	0.83	0.15	63,63,63,63	0
59	MG	DA	1771	1/1	0.83	0.12	60,60,60,60	0
59	MG	AA	3300	1/1	0.83	0.16	22,22,22,22	0
59	MG	C7	101	1/1	0.83	0.43	56,56,56,56	0
59	MG	CA	3629	1/1	0.84	0.08	55,55,55,55	0
59	MG	BA	1756	1/1	0.84	0.07	85,85,85,85	0
59	MG	AP	203	1/1	0.84	0.18	59,59,59,59	0
59	MG	CA	3633	1/1	0.84	0.26	68,68,68,68	0
59	MG	CA	3634	1/1	0.84	0.23	82,82,82,82	0
59	MG	CA	3432	1/1	0.84	0.27	32,32,32,32	0
59	MG	CA	3456	1/1	0.84	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
59	MG	AA	3792	1/1	0.84	0.13	48,48,48,48	0
59	MG	AA	3061	1/1	0.84	0.57	59,59,59,59	0
59	MG	BA	1772	1/1	0.84	0.12	66,66,66,66	0
59	MG	CA	3070	1/1	0.84	0.16	60,60,60,60	0
59	MG	AA	3808	1/1	0.84	0.40	72,72,72,72	0
59	MG	AA	3626	1/1	0.84	0.18	35,35,35,35	0
59	MG	AA	3544	1/1	0.84	0.22	26,26,26,26	0
59	MG	AA	3208	1/1	0.84	0.42	54,54,54,54	0
59	MG	CA	3200	1/1	0.84	0.30	51,51,51,51	0
59	MG	DA	1603	1/1	0.84	0.10	72,72,72,72	0
59	MG	AA	3026	1/1	0.84	0.23	47,47,47,47	0
59	MG	CA	3203	1/1	0.84	0.19	73,73,73,73	0
59	MG	CA	3081	1/1	0.84	0.31	63,63,63,63	0
59	MG	AA	3818	1/1	0.84	0.31	61,61,61,61	0
59	MG	DA	1618	1/1	0.84	0.64	91,91,91,91	0
59	MG	BA	1792	1/1	0.84	0.19	80,80,80,80	0
59	MG	CA	3521	1/1	0.84	0.22	74,74,74,74	0
59	MG	DA	1624	1/1	0.84	0.12	82,82,82,82	0
59	MG	BA	1682	1/1	0.84	0.82	70,70,70,70	0
59	MG	CA	3530	1/1	0.84	0.51	71,71,71,71	0
59	MG	AA	3169	1/1	0.84	0.34	35,35,35,35	0
59	MG	AA	3409	1/1	0.84	0.08	60,60,60,60	0
59	MG	AB	3001	1/1	0.84	0.37	74,74,74,74	0
59	MG	AA	3093	1/1	0.84	1.05	92,92,92,92	0
59	MG	BA	1696	1/1	0.84	0.16	98,98,98,98	0
59	MG	DA	1644	1/1	0.84	0.35	94,94,94,94	0
59	MG	CA	3273	1/1	0.84	0.35	58,58,58,58	0
59	MG	AA	3461	1/1	0.84	0.19	62,62,62,62	0
59	MG	CA	3284	1/1	0.84	0.17	75,75,75,75	0
59	MG	BA	1624	1/1	0.84	0.18	58,58,58,58	0
59	MG	DA	1665	1/1	0.84	0.20	63,63,63,63	0
59	MG	AB	3006	1/1	0.84	0.19	57,57,57,57	0
59	MG	CA	3296	1/1	0.84	0.15	79,79,79,79	0
59	MG	AA	3467	1/1	0.84	0.31	49,49,49,49	0
59	MG	CA	3120	1/1	0.84	0.21	42,42,42,42	0
59	MG	AA	3479	1/1	0.84	0.23	55,55,55,55	0
59	MG	CA	3124	1/1	0.84	0.26	65,65,65,65	0
59	MG	AA	3614	1/1	0.84	0.28	50,50,50,50	1
59	MG	AD	307	1/1	0.84	0.24	56,56,56,56	0
59	MG	CA	3581	1/1	0.84	0.12	38,38,38,38	0
59	MG	DA	1732	1/1	0.84	0.15	85,85,85,85	0
59	MG	BA	1719	1/1	0.84	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3363	1/1	0.84	0.17	88,88,88,88	0
59	MG	AA	3480	1/1	0.84	0.31	88,88,88,88	0
59	MG	AA	3010	1/1	0.84	0.45	46,46,46,46	0
59	MG	CA	3599	1/1	0.84	0.08	70,70,70,70	0
59	MG	BA	1729	1/1	0.84	0.16	53,53,53,53	0
59	MG	AA	3786	1/1	0.84	0.17	53,53,53,53	0
59	MG	CA	3603	1/1	0.84	0.35	49,49,49,49	0
59	MG	BA	1750	1/1	0.84	0.20	55,55,55,55	0
59	MG	BA	1646	1/1	0.84	0.95	66,66,66,66	0
59	MG	CA	3392	1/1	0.84	0.19	43,43,43,43	0
59	MG	CA	3153	1/1	0.84	0.23	73,73,73,73	0
59	MG	CF	301	1/1	0.85	0.47	61,61,61,61	0
59	MG	BA	1610	1/1	0.85	0.08	78,78,78,78	0
59	MG	AA	3634	1/1	0.85	0.19	76,76,76,76	0
59	MG	CA	3288	1/1	0.85	0.17	49,49,49,49	0
59	MG	CA	3069	1/1	0.85	0.72	81,81,81,81	0
59	MG	AA	3344	1/1	0.85	0.23	22,22,22,22	0
59	MG	AA	3180	1/1	0.85	0.26	69,69,69,69	0
59	MG	BA	1814	1/1	0.85	0.21	69,69,69,69	0
59	MG	BA	1815	1/1	0.85	0.22	53,53,53,53	0
59	MG	AA	3740	1/1	0.85	0.29	61,61,61,61	0
59	MG	BA	1727	1/1	0.85	0.09	77,77,77,77	0
59	MG	AA	3215	1/1	0.85	0.33	59,59,59,59	0
59	MG	BA	1625	1/1	0.85	0.15	86,86,86,86	0
59	MG	BA	1679	1/1	0.85	0.31	59,59,59,59	0
59	MG	CA	3352	1/1	0.85	0.18	79,79,79,79	0
59	MG	CA	3088	1/1	0.85	0.31	67,67,67,67	0
59	MG	AA	3649	1/1	0.85	0.33	62,62,62,62	0
59	MG	CA	3560	1/1	0.85	0.23	79,79,79,79	0
59	MG	CA	3373	1/1	0.85	0.29	58,58,58,58	0
59	MG	CA	3091	1/1	0.85	0.28	69,69,69,69	0
59	MG	CA	3184	1/1	0.85	0.33	77,77,77,77	0
59	MG	CA	3379	1/1	0.85	0.23	83,83,83,83	0
59	MG	DA	1643	1/1	0.85	0.24	79,79,79,79	0
59	MG	BA	1685	1/1	0.85	0.14	50,50,50,50	0
59	MG	CA	3577	1/1	0.85	0.16	51,51,51,51	1
59	MG	CA	3014	1/1	0.85	0.24	50,50,50,50	0
59	MG	AA	3542	1/1	0.85	0.23	58,58,58,58	0
59	MG	AA	3611	1/1	0.85	0.18	47,47,47,47	0
59	MG	AA	3083	1/1	0.85	0.38	61,61,61,61	0
59	MG	CA	3408	1/1	0.85	0.11	58,58,58,58	0
59	MG	AA	3551	1/1	0.85	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	1694	1/1	0.85	0.24	83,83,83,83	0
59	MG	CA	3111	1/1	0.85	0.24	79,79,79,79	0
59	MG	CA	3454	1/1	0.85	0.16	81,81,81,81	0
59	MG	CA	3210	1/1	0.85	0.34	62,62,62,62	0
59	MG	A0	103	1/1	0.85	0.10	70,70,70,70	0
59	MG	AA	3249	1/1	0.85	0.17	59,59,59,59	0
59	MG	CA	3226	1/1	0.85	0.33	52,52,52,52	0
59	MG	DA	1729	1/1	0.85	0.17	49,49,49,49	0
59	MG	CA	3229	1/1	0.85	0.19	53,53,53,53	0
59	MG	CA	3488	1/1	0.85	0.15	88,88,88,88	0
59	MG	AA	3041	1/1	0.85	0.26	37,37,37,37	0
59	MG	AA	3057	1/1	0.85	0.18	46,46,46,46	0
59	MG	AA	3575	1/1	0.85	0.14	35,35,35,35	0
59	MG	DA	1749	1/1	0.85	0.33	77,77,77,77	0
59	MG	BA	1791	1/1	0.85	0.18	72,72,72,72	0
59	MG	AA	3095	1/1	0.85	0.32	75,75,75,75	0
59	MG	CA	3251	1/1	0.85	0.18	82,82,82,82	0
59	MG	DA	1761	1/1	0.85	0.29	72,72,72,72	0
59	MG	CA	3647	1/1	0.85	0.15	85,85,85,85	0
59	MG	CA	3507	1/1	0.85	0.27	83,83,83,83	0
59	MG	CA	3510	1/1	0.85	0.11	95,95,95,95	0
59	MG	DE	202	1/1	0.85	0.08	100,100,100,100	0
59	MG	CA	3130	1/1	0.85	0.16	55,55,55,55	0
59	MG	CA	3276	1/1	0.85	0.18	44,44,44,44	0
59	MG	AA	3035	1/1	0.86	0.15	48,48,48,48	0
59	MG	AA	3213	1/1	0.86	0.65	76,76,76,76	0
59	MG	CA	3319	1/1	0.86	0.14	65,65,65,65	0
59	MG	BA	1695	1/1	0.86	0.08	83,83,83,83	0
59	MG	AA	3695	1/1	0.86	0.08	67,67,67,67	0
59	MG	CA	3540	1/1	0.86	0.07	54,54,54,54	0
59	MG	DA	1609	1/1	0.86	0.30	89,89,89,89	0
59	MG	BA	1803	1/1	0.86	0.12	64,64,64,64	0
59	MG	CA	3340	1/1	0.86	0.17	66,66,66,66	0
59	MG	CA	3544	1/1	0.86	0.32	60,60,60,60	0
59	MG	CA	3341	1/1	0.86	0.34	73,73,73,73	0
59	MG	AE	304	1/1	0.86	0.19	52,52,52,52	0
59	MG	AA	3705	1/1	0.86	0.57	53,53,53,53	1
59	MG	CA	3165	1/1	0.86	0.25	57,57,57,57	0
59	MG	BA	1700	1/1	0.86	0.14	52,52,52,52	0
59	MG	AA	3274	1/1	0.86	0.38	75,75,75,75	0
59	MG	AA	3275	1/1	0.86	0.34	89,89,89,89	0
59	MG	CA	3376	1/1	0.86	0.09	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3087	1/1	0.86	0.81	68,68,68,68	0
59	MG	DA	1636	1/1	0.86	0.50	62,62,62,62	0
59	MG	AA	3150	1/1	0.86	0.28	45,45,45,45	0
59	MG	BD	502	1/1	0.86	0.53	64,64,64,64	0
59	MG	AA	3202	1/1	0.86	0.11	61,61,61,61	0
59	MG	AA	3177	1/1	0.86	0.28	59,59,59,59	0
59	MG	BA	1652	1/1	0.86	0.12	59,59,59,59	0
59	MG	CA	3095	1/1	0.86	0.32	58,58,58,58	0
59	MG	CA	3395	1/1	0.86	0.42	50,50,50,50	0
59	MG	AA	3736	1/1	0.86	0.30	59,59,59,59	0
59	MG	DA	1662	1/1	0.86	0.23	75,75,75,75	0
59	MG	AA	3253	1/1	0.86	0.35	64,64,64,64	0
59	MG	AA	3158	1/1	0.86	0.88	68,68,68,68	0
59	MG	BA	1659	1/1	0.86	0.33	67,67,67,67	0
59	MG	CA	3016	1/1	0.86	0.25	52,52,52,52	0
59	MG	AA	3481	1/1	0.86	0.13	78,78,78,78	0
59	MG	BA	1662	1/1	0.86	0.72	70,70,70,70	0
59	MG	CA	3235	1/1	0.86	0.28	78,78,78,78	0
59	MG	CA	3115	1/1	0.86	0.41	67,67,67,67	0
59	MG	CA	3481	1/1	0.86	0.21	64,64,64,64	0
59	MG	CA	3612	1/1	0.86	0.36	83,83,83,83	0
59	MG	AA	3751	1/1	0.86	0.34	61,61,61,61	0
59	MG	AA	3237	1/1	0.86	0.38	76,76,76,76	0
59	MG	BA	1669	1/1	0.86	0.37	66,66,66,66	0
59	MG	AA	3603	1/1	0.86	0.62	76,76,76,76	0
59	MG	AA	3604	1/1	0.86	0.43	81,81,81,81	0
59	MG	CA	3256	1/1	0.86	0.29	65,65,65,65	0
59	MG	BA	1613	1/1	0.86	0.12	76,76,76,76	0
59	MG	AA	3657	1/1	0.86	0.17	63,63,63,63	0
59	MG	AA	3327	1/1	0.86	0.17	31,31,31,31	0
59	MG	AB	3020	1/1	0.86	0.18	62,62,62,62	0
59	MG	CA	3140	1/1	0.86	0.38	63,63,63,63	0
59	MG	CA	3656	1/1	0.86	0.57	63,63,63,63	0
59	MG	BA	1784	1/1	0.86	0.27	68,68,68,68	0
59	MG	CA	3291	1/1	0.86	0.41	48,48,48,48	0
59	MG	CA	3516	1/1	0.86	0.35	79,79,79,79	0
59	MG	AD	303	1/1	0.86	0.16	50,50,50,50	0
59	MG	AA	3331	1/1	0.86	0.16	15,15,15,15	0
59	MG	BA	1737	1/1	0.87	0.20	79,79,79,79	0
59	MG	CA	3478	1/1	0.87	0.31	65,65,65,65	0
59	MG	AA	3694	1/1	0.87	0.15	53,53,53,53	0
59	MG	BA	1630	1/1	0.87	0.29	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3153	1/1	0.87	0.32	59,59,59,59	0
59	MG	BA	1683	1/1	0.87	0.21	71,71,71,71	0
59	MG	AA	3157	1/1	0.87	0.48	91,91,91,91	0
59	MG	BA	1687	1/1	0.87	0.22	52,52,52,52	0
59	MG	AA	3264	1/1	0.87	0.41	51,51,51,51	0
59	MG	CA	3317	1/1	0.87	0.14	49,49,49,49	0
59	MG	DA	1641	1/1	0.87	0.25	74,74,74,74	0
59	MG	A2	3001	1/1	0.87	0.25	53,53,53,53	0
59	MG	A6	101	1/1	0.87	0.23	60,60,60,60	0
59	MG	CA	3098	1/1	0.87	0.14	70,70,70,70	0
59	MG	AA	3592	1/1	0.87	0.15	26,26,26,26	0
59	MG	CA	3511	1/1	0.87	0.20	81,81,81,81	0
59	MG	AA	3197	1/1	0.87	0.19	45,45,45,45	0
59	MG	AA	3229	1/1	0.87	0.36	67,67,67,67	0
59	MG	DA	1660	1/1	0.87	0.15	80,80,80,80	0
59	MG	AB	3021	1/1	0.87	0.26	65,65,65,65	0
59	MG	AA	3126	1/1	0.87	0.36	79,79,79,79	0
59	MG	CA	3204	1/1	0.87	0.19	54,54,54,54	0
59	MG	BA	1605	1/1	0.87	0.13	73,73,73,73	0
59	MG	DA	1681	1/1	0.87	0.37	70,70,70,70	0
59	MG	DA	1683	1/1	0.87	0.32	58,58,58,58	0
59	MG	DA	1686	1/1	0.87	0.19	56,56,56,56	0
59	MG	DA	1692	1/1	0.87	0.16	53,53,53,53	0
59	MG	CA	3116	1/1	0.87	0.32	52,52,52,52	0
59	MG	DA	1708	1/1	0.87	0.25	77,77,77,77	0
59	MG	AA	3164	1/1	0.87	0.63	71,71,71,71	0
59	MG	CA	3118	1/1	0.87	0.64	65,65,65,65	0
59	MG	CA	3059	1/1	0.87	0.43	58,58,58,58	0
59	MG	AA	3079	1/1	0.87	0.12	27,27,27,27	0
59	MG	BA	1658	1/1	0.87	0.61	66,66,66,66	0
59	MG	CA	3065	1/1	0.87	0.55	56,56,56,56	0
59	MG	CB	3012	1/1	0.87	0.26	62,62,62,62	0
59	MG	BA	1709	1/1	0.87	0.29	50,50,50,50	0
59	MG	CA	3545	1/1	0.87	0.46	86,86,86,86	0
59	MG	DA	1737	1/1	0.87	0.20	69,69,69,69	0
59	MG	BA	1712	1/1	0.87	0.40	57,57,57,57	0
59	MG	AA	3065	1/1	0.87	0.58	62,62,62,62	0
