wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 07:09 PM EST

PDB ID	:	4WQY
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with elongation factor G in the post-translocational state (without fusitic acid)
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:

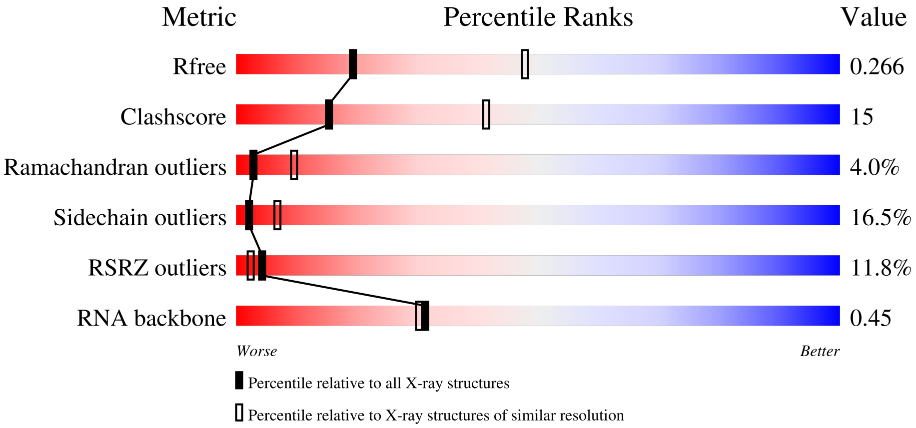
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

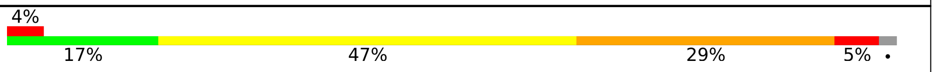
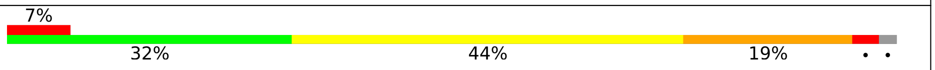
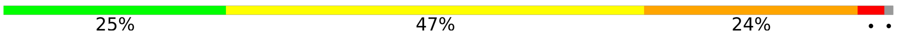
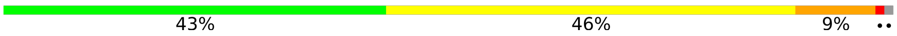
The reported resolution of this entry is 2.80 Å.

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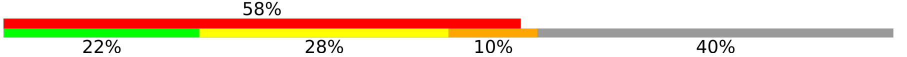
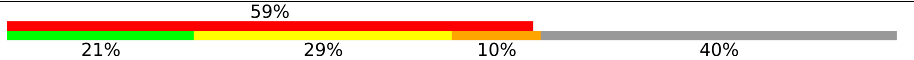
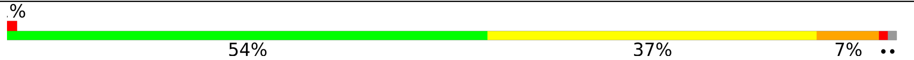
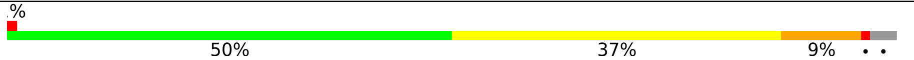
Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
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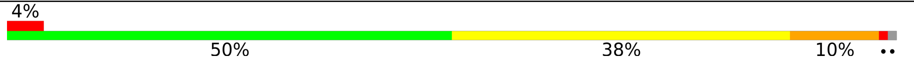
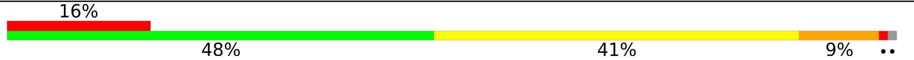
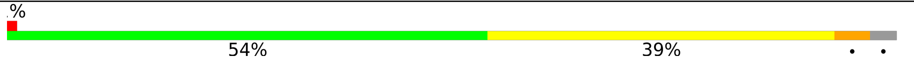
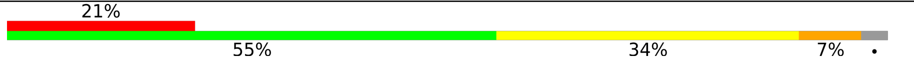
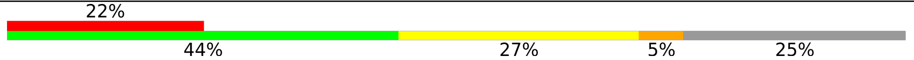
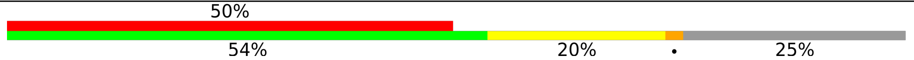
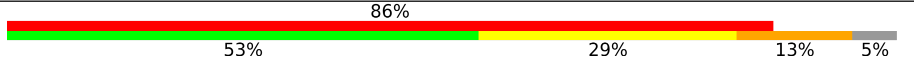
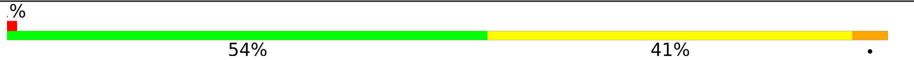
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
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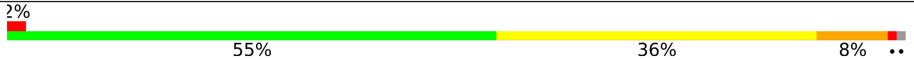
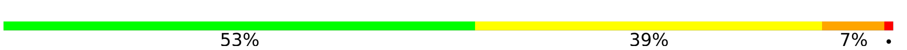
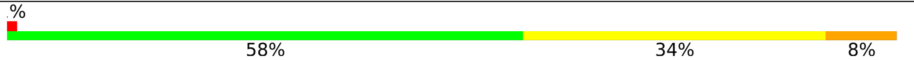
12	CO	122	
13	AP	150	
13	CP	150	
14	AQ	141	
14	CQ	141	
15	AR	118	

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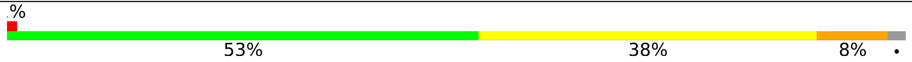
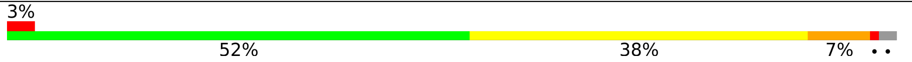
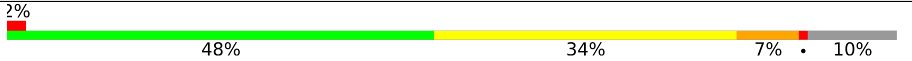
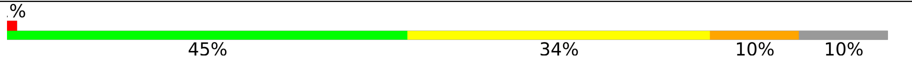
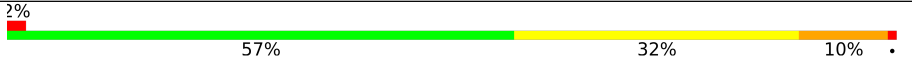
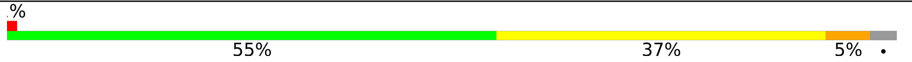
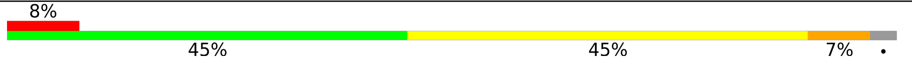
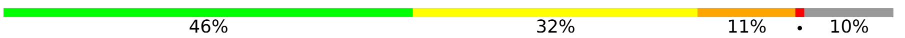
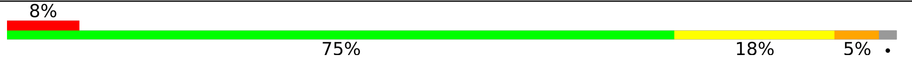
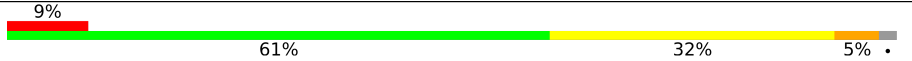
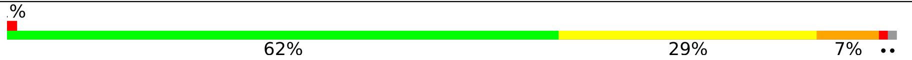
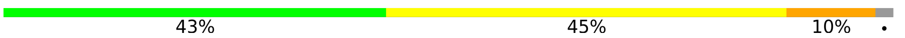
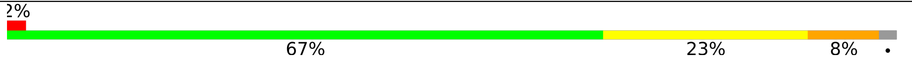
Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
25	C1	98	
26	A2	72	
26	C2	72	
27	A3	60	
27	C3	60	

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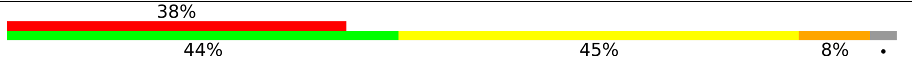
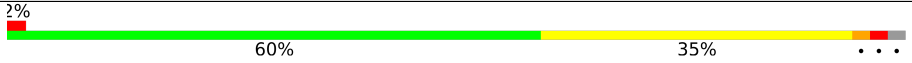
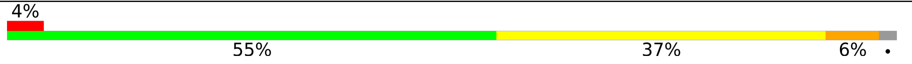
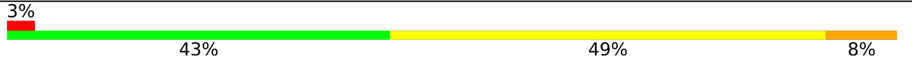
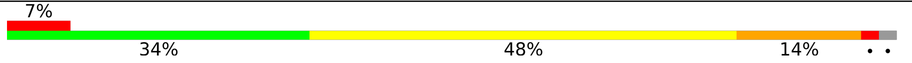
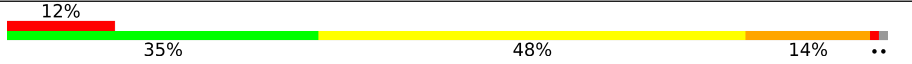
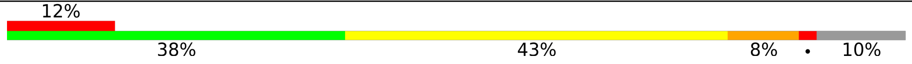
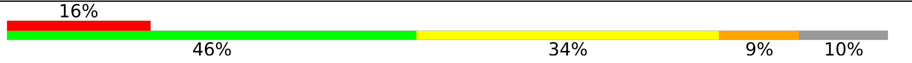
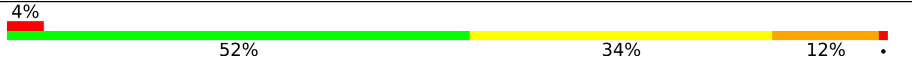
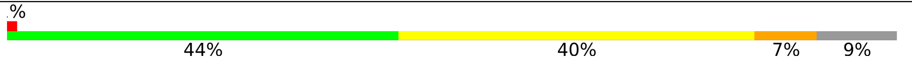
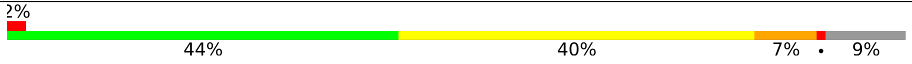
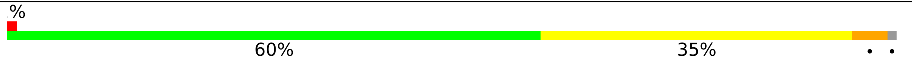
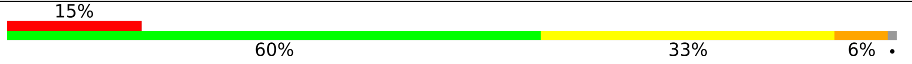
Mol	Chain	Length	Quality of chain
28	A4	71	
28	C4	71	
29	A5	60	
29	C5	60	
30	A6	54	
30	C6	54	
31	A7	49	
31	C7	49	
32	A8	65	
32	C8	65	
33	A9	37	
33	C9	37	
34	BA	1521	
34	DA	1521	
35	BB	256	
35	DB	256	
36	BC	239	
36	DC	239	
37	BD	209	
37	DD	209	
38	BE	162	
38	DE	162	
39	BF	101	
39	DF	101	
40	BG	156	