59	MG	AA	3444	1/1	0.87	0.24	66,66,66,66	0
59	MG	CQ	203	1/1	0.87	0.34	54,54,54,54	0
59	MG	CA	3551	1/1	0.87	0.07	63,63,63,63	0
59	MG	AA	3445	1/1	0.87	0.13	23,23,23,23	0
59	MG	CA	3246	1/1	0.87	0.50	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	CA	3411	1/1	0.87	0.24	57,57,57,57	0
59	MG	BA	1663	1/1	0.87	0.23	43,43,43,43	0
59	MG	AA	3677	1/1	0.87	0.10	69,69,69,69	0
59	MG	CA	3260	1/1	0.87	0.15	35,35,35,35	0
59	MG	BA	1622	1/1	0.87	0.51	65,65,65,65	0
59	MG	AA	3068	1/1	0.87	0.56	73,73,73,73	0
59	MG	AA	3025	1/1	0.87	0.43	68,68,68,68	0
59	MG	DZ	701	1/1	0.87	0.25	72,72,72,72	0
59	MG	CA	3114	1/1	0.88	0.19	66,66,66,66	0
59	MG	CA	3224	1/1	0.88	0.53	59,59,59,59	0
59	MG	AA	3659	1/1	0.88	0.18	73,73,73,73	0
59	MG	AA	3031	1/1	0.88	0.48	63,63,63,63	0
59	MG	AA	3664	1/1	0.88	0.20	62,62,62,62	0
59	MG	AA	3171	1/1	0.88	0.27	54,54,54,54	0
59	MG	AA	3175	1/1	0.88	0.56	63,63,63,63	0
59	MG	CA	3057	1/1	0.88	0.29	60,60,60,60	0
59	MG	AA	3619	1/1	0.88	0.12	47,47,47,47	0
59	MG	AA	3156	1/1	0.88	0.43	49,49,49,49	0
59	MG	CA	3569	1/1	0.88	0.19	41,41,41,41	0
59	MG	AA	3414	1/1	0.88	0.17	37,37,37,37	0
59	MG	DA	1638	1/1	0.88	0.29	80,80,80,80	0
59	MG	AE	305	1/1	0.88	0.35	48,48,48,48	0
59	MG	AF	302	1/1	0.88	0.11	41,41,41,41	0
59	MG	AA	3788	1/1	0.88	0.28	61,61,61,61	0
59	MG	AN	3003	1/1	0.88	0.08	55,55,55,55	0
59	MG	CA	3474	1/1	0.88	0.22	59,59,59,59	0
59	MG	DA	1646	1/1	0.88	0.12	57,57,57,57	0
59	MG	DA	1652	1/1	0.88	0.84	80,80,80,80	0
59	MG	CA	3264	1/1	0.88	0.19	60,60,60,60	0
59	MG	AP	202	1/1	0.88	0.18	44,44,44,44	0
59	MG	AA	3440	1/1	0.88	0.24	63,63,63,63	0
59	MG	BA	1703	1/1	0.88	0.30	51,51,51,51	0
59	MG	AR	201	1/1	0.88	0.16	28,28,28,28	0
59	MG	AA	3796	1/1	0.88	0.50	78,78,78,78	0
59	MG	DA	1663	1/1	0.88	0.42	91,91,91,91	0
59	MG	CA	3492	1/1	0.88	0.24	59,59,59,59	0
59	MG	AA	3699	1/1	0.88	0.27	71,71,71,71	0
59	MG	CA	3495	1/1	0.88	0.21	70,70,70,70	0
59	MG	DA	1679	1/1	0.88	0.12	70,70,70,70	0
59	MG	CA	3496	1/1	0.88	0.13	56,56,56,56	0
59	MG	AA	3047	1/1	0.88	0.18	29,29,29,29	0
59	MG	AA	3285	1/1	0.88	0.30	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	AA	3293	1/1	0.88	0.15	27,27,27,27	0
59	MG	CA	3503	1/1	0.88	0.35	52,52,52,52	0
59	MG	AA	3636	1/1	0.88	0.34	86,86,86,86	0
59	MG	AA	3142	1/1	0.88	0.25	64,64,64,64	0
59	MG	BW	503	1/1	0.88	0.20	60,60,60,60	0
59	MG	CA	3173	1/1	0.88	0.36	61,61,61,61	0
59	MG	CA	3090	1/1	0.88	0.28	77,77,77,77	0
59	MG	AA	3723	1/1	0.88	0.09	49,49,49,49	0
59	MG	CA	3328	1/1	0.88	0.20	35,35,35,35	0
59	MG	AA	3724	1/1	0.88	0.23	47,47,47,47	0
59	MG	CA	3336	1/1	0.88	0.09	64,64,64,64	0
59	MG	CB	3011	1/1	0.88	0.23	56,56,56,56	0
59	MG	DA	1735	1/1	0.88	0.12	73,73,73,73	0
59	MG	AA	3642	1/1	0.88	0.34	71,71,71,71	0
59	MG	CA	3189	1/1	0.88	0.14	50,50,50,50	0
59	MG	DA	1739	1/1	0.88	0.12	73,73,73,73	0
59	MG	CA	3191	1/1	0.88	0.22	46,46,46,46	0
59	MG	CE	301	1/1	0.88	0.32	53,53,53,53	0
59	MG	CA	3534	1/1	0.88	0.11	73,73,73,73	0
59	MG	CA	3535	1/1	0.88	0.22	77,77,77,77	0
59	MG	CQ	201	1/1	0.88	0.23	72,72,72,72	0
59	MG	AA	3464	1/1	0.88	0.40	66,66,66,66	0
59	MG	AA	3194	1/1	0.88	0.26	82,82,82,82	0
59	MG	AA	3015	1/1	0.88	0.35	57,57,57,57	0
59	MG	BA	1744	1/1	0.88	0.17	57,57,57,57	0
59	MG	BA	1609	1/1	0.88	0.12	62,62,62,62	0
59	MG	AA	3196	1/1	0.88	0.19	55,55,55,55	0
59	MG	CA	3035	1/1	0.88	0.28	69,69,69,69	0
59	MG	AA	3005	1/1	0.88	0.16	64,64,64,64	0
59	MG	AA	3235	1/1	0.88	0.45	93,93,93,93	0
59	MG	AA	3499	1/1	0.89	0.13	48,48,48,48	0
59	MG	BA	1730	1/1	0.89	0.18	53,53,53,53	0
59	MG	AA	3371	1/1	0.89	0.23	53,53,53,53	0
59	MG	BA	1607	1/1	0.89	0.27	64,64,64,64	0
59	MG	CA	3371	1/1	0.89	0.18	52,52,52,52	0
59	MG	AA	3616	1/1	0.89	0.17	57,57,57,57	0
59	MG	DA	1604	1/1	0.89	0.12	80,80,80,80	0
59	MG	AA	3385	1/1	0.89	0.21	49,49,49,49	0
59	MG	CA	3113	1/1	0.89	0.39	38,38,38,38	0
59	MG	CA	3215	1/1	0.89	0.07	54,54,54,54	0
59	MG	AA	3230	1/1	0.89	0.28	69,69,69,69	0
59	MG	CA	3385	1/1	0.89	0.37	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	1617	1/1	0.89	0.17	64,64,64,64	0
59	MG	CA	3223	1/1	0.89	0.15	59,59,59,59	0
59	MG	DA	1621	1/1	0.89	0.09	42,42,42,42	0
59	MG	BA	1671	1/1	0.89	0.21	101,101,101,101	0
59	MG	AA	3295	1/1	0.89	0.14	57,57,57,57	0
59	MG	AA	3418	1/1	0.89	0.13	74,74,74,74	0
59	MG	AA	3782	1/1	0.89	0.20	44,44,44,44	0
59	MG	DA	1627	1/1	0.89	0.08	77,77,77,77	0
59	MG	CA	3398	1/1	0.89	0.15	67,67,67,67	0
59	MG	CA	3046	1/1	0.89	0.29	68,68,68,68	0
59	MG	BA	1768	1/1	0.89	0.10	64,64,64,64	0
59	MG	AA	3233	1/1	0.89	0.18	46,46,46,46	0
59	MG	AA	3557	1/1	0.89	0.19	37,37,37,37	0
59	MG	CA	3417	1/1	0.89	0.21	56,56,56,56	0
59	MG	CA	3419	1/1	0.89	0.15	59,59,59,59	0
59	MG	CA	3241	1/1	0.89	0.18	72,72,72,72	0
59	MG	CA	3573	1/1	0.89	0.12	65,65,65,65	0
59	MG	CA	3426	1/1	0.89	0.20	38,38,38,38	0
59	MG	CA	3428	1/1	0.89	0.26	58,58,58,58	0
59	MG	AA	3209	1/1	0.89	0.30	62,62,62,62	0
59	MG	CA	3129	1/1	0.89	0.59	64,64,64,64	0
59	MG	CA	3582	1/1	0.89	0.08	99,99,99,99	0
59	MG	AA	3795	1/1	0.89	0.25	22,22,22,22	0
59	MG	BA	1779	1/1	0.89	0.19	85,85,85,85	0
59	MG	AA	3168	1/1	0.89	0.31	47,47,47,47	0
59	MG	CA	3593	1/1	0.89	0.60	61,61,61,61	0
59	MG	CA	3467	1/1	0.89	0.62	77,77,77,77	0
59	MG	CA	3257	1/1	0.89	0.16	35,35,35,35	0
59	MG	AA	3803	1/1	0.89	0.33	45,45,45,45	0
59	MG	DA	1666	1/1	0.89	0.19	53,53,53,53	0
59	MG	CA	3141	1/1	0.89	0.45	68,68,68,68	0
59	MG	CA	3270	1/1	0.89	0.28	76,76,76,76	0
59	MG	AA	3635	1/1	0.89	0.31	49,49,49,49	0
59	MG	AA	3055	1/1	0.89	0.28	65,65,65,65	0
59	MG	AA	3143	1/1	0.89	0.23	48,48,48,48	0
59	MG	DA	1684	1/1	0.89	0.18	69,69,69,69	0
59	MG	CA	3615	1/1	0.89	0.20	28,28,28,28	0
59	MG	DA	1689	1/1	0.89	0.17	56,56,56,56	0
59	MG	AW	3001	1/1	0.89	0.29	54,54,54,54	0
59	MG	DA	1702	1/1	0.89	0.13	63,63,63,63	0
59	MG	BA	1796	1/1	0.89	0.26	57,57,57,57	0
59	MG	CA	3625	1/1	0.89	0.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
59	MG	CA	3626	1/1	0.89	0.18	61,61,61,61	0
59	MG	CA	3628	1/1	0.89	0.18	54,54,54,54	0
59	MG	AA	3034	1/1	0.89	0.31	49,49,49,49	0
59	MG	BA	1641	1/1	0.89	0.20	54,54,54,54	0
59	MG	AA	3584	1/1	0.89	0.13	17,17,17,17	0
59	MG	CA	3632	1/1	0.89	0.18	74,74,74,74	0
59	MG	CA	3500	1/1	0.89	0.23	75,75,75,75	0
59	MG	AA	3162	1/1	0.89	0.26	67,67,67,67	0
59	MG	BA	1645	1/1	0.89	0.18	74,74,74,74	0
59	MG	AA	3027	1/1	0.89	0.51	75,75,75,75	0
59	MG	DA	1736	1/1	0.89	0.12	78,78,78,78	0
59	MG	CA	3310	1/1	0.89	0.17	47,47,47,47	0
59	MG	CA	3649	1/1	0.89	0.26	51,51,51,51	0
59	MG	AA	3357	1/1	0.89	0.15	55,55,55,55	0
59	MG	CA	3509	1/1	0.89	0.11	83,83,83,83	0
59	MG	CA	3663	1/1	0.89	0.11	64,64,64,64	0
59	MG	CB	3001	1/1	0.89	0.28	72,72,72,72	0
59	MG	CB	3007	1/1	0.89	0.22	52,52,52,52	0
59	MG	BA	1711	1/1	0.89	0.14	61,61,61,61	0
59	MG	A0	104	1/1	0.89	0.35	51,51,51,51	0
59	MG	AA	3825	1/1	0.89	0.40	63,63,63,63	0
59	MG	DA	1767	1/1	0.89	0.13	74,74,74,74	0
59	MG	AA	3655	1/1	0.89	0.33	55,55,55,55	0
59	MG	AA	3744	1/1	0.89	0.15	34,34,34,34	0
59	MG	AA	3088	1/1	0.89	0.42	39,39,39,39	0
59	MG	CE	304	1/1	0.89	0.36	75,75,75,75	0
59	MG	AA	3485	1/1	0.89	0.11	48,48,48,48	0
59	MG	AA	3492	1/1	0.89	0.18	26,26,26,26	0
59	MG	BA	1661	1/1	0.89	0.32	63,63,63,63	0
59	MG	AA	3267	1/1	0.90	0.35	53,53,53,53	0
59	MG	CR	201	1/1	0.90	0.26	34,34,34,34	0
59	MG	AA	3607	1/1	0.90	0.14	60,60,60,60	1
59	MG	CX	5001	1/1	0.90	0.14	65,65,65,65	0
59	MG	BA	1728	1/1	0.90	0.19	47,47,47,47	0
59	MG	AA	3608	1/1	0.90	0.36	60,60,60,60	0
59	MG	AA	3676	1/1	0.90	0.15	26,26,26,26	0
59	MG	CA	3539	1/1	0.90	0.18	90,90,90,90	0
59	MG	DA	1608	1/1	0.90	0.17	57,57,57,57	0
59	MG	AA	3783	1/1	0.90	0.49	53,53,53,53	1
59	MG	BA	1739	1/1	0.90	0.19	62,62,62,62	0
59	MG	AA	3105	1/1	0.90	0.15	52,52,52,52	0
59	MG	BA	1656	1/1	0.90	0.32	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	DA	1616	1/1	0.90	0.23	51,51,51,51	0
59	MG	AA	3787	1/1	0.90	0.20	82,82,82,82	0
59	MG	CA	3171	1/1	0.90	0.37	56,56,56,56	0
59	MG	AA	3679	1/1	0.90	0.08	36,36,36,36	0
59	MG	AA	3347	1/1	0.90	0.13	88,88,88,88	0
59	MG	AA	3683	1/1	0.90	0.27	62,62,62,62	0
59	MG	AA	3123	1/1	0.90	0.34	54,54,54,54	0
59	MG	CA	3066	1/1	0.90	0.16	69,69,69,69	0
59	MG	AA	3017	1/1	0.90	0.10	61,61,61,61	0
59	MG	AA	3618	1/1	0.90	0.15	72,72,72,72	0
59	MG	A0	105	1/1	0.90	0.08	30,30,30,30	0
59	MG	CA	3192	1/1	0.90	0.11	45,45,45,45	0
59	MG	BA	1774	1/1	0.90	0.27	50,50,50,50	0
59	MG	DA	1635	1/1	0.90	0.28	75,75,75,75	0
59	MG	AA	3183	1/1	0.90	0.35	58,58,58,58	0
59	MG	AA	3700	1/1	0.90	0.21	70,70,70,70	0
59	MG	AA	3810	1/1	0.90	0.27	67,67,67,67	0
59	MG	AA	3191	1/1	0.90	0.11	16,16,16,16	0
59	MG	AA	3280	1/1	0.90	0.29	53,53,53,53	0
59	MG	AA	3028	1/1	0.90	0.28	39,39,39,39	0
59	MG	AA	3282	1/1	0.90	0.12	33,33,33,33	0
59	MG	CA	3086	1/1	0.90	0.26	85,85,85,85	0
59	MG	AA	3715	1/1	0.90	0.54	33,33,33,33	1
59	MG	AA	3822	1/1	0.90	0.31	47,47,47,47	0
59	MG	CA	3586	1/1	0.90	0.17	93,93,93,93	0
59	MG	BA	1608	1/1	0.90	0.52	57,57,57,57	0
59	MG	DA	1658	1/1	0.90	0.33	51,51,51,51	0
59	MG	AA	3138	1/1	0.90	0.13	38,38,38,38	0
59	MG	BA	1797	1/1	0.90	0.17	59,59,59,59	0
59	MG	CA	3595	1/1	0.90	0.10	70,70,70,70	0
59	MG	AA	3633	1/1	0.90	0.16	48,48,48,48	0
59	MG	DA	1664	1/1	0.90	0.12	66,66,66,66	0
59	MG	CA	3450	1/1	0.90	0.11	54,54,54,54	0
59	MG	CA	3453	1/1	0.90	0.16	35,35,35,35	0
59	MG	DA	1667	1/1	0.90	0.06	66,66,66,66	0
59	MG	AA	3155	1/1	0.90	0.21	93,93,93,93	0
59	MG	BA	1806	1/1	0.90	0.33	55,55,55,55	0
59	MG	AA	3252	1/1	0.90	0.20	44,44,44,44	0
59	MG	CA	3458	1/1	0.90	0.22	54,54,54,54	0
59	MG	AA	3226	1/1	0.90	0.22	46,46,46,46	0
59	MG	CA	3465	1/1	0.90	0.30	70,70,70,70	0
59	MG	AA	3576	1/1	0.90	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3472	1/1	0.90	0.47	62,62,62,62	0