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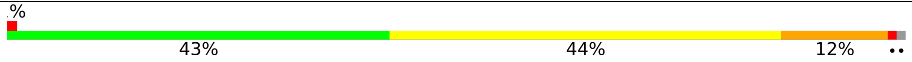
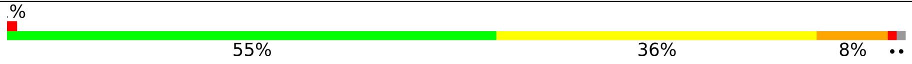
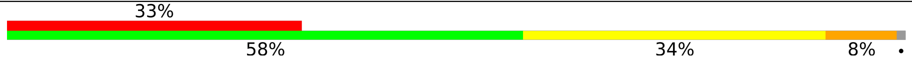
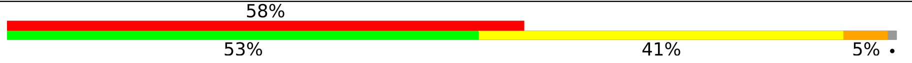
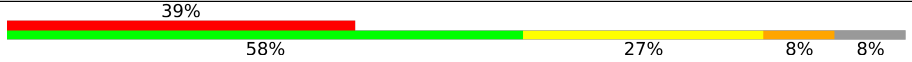
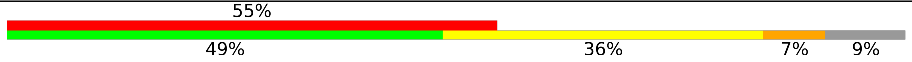
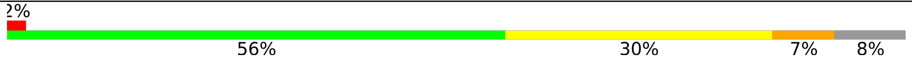
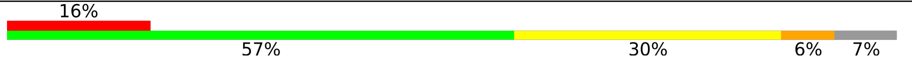
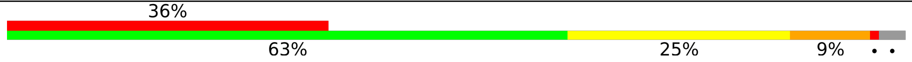
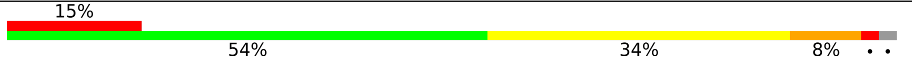
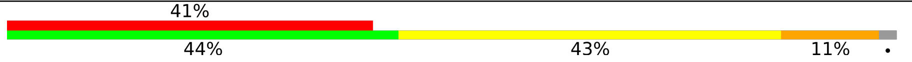
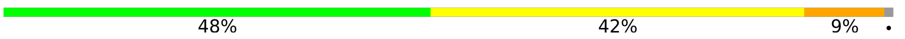
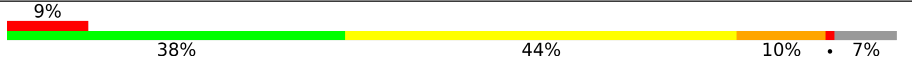
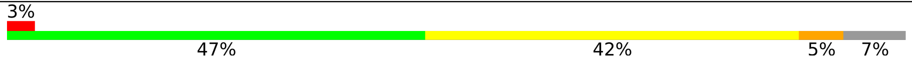
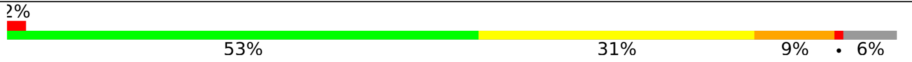
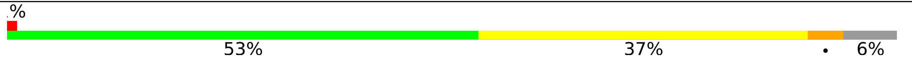
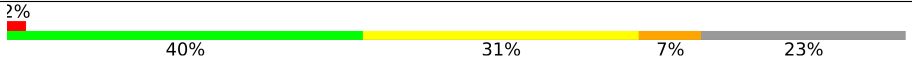
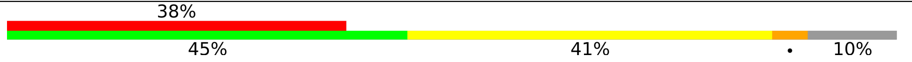
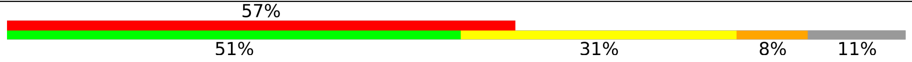
41	BH	138	
41	DH	138	
42	BI	128	
42	DI	128	
43	BJ	105	
43	DJ	105	
44	BK	129	
44	DK	129	
45	BL	132	
45	DL	132	
46	BM	126	
46	DM	126	
47	BN	61	
47	DN	61	
48	BO	89	
48	DO	89	
49	BP	88	
49	DP	88	
50	BQ	105	
50	DQ	105	
51	BR	88	
51	DR	88	
52	BS	93	
52	DS	93	

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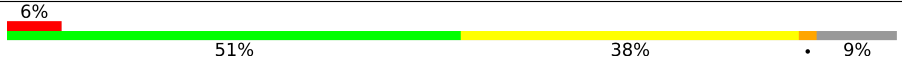
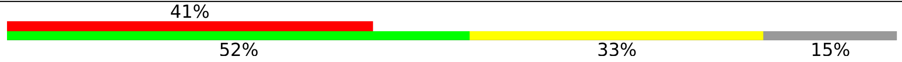
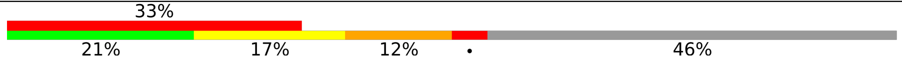
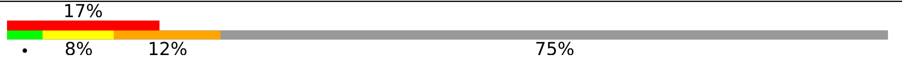
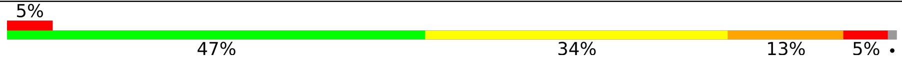
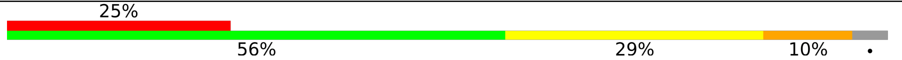
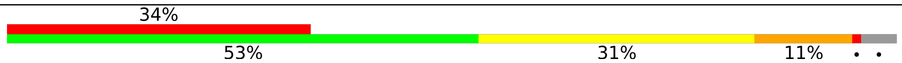
Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	24	
55	DV	24	
56	BX	77	
56	DX	77	
57	BZ	758	
57	DZ	758	

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
58	MG	AA	3018	-	-	-	X
58	MG	AA	3026	-	-	-	X
58	MG	AA	3088	-	-	-	X
58	MG	AA	3096	-	-	-	X
58	MG	AA	3109	-	-	-	X
58	MG	AA	3113	-	-	-	X
58	MG	AA	3122	-	-	-	X
58	MG	AA	3193	-	-	-	X
58	MG	AA	3641	-	-	-	X
58	MG	AA	3752	-	-	-	X
58	MG	AA	3784	-	-	-	X
58	MG	AB	3006	-	-	-	X
58	MG	AZ	301	-	-	-	X
58	MG	BA	3035	-	-	-	X
58	MG	BA	3088	-	-	-	X
58	MG	BA	3092	-	-	-	X
58	MG	BA	3106	-	-	-	X
58	MG	BA	3112	-	-	-	X
58	MG	BA	3169	-	-	-	X
58	MG	CA	3002	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	CA	3042	-	-	-	X
58	MG	CA	3067	-	-	-	X
58	MG	CA	3074	-	-	-	X
58	MG	CA	3094	-	-	-	X
58	MG	CA	3124	-	-	-	X
58	MG	CA	3130	-	-	-	X
58	MG	CA	3135	-	-	-	X
58	MG	CA	3141	-	-	-	X
58	MG	CA	3181	-	-	-	X
58	MG	CA	3184	-	-	-	X
58	MG	CA	3195	-	-	-	X
58	MG	CA	3209	-	-	-	X
58	MG	CA	3225	-	-	-	X
58	MG	CA	3232	-	-	-	X
58	MG	CA	3238	-	-	-	X
58	MG	CA	3286	-	-	-	X
58	MG	CA	3292	-	-	-	X
58	MG	CA	3461	-	-	-	X
58	MG	CA	3494	-	-	-	X
58	MG	CE	304	-	-	-	X
58	MG	DA	1605	-	-	-	X
58	MG	DA	1635	-	-	-	X
58	MG	DA	1659	-	-	-	X
58	MG	DA	1677	-	-	-	X
58	MG	DA	1704	-	-	-	X
58	MG	DA	1753	-	-	-	X
58	MG	DE	202	-	-	-	X
58	MG	DZ	701	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 305548 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	2852	Total C N O P 61426 27339 11489 19747 2851	0	0	0
1	CA	2848	Total C N O P 61337 27299 11470 19721 2847	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	AC	137	Total C N O S 1063 669 201 192 1	0	0	0
3	CC	137	Total C N O S 1063 669 201 192 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 C N O S 2136 1349 423 361 3	0	0	0
4	CD	275	Total C N O S 2142 1352 426 361 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	139	Total C N O S 1025 653 181 186 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CL	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			750	488	135	126	1			
21	CX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- 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	0	0	0
			806	517	152	131	6			
22	CY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- 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	0	0	0
			1451	927	258	264	2			
23	CZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- 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	0	0	0
			755	475	148	131	1			
25	C1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- 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	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	C2	70	Total C N O S 588 365 118 103 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 C N O 469 298 90 81	0	0	0
27	C3	59	Total C N O 464 296 90 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 C N O S 558 352 102 99 5	0	0	0
28	C4	69	Total C N O S 532 339 97 91 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 C N O S 455 285 89 76 5	0	0	0
29	C5	59	Total C N O S 455 285 89 76 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 C N O S 453 281 91 77 4	0	0	0
30	C6	53	Total C N O S 449 279 91 75 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 C N O S 418 257 104 55 2	0	0	0
31	C7	48	Total C N O S 418 257 104 55 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	0	0	0
			517	331	102	82	2			
32	C8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- 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	0	0	0
			307	188	68	47	4			
33	C9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- 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	0	0	0
			32141	14304	5958	10384	1495			
34	DA	1501	Total	C	N	O	P	0	0	0
			32268	14361	5980	10426	1501			

- 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	0	0	0
			1846	1179	331	331	5			
35	DB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- 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	0	0	0
			1552	976	302	273	1			
36	DC	206	Total	C	N	O	S	0	0	0
			1544	970	300	273	1			

- 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
42	DI	127	Total 978	C 619	N 190	O 169	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BM	117	Total 923	C 570	N 191	O 160	S 2	0	0	0
46	DM	122	Total 950	C 586	N 197	O 165	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0
47	DN	60	Total 492	C 312	N 104	O 72	S 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
			Total	C	N	O	S			
53	BT	96	728	446	156	124	2	0	0	0
53	DT	96	731	449	156	124	2	0	0	0

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

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

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
55	BV	13	277	125	51	88	13	0	0	0
55	DV	6	128	59	27	37	5	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
56	BX	76	1625	725	294	529	76	1	0	0	0
56	DX	76	1621	723	292	529	76	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	BZ	730	4869	3031	886	942	10	0	0	0
57	DZ	730	4867	3029	886	942	10	0	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	AA	836	836	836	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AB	23	Total Mg 23 23	0	0
58	AD	10	Total Mg 10 10	0	0
58	AE	4	Total Mg 4 4	0	0
58	AF	5	Total Mg 5 5	0	0
58	AG	2	Total Mg 2 2	0	0
58	AH	2	Total Mg 2 2	0	0
58	AN	3	Total Mg 3 3	0	0
58	AO	1	Total Mg 1 1	0	0
58	AP	2	Total Mg 2 2	0	0
58	AQ	2	Total Mg 2 2	0	0
58	AR	1	Total Mg 1 1	0	0
58	AU	3	Total Mg 3 3	0	0
58	AV	2	Total Mg 2 2	0	0
58	AW	4	Total Mg 4 4	0	0
58	AX	2	Total Mg 2 2	0	0
58	AZ	2	Total Mg 2 2	0	0
58	A0	4	Total Mg 4 4	0	0
58	A1	1	Total Mg 1 1	0	0
58	A2	1	Total Mg 1 1	0	0
58	A4	1	Total Mg 1 1	0	0
58	A5	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	A6	2	Total Mg 2 2	0	0
58	A7	1	Total Mg 1 1	0	0
58	A8	2	Total Mg 2 2	0	0
58	A9	1	Total Mg 1 1	0	0
58	BA	212	Total Mg 212 212	0	0
58	BB	1	Total Mg 1 1	0	0
58	BD	1	Total Mg 1 1	0	0
58	BE	1	Total Mg 1 1	0	0
58	BF	1	Total Mg 1 1	0	0
58	BK	1	Total Mg 1 1	0	0
58	BL	4	Total Mg 4 4	0	0
58	BN	2	Total Mg 2 2	0	0
58	BT	1	Total Mg 1 1	0	0
58	BV	1	Total Mg 1 1	0	0
58	BX	10	Total Mg 10 10	0	0
58	BZ	1	Total Mg 1 1	0	0
58	CA	666	Total Mg 666 666	0	0
58	CB	13	Total Mg 13 13	0	0
58	CD	3	Total Mg 3 3	0	0
58	CE	7	Total Mg 7 7	0	0
58	CF	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	CG	1	Total Mg 1 1	0	0
58	CN	1	Total Mg 1 1	0	0
58	CO	2	Total Mg 2 2	0	0
58	CQ	4	Total Mg 4 4	0	0
58	CR	1	Total Mg 1 1	0	0
58	CU	2	Total Mg 2 2	0	0
58	CV	2	Total Mg 2 2	0	0
58	CY	1	Total Mg 1 1	0	0
58	C0	1	Total Mg 1 1	0	0
58	C1	1	Total Mg 1 1	0	0
58	C3	1	Total Mg 1 1	0	0
58	C7	1	Total Mg 1 1	0	0
58	C8	1	Total Mg 1 1	0	0
58	DA	166	Total Mg 166 166	0	0
58	DD	1	Total Mg 1 1	0	0
58	DE	2	Total Mg 2 2	0	0
58	DF	1	Total Mg 1 1	0	0
58	DJ	1	Total Mg 1 1	0	0
58	DK	1	Total Mg 1 1	0	0
58	DL	2	Total Mg 2 2	0	0
58	DT	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	DZ	3	Total Mg 3 3	0	0

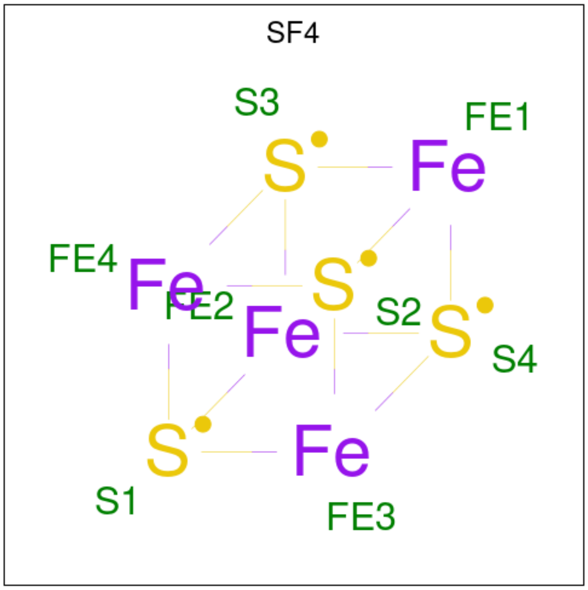
- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AA	1	Total K 1 1	0	0

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

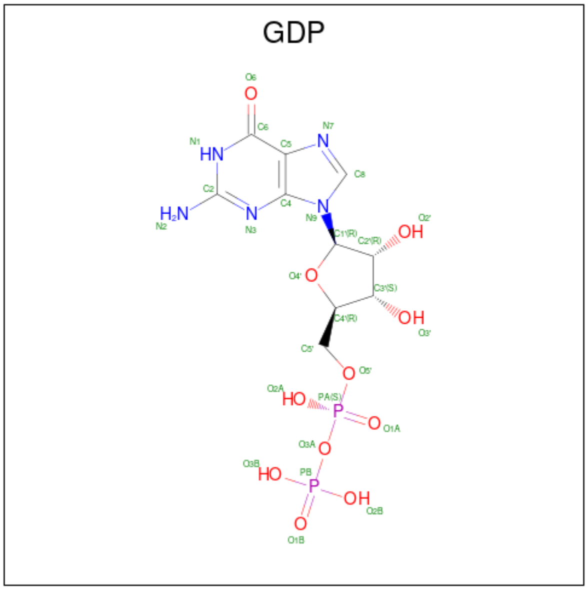
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AY	1	Total Zn 1 1	0	0
60	A4	1	Total Zn 1 1	0	0
60	A5	1	Total Zn 1 1	0	0
60	A6	1	Total Zn 1 1	0	0
60	A9	1	Total Zn 1 1	0	0
60	BN	1	Total Zn 1 1	0	0
60	CY	1	Total Zn 1 1	0	0
60	C4	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0
60	C6	1	Total Zn 1 1	0	0
60	C9	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	1406	Total O 1406 1406	0	0
63	AB	37	Total O 37 37	0	0
63	AD	16	Total O 16 16	0	0
63	AE	14	Total O 14 14	0	0
63	AF	6	Total O 6 6	0	0
63	AG	3	Total O 3 3	0	0
63	AH	1	Total O 1 1	0	0
63	AN	3	Total O 3 3	0	0
63	AO	1	Total O 1 1	0	0
63	AP	18	Total O 18 18	0	0
63	AQ	5	Total O 5 5	0	0
63	AR	2	Total O 2 2	0	0
63	AS	1	Total O 1 1	0	0
63	AT	3	Total O 3 3	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	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	AZ	1	Total O 1 1	0	0
63	A0	9	Total O 9 9	0	0
63	A1	2	Total O 2 2	0	0
63	A2	1	Total O 1 1	0	0
63	A3	2	Total O 2 2	0	0
63	A5	4	Total O 4 4	0	0
63	A7	4	Total O 4 4	0	0
63	A8	9	Total O 9 9	0	0
63	A9	1	Total O 1 1	0	0
63	BA	203	Total O 203 203	0	0
63	BD	3	Total O 3 3	0	0
63	BE	2	Total O 2 2	0	0
63	BG	1	Total O 1 1	0	0
63	BJ	1	Total O 1 1	0	0
63	BL	1	Total O 1 1	0	0
63	BM	1	Total O 1 1	0	0
63	BO	2	Total O 2 2	0	0
63	BP	1	Total O 1 1	0	0
63	BV	3	Total O 3 3	0	0
63	BX	5	Total O 5 5	0	0
63	BZ	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	CA	974	Total O 974 974	0	0
63	CB	9	Total O 9 9	0	0
63	CD	17	Total O 17 17	0	0
63	CE	14	Total O 14 14	0	0
63	CF	6	Total O 6 6	0	0
63	CN	2	Total O 2 2	0	0
63	CP	12	Total O 12 12	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	2	Total O 2 2	0	0
63	CW	1	Total O 1 1	0	0
63	CX	2	Total O 2 2	0	0
63	CY	2	Total O 2 2	0	0
63	C0	5	Total O 5 5	0	0
63	C1	1	Total O 1 1	0	0
63	C3	2	Total O 2 2	0	0
63	C6	1	Total O 1 1	0	0
63	C7	1	Total O 1 1	0	0
63	C8	3	Total O 3 3	0	0
63	DA	154	Total O 154 154	0	0

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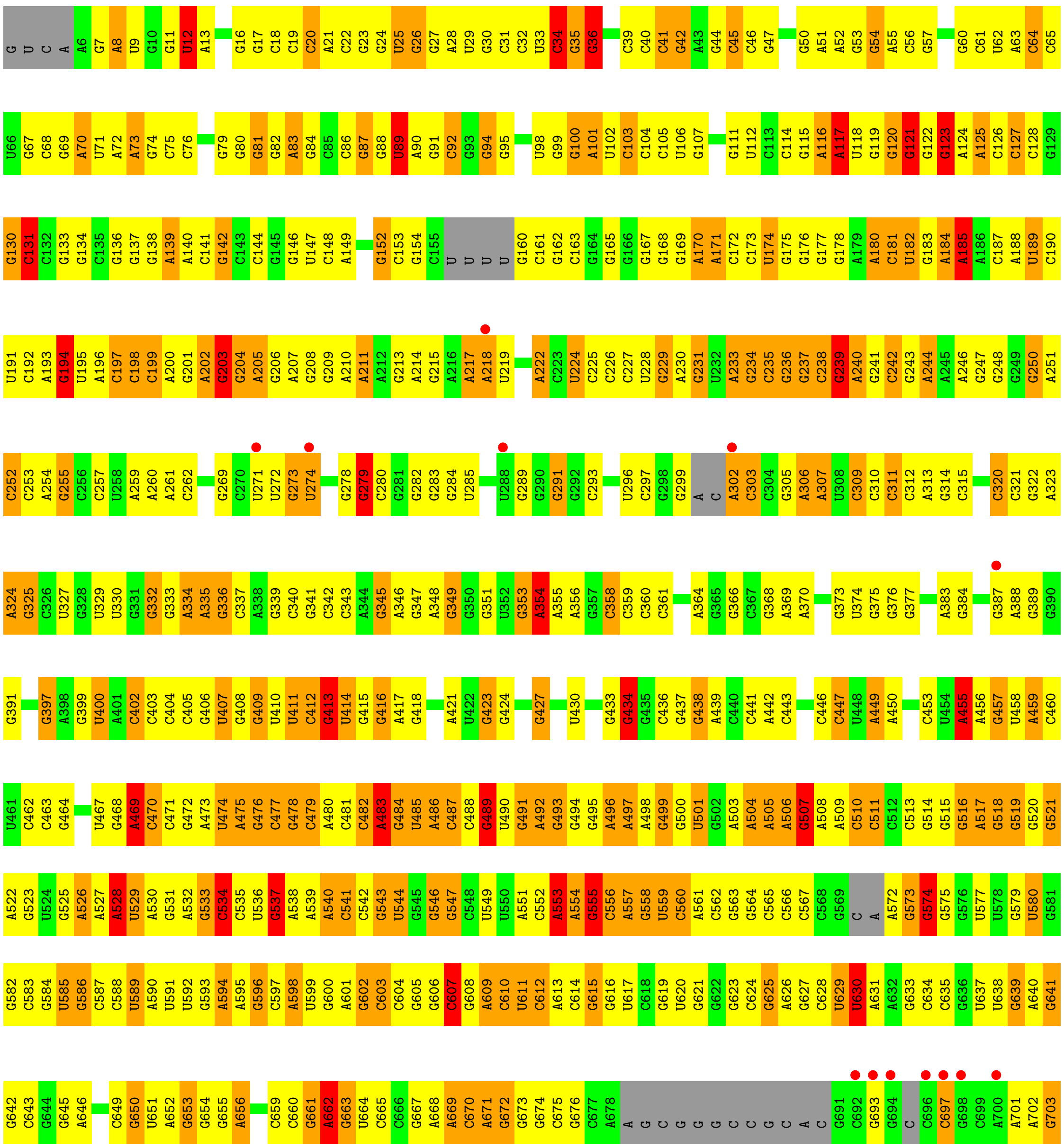
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	DE	3	Total O 3 3	0	0
63	DH	1	Total O 1 1	0	0
63	DJ	1	Total O 1 1	0	0
63	DK	2	Total O 2 2	0	0
63	DP	1	Total O 1 1	0	0
63	DT	1	Total O 1 1	0	0
63	DV	1	Total O 1 1	0	0
63	DZ	1	Total O 1 1	0	0