59	MG	BA	1813	1/1	0.90	0.07	55,55,55,55	0
59	MG	AA	3256	1/1	0.90	0.34	49,49,49,49	0
59	MG	DA	1703	1/1	0.90	0.21	89,89,89,89	0
59	MG	AA	3308	1/1	0.90	0.22	18,18,18,18	0
59	MG	AA	3313	1/1	0.90	0.16	39,39,39,39	0
59	MG	CA	3249	1/1	0.90	0.15	61,61,61,61	0
59	MG	CA	3250	1/1	0.90	0.14	38,38,38,38	0
59	MG	AA	3466	1/1	0.90	0.20	76,76,76,76	0
59	MG	BA	1701	1/1	0.90	0.09	54,54,54,54	0
59	MG	AD	301	1/1	0.90	0.71	58,58,58,58	0
59	MG	BW	502	1/1	0.90	0.10	59,59,59,59	0
59	MG	AD	302	1/1	0.90	0.15	17,17,17,17	0
59	MG	DA	1730	1/1	0.90	0.25	71,71,71,71	0
59	MG	BA	1705	1/1	0.90	0.23	53,53,53,53	0
59	MG	AA	3591	1/1	0.90	0.26	52,52,52,52	0
59	MG	AA	3756	1/1	0.90	0.14	49,49,49,49	0
59	MG	AD	306	1/1	0.90	0.14	65,65,65,65	0
59	MG	CA	3280	1/1	0.90	0.15	48,48,48,48	0
59	MG	AA	3139	1/1	0.90	0.33	60,60,60,60	0
59	MG	CB	3002	1/1	0.90	0.10	63,63,63,63	0
59	MG	CB	3003	1/1	0.90	0.09	65,65,65,65	0
59	MG	CA	3506	1/1	0.90	0.12	63,63,63,63	0
59	MG	AA	3763	1/1	0.90	0.26	47,47,47,47	0
59	MG	DA	1753	1/1	0.90	0.29	79,79,79,79	0
59	MG	CA	3020	1/1	0.90	0.18	47,47,47,47	0
59	MG	CA	3021	1/1	0.90	0.44	69,69,69,69	0
59	MG	AA	3472	1/1	0.90	0.23	42,42,42,42	0
59	MG	CA	3512	1/1	0.90	0.15	53,53,53,53	0
59	MG	CA	3134	1/1	0.90	0.66	71,71,71,71	0
59	MG	CA	3298	1/1	0.90	0.36	57,57,57,57	0
59	MG	BA	1642	1/1	0.90	0.15	60,60,60,60	0
59	MG	CF	302	1/1	0.90	0.53	69,69,69,69	0
59	MG	CA	3031	1/1	0.90	0.48	68,68,68,68	0
59	MG	DF	3001	1/1	0.90	0.20	54,54,54,54	0
59	MG	CA	3033	1/1	0.90	0.40	55,55,55,55	0
59	MG	AA	3199	1/1	0.90	0.34	41,41,41,41	0
59	MG	AA	3120	1/1	0.90	0.24	33,33,33,33	0
59	MG	CA	3271	1/1	0.91	0.18	48,48,48,48	0
59	MG	AA	3781	1/1	0.91	0.20	72,72,72,72	0
59	MG	CA	3274	1/1	0.91	0.15	52,52,52,52	0
59	MG	AF	301	1/1	0.91	0.21	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3278	1/1	0.91	0.12	58,58,58,58	0
59	MG	AA	3339	1/1	0.91	0.17	49,49,49,49	0
59	MG	AA	3090	1/1	0.91	0.38	53,53,53,53	0
59	MG	AA	3211	1/1	0.91	0.27	56,56,56,56	0
59	MG	AA	3612	1/1	0.91	0.14	68,68,68,68	0
59	MG	AA	3486	1/1	0.91	0.21	67,67,67,67	0
59	MG	CA	3126	1/1	0.91	0.31	62,62,62,62	0
59	MG	DA	1601	1/1	0.91	0.42	74,74,74,74	0
59	MG	BA	1647	1/1	0.91	0.51	57,57,57,57	0
59	MG	BA	1724	1/1	0.91	0.19	67,67,67,67	0
59	MG	CA	3524	1/1	0.91	0.24	52,52,52,52	0
59	MG	DA	1606	1/1	0.91	0.30	85,85,85,85	0
59	MG	AQ	203	1/1	0.91	0.29	32,32,32,32	0
59	MG	BA	1649	1/1	0.91	0.16	35,35,35,35	0
59	MG	AA	3078	1/1	0.91	0.32	70,70,70,70	0
59	MG	CA	3137	1/1	0.91	0.23	69,69,69,69	0
59	MG	CA	3314	1/1	0.91	0.29	57,57,57,57	0
59	MG	CA	3032	1/1	0.91	0.55	100,100,100,100	0
59	MG	AA	3166	1/1	0.91	0.41	40,40,40,40	0
59	MG	BA	1733	1/1	0.91	0.20	78,78,78,78	0
59	MG	DA	1620	1/1	0.91	0.21	57,57,57,57	0
59	MG	BA	1736	1/1	0.91	0.17	67,67,67,67	0
59	MG	CA	3036	1/1	0.91	0.28	32,32,32,32	0
59	MG	CA	3148	1/1	0.91	0.34	62,62,62,62	0
59	MG	AA	3516	1/1	0.91	0.23	65,65,65,65	0
59	MG	BA	1738	1/1	0.91	0.08	66,66,66,66	0
59	MG	AA	3358	1/1	0.91	0.12	45,45,45,45	0
59	MG	CA	3343	1/1	0.91	0.12	32,32,32,32	0
59	MG	AY	502	1/1	0.91	0.28	60,60,60,60	0
59	MG	CA	3042	1/1	0.91	0.31	65,65,65,65	0
59	MG	AA	3043	1/1	0.91	0.30	45,45,45,45	0
59	MG	BA	1746	1/1	0.91	0.12	33,33,33,33	0
59	MG	AA	3701	1/1	0.91	0.15	81,81,81,81	0
59	MG	BA	1753	1/1	0.91	0.11	48,48,48,48	0
59	MG	AA	3624	1/1	0.91	0.12	42,42,42,42	0
59	MG	CA	3374	1/1	0.91	0.30	60,60,60,60	0
59	MG	AA	3246	1/1	0.91	0.13	52,52,52,52	0
59	MG	AA	3373	1/1	0.91	0.16	48,48,48,48	0
59	MG	CA	3174	1/1	0.91	0.52	50,50,50,50	0
59	MG	AA	3284	1/1	0.91	0.58	60,60,60,60	0
59	MG	AA	3391	1/1	0.91	0.20	19,19,19,19	0
59	MG	AA	3630	1/1	0.91	0.34	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
59	MG	AA	3722	1/1	0.91	0.12	37,37,37,37	0
59	MG	CA	3580	1/1	0.91	0.23	76,76,76,76	0
59	MG	CA	3187	1/1	0.91	0.22	37,37,37,37	0
59	MG	CA	3067	1/1	0.91	0.19	63,63,63,63	0
59	MG	AA	3009	1/1	0.91	0.09	22,22,22,22	0
59	MG	AA	3288	1/1	0.91	0.27	39,39,39,39	0
59	MG	AA	3826	1/1	0.91	0.28	46,46,46,46	0
59	MG	CA	3071	1/1	0.91	0.27	45,45,45,45	0
59	MG	CA	3409	1/1	0.91	0.28	42,42,42,42	0
59	MG	CA	3594	1/1	0.91	0.11	73,73,73,73	0
59	MG	CA	3199	1/1	0.91	0.22	55,55,55,55	0
59	MG	CA	3597	1/1	0.91	0.21	58,58,58,58	0
59	MG	DA	1672	1/1	0.91	0.23	77,77,77,77	0
59	MG	AA	3224	1/1	0.91	0.24	56,56,56,56	0
59	MG	DA	1677	1/1	0.91	0.42	78,78,78,78	0
59	MG	AA	3106	1/1	0.91	0.17	33,33,33,33	0
59	MG	AA	3638	1/1	0.91	0.35	71,71,71,71	0
59	MG	AA	3135	1/1	0.91	0.55	55,55,55,55	0
59	MG	CA	3079	1/1	0.91	0.10	41,41,41,41	0
59	MG	CA	3604	1/1	0.91	0.09	62,62,62,62	0
59	MG	AA	3579	1/1	0.91	0.18	54,54,54,54	0
59	MG	AA	3069	1/1	0.91	0.09	28,28,28,28	0
59	MG	DA	1694	1/1	0.91	0.35	106,106,106,106	0
59	MG	DA	1699	1/1	0.91	0.19	74,74,74,74	0
59	MG	DA	1701	1/1	0.91	0.24	68,68,68,68	0
59	MG	CA	3610	1/1	0.91	0.13	69,69,69,69	0
59	MG	CA	3442	1/1	0.91	0.59	74,74,74,74	0
59	MG	CA	3444	1/1	0.91	0.10	67,67,67,67	0
59	MG	DA	1705	1/1	0.91	0.10	68,68,68,68	0
59	MG	CA	3616	1/1	0.91	0.64	74,74,74,74	0
59	MG	CA	3448	1/1	0.91	0.21	37,37,37,37	0
59	MG	CA	3623	1/1	0.91	0.15	64,64,64,64	0
59	MG	AB	3009	1/1	0.91	0.09	50,50,50,50	0
59	MG	AA	3446	1/1	0.91	0.09	59,59,59,59	0
59	MG	CA	3221	1/1	0.91	0.58	65,65,65,65	0
59	MG	BA	1794	1/1	0.91	0.07	38,38,38,38	0
59	MG	AA	3449	1/1	0.91	0.23	50,50,50,50	0
59	MG	AA	3014	1/1	0.91	0.12	31,31,31,31	0
59	MG	BA	1620	1/1	0.91	0.17	52,52,52,52	0
59	MG	AA	3654	1/1	0.91	0.06	67,67,67,67	0
59	MG	CA	3234	1/1	0.91	0.35	50,50,50,50	0
59	MG	AA	3310	1/1	0.91	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3636	1/1	0.91	0.19	64,64,64,64	0
59	MG	CA	3638	1/1	0.91	0.34	76,76,76,76	0
59	MG	CA	3473	1/1	0.91	0.16	51,51,51,51	0
59	MG	BA	1807	1/1	0.91	0.12	61,61,61,61	0
59	MG	CA	3477	1/1	0.91	0.14	69,69,69,69	0
59	MG	AA	3205	1/1	0.91	0.15	42,42,42,42	0
59	MG	CA	3239	1/1	0.91	0.17	69,69,69,69	0
59	MG	BA	1699	1/1	0.91	0.18	72,72,72,72	0
59	MG	AA	3232	1/1	0.91	0.25	58,58,58,58	0
59	MG	AA	3179	1/1	0.91	0.50	45,45,45,45	1
59	MG	AA	3772	1/1	0.91	0.62	61,61,61,61	1
59	MG	AA	3602	1/1	0.91	0.15	51,51,51,51	0
59	MG	AA	3270	1/1	0.91	0.55	55,55,55,55	0
59	MG	BA	1706	1/1	0.91	0.20	63,63,63,63	0
59	MG	CA	3110	1/1	0.91	0.26	56,56,56,56	0
59	MG	AA	3118	1/1	0.91	0.40	76,76,76,76	0
59	MG	BN	502	1/1	0.91	0.17	87,87,87,87	0
59	MG	BN	503	1/1	0.91	0.14	62,62,62,62	0
59	MG	BA	1708	1/1	0.91	0.22	64,64,64,64	0
59	MG	DW	503	1/1	0.91	0.22	85,85,85,85	0
59	MG	BA	1637	1/1	0.91	0.46	72,72,72,72	0
59	MG	BA	1718	1/1	0.92	0.09	63,63,63,63	0
59	MG	BA	1650	1/1	0.92	0.15	55,55,55,55	0
59	MG	AA	3134	1/1	0.92	0.23	62,62,62,62	0
59	MG	CA	3207	1/1	0.92	0.28	75,75,75,75	0
59	MG	AA	3203	1/1	0.92	0.07	59,59,59,59	0
59	MG	AA	3268	1/1	0.92	0.07	66,66,66,66	0
59	MG	CA	3212	1/1	0.92	0.24	84,84,84,84	0
59	MG	CA	3549	1/1	0.92	0.16	70,70,70,70	0
59	MG	CA	3387	1/1	0.92	0.33	50,50,50,50	0
59	MG	AA	3427	1/1	0.92	0.12	61,61,61,61	0
59	MG	DA	1613	1/1	0.92	0.24	48,48,48,48	0
59	MG	AA	3746	1/1	0.92	0.17	73,73,73,73	0
59	MG	A6	103	1/1	0.92	0.36	72,72,72,72	0
59	MG	CA	3391	1/1	0.92	0.07	51,51,51,51	0
59	MG	CA	3558	1/1	0.92	0.09	64,64,64,64	0
59	MG	CA	3222	1/1	0.92	0.34	57,57,57,57	0
59	MG	AA	3110	1/1	0.92	0.48	52,52,52,52	0
59	MG	CA	3396	1/1	0.92	0.23	39,39,39,39	0
59	MG	BA	1731	1/1	0.92	0.17	45,45,45,45	0
59	MG	CA	3403	1/1	0.92	0.07	70,70,70,70	0
59	MG	DA	1625	1/1	0.92	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3749	1/1	0.92	0.17	73,73,73,73	0
59	MG	AA	3115	1/1	0.92	0.34	44,44,44,44	0
59	MG	AA	3319	1/1	0.92	0.19	58,58,58,58	0
59	MG	AA	3085	1/1	0.92	0.20	46,46,46,46	0
59	MG	CA	3576	1/1	0.92	0.11	71,71,71,71	0
59	MG	AA	3447	1/1	0.92	0.34	56,56,56,56	0
59	MG	CA	3026	1/1	0.92	0.22	32,32,32,32	1
59	MG	BA	1666	1/1	0.92	0.37	61,61,61,61	0
59	MG	DA	1637	1/1	0.92	0.39	68,68,68,68	0
59	MG	CA	3238	1/1	0.92	0.24	69,69,69,69	0
59	MG	BA	1667	1/1	0.92	0.25	74,74,74,74	0
59	MG	AA	3678	1/1	0.92	0.15	77,77,77,77	0
59	MG	CA	3585	1/1	0.92	0.16	36,36,36,36	1
59	MG	CA	3431	1/1	0.92	0.20	75,75,75,75	0
59	MG	BA	1748	1/1	0.92	0.14	63,63,63,63	0
59	MG	CA	3589	1/1	0.92	0.23	71,71,71,71	0
59	MG	AB	3010	1/1	0.92	0.11	62,62,62,62	0
59	MG	CA	3243	1/1	0.92	0.28	58,58,58,58	0
59	MG	AA	3161	1/1	0.92	0.23	43,43,43,43	0
59	MG	BA	1754	1/1	0.92	0.13	49,49,49,49	0
59	MG	CA	3596	1/1	0.92	0.12	51,51,51,51	0
59	MG	CA	3247	1/1	0.92	0.28	39,39,39,39	0
59	MG	AA	3102	1/1	0.92	0.23	47,47,47,47	0
59	MG	DA	1661	1/1	0.92	0.18	66,66,66,66	0
59	MG	CA	3128	1/1	0.92	0.39	50,50,50,50	0
59	MG	BA	1611	1/1	0.92	0.13	31,31,31,31	0
59	MG	BA	1675	1/1	0.92	0.07	100,100,100,100	0
59	MG	CA	3131	1/1	0.92	0.23	26,26,26,26	0
59	MG	CA	3462	1/1	0.92	0.11	63,63,63,63	0
59	MG	CA	3259	1/1	0.92	0.26	80,80,80,80	0
59	MG	BA	1760	1/1	0.92	0.17	53,53,53,53	0
59	MG	DA	1670	1/1	0.92	0.12	49,49,49,49	0
59	MG	CA	3609	1/1	0.92	0.16	52,52,52,52	0
59	MG	BA	1676	1/1	0.92	0.20	61,61,61,61	0
59	MG	DA	1675	1/1	0.92	0.41	70,70,70,70	0
59	MG	CA	3043	1/1	0.92	0.41	61,61,61,61	0
59	MG	DA	1678	1/1	0.92	0.28	66,66,66,66	0
59	MG	AA	3184	1/1	0.92	0.24	75,75,75,75	0
59	MG	AA	3771	1/1	0.92	0.24	60,60,60,60	0
59	MG	CA	3619	1/1	0.92	0.38	40,40,40,40	0
59	MG	AA	3186	1/1	0.92	0.29	48,48,48,48	0
59	MG	CA	3143	1/1	0.92	0.56	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3244	1/1	0.92	0.25	52,52,52,52	0
59	MG	DA	1691	1/1	0.92	0.18	63,63,63,63	0
59	MG	BA	1618	1/1	0.92	0.31	52,52,52,52	0
59	MG	AA	3189	1/1	0.92	0.20	62,62,62,62	0
59	MG	AA	3696	1/1	0.92	0.17	66,66,66,66	0
59	MG	AA	3698	1/1	0.92	0.16	41,41,41,41	0