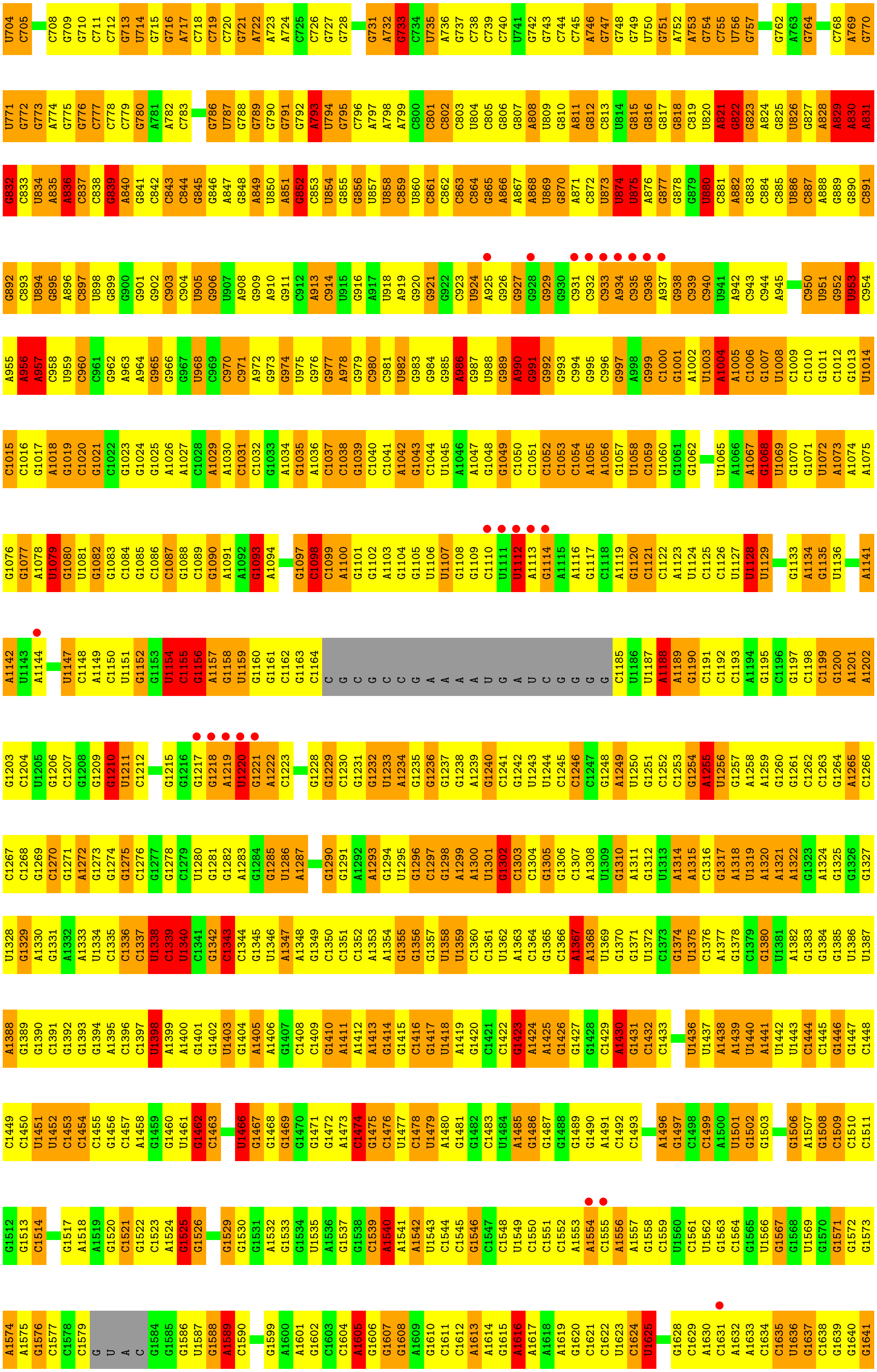
3 Residue-property plots ⓘ

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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U771 G772 G773 A774 G775 G776 C777 C778 C779 G780 A781 A782 C783 G786 U787 G788 G789 G790 G791 G792 A793 U794 G795 C796 A797 A798 A799 C800 C801 C802 C803 U804 C805 G806 G807 A808 U809 G810 A811 G812 C813 U814 G815 G816 G817 G818 C819 U820 A821 G822 G823 A824 G825 U826 G827 A828 A829 A830 A831
G832 C833 U834 A835 A836 C837 C838 G839 A840 G841 C842 C843 C844 G845 G846 A847 G848 A849 U850 A851 G852 C853 U854 G855 G856 U857 U858 C859 U860 C861 C862 C863 C864 G865 A866 A867 A868 U869 G870 A871 C872 U873 U874 U875 A876 G877 G878 G879 U880 C881 A882 G883 C884 G885 U886 C887 A888 G889 G890 C891
G892 C893 U894 G895 A896 C897 U898 G899 G900 G901 G902 C903 C904 U905 G906 U907 A908 G909 A910 G911 C912 A913 C914 U915 G916 A917 U918 A919 G920 G921 G922 C923 U924 A925 G926 G927 G928 G929 G930 C931 C932 C933 A934 C935 C936 A937 G938 C939 C940 U941 A942 G943 C944 A945 C950 U951 G952 U953 C954
A955 A956 A957 C958 U959 C960 C961 G962 A963 A964 G965 G966 G967 U968 C969 C970 C971 A972 G973 G974 U975 G976 G977 A978 G979 C980 C981 U982 G983 G984 G985 A986 G987 U988 G989 A990 G991 G992 G993 C994 G995 C996 G997 A998 G999 C1000 G1001 A1002 U1003 A1004 A1005 C1006 G1007 U1008 C1009 C1010 G1011 C1012 G1013 U1014
C1015 C1016 G1017 A1018 G1019 C1020 G1021 C1022 G1023 G1024 G1025 A1026 A1027 C1028 A1029 A1030 C1031 C1032 G1033 A1034 G1035 A1036 C1037 C1038 G1039 C1040 C1041 A1042 G1043 C1044 U1045 A1046 A1047 G1048 G1049 C1050 C1051 C1052 C1053 C1054 A1055 A1056 G1057 U1058 C1059 U1060 G1061 G1062 U1065 A1066 A1067 G1068 U1069 G1070 G1071 U1072 A1073 A1074 A1075
G1076 G1077 A1078 U1079 G1080 U1081 G1082 G1083 C1084 G1085 C1086 C1087 G1088 C1089 G1090 A1091 A1092 G1093 A1094 G1097 C1098 C1099 A1100 G1101 G1102 A1103 G1104 G1105 U1106 U1107 G1108 G1109 C1110 U1111 U1112 A1113 G1114 A1115 A1116 G1117 C1118 A1119 G1120 C1121 C1122 A1123 U1124 C1125 C1126 U1127 U1128 U1129 G1133 A1134 G1135 U1136 A1141
A1142 U1143 A1144 U1147 C1148 A1149 C1150 U1151 G1152 G1153 U1154 C1155 G1156 A1157 G1158 U1159 G1160 G1161 C1162 G1163 C1164 C G C G C C G A A A A U G A U C G G G G C1185 U1186 U1187 A1188 A1189 G1190 C1191 C1192 C1193 A1194 G1195 C1196 C1197 C1198 C1199 G1200 A1201 A1202
G1203 C1204 U1205 G1206 C1207 G1208 G1209 G1210 U1211 C1212 G1215 G1216 G1217 G1218 A1219 U1220 G1221 A1222 C1223 G1228 G1229 C1230 G1231 G1232 U1233 A1234 G1235 G1236 G1237 G1238 A1239 G1240 C1241 G1242 U1243 U1244 C1245 C1246 C1247 G1248 A1249 U1250 G1251 C1252 C1253 G1254 A1255 U1256 G1257 A1258 A1259 G1260 G1261 C1262 C1263 G1264 A1265 C1266
C1267 C1268 G1269 C1270 G1271 A1272 G1273 G1274 G1275 C1276 G1277 G1278 C1279 U1280 G1281 G1282 A1283 G1284 G1285 U1286 A1287 G1290 G1291 A1292 A1293 G1294 U1295 G1296 C1297 G1298 G1299 A1300 U1301 G1302 C1303 C1304 G1305 G1306 C1307 A1308 U1309 G1310 A1311 G1312 U1313 A1314 A1315 C1316 G1317 A1318 U1319 A1320 A1321 A1322 G1323 A1324 G1325 G1326 G1327
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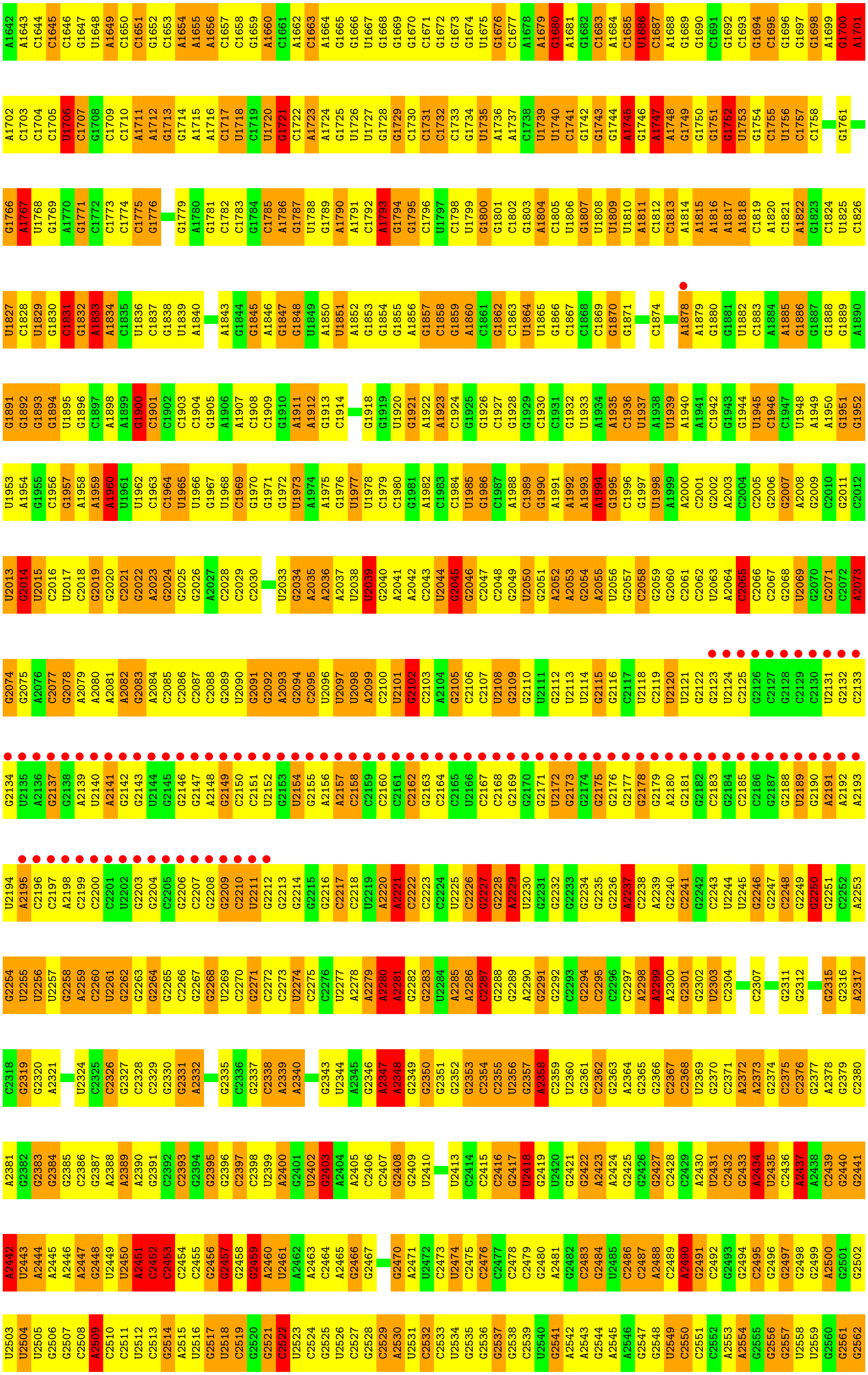
C1449 C1450 U1451 U1452 C1453 C1454 C1455 G1456 C1457 A1458 G1459 G1460 U1461 G1462 C1463 U1466 G1467 G1468 G1469 G1470 G1471 G1472 A1473 C1474 G1475 C1476 U1477 C1478 U1479 A1480 G1481 G1482 C1483 U1484 A1485 G1486 G1487 G1488 G1489 G1490 A1491 C1492 C1493 A1496 G1497 C1498 C1499 A1500 U1501 G1502 G1503 G1506 A1507 G1508 C1509 C1510 C1511
G1512 G1513 C1514 G1517 A1518 A1519 G1520 C1521 G1522 C1523 A1524 G1525 G1526 G1529 G1530 G1531 A1532 G1533 G1534 U1535 A1536 G1537 G1538 C1539 A1540 A1541 A1542 U1543 C1544 C1545 G1546 C1547 C1548 U1549 C1550 C1551 C1552 A1553 A1554 C1555 A1556 A1557 G1558 C1559 U1560 C1561 U1562 G1563 C1564 G1565 U1566 G1567 G1568 U1569 G1570 G1571 G1572 G1573
A1574 A1575 G1576 C1577 C1578 C1579 G U A C G1584 G1585 G1586 U1587 G1588 A1589 C1590 G1599 A1600 A1601 G1602 C1603 C1604 A1605 G1606 G1607 G1608 A1609 G1610 C1611 C1612 A1613 A1614 G1615 A1616 A1617 A1618 G1619 G1620 C1621 C1622 U1623 C1624 U1625 G1628 C1629 A1630 C1631 A1632 A1633 C1634 C1635 U1636 G1637 C1638 G1639 G1640 G1641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U1953 A1954 G1955 C1956 G1957 A1958 A1959 A1960 U1961 C1962 C1963 C1964 U1965 U1966 G1967 U1968 C1969 G1970 C1971 G1972 U1973 A1974 A1975 G1976 U1977 U1978 C1979 C1980 G1981 A1982 C1983 C1984 U1985 G1986 C1987 A1988 C1989 G1990 A1991 A1992 A1993 A1994 G1995 C1996 G1997 U1998 A1999 A2000 C2001 G2002 A2003 C2004 C2005 G2006 G2007 A2008 G2009 C2010 G2011 C2012
U2013 G2014 U2015 C2016 U2017 C2018 G2019 G2020 C2021 G2022 A2023 G2024 G2025 G2026 A2027 C2028 C2029 C2030 U2033 G2034 A2035 A2036 A2037 U2038 U2039 G2040 A2041 A2042 C2043 U2044 G2045 G2046 C2047 C2048 G2049 U2050 G2051 A2052 A2053 G2054 A2055 U2056 G2057 C2058 G2059 C2060 C2061 C2062 U2063 A2064 C2065 C2066 C2067 C2068 U2069 G2070 C2071 C2072 A2073
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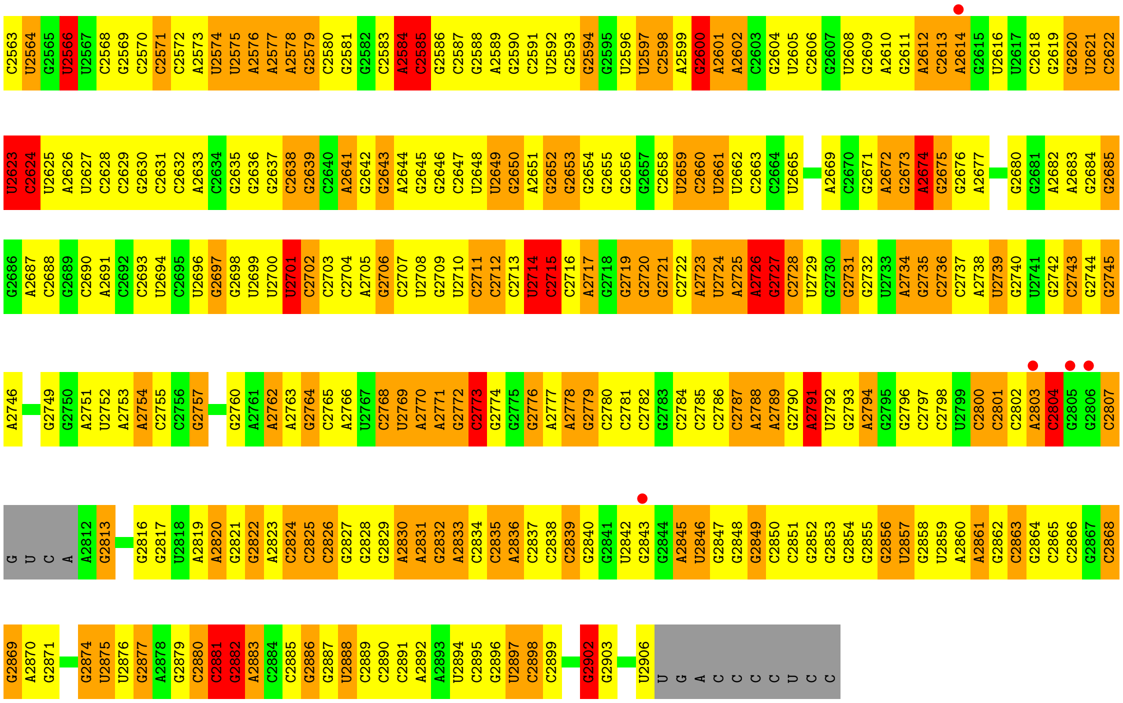

- Molecule 1: 23S Ribosomal RNA

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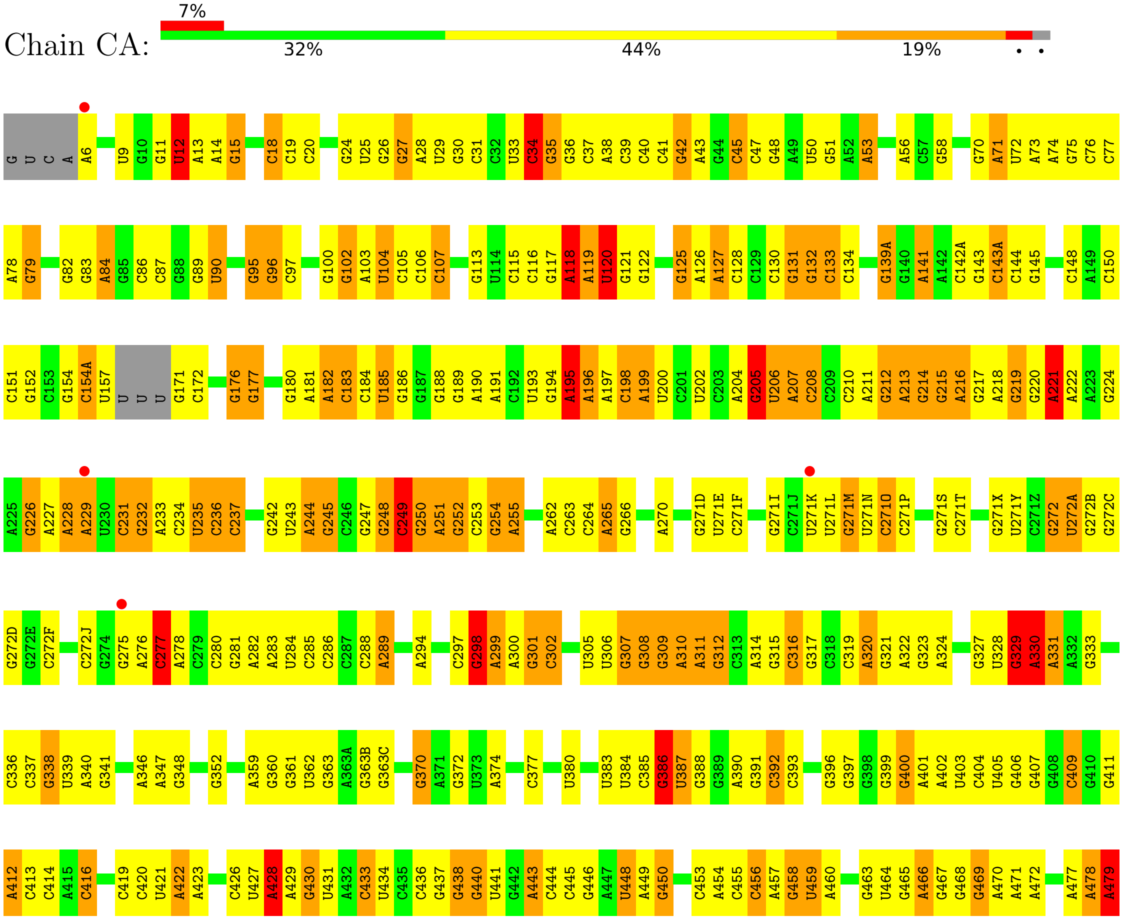

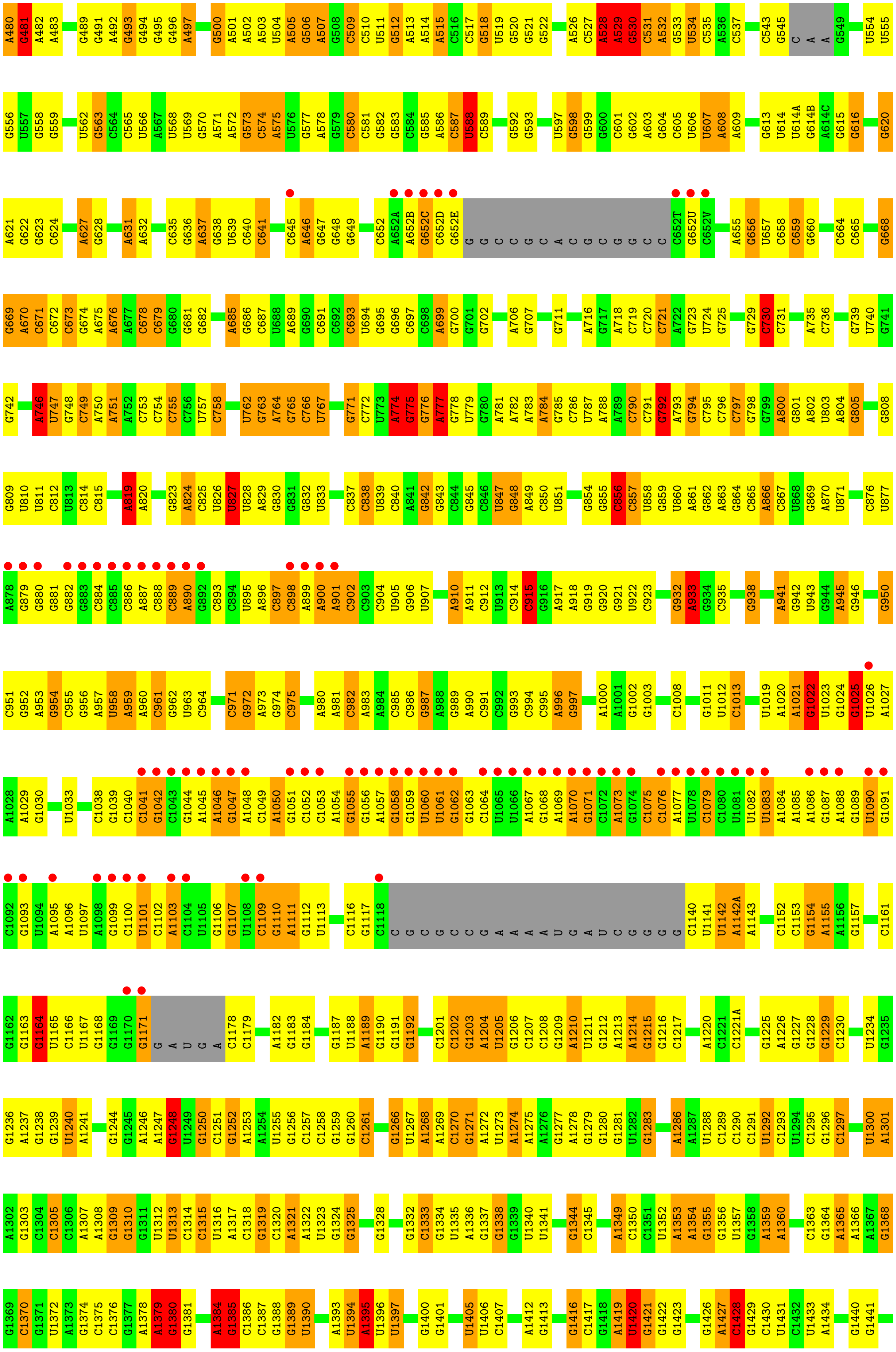
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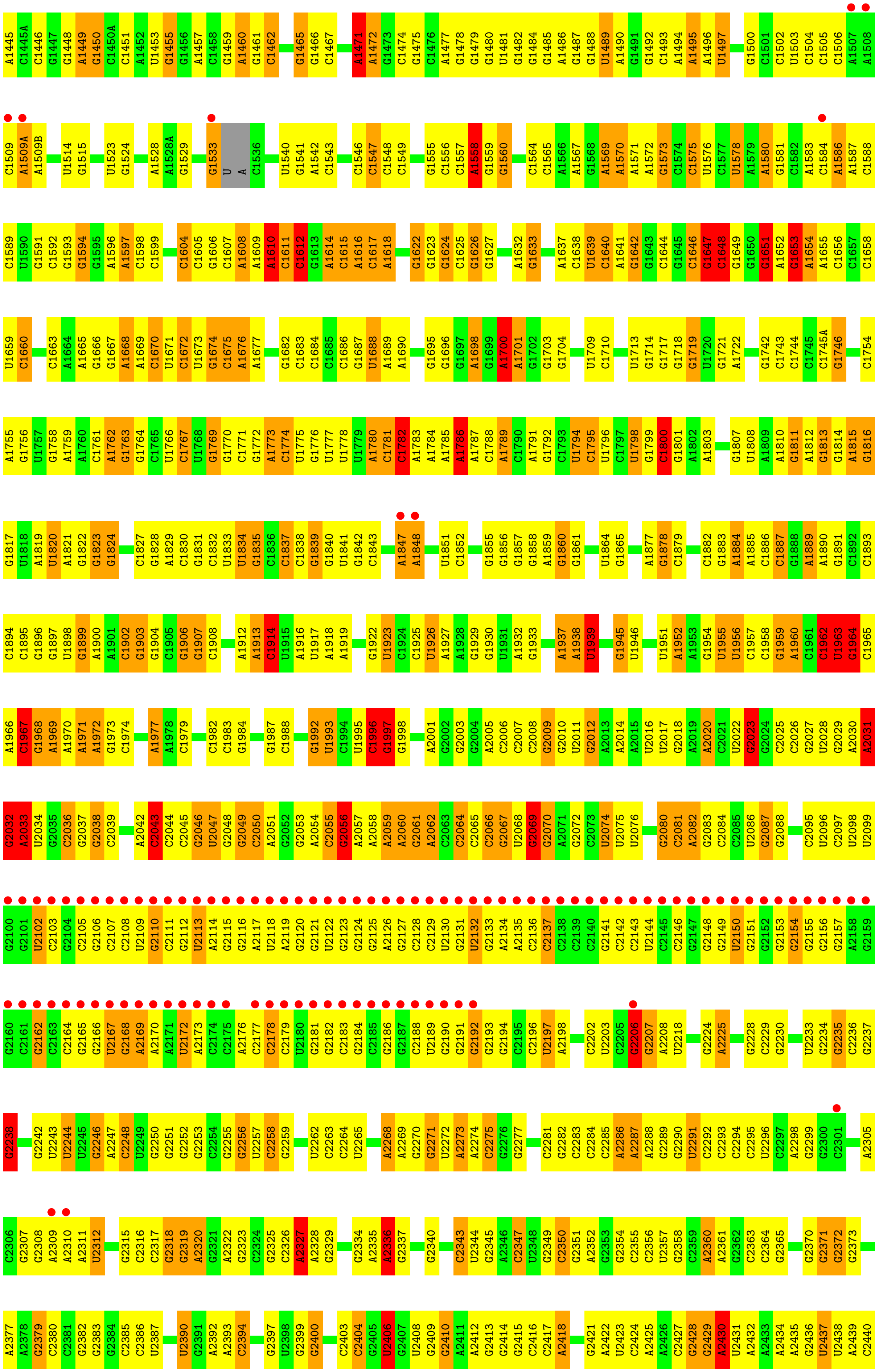
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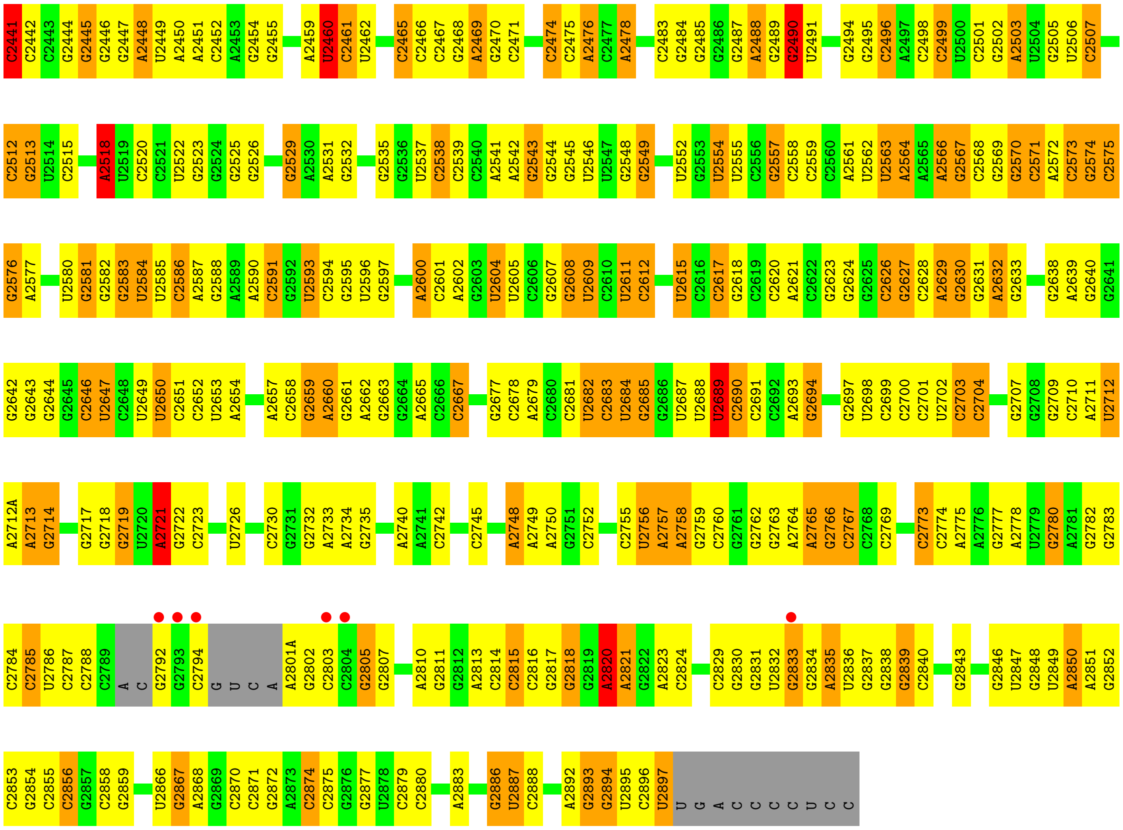

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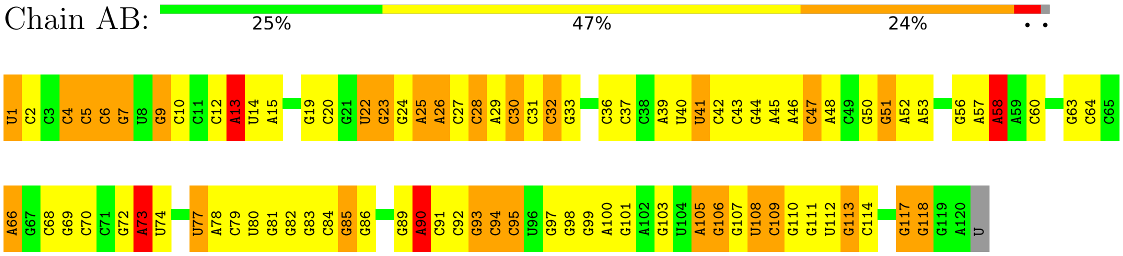
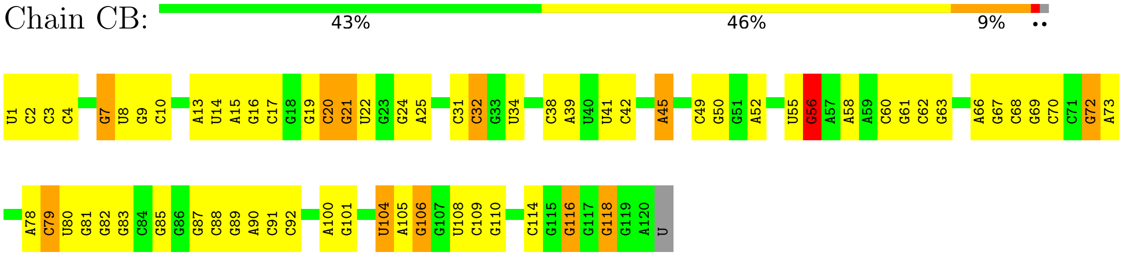


- Molecule 2: 5S Ribosomal RNA



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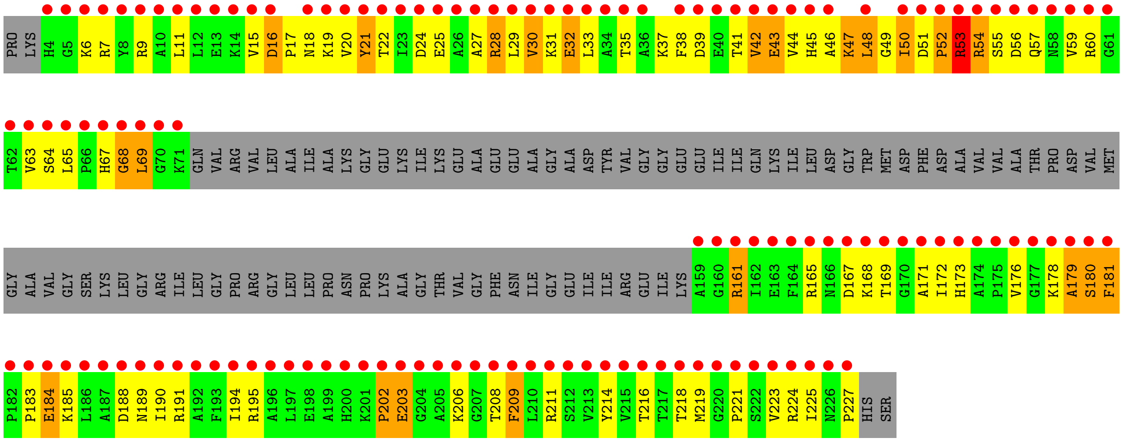