59	MG	BA	1623	1/1	0.92	0.62	67,67,67,67	0
59	MG	AA	3141	1/1	0.92	0.09	68,68,68,68	0
59	MG	AA	3476	1/1	0.92	0.17	28,28,28,28	0
59	MG	AA	3033	1/1	0.92	0.27	55,55,55,55	0
59	MG	BA	1629	1/1	0.92	0.28	61,61,61,61	0
59	MG	DA	1713	1/1	0.92	0.17	49,49,49,49	0
59	MG	CA	3301	1/1	0.92	0.19	60,60,60,60	0
59	MG	AA	3287	1/1	0.92	0.39	43,43,43,43	0
59	MG	AA	3707	1/1	0.92	0.09	59,59,59,59	0
59	MG	CA	3168	1/1	0.92	0.42	58,58,58,58	0
59	MG	CA	3312	1/1	0.92	0.18	38,38,38,38	0
59	MG	DA	1726	1/1	0.92	0.29	60,60,60,60	0
59	MG	AA	3045	1/1	0.92	0.32	55,55,55,55	0
59	MG	DA	1728	1/1	0.92	0.08	71,71,71,71	0
59	MG	CA	3508	1/1	0.92	0.18	52,52,52,52	0
59	MG	AA	3641	1/1	0.92	0.28	51,51,51,51	0
59	MG	BA	1800	1/1	0.92	0.46	77,77,77,77	0
59	MG	AN	3001	1/1	0.92	0.32	58,58,58,58	0
59	MG	AA	3483	1/1	0.92	0.20	46,46,46,46	0
59	MG	BA	1805	1/1	0.92	0.25	71,71,71,71	0
59	MG	AA	3797	1/1	0.92	0.17	52,52,52,52	0
59	MG	CA	3515	1/1	0.92	0.20	54,54,54,54	0
59	MG	AA	3800	1/1	0.92	0.16	35,35,35,35	0
59	MG	DA	1741	1/1	0.92	0.35	67,67,67,67	0
59	MG	AA	3080	1/1	0.92	0.50	61,61,61,61	0
59	MG	CA	3083	1/1	0.92	0.41	61,61,61,61	0
59	MG	DA	1748	1/1	0.92	0.18	70,70,70,70	0
59	MG	CA	3520	1/1	0.92	0.16	73,73,73,73	0
59	MG	DA	1751	1/1	0.92	0.16	64,64,64,64	0
59	MG	CD	303	1/1	0.92	0.08	70,70,70,70	0
59	MG	AA	3716	1/1	0.92	0.24	66,66,66,66	0
59	MG	CE	303	1/1	0.92	0.40	51,51,51,51	0
59	MG	CA	3345	1/1	0.92	0.17	46,46,46,46	0
59	MG	CA	3527	1/1	0.92	0.14	76,76,76,76	0
59	MG	AA	3077	1/1	0.92	0.27	43,43,43,43	0
59	MG	CA	3529	1/1	0.92	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3718	1/1	0.92	0.21	42,42,42,42	0
59	MG	CA	3532	1/1	0.92	0.23	49,49,49,49	0
59	MG	DE	201	1/1	0.92	0.17	84,84,84,84	0
59	MG	AA	3645	1/1	0.92	0.21	58,58,58,58	0
59	MG	AA	3487	1/1	0.92	0.03	49,49,49,49	0
59	MG	AA	3133	1/1	0.92	0.33	50,50,50,50	0
59	MG	CA	3368	1/1	0.92	0.16	44,44,44,44	0
59	MG	DW	502	1/1	0.92	0.08	58,58,58,58	0
59	MG	AA	3394	1/1	0.92	0.16	39,39,39,39	0
59	MG	C3	3001	1/1	0.92	0.39	72,72,72,72	0
60	ZN	C4	501	1/1	0.92	0.11	194,194,194,194	0
59	MG	DA	1607	1/1	0.93	0.10	86,86,86,86	0
59	MG	AQ	202	1/1	0.93	0.25	35,35,35,35	0
59	MG	BA	1710	1/1	0.93	0.25	81,81,81,81	0
59	MG	AA	3024	1/1	0.93	0.13	48,48,48,48	0
59	MG	AA	3646	1/1	0.93	0.22	53,53,53,53	0
59	MG	AA	3648	1/1	0.93	0.17	41,41,41,41	0
59	MG	AA	3304	1/1	0.93	0.15	47,47,47,47	0
59	MG	AA	3651	1/1	0.93	0.22	77,77,77,77	0
59	MG	AA	3234	1/1	0.93	0.29	36,36,36,36	0
59	MG	AZ	301	1/1	0.93	0.14	55,55,55,55	0
59	MG	BA	1720	1/1	0.93	0.21	61,61,61,61	0
59	MG	CA	3402	1/1	0.93	0.09	66,66,66,66	0
59	MG	CA	3094	1/1	0.93	0.21	59,59,59,59	0
59	MG	AA	3038	1/1	0.93	0.45	29,29,29,29	1
59	MG	BE	3001	1/1	0.93	0.11	78,78,78,78	0
59	MG	BK	201	1/1	0.93	0.10	44,44,44,44	0
59	MG	AA	3731	1/1	0.93	0.14	51,51,51,51	0
59	MG	CA	3412	1/1	0.93	0.18	59,59,59,59	0
59	MG	DA	1629	1/1	0.93	0.42	59,59,59,59	0
59	MG	AA	3058	1/1	0.93	0.14	22,22,22,22	0
59	MG	CA	3414	1/1	0.93	0.19	34,34,34,34	1
59	MG	CA	3233	1/1	0.93	0.12	59,59,59,59	0
59	MG	AA	3733	1/1	0.93	0.15	49,49,49,49	0
59	MG	AA	3609	1/1	0.93	0.11	58,58,58,58	0
59	MG	AA	3738	1/1	0.93	0.19	24,24,24,24	0
59	MG	AA	3514	1/1	0.93	0.18	42,42,42,42	0
59	MG	CA	3430	1/1	0.93	0.36	41,41,41,41	0
59	MG	AA	3823	1/1	0.93	0.48	39,39,39,39	0
59	MG	BA	1732	1/1	0.93	0.25	70,70,70,70	0
59	MG	CA	3588	1/1	0.93	0.12	32,32,32,32	0
59	MG	CA	3434	1/1	0.93	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3436	1/1	0.93	0.11	64,64,64,64	0
59	MG	AA	3314	1/1	0.93	0.26	57,57,57,57	0
59	MG	DA	1650	1/1	0.93	0.28	50,50,50,50	0
59	MG	BA	1734	1/1	0.93	0.13	61,61,61,61	0
59	MG	AA	3429	1/1	0.93	0.19	31,31,31,31	0
59	MG	AA	3661	1/1	0.93	0.24	41,41,41,41	1
59	MG	AA	3832	1/1	0.93	0.42	55,55,55,55	0
59	MG	CA	3245	1/1	0.93	0.41	62,62,62,62	0
59	MG	AA	3046	1/1	0.93	0.33	35,35,35,35	0
59	MG	CA	3022	1/1	0.93	0.52	69,69,69,69	0
59	MG	AB	3002	1/1	0.93	0.17	52,52,52,52	0
59	MG	AA	3748	1/1	0.93	0.20	45,45,45,45	0
59	MG	CA	3029	1/1	0.93	0.09	56,56,56,56	0
59	MG	CA	3463	1/1	0.93	0.23	56,56,56,56	0
59	MG	CA	3254	1/1	0.93	0.16	85,85,85,85	0
59	MG	AA	3667	1/1	0.93	0.29	41,41,41,41	0
59	MG	AA	3669	1/1	0.93	0.18	81,81,81,81	0
59	MG	DA	1668	1/1	0.93	0.38	65,65,65,65	0
59	MG	AA	3673	1/1	0.93	0.11	38,38,38,38	0
59	MG	CA	3614	1/1	0.93	0.24	62,62,62,62	0
59	MG	BA	1672	1/1	0.93	0.30	65,65,65,65	0
59	MG	CA	3476	1/1	0.93	0.17	38,38,38,38	0
59	MG	AA	3062	1/1	0.93	0.17	47,47,47,47	0
59	MG	AA	3096	1/1	0.93	0.20	59,59,59,59	0
59	MG	AA	3172	1/1	0.93	0.22	47,47,47,47	0
59	MG	CA	3484	1/1	0.93	0.26	78,78,78,78	0
59	MG	DA	1680	1/1	0.93	0.17	56,56,56,56	0
59	MG	BA	1757	1/1	0.93	0.22	43,43,43,43	0
59	MG	DA	1682	1/1	0.93	0.33	52,52,52,52	0
59	MG	AA	3764	1/1	0.93	0.16	73,73,73,73	0
59	MG	CA	3275	1/1	0.93	0.10	61,61,61,61	0
59	MG	BA	1759	1/1	0.93	0.32	63,63,63,63	0
59	MG	DA	1688	1/1	0.93	0.25	51,51,51,51	0
59	MG	AA	3101	1/1	0.93	0.64	68,68,68,68	0
59	MG	DA	1690	1/1	0.93	0.19	73,73,73,73	0
59	MG	BA	1763	1/1	0.93	0.17	76,76,76,76	0
59	MG	BA	1617	1/1	0.93	0.12	118,118,118,118	0
59	MG	AA	3063	1/1	0.93	0.26	54,54,54,54	0
59	MG	AA	3198	1/1	0.93	0.15	63,63,63,63	0
59	MG	DA	1700	1/1	0.93	0.16	61,61,61,61	0
59	MG	AA	3454	1/1	0.93	0.24	61,61,61,61	0
59	MG	CA	3051	1/1	0.93	0.74	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	CA	3642	1/1	0.93	0.52	52,52,52,52	0
59	MG	CA	3293	1/1	0.93	0.16	60,60,60,60	0
59	MG	CA	3052	1/1	0.93	0.18	44,44,44,44	0
59	MG	BA	1621	1/1	0.93	0.11	51,51,51,51	0
59	MG	CA	3056	1/1	0.93	0.09	63,63,63,63	0
59	MG	CA	3651	1/1	0.93	0.53	76,76,76,76	0
59	MG	AA	3456	1/1	0.93	0.14	56,56,56,56	0
59	MG	CA	3655	1/1	0.93	0.41	52,52,52,52	0
59	MG	CA	3156	1/1	0.93	0.38	52,52,52,52	0
59	MG	CA	3658	1/1	0.93	0.39	64,64,64,64	0
59	MG	CA	3660	1/1	0.93	0.19	60,60,60,60	0
59	MG	CA	3157	1/1	0.93	0.55	81,81,81,81	0
59	MG	AA	3178	1/1	0.93	0.36	48,48,48,48	0
59	MG	AA	3775	1/1	0.93	0.59	25,25,25,25	1
59	MG	CA	3313	1/1	0.93	0.26	38,38,38,38	0
59	MG	CB	3004	1/1	0.93	0.13	55,55,55,55	0
59	MG	CB	3005	1/1	0.93	0.38	63,63,63,63	0
59	MG	CA	3161	1/1	0.93	0.25	57,57,57,57	0
59	MG	CA	3164	1/1	0.93	0.56	64,64,64,64	0
59	MG	AD	308	1/1	0.93	0.42	46,46,46,46	0
59	MG	CA	3167	1/1	0.93	0.08	50,50,50,50	0
59	MG	BA	1780	1/1	0.93	0.36	60,60,60,60	0
59	MG	BA	1782	1/1	0.93	0.19	47,47,47,47	0
59	MG	AA	3577	1/1	0.93	0.08	42,42,42,42	0
59	MG	DA	1744	1/1	0.93	0.22	66,66,66,66	0
59	MG	AA	3086	1/1	0.93	0.40	55,55,55,55	0
59	MG	BA	1787	1/1	0.93	0.27	55,55,55,55	0
59	MG	CA	3526	1/1	0.93	0.21	58,58,58,58	0
59	MG	AA	3356	1/1	0.93	0.15	80,80,80,80	0
59	MG	CA	3177	1/1	0.93	0.15	29,29,29,29	0
59	MG	CF	303	1/1	0.93	0.14	51,51,51,51	0
59	MG	DA	1755	1/1	0.93	0.51	88,88,88,88	0
59	MG	CN	5001	1/1	0.93	0.16	65,65,65,65	0
59	MG	CA	3178	1/1	0.93	0.13	54,54,54,54	0
59	MG	DA	1758	1/1	0.93	0.17	75,75,75,75	0
59	MG	DA	1759	1/1	0.93	0.17	53,53,53,53	0
59	MG	AA	3286	1/1	0.93	0.45	40,40,40,40	0
59	MG	AA	3124	1/1	0.93	0.73	62,62,62,62	0
59	MG	AA	3204	1/1	0.93	0.33	54,54,54,54	0
59	MG	CA	3073	1/1	0.93	0.26	49,49,49,49	0
59	MG	BA	1793	1/1	0.93	0.09	65,65,65,65	0
59	MG	CA	3076	1/1	0.93	0.34	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3589	1/1	0.93	0.08	55,55,55,55	0
59	MG	AA	3261	1/1	0.93	0.31	25,25,25,25	0
59	MG	DJ	5001	1/1	0.93	0.32	82,82,82,82	0
59	MG	AA	3231	1/1	0.93	0.21	64,64,64,64	0
59	MG	BA	1639	1/1	0.93	0.46	61,61,61,61	0
59	MG	AA	3376	1/1	0.93	0.21	35,35,35,35	0
59	MG	CA	3201	1/1	0.93	0.23	45,45,45,45	0
59	MG	AA	3163	1/1	0.93	0.25	72,72,72,72	0
60	ZN	BN	501	1/1	0.93	0.10	132,132,132,132	0
59	MG	CA	3547	1/1	0.93	0.13	69,69,69,69	0
59	MG	AA	3276	1/1	0.94	0.24	67,67,67,67	0
59	MG	AA	3089	1/1	0.94	0.28	49,49,49,49	0
59	MG	AA	3278	1/1	0.94	0.21	60,60,60,60	0
59	MG	CA	3018	1/1	0.94	0.08	41,41,41,41	0
59	MG	AA	3828	1/1	0.94	0.38	38,38,38,38	0
59	MG	CA	3142	1/1	0.94	0.43	61,61,61,61	0
59	MG	AA	3711	1/1	0.94	0.35	43,43,43,43	1
59	MG	AA	3615	1/1	0.94	0.25	43,43,43,43	0
59	MG	C1	101	1/1	0.94	0.18	57,57,57,57	0
59	MG	BA	1726	1/1	0.94	0.20	46,46,46,46	0
59	MG	AA	3351	1/1	0.94	0.21	29,29,29,29	0
59	MG	CA	3522	1/1	0.94	0.13	54,54,54,54	0
59	MG	DA	1602	1/1	0.94	0.10	45,45,45,45	0
59	MG	AA	3474	1/1	0.94	0.15	18,18,18,18	1
59	MG	AA	3279	1/1	0.94	0.23	34,34,34,34	0
59	MG	CA	3151	1/1	0.94	0.16	38,38,38,38	0
59	MG	AA	3245	1/1	0.94	0.17	11,11,11,11	0
59	MG	CA	3316	1/1	0.94	0.17	43,43,43,43	0
59	MG	AA	3620	1/1	0.94	0.11	22,22,22,22	0
59	MG	CA	3531	1/1	0.94	0.09	47,47,47,47	0
59	MG	BA	1636	1/1	0.94	0.17	57,57,57,57	0
59	MG	CA	3533	1/1	0.94	0.18	45,45,45,45	0
59	MG	DA	1612	1/1	0.94	0.13	57,57,57,57	0
59	MG	AA	3719	1/1	0.94	0.10	59,59,59,59	0
59	MG	AA	3030	1/1	0.94	0.29	24,24,24,24	1
59	MG	AA	3081	1/1	0.94	0.21	56,56,56,56	0
59	MG	AB	3018	1/1	0.94	0.22	69,69,69,69	0
59	MG	AA	3359	1/1	0.94	0.18	31,31,31,31	0
59	MG	AA	3361	1/1	0.94	0.16	53,53,53,53	0
59	MG	AA	3251	1/1	0.94	0.35	56,56,56,56	0
59	MG	BA	1742	1/1	0.94	0.18	48,48,48,48	0
59	MG	CA	3166	1/1	0.94	0.31	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	AA	3628	1/1	0.94	0.23	70,70,70,70	0
59	MG	BA	1745	1/1	0.94	0.20	46,46,46,46	0
59	MG	CA	3170	1/1	0.94	0.15	32,32,32,32	0
59	MG	CA	3357	1/1	0.94	0.12	66,66,66,66	0
59	MG	CA	3359	1/1	0.94	0.08	33,33,33,33	0
59	MG	AA	3365	1/1	0.94	0.39	77,77,77,77	0
59	MG	CA	3048	1/1	0.94	0.10	47,47,47,47	0
59	MG	AA	3490	1/1	0.94	0.16	27,27,27,27	0
59	MG	CA	3370	1/1	0.94	0.14	41,41,41,41	0
59	MG	AA	3367	1/1	0.94	0.17	60,60,60,60	0
59	MG	AA	3495	1/1	0.94	0.15	35,35,35,35	0