- Molecule 3: 50S ribosomal protein L1

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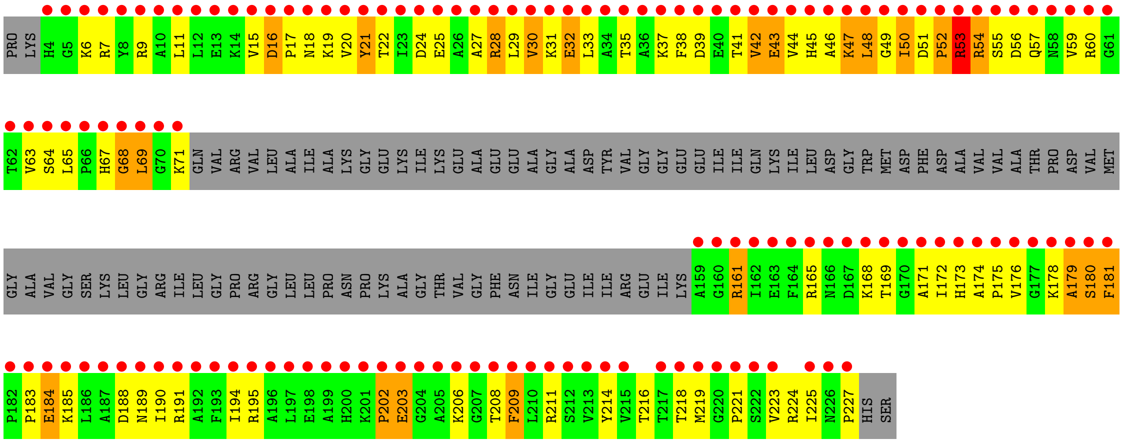

- Molecule 4: 50S ribosomal protein L2

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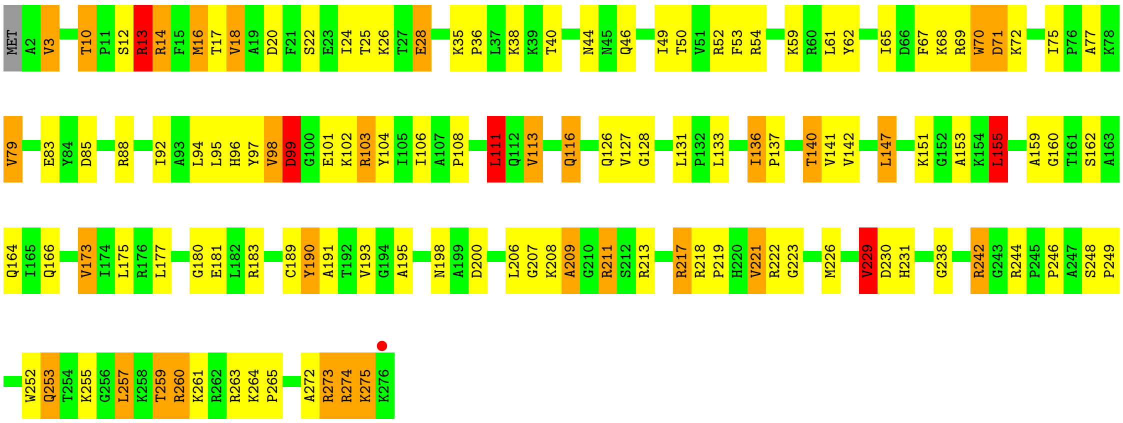
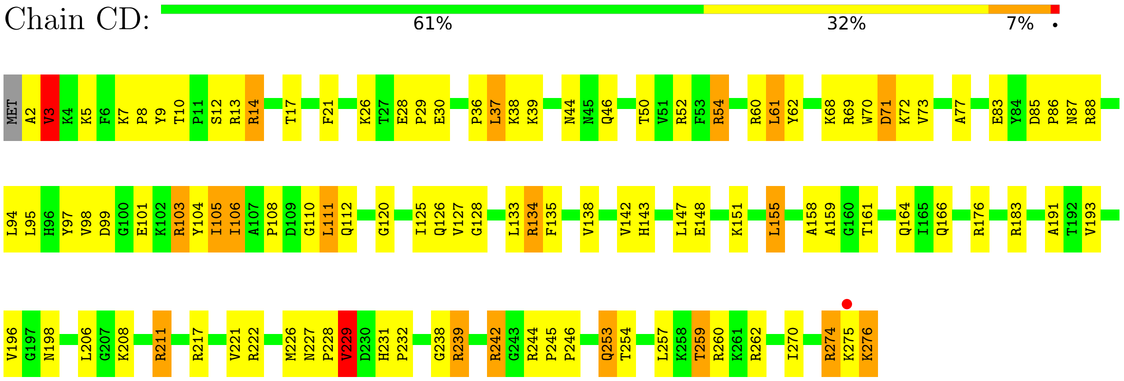
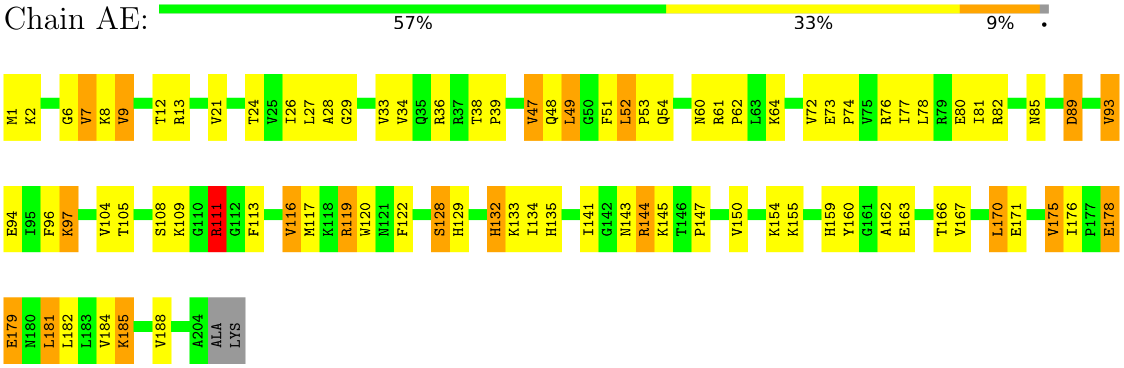


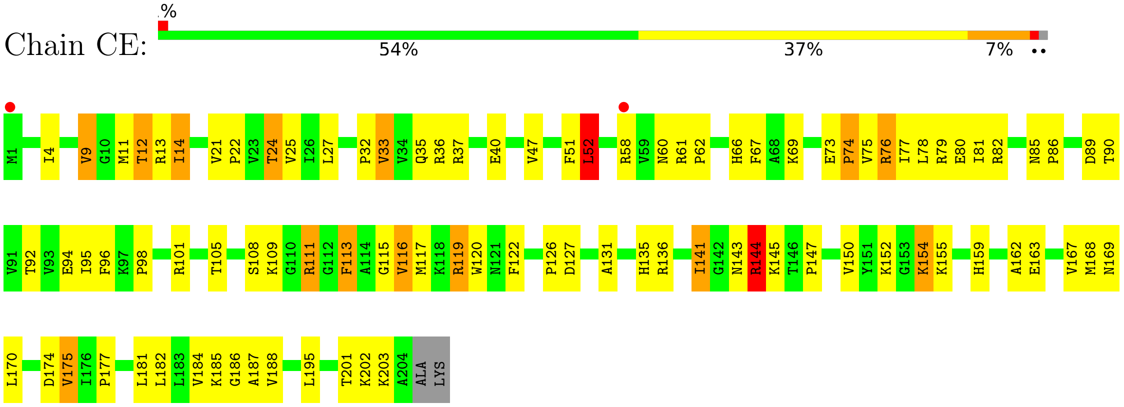
- Molecule 4: 50S ribosomal protein L2


Chain CD:

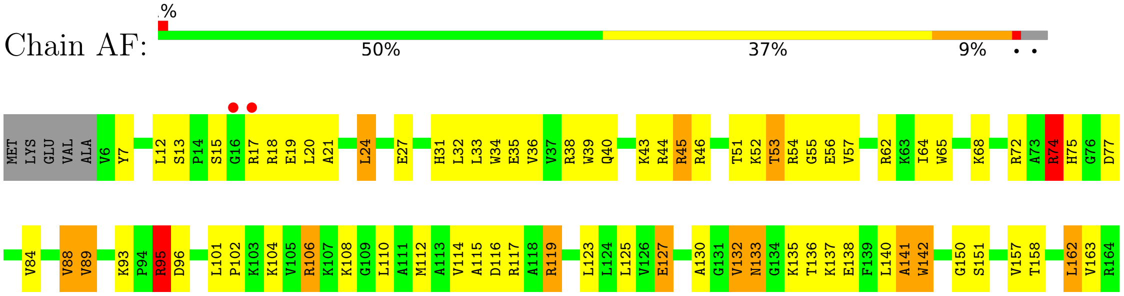
- Molecule 5: 50S ribosomal protein L3

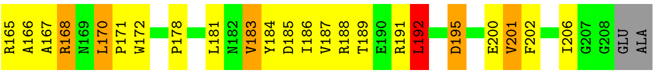

Chain AE:

- Molecule 5: 50S ribosomal protein L3


Chain CE:

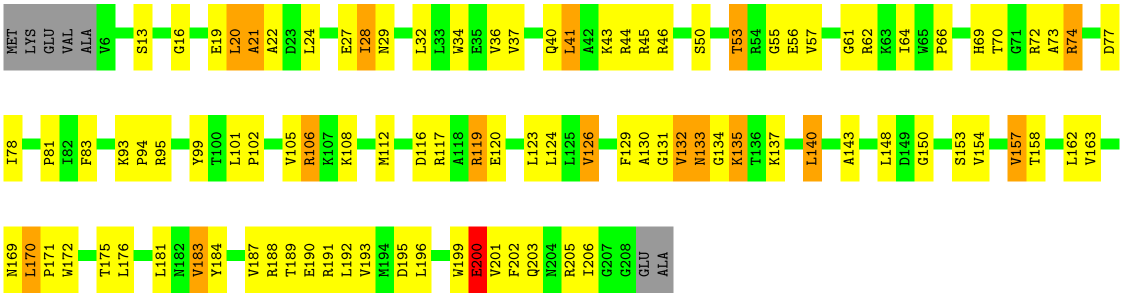
- Molecule 6: 50S ribosomal protein L4


Chain AF:



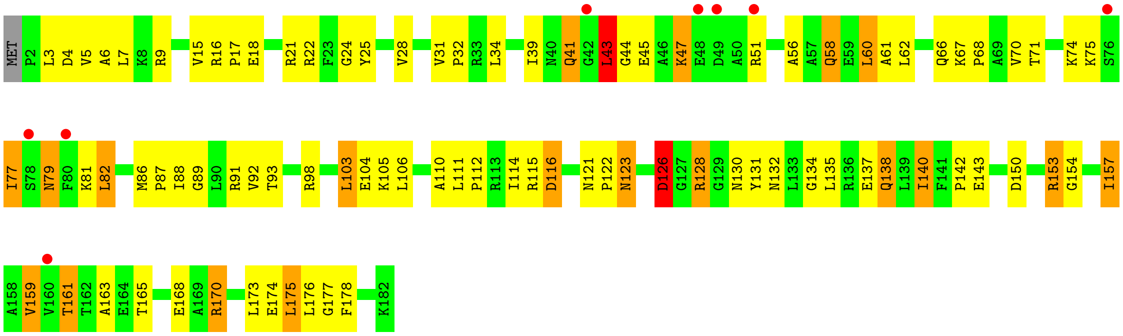
- Molecule 6: 50S ribosomal protein L4

Chain CF:



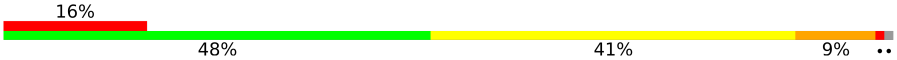
- Molecule 7: 50S ribosomal protein L5

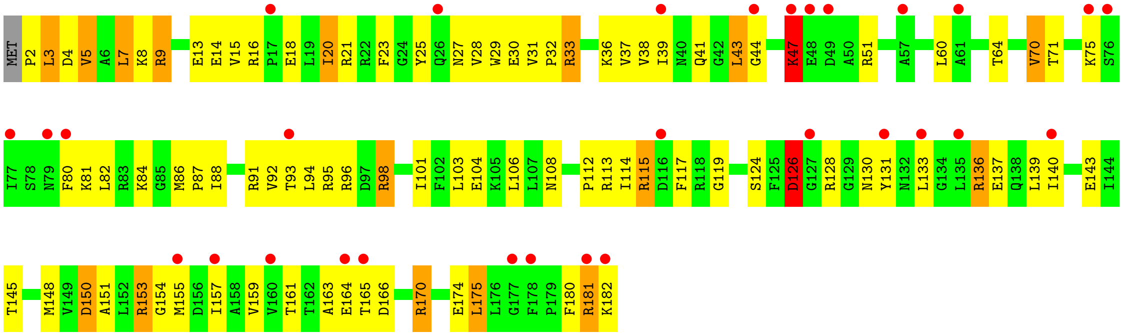
Chain AG:



- Molecule 7: 50S ribosomal protein L5

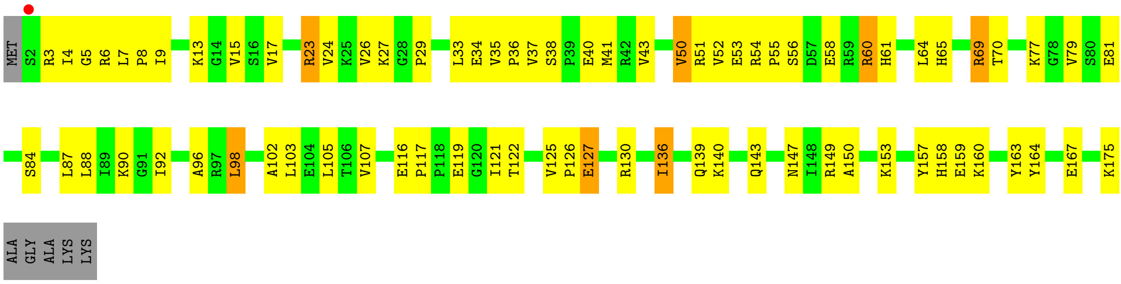
Chain CG:





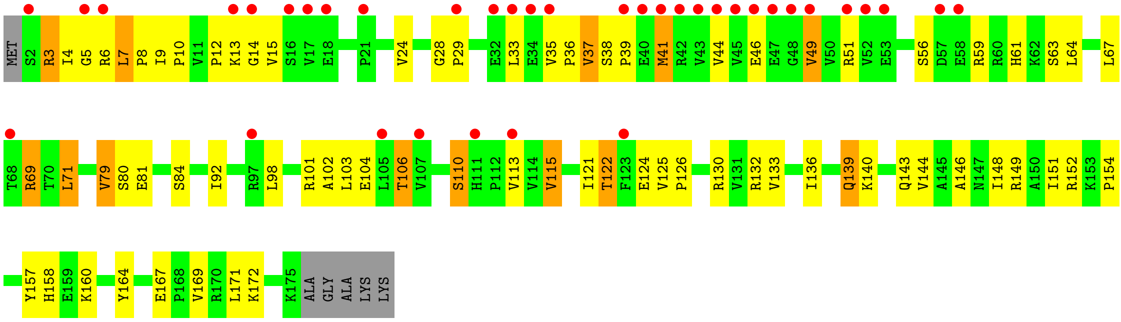
- Molecule 8: 50S ribosomal protein L6

Chain AH:



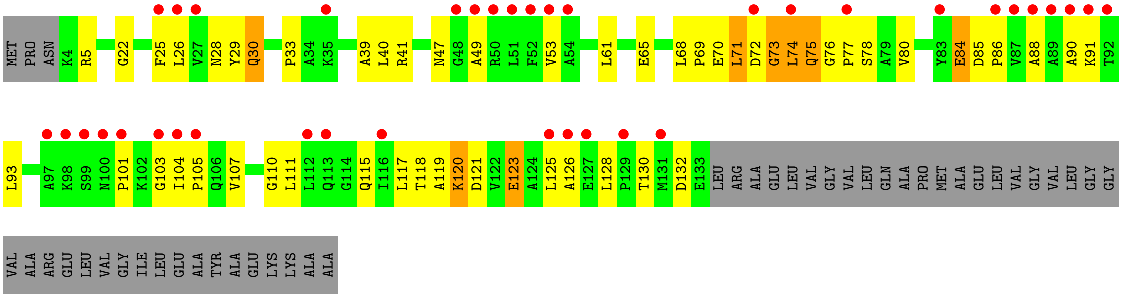
- Molecule 8: 50S ribosomal protein L6

Chain CH:



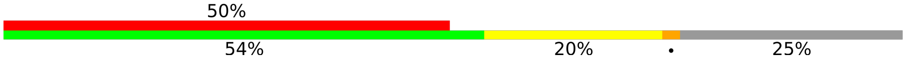
- Molecule 9: 50S ribosomal protein L10

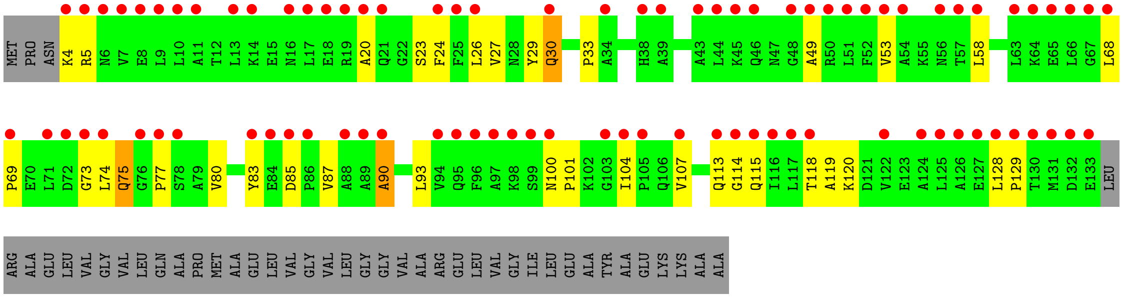
Chain AK:



- Molecule 9: 50S ribosomal protein L10

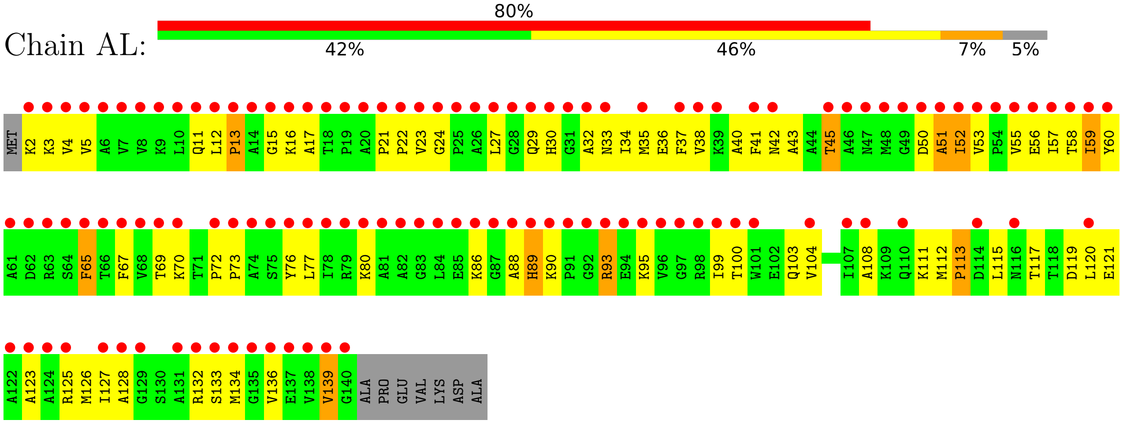
Chain CK:





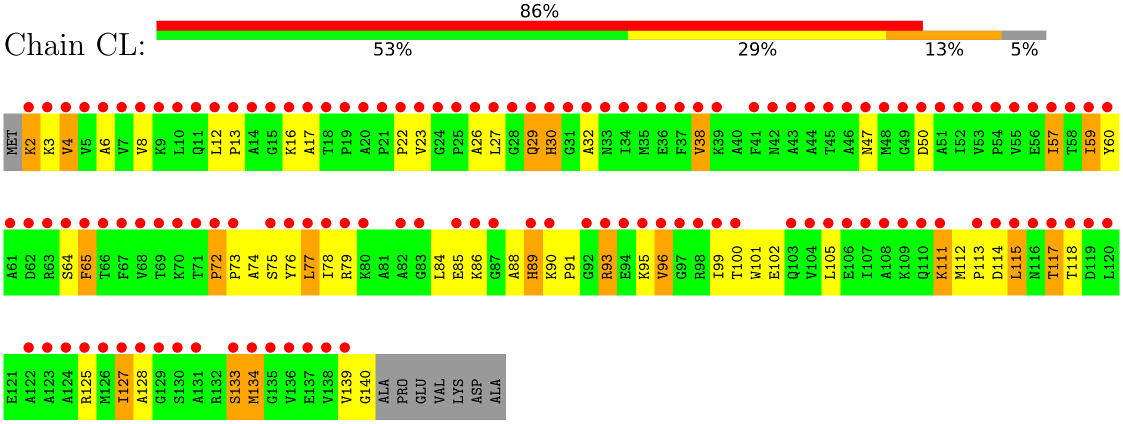
- Molecule 10: 50S ribosomal protein L11

Chain AL:



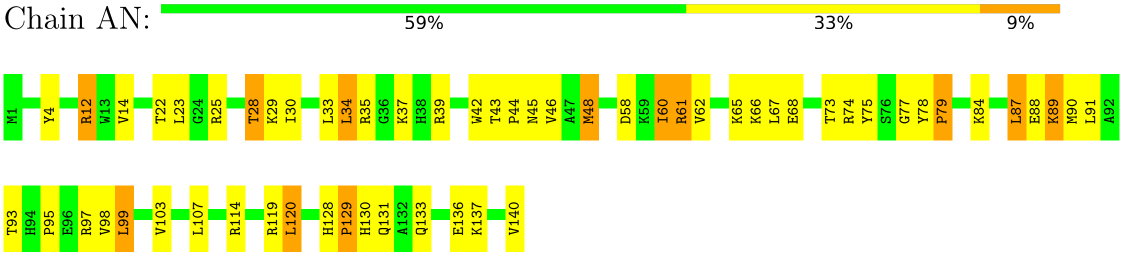
- Molecule 10: 50S ribosomal protein L11

Chain CL:



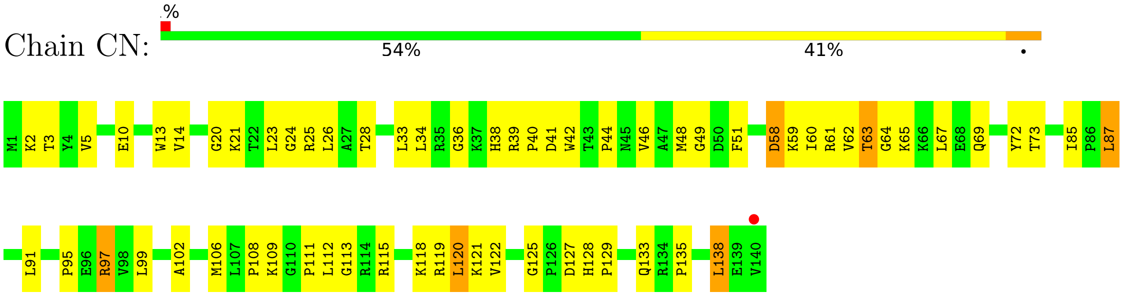
- Molecule 11: 50S ribosomal protein L13

Chain AN:



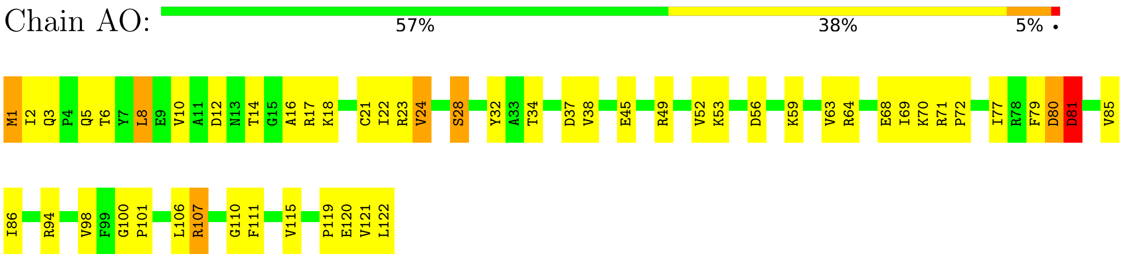
- Molecule 11: 50S ribosomal protein L13

Chain CN:



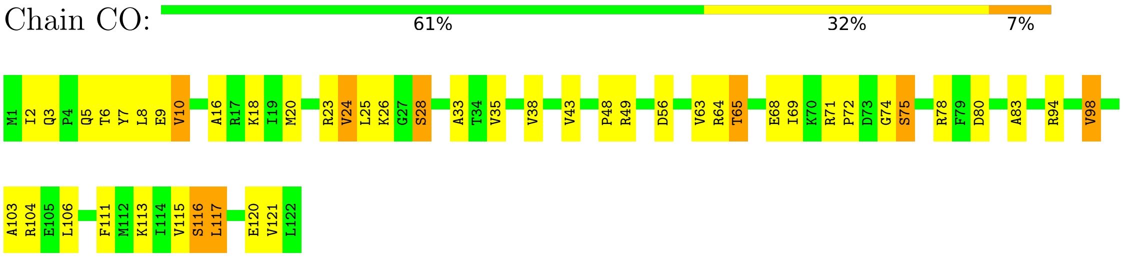
- Molecule 12: 50S ribosomal protein L14

Chain AO:



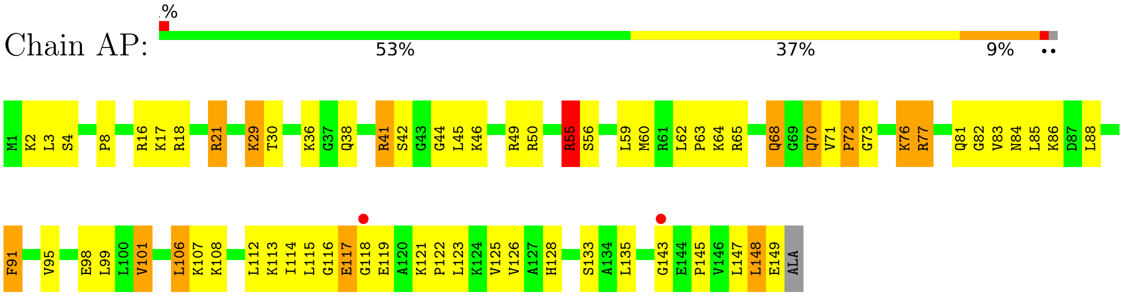
- Molecule 12: 50S ribosomal protein L14

Chain CO:



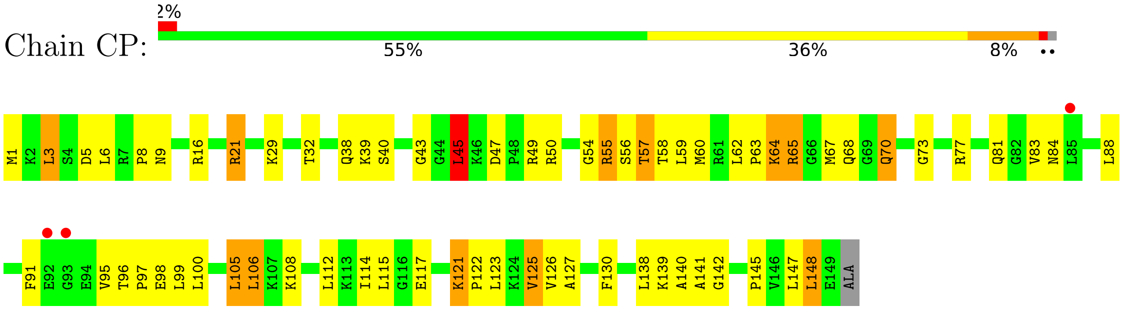
- Molecule 13: 50S ribosomal protein L15

Chain AP:



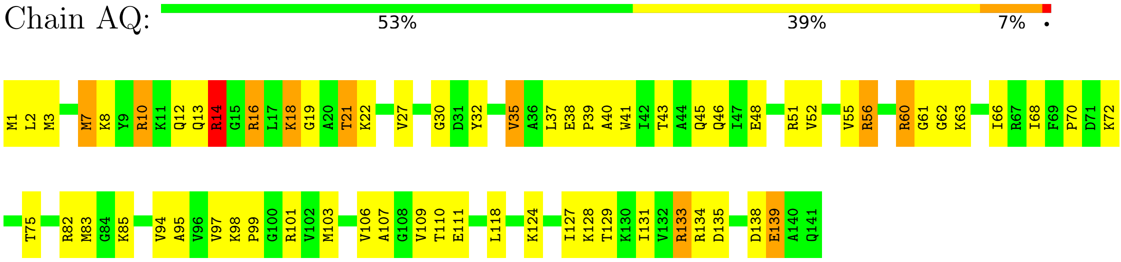
- Molecule 13: 50S ribosomal protein L15