59	MG	AA	3743	1/1	0.94	0.16	67,67,67,67	0
59	MG	BA	1651	1/1	0.94	0.33	55,55,55,55	0
59	MG	CA	3561	1/1	0.94	0.14	41,41,41,41	1
59	MG	DA	1640	1/1	0.94	0.31	77,77,77,77	0
59	MG	AD	309	1/1	0.94	0.25	37,37,37,37	0
59	MG	CA	3182	1/1	0.94	0.31	38,38,38,38	0
59	MG	CA	3183	1/1	0.94	0.21	49,49,49,49	0
59	MG	CA	3568	1/1	0.94	0.10	39,39,39,39	0
59	MG	AD	310	1/1	0.94	0.39	78,78,78,78	0
59	MG	DA	1647	1/1	0.94	0.15	51,51,51,51	0
59	MG	AA	3370	1/1	0.94	0.15	47,47,47,47	0
59	MG	AA	3170	1/1	0.94	0.19	54,54,54,54	0
59	MG	CA	3188	1/1	0.94	0.80	94,94,94,94	0
59	MG	AA	3004	1/1	0.94	0.15	21,21,21,21	0
59	MG	CA	3190	1/1	0.94	0.23	66,66,66,66	0
59	MG	CA	3578	1/1	0.94	0.09	38,38,38,38	0
59	MG	CA	3063	1/1	0.94	0.10	34,34,34,34	0
59	MG	CA	3393	1/1	0.94	0.07	68,68,68,68	0
59	MG	AA	3518	1/1	0.94	0.17	14,14,14,14	0
59	MG	AA	3374	1/1	0.94	0.31	49,49,49,49	0
59	MG	AA	3254	1/1	0.94	0.25	52,52,52,52	0
59	MG	CA	3399	1/1	0.94	0.07	57,57,57,57	0
59	MG	CA	3196	1/1	0.94	0.66	68,68,68,68	0
59	MG	AA	3378	1/1	0.94	0.17	56,56,56,56	0
59	MG	AA	3255	1/1	0.94	0.22	38,38,38,38	0
59	MG	AA	3759	1/1	0.94	0.10	57,57,57,57	0
59	MG	CA	3590	1/1	0.94	0.10	59,59,59,59	0
59	MG	BA	1664	1/1	0.94	0.14	56,56,56,56	0
59	MG	CA	3410	1/1	0.94	0.22	25,25,25,25	0
59	MG	AA	3549	1/1	0.94	0.05	66,66,66,66	0
59	MG	AA	3387	1/1	0.94	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3555	1/1	0.94	0.15	45,45,45,45	0
59	MG	AA	3766	1/1	0.94	0.17	54,54,54,54	0
59	MG	BA	1781	1/1	0.94	0.14	63,63,63,63	0
59	MG	AQ	204	1/1	0.94	0.23	86,86,86,86	0
59	MG	AA	3289	1/1	0.94	0.43	53,53,53,53	0
59	MG	CA	3421	1/1	0.94	0.20	57,57,57,57	0
59	MG	AA	3071	1/1	0.94	0.60	40,40,40,40	0
59	MG	AA	3408	1/1	0.94	0.34	41,41,41,41	0
59	MG	CA	3429	1/1	0.94	0.26	59,59,59,59	0
59	MG	CA	3606	1/1	0.94	0.48	73,73,73,73	0
59	MG	CA	3607	1/1	0.94	0.09	64,64,64,64	0
59	MG	AA	3257	1/1	0.94	0.32	54,54,54,54	0
59	MG	BA	1789	1/1	0.94	0.15	72,72,72,72	0
59	MG	AA	3572	1/1	0.94	0.20	17,17,17,17	0
59	MG	AA	3573	1/1	0.94	0.16	12,12,12,12	0
59	MG	DA	1695	1/1	0.94	0.17	63,63,63,63	0
59	MG	DA	1698	1/1	0.94	0.33	97,97,97,97	0
59	MG	AA	3413	1/1	0.94	0.19	25,25,25,25	0
59	MG	CA	3441	1/1	0.94	0.23	56,56,56,56	0
59	MG	AA	3207	1/1	0.94	0.20	60,60,60,60	0
59	MG	AA	3190	1/1	0.94	0.13	24,24,24,24	0
59	MG	BA	1795	1/1	0.94	0.10	59,59,59,59	0
59	MG	CA	3621	1/1	0.94	0.21	61,61,61,61	0
59	MG	CA	3622	1/1	0.94	0.17	50,50,50,50	0
59	MG	DA	1706	1/1	0.94	0.33	66,66,66,66	0
59	MG	AA	3173	1/1	0.94	0.29	46,46,46,46	0
59	MG	DA	1709	1/1	0.94	0.16	70,70,70,70	0
59	MG	DA	1710	1/1	0.94	0.25	104,104,104,104	0
59	MG	CA	3452	1/1	0.94	0.20	36,36,36,36	0
59	MG	AA	3662	1/1	0.94	0.07	60,60,60,60	0
59	MG	AA	3580	1/1	0.94	0.22	54,54,54,54	0
59	MG	BA	1801	1/1	0.94	0.09	65,65,65,65	0
59	MG	A5	502	1/1	0.94	0.16	51,51,51,51	0
59	MG	DA	1723	1/1	0.94	0.13	53,53,53,53	0
59	MG	AA	3784	1/1	0.94	0.21	59,59,59,59	0
59	MG	AA	3265	1/1	0.94	0.17	43,43,43,43	0
59	MG	AA	3174	1/1	0.94	0.44	59,59,59,59	0
59	MG	A8	5001	1/1	0.94	0.27	30,30,30,30	0
59	MG	AA	3672	1/1	0.94	0.15	48,48,48,48	0
59	MG	CA	3635	1/1	0.94	0.23	48,48,48,48	0
59	MG	CA	3104	1/1	0.94	0.15	80,80,80,80	0
59	MG	CA	3470	1/1	0.94	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3443	1/1	0.94	0.19	33,33,33,33	0
59	MG	CA	3643	1/1	0.94	0.17	79,79,79,79	0
59	MG	AA	3148	1/1	0.94	0.45	29,29,29,29	1
59	MG	AA	3236	1/1	0.94	0.14	57,57,57,57	0
59	MG	CA	3248	1/1	0.94	0.42	53,53,53,53	0
59	MG	AA	3050	1/1	0.94	0.27	28,28,28,28	0
59	MG	AA	3001	1/1	0.94	0.14	25,25,25,25	0
59	MG	DA	1743	1/1	0.94	0.13	59,59,59,59	0
59	MG	AA	3594	1/1	0.94	0.24	56,56,56,56	0
59	MG	CA	3483	1/1	0.94	0.32	64,64,64,64	0
59	MG	CA	3253	1/1	0.94	0.17	70,70,70,70	0
59	MG	AA	3448	1/1	0.94	0.12	62,62,62,62	0
59	MG	AA	3217	1/1	0.94	0.44	29,29,29,29	1
59	MG	CA	3661	1/1	0.94	0.23	27,27,27,27	0
59	MG	AA	3324	1/1	0.94	0.14	15,15,15,15	0
59	MG	CA	3664	1/1	0.94	0.13	48,48,48,48	0
59	MG	CA	3489	1/1	0.94	0.10	39,39,39,39	0
59	MG	AA	3451	1/1	0.94	0.07	57,57,57,57	0
59	MG	AA	3218	1/1	0.94	0.09	67,67,67,67	0
59	MG	CA	3493	1/1	0.94	0.52	65,65,65,65	0
59	MG	AA	3606	1/1	0.94	0.24	34,34,34,34	0
59	MG	DA	1762	1/1	0.94	0.20	61,61,61,61	0
59	MG	CA	3269	1/1	0.94	0.14	81,81,81,81	0
59	MG	DA	1768	1/1	0.94	0.07	59,59,59,59	0
59	MG	AA	3455	1/1	0.94	0.20	32,32,32,32	1
59	MG	BW	501	1/1	0.94	0.22	47,47,47,47	0
59	MG	AA	3039	1/1	0.94	0.52	34,34,34,34	1
59	MG	AA	3819	1/1	0.94	0.51	57,57,57,57	0
59	MG	AA	3337	1/1	0.94	0.16	75,75,75,75	0
59	MG	CA	3003	1/1	0.94	0.30	62,62,62,62	0
59	MG	CD	304	1/1	0.94	0.29	28,28,28,28	0
59	MG	CA	3504	1/1	0.94	0.13	79,79,79,79	0
59	MG	AA	3610	1/1	0.94	0.22	59,59,59,59	0
59	MG	AA	3704	1/1	0.94	0.19	49,49,49,49	0
59	MG	CA	3132	1/1	0.94	0.16	48,48,48,48	0
59	MG	CA	3283	1/1	0.94	0.12	31,31,31,31	0
60	ZN	A4	501	1/1	0.94	0.07	117,117,117,117	0
59	MG	CA	3008	1/1	0.94	0.38	46,46,46,46	0
59	MG	CA	3285	1/1	0.94	0.19	63,63,63,63	0
59	MG	CA	3147	1/1	0.95	0.29	55,55,55,55	0
59	MG	AA	3022	1/1	0.95	0.12	5,5,5,5	0
59	MG	C5	101	1/1	0.95	0.49	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3099	1/1	0.95	0.10	53,53,53,53	0
59	MG	CA	3009	1/1	0.95	0.10	27,27,27,27	0
59	MG	CA	3318	1/1	0.95	0.21	24,24,24,24	0
59	MG	CA	3012	1/1	0.95	0.15	65,65,65,65	0
59	MG	CA	3321	1/1	0.95	0.13	28,28,28,28	0
59	MG	AA	3187	1/1	0.95	0.29	56,56,56,56	0
59	MG	AA	3671	1/1	0.95	0.23	19,19,19,19	0
59	MG	AA	3588	1/1	0.95	0.15	47,47,47,47	0
59	MG	AA	3785	1/1	0.95	0.15	61,61,61,61	0
59	MG	AA	3271	1/1	0.95	0.33	34,34,34,34	0
59	MG	CA	3337	1/1	0.95	0.14	20,20,20,20	0
59	MG	A9	502	1/1	0.95	0.24	41,41,41,41	0
59	MG	AA	3674	1/1	0.95	0.14	30,30,30,30	0
59	MG	AA	3590	1/1	0.95	0.17	60,60,60,60	0
59	MG	CA	3024	1/1	0.95	0.29	100,100,100,100	0
59	MG	DA	1615	1/1	0.95	0.25	58,58,58,58	0
59	MG	CA	3346	1/1	0.95	0.19	30,30,30,30	0
59	MG	CA	3543	1/1	0.95	0.19	71,71,71,71	0
59	MG	AA	3790	1/1	0.95	0.46	57,57,57,57	0
59	MG	DA	1619	1/1	0.95	0.59	59,59,59,59	0
59	MG	CA	3349	1/1	0.95	0.20	23,23,23,23	0
59	MG	AA	3188	1/1	0.95	0.18	31,31,31,31	0
59	MG	BA	1717	1/1	0.95	0.18	78,78,78,78	0
59	MG	CA	3354	1/1	0.95	0.25	49,49,49,49	0
59	MG	CA	3356	1/1	0.95	0.19	44,44,44,44	0
59	MG	AA	3794	1/1	0.95	0.42	60,60,60,60	0
59	MG	AA	3384	1/1	0.95	0.21	22,22,22,22	0
59	MG	CA	3552	1/1	0.95	0.18	30,30,30,30	0
59	MG	AA	3478	1/1	0.95	0.24	33,33,33,33	0
59	MG	AA	3006	1/1	0.95	0.34	52,52,52,52	0
59	MG	AA	3048	1/1	0.95	0.16	28,28,28,28	0
59	MG	AA	3104	1/1	0.95	0.32	54,54,54,54	0
59	MG	AA	3804	1/1	0.95	0.18	50,50,50,50	0
59	MG	AA	3806	1/1	0.95	0.18	42,42,42,42	0
59	MG	AA	3684	1/1	0.95	0.25	51,51,51,51	0
59	MG	CA	3562	1/1	0.95	0.14	29,29,29,29	0
59	MG	CA	3375	1/1	0.95	0.34	68,68,68,68	0
59	MG	AA	3685	1/1	0.95	0.19	72,72,72,72	0
59	MG	AA	3686	1/1	0.95	0.20	61,61,61,61	0
59	MG	AA	3687	1/1	0.95	0.29	52,52,52,52	0
59	MG	AA	3812	1/1	0.95	0.17	41,41,41,41	0
59	MG	AA	3689	1/1	0.95	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
59	MG	CA	3185	1/1	0.95	0.29	48,48,48,48	0
59	MG	AA	3392	1/1	0.95	0.24	17,17,17,17	0
59	MG	AA	3393	1/1	0.95	0.20	23,23,23,23	0
59	MG	AA	3193	1/1	0.95	0.20	40,40,40,40	0
59	MG	AA	3400	1/1	0.95	0.17	13,13,13,13	0
59	MG	AA	3697	1/1	0.95	0.23	40,40,40,40	0
59	MG	BA	1626	1/1	0.95	0.12	41,41,41,41	0
59	MG	BA	1627	1/1	0.95	0.23	51,51,51,51	0
59	MG	AA	3325	1/1	0.95	0.16	70,70,70,70	0
59	MG	CA	3397	1/1	0.95	0.15	57,57,57,57	0
59	MG	AA	3013	1/1	0.95	0.18	28,28,28,28	0
59	MG	AA	3824	1/1	0.95	0.58	72,72,72,72	0
59	MG	CA	3198	1/1	0.95	0.23	34,34,34,34	0
59	MG	AA	3493	1/1	0.95	0.10	77,77,77,77	0
59	MG	BA	1749	1/1	0.95	0.32	61,61,61,61	0
59	MG	AA	3494	1/1	0.95	0.09	34,34,34,34	0
59	MG	AA	3330	1/1	0.95	0.06	66,66,66,66	0
59	MG	AA	3221	1/1	0.95	0.15	30,30,30,30	0
59	MG	AA	3829	1/1	0.95	0.24	47,47,47,47	0
59	MG	AA	3706	1/1	0.95	0.54	41,41,41,41	1
59	MG	AA	3501	1/1	0.95	0.06	49,49,49,49	0
59	MG	AA	3502	1/1	0.95	0.13	29,29,29,29	1
59	MG	CA	3416	1/1	0.95	0.14	44,44,44,44	0
59	MG	AA	3503	1/1	0.95	0.06	54,54,54,54	0
59	MG	AA	3504	1/1	0.95	0.09	29,29,29,29	0
59	MG	CA	3601	1/1	0.95	0.13	57,57,57,57	0
59	MG	CA	3213	1/1	0.95	0.27	51,51,51,51	0
59	MG	AA	3508	1/1	0.95	0.18	43,43,43,43	0
59	MG	AA	3509	1/1	0.95	0.16	40,40,40,40	0
59	MG	AA	3510	1/1	0.95	0.24	17,17,17,17	0
59	MG	AA	3513	1/1	0.95	0.10	41,41,41,41	0
59	MG	BA	1771	1/1	0.95	0.21	65,65,65,65	0
59	MG	DA	1685	1/1	0.95	0.10	46,46,46,46	0
59	MG	AB	3013	1/1	0.95	0.15	53,53,53,53	0
59	MG	DA	1687	1/1	0.95	0.42	56,56,56,56	0
59	MG	AA	3417	1/1	0.95	0.18	25,25,25,25	0
59	MG	AA	3333	1/1	0.95	0.20	11,11,11,11	0
59	MG	AA	3420	1/1	0.95	0.15	25,25,25,25	1
59	MG	CA	3440	1/1	0.95	0.31	49,49,49,49	0
59	MG	AA	3520	1/1	0.95	0.14	17,17,17,17	0
59	MG	AB	3022	1/1	0.95	0.12	61,61,61,61	0
59	MG	AA	3521	1/1	0.95	0.18	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3445	1/1	0.95	0.20	22,22,22,22	0
59	MG	AA	3522	1/1	0.95	0.16	30,30,30,30	0
59	MG	AA	3632	1/1	0.95	0.20	54,54,54,54	0
59	MG	CA	3451	1/1	0.95	0.21	62,62,62,62	0
59	MG	BA	1783	1/1	0.95	0.18	57,57,57,57	0
59	MG	AD	304	1/1	0.95	0.35	41,41,41,41	0
59	MG	AA	3530	1/1	0.95	0.19	20,20,20,20	1
59	MG	CA	3455	1/1	0.95	0.28	49,49,49,49	0
59	MG	AA	3533	1/1	0.95	0.17	22,22,22,22	0
59	MG	DA	1707	1/1	0.95	0.07	61,61,61,61	0
59	MG	AA	3737	1/1	0.95	0.16	54,54,54,54	0
59	MG	AA	3425	1/1	0.95	0.05	77,77,77,77	0
59	MG	AA	3036	1/1	0.95	0.24	25,25,25,25	0
59	MG	AA	3637	1/1	0.95	0.33	17,17,17,17	1
59	MG	AA	3132	1/1	0.95	0.21	41,41,41,41	0
59	MG	AA	3431	1/1	0.95	0.15	25,25,25,25	0
59	MG	AA	3548	1/1	0.95	0.11	7,7,7,7	0
59	MG	DA	1719	1/1	0.95	0.38	61,61,61,61	0
59	MG	CA	3469	1/1	0.95	0.22	61,61,61,61	0
59	MG	CA	3639	1/1	0.95	0.59	61,61,61,61	0
59	MG	AA	3064	1/1	0.95	0.13	32,32,32,32	0
59	MG	DA	1725	1/1	0.95	0.17	58,58,58,58	0
59	MG	CA	3107	1/1	0.95	0.26	77,77,77,77	0
59	MG	AA	3441	1/1	0.95	0.29	58,58,58,58	0
59	MG	CA	3645	1/1	0.95	0.11	69,69,69,69	0
59	MG	CA	3252	1/1	0.95	0.19	62,62,62,62	0
59	MG	AA	3052	1/1	0.95	0.16	11,11,11,11	0
59	MG	BA	1799	1/1	0.95	0.13	64,64,64,64	0
59	MG	AA	3348	1/1	0.95	0.06	53,53,53,53	0
59	MG	DA	1734	1/1	0.95	0.14	65,65,65,65	0
59	MG	CA	3480	1/1	0.95	0.21	50,50,50,50	0
59	MG	AF	306	1/1	0.95	0.24	57,57,57,57	0
59	MG	AG	202	1/1	0.95	0.06	54,54,54,54	0
59	MG	AH	201	1/1	0.95	0.85	64,64,64,64	0
59	MG	CA	3263	1/1	0.95	0.14	64,64,64,64	0
59	MG	BA	1674	1/1	0.95	0.57	48,48,48,48	0
59	MG	CA	3265	1/1	0.95	0.29	61,61,61,61	0
59	MG	CA	3268	1/1	0.95	0.17	52,52,52,52	0
59	MG	AA	3176	1/1	0.95	0.32	70,70,70,70	0
59	MG	AA	3200	1/1	0.95	0.22	30,30,30,30	0
59	MG	DA	1747	1/1	0.95	0.14	48,48,48,48	0
59	MG	BA	1809	1/1	0.95	0.23	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3121	1/1	0.95	0.13	49,49,49,49	0
59	MG	DA	1750	1/1	0.95	0.08	67,67,67,67	0
59	MG	AO	5001	1/1	0.95	0.09	34,34,34,34	0
59	MG	DA	1752	1/1	0.95	0.16	52,52,52,52	0
59	MG	BA	1680	1/1	0.95	0.19	40,40,40,40	0
59	MG	AA	3757	1/1	0.95	0.07	14,14,14,14	0
59	MG	AA	3560	1/1	0.95	0.13	29,29,29,29	0
59	MG	AA	3044	1/1	0.95	0.37	52,52,52,52	0
59	MG	AA	3762	1/1	0.95	0.14	23,23,23,23	0
59	MG	CA	3281	1/1	0.95	0.23	21,21,21,21	0
59	MG	AA	3652	1/1	0.95	0.14	53,53,53,53	0
59	MG	DA	1760	1/1	0.95	0.14	61,61,61,61	0
59	MG	AA	3260	1/1	0.95	0.17	21,21,21,21	0
59	MG	AU	205	1/1	0.95	0.26	45,45,45,45	0
59	MG	DA	1763	1/1	0.95	0.30	76,76,76,76	0
59	MG	DA	1766	1/1	0.95	0.12	74,74,74,74	0
59	MG	BA	1692	1/1	0.95	0.28	55,55,55,55	0
59	MG	AA	3160	1/1	0.95	0.15	30,30,30,30	0
59	MG	CE	305	1/1	0.95	0.04	58,58,58,58	0
59	MG	AA	3574	1/1	0.95	0.17	12,12,12,12	0
59	MG	AW	3003	1/1	0.95	0.25	28,28,28,28	0
59	MG	AA	3290	1/1	0.95	0.13	64,64,64,64	0
59	MG	AA	3137	1/1	0.95	0.63	53,53,53,53	0
59	MG	AA	3658	1/1	0.95	0.21	42,42,42,42	0
59	MG	AA	3112	1/1	0.95	0.14	61,61,61,61	0
59	MG	CA	3303	1/1	0.95	0.35	43,43,43,43	0
59	MG	AA	3021	1/1	0.95	0.13	33,33,33,33	0
59	MG	CA	3305	1/1	0.95	0.27	48,48,48,48	0
59	MG	CA	3144	1/1	0.95	0.23	40,40,40,40	0
59	MG	CU	201	1/1	0.95	0.48	74,74,74,74	0
59	MG	AA	3299	1/1	0.95	0.26	47,47,47,47	0
59	MG	CW	201	1/1	0.95	0.36	46,46,46,46	0
59	MG	AA	3117	1/1	0.95	0.24	25,25,25,25	1
59	MG	CA	3471	1/1	0.96	0.19	33,33,33,33	0
59	MG	AA	3116	1/1	0.96	0.63	35,35,35,35	0
59	MG	AA	3259	1/1	0.96	0.34	41,41,41,41	1
59	MG	AA	3353	1/1	0.96	0.22	39,39,39,39	0
59	MG	AA	3008	1/1	0.96	0.21	26,26,26,26	0
59	MG	AA	3185	1/1	0.96	0.16	76,76,76,76	0
59	MG	AA	3291	1/1	0.96	0.28	45,45,45,45	0
59	MG	AA	3813	1/1	0.96	0.19	29,29,29,29	1
59	MG	AA	3262	1/1	0.96	0.14	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CG	3001	1/1	0.96	0.10	65,65,65,65	0
59	MG	AA	3581	1/1	0.96	0.17	52,52,52,52	0
59	MG	CO	5001	1/1	0.96	0.17	50,50,50,50	0
59	MG	AA	3462	1/1	0.96	0.09	54,54,54,54	0
59	MG	CA	3255	1/1	0.96	0.24	28,28,28,28	0
59	MG	BA	1766	1/1	0.96	0.14	62,62,62,62	0
59	MG	BA	1632	1/1	0.96	0.08	48,48,48,48	0
59	MG	AA	3263	1/1	0.96	0.42	24,24,24,24	1
59	MG	BA	1770	1/1	0.96	0.12	54,54,54,54	0
59	MG	CA	3491	1/1	0.96	0.06	44,44,44,44	0
59	MG	CA	3262	1/1	0.96	0.12	11,11,11,11	0
59	MG	AA	3007	1/1	0.96	0.14	12,12,12,12	0
59	MG	AA	3688	1/1	0.96	0.15	25,25,25,25	0
59	MG	C0	101	1/1	0.96	0.17	59,59,59,59	0
59	MG	AA	3119	1/1	0.96	0.31	47,47,47,47	0
59	MG	AA	3690	1/1	0.96	0.20	50,50,50,50	0
59	MG	AA	3692	1/1	0.96	0.15	36,36,36,36	1
59	MG	AA	3468	1/1	0.96	0.06	55,55,55,55	0
59	MG	AA	3469	1/1	0.96	0.12	32,32,32,32	0
59	MG	CA	3099	1/1	0.96	0.25	58,58,58,58	0
59	MG	AA	3471	1/1	0.96	0.08	56,56,56,56	0
59	MG	AA	3092	1/1	0.96	0.17	39,39,39,39	0
59	MG	CA	3102	1/1	0.96	0.50	62,62,62,62	0
59	MG	CA	3277	1/1	0.96	0.18	55,55,55,55	0
59	MG	AA	3301	1/1	0.96	0.30	39,39,39,39	0
59	MG	CA	3106	1/1	0.96	0.13	66,66,66,66	0
59	MG	AA	3593	1/1	0.96	0.22	15,15,15,15	1
59	MG	AA	3210	1/1	0.96	0.31	59,59,59,59	1
59	MG	AA	3305	1/1	0.96	0.16	25,25,25,25	0
59	MG	AA	3599	1/1	0.96	0.16	59,59,59,59	0
59	MG	AA	3703	1/1	0.96	0.23	56,56,56,56	0
59	MG	CA	3286	1/1	0.96	0.20	58,58,58,58	0
59	MG	AA	3306	1/1	0.96	0.25	52,52,52,52	0
59	MG	AB	3007	1/1	0.96	0.07	39,39,39,39	0
59	MG	CA	3290	1/1	0.96	0.33	34,34,34,34	0
59	MG	AA	3375	1/1	0.96	0.29	48,48,48,48	0
59	MG	CA	3519	1/1	0.96	0.22	48,48,48,48	0
59	MG	BA	1653	1/1	0.96	0.10	56,56,56,56	0
59	MG	AA	3307	1/1	0.96	0.34	61,61,61,61	0
59	MG	CA	3295	1/1	0.96	0.26	66,66,66,66	0
59	MG	AA	3121	1/1	0.96	0.16	53,53,53,53	0
59	MG	AA	3605	1/1	0.96	0.32	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3299	1/1	0.96	0.14	64,64,64,64	0
59	MG	CA	3300	1/1	0.96	0.12	47,47,47,47	0
59	MG	AA	3710	1/1	0.96	0.51	29,29,29,29	1
59	MG	DA	1628	1/1	0.96	0.09	39,39,39,39	0
59	MG	AA	3382	1/1	0.96	0.12	37,37,37,37	0
59	MG	DA	1630	1/1	0.96	0.71	62,62,62,62	0
59	MG	CA	3123	1/1	0.96	0.09	29,29,29,29	0
59	MG	BA	1798	1/1	0.96	0.41	73,73,73,73	0
59	MG	AA	3383	1/1	0.96	0.16	20,20,20,20	0
59	MG	AA	3239	1/1	0.96	0.27	25,25,25,25	1
59	MG	AA	3312	1/1	0.96	0.10	23,23,23,23	0
59	MG	AB	3023	1/1	0.96	0.35	54,54,54,54	0
59	MG	AA	3491	1/1	0.96	0.09	46,46,46,46	0
59	MG	AA	3386	1/1	0.96	0.12	45,45,45,45	0
59	MG	AA	3084	1/1	0.96	0.10	23,23,23,23	0
59	MG	AA	3388	1/1	0.96	0.08	28,28,28,28	0
59	MG	BA	1808	1/1	0.96	0.16	54,54,54,54	0
59	MG	CA	3320	1/1	0.96	0.16	36,36,36,36	0
59	MG	AA	3720	1/1	0.96	0.16	55,55,55,55	0
59	MG	AA	3389	1/1	0.96	0.15	25,25,25,25	0
59	MG	DA	1645	1/1	0.96	0.10	58,58,58,58	0
59	MG	CA	3324	1/1	0.96	0.17	26,26,26,26	0
59	MG	AA	3107	1/1	0.96	0.12	49,49,49,49	0
59	MG	DA	1649	1/1	0.96	0.33	69,69,69,69	0
59	MG	CA	3326	1/1	0.96	0.24	28,28,28,28	0
59	MG	CA	3327	1/1	0.96	0.16	38,38,38,38	0
59	MG	AA	3500	1/1	0.96	0.12	59,59,59,59	0
59	MG	CA	3330	1/1	0.96	0.21	36,36,36,36	0
59	MG	AA	3725	1/1	0.96	0.15	13,13,13,13	0
59	MG	CA	3335	1/1	0.96	0.20	66,66,66,66	0
59	MG	AA	3728	1/1	0.96	0.26	29,29,29,29	0
59	MG	AA	3272	1/1	0.96	0.16	55,55,55,55	0
59	MG	CA	3338	1/1	0.96	0.14	64,64,64,64	0
59	MG	AA	3318	1/1	0.96	0.16	23,23,23,23	0
59	MG	AA	3094	1/1	0.96	0.24	80,80,80,80	0
59	MG	AA	3621	1/1	0.96	0.07	17,17,17,17	0
59	MG	CA	3344	1/1	0.96	0.07	68,68,68,68	0
59	MG	BF	3001	1/1	0.96	0.17	49,49,49,49	0
59	MG	BA	1678	1/1	0.96	0.21	54,54,54,54	0
59	MG	CA	3347	1/1	0.96	0.15	45,45,45,45	0
59	MG	AA	3396	1/1	0.96	0.17	16,16,16,16	0
59	MG	BL	202	1/1	0.96	0.17	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
59	MG	DA	1671	1/1	0.96	0.36	56,56,56,56	0
59	MG	BM	201	1/1	0.96	0.04	62,62,62,62	0
59	MG	AA	3506	1/1	0.96	0.10	48,48,48,48	0
59	MG	CA	3574	1/1	0.96	0.15	37,37,37,37	0
59	MG	BA	1681	1/1	0.96	0.09	53,53,53,53	0
59	MG	CA	3355	1/1	0.96	0.14	35,35,35,35	0
59	MG	AF	304	1/1	0.96	0.29	36,36,36,36	0
59	MG	BT	3001	1/1	0.96	0.12	46,46,46,46	0
59	MG	AA	3507	1/1	0.96	0.15	50,50,50,50	0
59	MG	CA	3360	1/1	0.96	0.17	38,38,38,38	0
59	MG	CA	3362	1/1	0.96	0.12	43,43,43,43	0
59	MG	BA	1684	1/1	0.96	0.27	61,61,61,61	0
59	MG	CA	3366	1/1	0.96	0.16	49,49,49,49	0
59	MG	CA	3584	1/1	0.96	0.15	32,32,32,32	0
59	MG	AA	3399	1/1	0.96	0.15	16,16,16,16	0
59	MG	BZ	701	1/1	0.96	0.19	49,49,49,49	0
59	MG	CA	3160	1/1	0.96	0.39	57,57,57,57	0
59	MG	AA	3742	1/1	0.96	0.12	68,68,68,68	0
59	MG	CA	3162	1/1	0.96	0.39	31,31,31,31	0
59	MG	AA	3322	1/1	0.96	0.20	61,61,61,61	0
59	MG	DA	1693	1/1	0.96	0.14	67,67,67,67	0
59	MG	CA	3004	1/1	0.96	0.14	49,49,49,49	0
59	MG	AA	3403	1/1	0.96	0.34	42,42,42,42	0
59	MG	DA	1696	1/1	0.96	0.17	53,53,53,53	0
59	MG	AN	3002	1/1	0.96	0.45	69,69,69,69	0
59	MG	AA	3511	1/1	0.96	0.20	14,14,14,14	0
59	MG	AA	3404	1/1	0.96	0.20	27,27,27,27	0
59	MG	CA	3381	1/1	0.96	0.14	50,50,50,50	0
59	MG	CA	3010	1/1	0.96	0.19	43,43,43,43	0
59	MG	AP	201	1/1	0.96	0.32	21,21,21,21	1
59	MG	AA	3059	1/1	0.96	0.36	40,40,40,40	0
59	MG	AA	3032	1/1	0.96	0.33	59,59,59,59	0
59	MG	AA	3750	1/1	0.96	0.33	51,51,51,51	0
59	MG	AA	3129	1/1	0.96	0.18	34,34,34,34	1
59	MG	AA	3247	1/1	0.96	0.16	55,55,55,55	0
59	MG	AA	3329	1/1	0.96	0.08	40,40,40,40	1
59	MG	CA	3394	1/1	0.96	0.12	69,69,69,69	0
59	MG	DA	1711	1/1	0.96	0.12	60,60,60,60	0
59	MG	AU	202	1/1	0.96	0.45	82,82,82,82	0
59	MG	DA	1714	1/1	0.96	0.15	68,68,68,68	0
59	MG	AA	3131	1/1	0.96	0.26	63,63,63,63	0
59	MG	DA	1716	1/1	0.96	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AV	202	1/1	0.96	0.23	33,33,33,33	0
59	MG	AA	3758	1/1	0.96	0.28	43,43,43,43	1
59	MG	CA	3611	1/1	0.96	0.15	59,59,59,59	0
59	MG	DA	1720	1/1	0.96	0.10	60,60,60,60	0
59	MG	DA	1721	1/1	0.96	0.09	80,80,80,80	0
59	MG	CA	3028	1/1	0.96	0.63	51,51,51,51	0
59	MG	AA	3529	1/1	0.96	0.20	30,30,30,30	0
59	MG	AA	3042	1/1	0.96	0.24	32,32,32,32	0
59	MG	AA	3531	1/1	0.96	0.13	24,24,24,24	0
59	MG	CA	3617	1/1	0.96	0.13	41,41,41,41	0
59	MG	AA	3532	1/1	0.96	0.20	20,20,20,20	0
59	MG	AA	3423	1/1	0.96	0.20	16,16,16,16	0
59	MG	AA	3113	1/1	0.96	0.32	45,45,45,45	0
59	MG	AA	3537	1/1	0.96	0.17	20,20,20,20	0
59	MG	DA	1731	1/1	0.96	0.09	49,49,49,49	0
59	MG	AA	3538	1/1	0.96	0.15	15,15,15,15	0
59	MG	AA	3647	1/1	0.96	0.11	43,43,43,43	0
59	MG	BA	1715	1/1	0.96	0.11	60,60,60,60	0
59	MG	AA	3426	1/1	0.96	0.17	20,20,20,20	0
59	MG	AA	3336	1/1	0.96	0.14	51,51,51,51	0
59	MG	CA	3418	1/1	0.96	0.29	34,34,34,34	0
59	MG	AA	3114	1/1	0.96	0.21	26,26,26,26	0
59	MG	AA	3546	1/1	0.96	0.14	60,60,60,60	0
59	MG	DA	1740	1/1	0.96	0.57	68,68,68,68	0
59	MG	AA	3547	1/1	0.96	0.26	60,60,60,60	0
59	MG	AA	3201	1/1	0.96	0.09	53,53,53,53	0
59	MG	CA	3047	1/1	0.96	0.16	84,84,84,84	0
59	MG	AA	3435	1/1	0.96	0.17	52,52,52,52	0
59	MG	AA	3550	1/1	0.96	0.20	38,38,38,38	0
59	MG	CA	3637	1/1	0.96	0.47	61,61,61,61	0
59	MG	AA	3340	1/1	0.96	0.22	3,3,3,3	0
59	MG	AA	3341	1/1	0.96	0.19	25,25,25,25	0
59	MG	CA	3054	1/1	0.96	0.25	36,36,36,36	0
59	MG	AA	3343	1/1	0.96	0.10	46,46,46,46	0
59	MG	CA	3439	1/1	0.96	0.23	32,32,32,32	0
59	MG	AA	3228	1/1	0.96	0.30	32,32,32,32	0
59	MG	CA	3218	1/1	0.96	0.36	40,40,40,40	0
59	MG	AA	3029	1/1	0.96	0.24	28,28,28,28	0
59	MG	BA	1606	1/1	0.96	0.28	126,126,126,126	0
59	MG	AA	3136	1/1	0.96	0.64	63,63,63,63	0
59	MG	AA	3564	1/1	0.96	0.20	44,44,44,44	0
59	MG	AA	3791	1/1	0.96	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3062	1/1	0.96	0.29	38,38,38,38	0
59	MG	AA	3566	1/1	0.96	0.05	56,56,56,56	0
59	MG	CA	3659	1/1	0.96	0.10	55,55,55,55	0
59	MG	CA	3232	1/1	0.96	0.17	54,54,54,54	0
59	MG	DA	1764	1/1	0.96	0.08	71,71,71,71	0
59	MG	DA	1765	1/1	0.96	0.13	64,64,64,64	0
59	MG	AA	3668	1/1	0.96	0.17	54,54,54,54	0
59	MG	CA	3662	1/1	0.96	0.32	33,33,33,33	0
59	MG	AA	3567	1/1	0.96	0.11	26,26,26,26	0
59	MG	AA	3670	1/1	0.96	0.08	54,54,54,54	0
59	MG	AA	3568	1/1	0.96	0.18	15,15,15,15	0
59	MG	BA	1615	1/1	0.96	0.28	62,62,62,62	0
59	MG	DD	502	1/1	0.96	0.48	50,50,50,50	0
59	MG	AA	3798	1/1	0.96	0.22	25,25,25,25	0
59	MG	CA	3461	1/1	0.96	0.15	34,34,34,34	0
59	MG	AA	3570	1/1	0.96	0.15	14,14,14,14	0
59	MG	CB	3006	1/1	0.96	0.06	71,71,71,71	0
59	MG	AA	3802	1/1	0.96	0.15	86,86,86,86	0
59	MG	CA	3464	1/1	0.96	0.18	36,36,36,36	0
59	MG	CB	3010	1/1	0.96	0.13	51,51,51,51	0
59	MG	AA	3349	1/1	0.96	0.17	47,47,47,47	0
59	MG	CA	3074	1/1	0.96	0.33	49,49,49,49	0
59	MG	DZ	702	1/1	0.96	0.22	57,57,57,57	0
59	MG	AA	3350	1/1	0.96	0.08	36,36,36,36	0
59	MG	CD	301	1/1	0.96	0.44	43,43,43,43	0
59	MG	AA	3805	1/1	0.96	0.21	58,58,58,58	0
60	ZN	DN	501	1/1	0.96	0.08	117,117,117,117	0
62	GDP	DZ	703	28/28	0.96	0.14	66,66,66,66	1
59	MG	AA	3159	1/1	0.97	0.27	55,55,55,55	0
59	MG	CA	3053	1/1	0.97	0.45	32,32,32,32	0
59	MG	BA	1761	1/1	0.97	0.16	62,62,62,62	0
59	MG	BA	1762	1/1	0.97	0.06	74,74,74,74	0
59	MG	CA	3351	1/1	0.97	0.14	46,46,46,46	0
59	MG	CA	3537	1/1	0.97	0.30	59,59,59,59	0
59	MG	AA	3515	1/1	0.97	0.22	12,12,12,12	0
59	MG	AA	3453	1/1	0.97	0.23	39,39,39,39	0
59	MG	AA	3517	1/1	0.97	0.07	23,23,23,23	0
59	MG	AA	3100	1/1	0.97	0.24	29,29,29,29	0
59	MG	AA	3598	1/1	0.97	0.24	51,51,51,51	0
59	MG	BA	1769	1/1	0.97	0.10	58,58,58,58	0
59	MG	AA	3770	1/1	0.97	0.12	43,43,43,43	0
59	MG	AA	3519	1/1	0.97	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
59	MG	CA	3197	1/1	0.97	0.40	45,45,45,45	0
59	MG	CA	3364	1/1	0.97	0.10	22,22,22,22	0
59	MG	CA	3365	1/1	0.97	0.19	55,55,55,55	0
59	MG	CA	3064	1/1	0.97	0.09	48,48,48,48	0
59	MG	AA	3355	1/1	0.97	0.16	57,57,57,57	0
59	MG	BA	1773	1/1	0.97	0.13	40,40,40,40	0
59	MG	AG	201	1/1	0.97	0.07	38,38,38,38	0
59	MG	AA	3395	1/1	0.97	0.17	54,54,54,54	0
59	MG	CA	3554	1/1	0.97	0.09	66,66,66,66	0
59	MG	AA	3459	1/1	0.97	0.20	53,53,53,53	0
59	MG	CA	3556	1/1	0.97	0.18	62,62,62,62	0
59	MG	BA	1777	1/1	0.97	0.29	71,71,71,71	0
59	MG	AA	3524	1/1	0.97	0.19	41,41,41,41	0
59	MG	AA	3779	1/1	0.97	0.12	22,22,22,22	0
59	MG	AA	3681	1/1	0.97	0.13	42,42,42,42	0
59	MG	AA	3682	1/1	0.97	0.17	31,31,31,31	0
59	MG	CA	3211	1/1	0.97	0.09	29,29,29,29	0
59	MG	AA	3525	1/1	0.97	0.18	35,35,35,35	0
59	MG	CA	3564	1/1	0.97	0.13	80,80,80,80	0
59	MG	AA	3527	1/1	0.97	0.16	27,27,27,27	0
59	MG	CA	3386	1/1	0.97	0.20	50,50,50,50	0
59	MG	AA	3460	1/1	0.97	0.14	27,27,27,27	0
59	MG	BA	1785	1/1	0.97	0.17	62,62,62,62	0
59	MG	CA	3571	1/1	0.97	0.26	45,45,45,45	0
59	MG	CA	3217	1/1	0.97	0.26	62,62,62,62	0
59	MG	AQ	201	1/1	0.97	0.44	48,48,48,48	0
59	MG	CA	3219	1/1	0.97	0.25	42,42,42,42	0
59	MG	CA	3220	1/1	0.97	0.07	59,59,59,59	0
59	MG	AA	3054	1/1	0.97	0.17	21,21,21,21	0
59	MG	AA	3397	1/1	0.97	0.13	13,13,13,13	0
59	MG	AA	3463	1/1	0.97	0.16	15,15,15,15	0
59	MG	AA	3398	1/1	0.97	0.22	31,31,31,31	0
59	MG	AU	201	1/1	0.97	0.19	25,25,25,25	0
59	MG	AA	3534	1/1	0.97	0.19	14,14,14,14	0
59	MG	AU	203	1/1	0.97	0.21	31,31,31,31	0
59	MG	DA	1657	1/1	0.97	0.10	23,23,23,23	0
59	MG	CA	3230	1/1	0.97	0.33	49,49,49,49	0
59	MG	CA	3231	1/1	0.97	0.72	60,60,60,60	0
59	MG	CA	3404	1/1	0.97	0.16	65,65,65,65	0
59	MG	AU	204	1/1	0.97	0.38	25,25,25,25	0
59	MG	CA	3407	1/1	0.97	0.19	36,36,36,36	0
59	MG	AA	3691	1/1	0.97	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	AA	3613	1/1	0.97	0.17	48,48,48,48	0
59	MG	AA	3535	1/1	0.97	0.13	48,48,48,48	0
59	MG	AA	3111	1/1	0.97	0.23	24,24,24,24	0
59	MG	AA	3144	1/1	0.97	0.35	50,50,50,50	0
59	MG	AA	3145	1/1	0.97	0.29	44,44,44,44	0
59	MG	AA	3539	1/1	0.97	0.14	34,34,34,34	0
59	MG	AA	3360	1/1	0.97	0.23	22,22,22,22	0
59	MG	AA	3406	1/1	0.97	0.09	20,20,20,20	0
59	MG	BA	1804	1/1	0.97	0.10	45,45,45,45	0
59	MG	AA	3543	1/1	0.97	0.22	32,32,32,32	0
59	MG	AA	3326	1/1	0.97	0.09	36,36,36,36	1
59	MG	DA	1676	1/1	0.97	0.15	74,74,74,74	0
59	MG	AA	3623	1/1	0.97	0.17	28,28,28,28	0
59	MG	CA	3422	1/1	0.97	0.24	43,43,43,43	0
59	MG	CA	3424	1/1	0.97	0.19	66,66,66,66	0
59	MG	CA	3425	1/1	0.97	0.12	50,50,50,50	0
59	MG	AA	3473	1/1	0.97	0.07	53,53,53,53	0
59	MG	CA	3103	1/1	0.97	0.19	53,53,53,53	0
59	MG	AA	3147	1/1	0.97	0.52	40,40,40,40	1
59	MG	CA	3105	1/1	0.97	0.25	39,39,39,39	0
59	MG	AA	3298	1/1	0.97	0.15	58,58,58,58	0
59	MG	AA	3366	1/1	0.97	0.23	35,35,35,35	1
59	MG	AA	3214	1/1	0.97	0.81	58,58,58,58	1
59	MG	CA	3109	1/1	0.97	0.22	35,35,35,35	0
59	MG	CA	3437	1/1	0.97	0.18	64,64,64,64	0
59	MG	AA	3811	1/1	0.97	0.15	56,56,56,56	0
59	MG	AA	3369	1/1	0.97	0.12	47,47,47,47	0
59	MG	AA	3552	1/1	0.97	0.18	63,63,63,63	0
59	MG	BA	1702	1/1	0.97	0.19	46,46,46,46	0
59	MG	AA	3554	1/1	0.97	0.19	40,40,40,40	0
59	MG	AA	3815	1/1	0.97	0.17	30,30,30,30	0
59	MG	CA	3447	1/1	0.97	0.25	73,73,73,73	0
59	MG	AA	3713	1/1	0.97	0.22	27,27,27,27	0
59	MG	CA	3449	1/1	0.97	0.07	55,55,55,55	0
59	MG	AA	3419	1/1	0.97	0.17	20,20,20,20	0
59	MG	AA	3049	1/1	0.97	0.18	35,35,35,35	0
59	MG	CA	3627	1/1	0.97	0.19	60,60,60,60	0
59	MG	CA	3119	1/1	0.97	0.54	55,55,55,55	0
59	MG	AA	3422	1/1	0.97	0.18	23,23,23,23	0
59	MG	AA	3216	1/1	0.97	0.60	38,38,38,38	0
59	MG	AA	3821	1/1	0.97	0.19	38,38,38,38	0
59	MG	AA	3559	1/1	0.97	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3272	1/1	0.97	0.32	49,49,49,49	0
59	MG	AA	3424	1/1	0.97	0.18	14,14,14,14	0
59	MG	AA	3639	1/1	0.97	0.13	18,18,18,18	0
59	MG	AA	3721	1/1	0.97	0.20	40,40,40,40	0
59	MG	AA	3562	1/1	0.97	0.09	56,56,56,56	0
59	MG	AA	3563	1/1	0.97	0.21	34,34,34,34	0
59	MG	AA	3489	1/1	0.97	0.18	15,15,15,15	0
59	MG	CA	3641	1/1	0.97	0.21	46,46,46,46	0
59	MG	AA	3565	1/1	0.97	0.21	44,44,44,44	0
59	MG	CA	3002	1/1	0.97	0.23	28,28,28,28	0
59	MG	CA	3468	1/1	0.97	0.06	53,53,53,53	0
59	MG	AA	3830	1/1	0.97	0.27	47,47,47,47	0
59	MG	CA	3133	1/1	0.97	0.20	85,85,85,85	0
59	MG	AA	3334	1/1	0.97	0.14	63,63,63,63	0
59	MG	AA	3730	1/1	0.97	0.17	75,75,75,75	0
59	MG	CA	3136	1/1	0.97	0.10	63,63,63,63	0
59	MG	CA	3652	1/1	0.97	0.13	23,23,23,23	0
59	MG	CA	3653	1/1	0.97	0.20	32,32,32,32	0
59	MG	CA	3006	1/1	0.97	0.08	22,22,22,22	0
59	MG	CA	3475	1/1	0.97	0.25	50,50,50,50	0
59	MG	CA	3138	1/1	0.97	0.04	86,86,86,86	0
59	MG	CA	3657	1/1	0.97	0.39	41,41,41,41	0
59	MG	AA	3073	1/1	0.97	0.14	31,31,31,31	0
59	MG	AA	3074	1/1	0.97	0.29	14,14,14,14	0
59	MG	BA	1725	1/1	0.97	0.24	54,54,54,54	0
59	MG	AA	3428	1/1	0.97	0.19	18,18,18,18	0
59	MG	CA	3482	1/1	0.97	0.17	61,61,61,61	0
59	MG	CA	3011	1/1	0.97	0.38	63,63,63,63	0
59	MG	AB	3005	1/1	0.97	0.20	44,44,44,44	0
59	MG	CA	3297	1/1	0.97	0.34	36,36,36,36	0
59	MG	AA	3075	1/1	0.97	0.28	49,49,49,49	0
59	MG	CA	3487	1/1	0.97	0.20	60,60,60,60	0
59	MG	AA	3430	1/1	0.97	0.16	39,39,39,39	0
59	MG	AA	3650	1/1	0.97	0.11	49,49,49,49	0
59	MG	CA	3017	1/1	0.97	0.14	30,30,30,30	0
59	MG	AA	3496	1/1	0.97	0.36	31,31,31,31	0
59	MG	CA	3019	1/1	0.97	0.11	22,22,22,22	0
59	MG	CB	3009	1/1	0.97	0.18	67,67,67,67	0
59	MG	AA	3497	1/1	0.97	0.13	44,44,44,44	0
59	MG	AB	3011	1/1	0.97	0.16	29,29,29,29	0
59	MG	CA	3309	1/1	0.97	0.24	22,22,22,22	0
59	MG	AA	3125	1/1	0.97	0.16	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3497	1/1	0.97	0.09	45,45,45,45	0
59	MG	CA	3498	1/1	0.97	0.12	49,49,49,49	0
59	MG	BA	1735	1/1	0.97	0.20	41,41,41,41	0
59	MG	AB	3015	1/1	0.97	0.14	28,28,28,28	0
59	MG	AB	3016	1/1	0.97	0.14	34,34,34,34	0
59	MG	CE	302	1/1	0.97	0.13	64,64,64,64	0
59	MG	CA	3315	1/1	0.97	0.13	47,47,47,47	0
59	MG	CA	3027	1/1	0.97	0.06	31,31,31,31	0
59	MG	AA	3379	1/1	0.97	0.26	23,23,23,23	0
59	MG	AA	3222	1/1	0.97	0.17	4,4,4,4	0
59	MG	AB	3019	1/1	0.97	0.12	70,70,70,70	0
59	MG	AA	3578	1/1	0.97	0.13	28,28,28,28	0
59	MG	CF	304	1/1	0.97	0.13	65,65,65,65	0
59	MG	BA	1743	1/1	0.97	0.06	41,41,41,41	0
59	MG	CA	3163	1/1	0.97	0.30	30,30,30,30	0
59	MG	AA	3342	1/1	0.97	0.23	51,51,51,51	0
59	MG	AA	3442	1/1	0.97	0.14	23,23,23,23	0
59	MG	AA	3309	1/1	0.97	0.25	46,46,46,46	0
59	MG	BA	1747	1/1	0.97	0.19	65,65,65,65	0
59	MG	AA	3283	1/1	0.97	0.33	43,43,43,43	0
59	MG	AA	3223	1/1	0.97	0.11	15,15,15,15	0
59	MG	CA	3332	1/1	0.97	0.24	29,29,29,29	0
59	MG	AA	3098	1/1	0.97	0.27	51,51,51,51	0
59	MG	CA	3334	1/1	0.97	0.21	47,47,47,47	0
59	MG	BA	1751	1/1	0.97	0.12	48,48,48,48	0
59	MG	BA	1752	1/1	0.97	0.27	59,59,59,59	0
59	MG	AA	3755	1/1	0.97	0.64	78,78,78,78	0
59	MG	CA	3175	1/1	0.97	0.19	31,31,31,31	0
59	MG	CA	3339	1/1	0.97	0.14	24,24,24,24	0
59	MG	AA	3127	1/1	0.97	0.34	57,57,57,57	0
59	MG	AA	3665	1/1	0.97	0.30	40,40,40,40	0
59	MG	C8	5001	1/1	0.97	0.34	37,37,37,37	0
59	MG	AA	3666	1/1	0.97	0.14	41,41,41,41	0
60	ZN	CY	501	1/1	0.97	0.06	101,101,101,101	0
59	MG	AA	3060	1/1	0.97	0.32	20,20,20,20	0
60	ZN	C5	102	1/1	0.97	0.10	66,66,66,66	0
60	ZN	C6	501	1/1	0.97	0.10	66,66,66,66	0
59	MG	AA	3390	1/1	0.97	0.16	23,23,23,23	0
62	GDP	BZ	702	28/28	0.97	0.12	57,57,57,57	0
59	MG	AA	3317	1/1	0.97	0.16	24,24,24,24	0
59	MG	DA	1651	1/1	0.98	0.11	63,63,63,63	0
59	MG	CA	3361	1/1	0.98	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	DA	1653	1/1	0.98	0.30	55,55,55,55	0
59	MG	AA	3316	1/1	0.98	0.23	36,36,36,36	0
59	MG	AA	3182	1/1	0.98	0.22	46,46,46,46	0
59	MG	AA	3421	1/1	0.98	0.21	28,28,28,28	0
59	MG	AA	3523	1/1	0.98	0.16	13,13,13,13	0
59	MG	AA	3381	1/1	0.98	0.16	16,16,16,16	0
59	MG	AA	3470	1/1	0.98	0.08	39,39,39,39	0
59	MG	AE	303	1/1	0.98	0.21	19,19,19,19	0
59	MG	CA	3369	1/1	0.98	0.14	48,48,48,48	0
59	MG	AA	3294	1/1	0.98	0.17	37,37,37,37	0
59	MG	AA	3789	1/1	0.98	0.21	44,44,44,44	0
59	MG	AA	3585	1/1	0.98	0.17	35,35,35,35	0
59	MG	AA	3528	1/1	0.98	0.16	19,19,19,19	0
59	MG	CA	3258	1/1	0.98	0.36	51,51,51,51	0
59	MG	BA	1722	1/1	0.98	0.29	51,51,51,51	0
59	MG	CA	3640	1/1	0.98	0.28	43,43,43,43	0
59	MG	AF	303	1/1	0.98	0.20	19,19,19,19	0
59	MG	AA	3587	1/1	0.98	0.14	28,28,28,28	0
59	MG	BA	1640	1/1	0.98	0.44	52,52,52,52	0
59	MG	AA	3793	1/1	0.98	0.22	7,7,7,7	0
59	MG	DA	1673	1/1	0.98	0.13	82,82,82,82	0
59	MG	CA	3382	1/1	0.98	0.22	38,38,38,38	0
59	MG	CA	3383	1/1	0.98	0.20	30,30,30,30	0
59	MG	CA	3384	1/1	0.98	0.11	55,55,55,55	0
59	MG	CA	3648	1/1	0.98	0.34	52,52,52,52	0
59	MG	AA	3037	1/1	0.98	0.11	4,4,4,4	0
59	MG	CA	3650	1/1	0.98	0.25	14,14,14,14	0
59	MG	CA	3266	1/1	0.98	0.15	36,36,36,36	0
59	MG	CA	3267	1/1	0.98	0.13	38,38,38,38	0
59	MG	AA	3320	1/1	0.98	0.13	37,37,37,37	0
59	MG	AA	3082	1/1	0.98	0.27	60,60,60,60	0
59	MG	AA	3243	1/1	0.98	0.23	43,43,43,43	0
59	MG	AA	3020	1/1	0.98	0.18	11,11,11,11	0
59	MG	CA	3169	1/1	0.98	0.21	34,34,34,34	0
59	MG	AA	3130	1/1	0.98	0.23	34,34,34,34	0
59	MG	CA	3523	1/1	0.98	0.14	37,37,37,37	0
59	MG	AA	3097	1/1	0.98	0.20	22,22,22,22	0
59	MG	CA	3525	1/1	0.98	0.28	23,23,23,23	0
59	MG	AA	3595	1/1	0.98	0.15	42,42,42,42	0
59	MG	AA	3302	1/1	0.98	0.06	51,51,51,51	0
59	MG	AA	3597	1/1	0.98	0.11	33,33,33,33	0
59	MG	AA	3432	1/1	0.98	0.23	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
59	MG	AA	3727	1/1	0.98	0.14	23,23,23,23	0
59	MG	CA	3400	1/1	0.98	0.13	57,57,57,57	0
59	MG	DA	1697	1/1	0.98	0.17	48,48,48,48	0
59	MG	CA	3401	1/1	0.98	0.22	28,28,28,28	0
59	MG	AA	3484	1/1	0.98	0.11	53,53,53,53	0
59	MG	BA	1740	1/1	0.98	0.30	50,50,50,50	0
59	MG	CA	3179	1/1	0.98	0.32	60,60,60,60	0
59	MG	CA	3405	1/1	0.98	0.10	55,55,55,55	0
59	MG	AA	3729	1/1	0.98	0.20	41,41,41,41	0
59	MG	AA	3600	1/1	0.98	0.15	25,25,25,25	0
59	MG	AA	3663	1/1	0.98	0.19	11,11,11,11	0
59	MG	CA	3287	1/1	0.98	0.22	45,45,45,45	0
59	MG	AA	3433	1/1	0.98	0.14	37,37,37,37	0
59	MG	AA	3434	1/1	0.98	0.06	17,17,17,17	0
59	MG	AA	3734	1/1	0.98	0.24	26,26,26,26	0
59	MG	AA	3152	1/1	0.98	0.24	10,10,10,10	0
59	MG	CA	3292	1/1	0.98	0.09	12,12,12,12	0
59	MG	CA	3415	1/1	0.98	0.26	34,34,34,34	0
59	MG	AA	3488	1/1	0.98	0.18	36,36,36,36	0
59	MG	AA	3436	1/1	0.98	0.17	12,12,12,12	0
59	MG	AA	3545	1/1	0.98	0.19	43,43,43,43	0
59	MG	AA	3437	1/1	0.98	0.18	17,17,17,17	0
59	MG	AA	3439	1/1	0.98	0.28	37,37,37,37	0
59	MG	AA	3072	1/1	0.98	0.08	19,19,19,19	0
59	MG	AA	3250	1/1	0.98	0.18	123,123,123,123	0
59	MG	CA	3195	1/1	0.98	0.31	47,47,47,47	0
59	MG	AA	3332	1/1	0.98	0.18	17,17,17,17	0
59	MG	CA	3302	1/1	0.98	0.28	37,37,37,37	0
59	MG	CA	3427	1/1	0.98	0.19	37,37,37,37	0
59	MG	AA	3362	1/1	0.98	0.16	46,46,46,46	0
59	MG	AA	3165	1/1	0.98	0.16	52,52,52,52	0
59	MG	AA	3553	1/1	0.98	0.05	43,43,43,43	0
59	MG	CA	3306	1/1	0.98	0.08	24,24,24,24	0
59	MG	AA	3154	1/1	0.98	0.18	57,57,57,57	0
59	MG	CA	3308	1/1	0.98	0.10	39,39,39,39	0
59	MG	CA	3435	1/1	0.98	0.11	55,55,55,55	0
59	MG	AA	3498	1/1	0.98	0.24	47,47,47,47	0
59	MG	CV	202	1/1	0.98	0.21	38,38,38,38	0
59	MG	AA	3752	1/1	0.98	0.12	42,42,42,42	0
59	MG	CA	3567	1/1	0.98	0.22	26,26,26,26	0
59	MG	CA	3438	1/1	0.98	0.14	24,24,24,24	0
59	MG	AA	3753	1/1	0.98	0.15	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
59	MG	BA	1677	1/1	0.98	0.17	28,28,28,28	0
59	MG	AA	3831	1/1	0.98	0.20	37,37,37,37	0
59	MG	CA	3206	1/1	0.98	0.40	44,44,44,44	0
59	MG	CA	3443	1/1	0.98	0.18	28,28,28,28	0
59	MG	BA	1765	1/1	0.98	0.23	54,54,54,54	0
59	MG	AA	3335	1/1	0.98	0.24	15,15,15,15	0
59	MG	CA	3446	1/1	0.98	0.18	33,33,33,33	0
59	MG	CA	3209	1/1	0.98	0.13	73,73,73,73	0
59	MG	AA	3220	1/1	0.98	0.15	62,62,62,62	0
59	MG	AA	3368	1/1	0.98	0.24	49,49,49,49	0
59	MG	CA	3025	1/1	0.98	0.39	59,59,59,59	0
59	MG	AA	3192	1/1	0.98	0.23	30,30,30,30	0
59	MG	CA	3214	1/1	0.98	0.11	22,22,22,22	0
59	MG	AA	3338	1/1	0.98	0.08	28,28,28,28	0
59	MG	AA	3561	1/1	0.98	0.20	21,21,21,21	0
59	MG	AA	3760	1/1	0.98	0.37	55,55,55,55	0
59	MG	BA	1686	1/1	0.98	0.15	36,36,36,36	0
59	MG	CA	3329	1/1	0.98	0.14	21,21,21,21	0
59	MG	AA	3311	1/1	0.98	0.14	2,2,2,2	0
59	MG	CA	3459	1/1	0.98	0.09	28,28,28,28	0
59	MG	CA	3331	1/1	0.98	0.26	52,52,52,52	0
59	MG	CA	3592	1/1	0.98	0.14	64,64,64,64	0
59	MG	AA	3505	1/1	0.98	0.15	30,30,30,30	0
59	MG	AA	3452	1/1	0.98	0.14	14,14,14,14	0
59	MG	AA	3407	1/1	0.98	0.20	10,10,10,10	0
59	MG	AA	3765	1/1	0.98	0.38	60,60,60,60	0
59	MG	AB	3012	1/1	0.98	0.15	23,23,23,23	1
59	MG	CA	3466	1/1	0.98	0.40	56,56,56,56	0
59	MG	AA	3372	1/1	0.98	0.23	37,37,37,37	0
59	MG	AB	3014	1/1	0.98	0.11	56,56,56,56	0
59	MG	CA	3228	1/1	0.98	0.36	59,59,59,59	0
59	MG	CA	3039	1/1	0.98	0.28	37,37,37,37	0
59	MG	AA	3091	1/1	0.98	0.75	47,47,47,47	1
59	MG	CA	3342	1/1	0.98	0.11	33,33,33,33	0
59	MG	AA	3411	1/1	0.98	0.14	12,12,12,12	0
59	MG	AA	3569	1/1	0.98	0.22	17,17,17,17	0
59	MG	AA	3631	1/1	0.98	0.18	46,46,46,46	0
59	MG	AA	3457	1/1	0.98	0.13	30,30,30,30	0
59	MG	CA	3045	1/1	0.98	0.17	60,60,60,60	0
59	MG	AA	3412	1/1	0.98	0.20	39,39,39,39	0
59	MG	DW	501	1/1	0.98	0.17	44,44,44,44	0
59	MG	AA	3023	1/1	0.98	0.62	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3774	1/1	0.98	0.35	25,25,25,25	1
59	MG	CA	3613	1/1	0.98	0.22	57,57,57,57	0
59	MG	CA	3049	1/1	0.98	0.36	46,46,46,46	0
59	MG	AA	3003	1/1	0.98	0.06	8,8,8,8	0
59	MG	CA	3353	1/1	0.98	0.22	45,45,45,45	0
59	MG	AA	3416	1/1	0.98	0.14	14,14,14,14	0
59	MG	AA	3777	1/1	0.98	0.12	41,41,41,41	0
59	MG	AA	3778	1/1	0.98	0.14	43,43,43,43	0
59	MG	AA	3292	1/1	0.98	0.20	24,24,24,24	0
60	ZN	C9	501	1/1	0.98	0.09	75,75,75,75	0
59	MG	CA	3358	1/1	0.98	0.29	36,36,36,36	0
61	SF4	BD	501	8/8	0.98	0.10	78,78,78,78	0
61	SF4	DD	501	8/8	0.98	0.11	82,82,82,82	1
59	MG	AA	3377	1/1	0.98	0.06	20,20,20,20	0
59	MG	AA	3465	1/1	0.98	0.20	42,42,42,42	0
59	MG	AA	3438	1/1	0.99	0.15	17,17,17,17	0
59	MG	CA	3372	1/1	0.99	0.18	35,35,35,35	0
59	MG	AA	3380	1/1	0.99	0.12	18,18,18,18	0
59	MG	CA	3423	1/1	0.99	0.23	46,46,46,46	0
59	MG	AA	3248	1/1	0.99	0.14	22,22,22,22	0
59	MG	AA	3146	1/1	0.99	0.08	29,29,29,29	0
59	MG	DA	1745	1/1	0.99	0.38	50,50,50,50	0
59	MG	AA	3328	1/1	0.99	0.16	42,42,42,42	0
59	MG	CA	3282	1/1	0.99	0.18	36,36,36,36	0
59	MG	CA	3479	1/1	0.99	0.17	50,50,50,50	0
59	MG	AA	3053	1/1	0.99	0.18	19,19,19,19	0
59	MG	AA	3401	1/1	0.99	0.14	21,21,21,21	0
59	MG	CA	3380	1/1	0.99	0.21	59,59,59,59	0
59	MG	AA	3726	1/1	0.99	0.16	12,12,12,12	0
59	MG	AA	3402	1/1	0.99	0.13	27,27,27,27	0
59	MG	CA	3433	1/1	0.99	0.12	82,82,82,82	0
59	MG	AA	3354	1/1	0.99	0.12	27,27,27,27	0
59	MG	AA	3799	1/1	0.99	0.33	42,42,42,42	0
59	MG	AA	3103	1/1	0.99	0.03	5,5,5,5	0
59	MG	AA	3801	1/1	0.99	0.15	27,27,27,27	0
59	MG	AA	3405	1/1	0.99	0.27	44,44,44,44	0
59	MG	DA	1648	1/1	0.99	0.12	40,40,40,40	0
59	MG	AA	3076	1/1	0.99	0.13	0,0,0,0	0
59	MG	AA	3526	1/1	0.99	0.20	19,19,19,19	0
59	MG	AA	3321	1/1	0.99	0.10	61,61,61,61	0
59	MG	AA	3702	1/1	0.99	0.20	14,14,14,14	0
59	MG	AA	3735	1/1	0.99	0.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3085	1/1	0.99	0.16	25,25,25,25	0
59	MG	AA	3303	1/1	0.99	0.15	24,24,24,24	0
59	MG	AA	3475	1/1	0.99	0.25	45,45,45,45	0
59	MG	DA	1712	1/1	0.99	0.33	53,53,53,53	0
59	MG	AA	3345	1/1	0.99	0.13	6,6,6,6	0
59	MG	AA	3477	1/1	0.99	0.18	14,14,14,14	0
59	MG	AA	3410	1/1	0.99	0.14	57,57,57,57	0
59	MG	AA	3741	1/1	0.99	0.10	21,21,21,21	0
59	MG	AA	3346	1/1	0.99	0.13	59,59,59,59	0
59	MG	AA	3709	1/1	0.99	0.42	23,23,23,23	1
59	MG	CA	3261	1/1	0.99	0.16	47,47,47,47	0
59	MG	BA	1688	1/1	0.99	0.43	61,61,61,61	0
59	MG	AA	3011	1/1	0.99	0.08	16,16,16,16	0
59	MG	CA	3015	1/1	0.99	0.28	51,51,51,51	0
59	MG	AA	3745	1/1	0.99	0.18	68,68,68,68	0
59	MG	CA	3311	1/1	0.99	0.14	50,50,50,50	0
59	MG	AA	3151	1/1	0.99	0.23	62,62,62,62	0
59	MG	CA	3181	1/1	0.99	0.16	40,40,40,40	0
60	ZN	AY	501	1/1	0.99	0.09	61,61,61,61	0
59	MG	CA	3618	1/1	0.99	0.30	40,40,40,40	0
60	ZN	A5	501	1/1	0.99	0.13	30,30,30,30	0
60	ZN	A6	102	1/1	0.99	0.12	40,40,40,40	0
59	MG	AA	3482	1/1	0.99	0.11	41,41,41,41	0
59	MG	AA	3297	1/1	0.99	0.23	27,27,27,27	0
59	MG	AA	3458	1/1	0.99	0.09	40,40,40,40	0
59	MG	CA	3227	1/1	0.99	0.22	41,41,41,41	0
59	MG	AA	3415	1/1	0.99	0.23	62,62,62,62	0
59	MG	CA	3570	1/1	0.99	0.12	36,36,36,36	0
59	MG	AV	201	1/1	0.99	0.25	42,42,42,42	0
59	MG	AA	3540	1/1	0.99	0.09	36,36,36,36	0
59	MG	AA	3512	1/1	0.99	0.15	38,38,38,38	0
59	MG	CA	3322	1/1	0.99	0.26	40,40,40,40	0
59	MG	AA	3364	1/1	0.99	0.18	23,23,23,23	0
60	ZN	A9	501	1/1	1.00	0.12	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.