Chain CP:



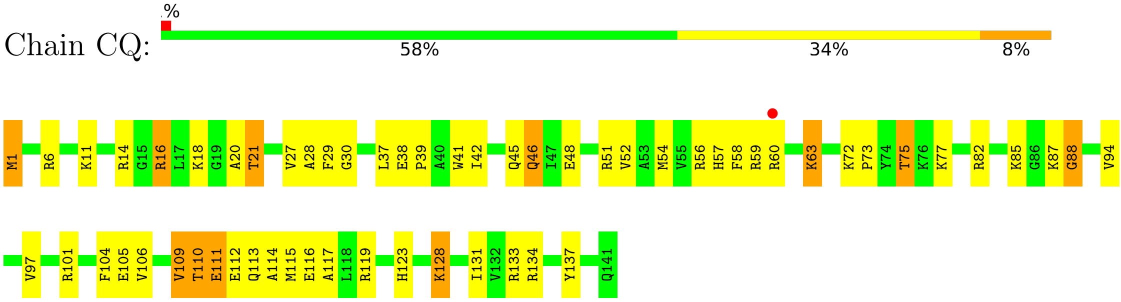
- Molecule 14: 50S ribosomal protein L16

Chain AQ:



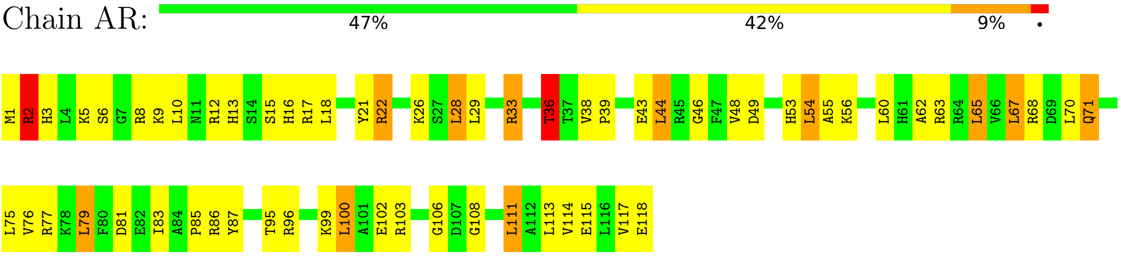
- Molecule 14: 50S ribosomal protein L16

Chain CQ:



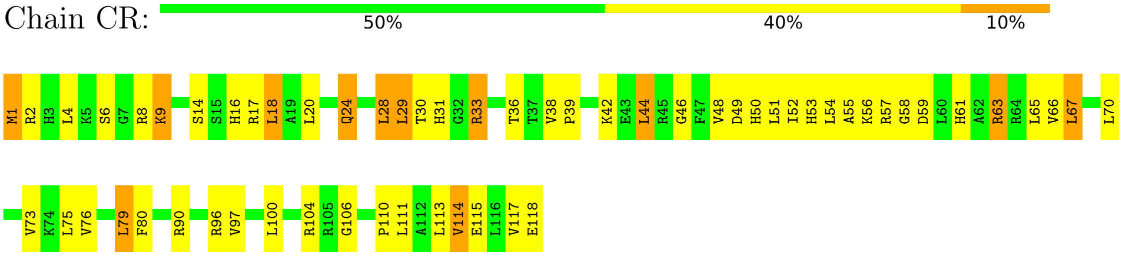
- Molecule 15: 50S ribosomal protein L17

Chain AR:



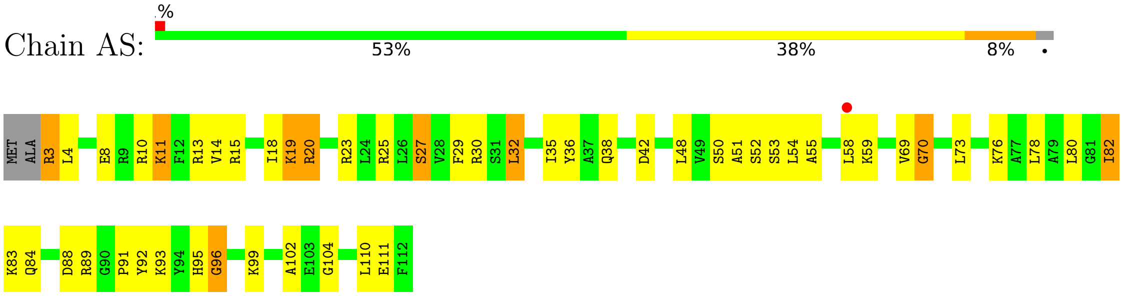
- Molecule 15: 50S ribosomal protein L17

Chain CR:



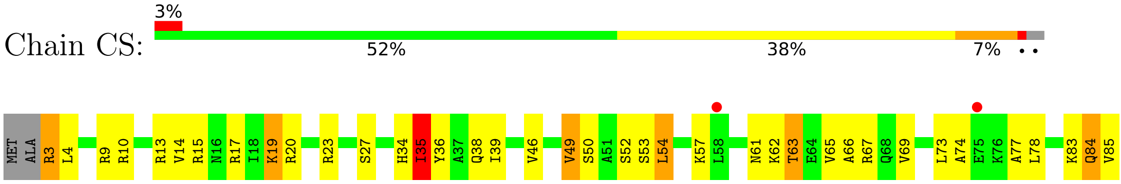
- Molecule 16: 50S ribosomal protein L18

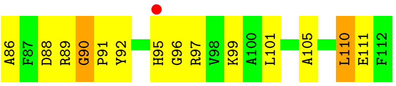
Chain AS:



- Molecule 16: 50S ribosomal protein L18

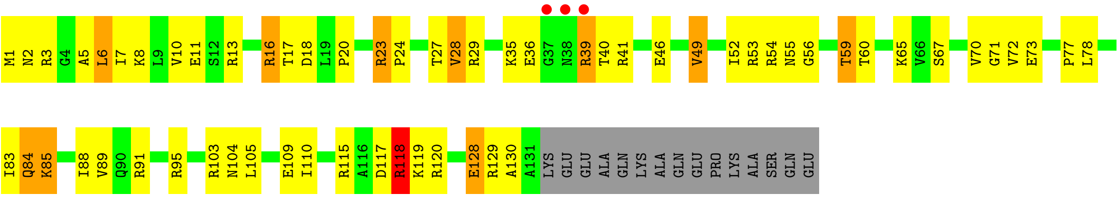
Chain CS:





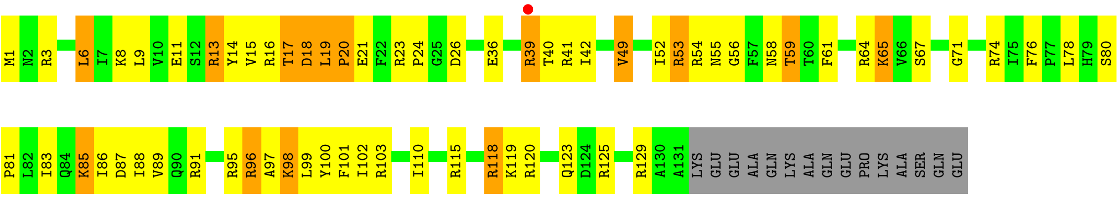
- Molecule 17: 50S ribosomal protein L19

Chain AT:



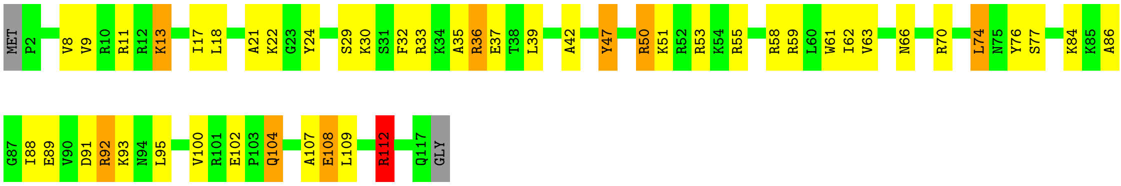
- Molecule 17: 50S ribosomal protein L19

Chain CT:



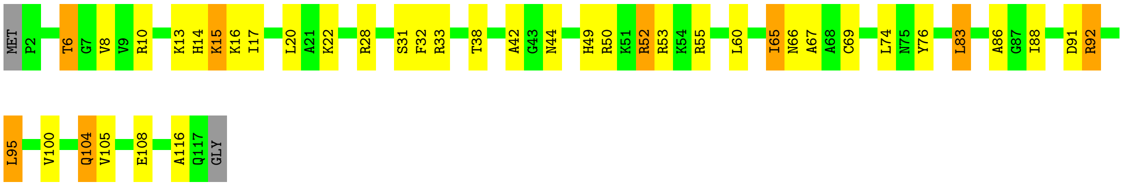
- Molecule 18: 50S ribosomal protein L20

Chain AU:



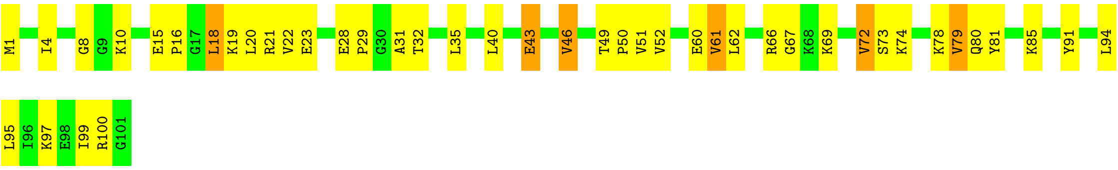
- Molecule 18: 50S ribosomal protein L20

Chain CU:



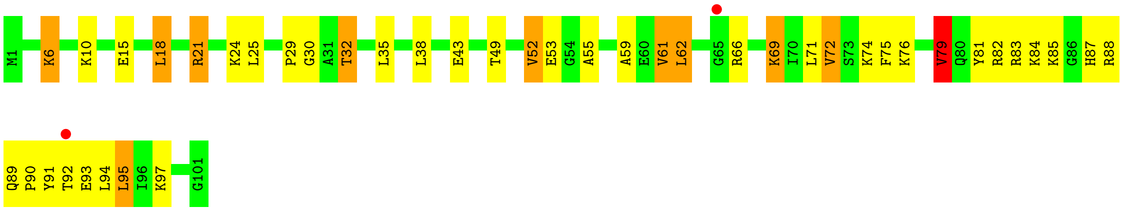
- Molecule 19: 50S ribosomal protein L21

Chain AV:



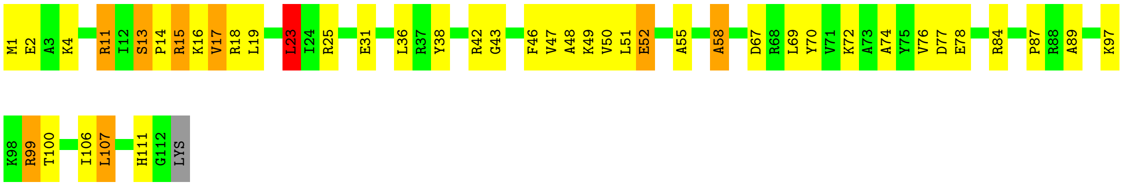
- Molecule 19: 50S ribosomal protein L21

Chain CV:



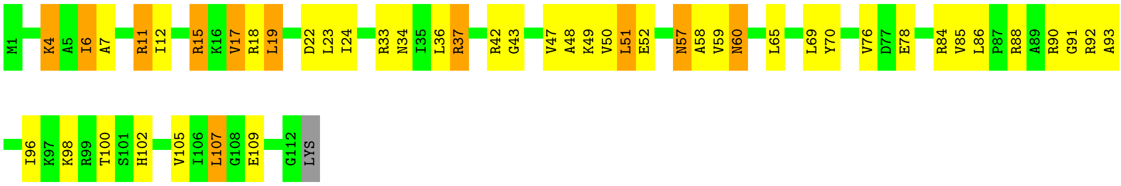
- Molecule 20: 50S ribosomal protein L22

Chain AW:



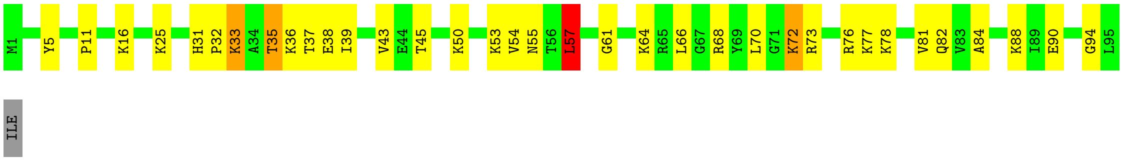
- Molecule 20: 50S ribosomal protein L22

Chain CW:



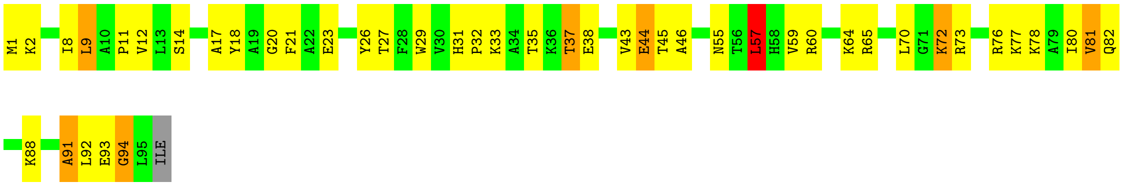
- Molecule 21: 50S ribosomal protein L23

Chain AX:

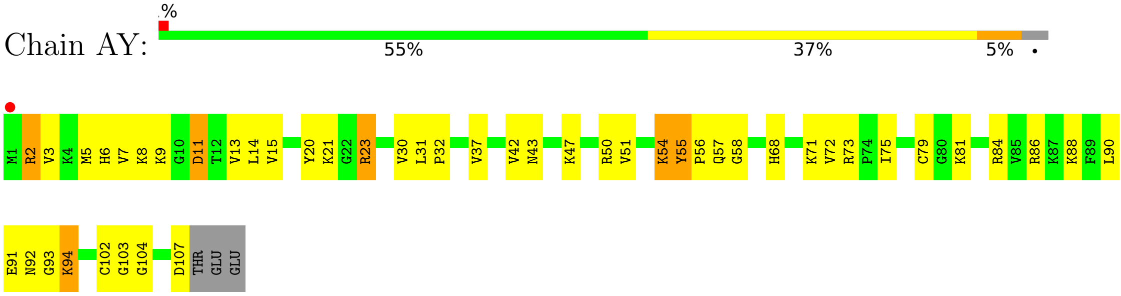


- Molecule 21: 50S ribosomal protein L23

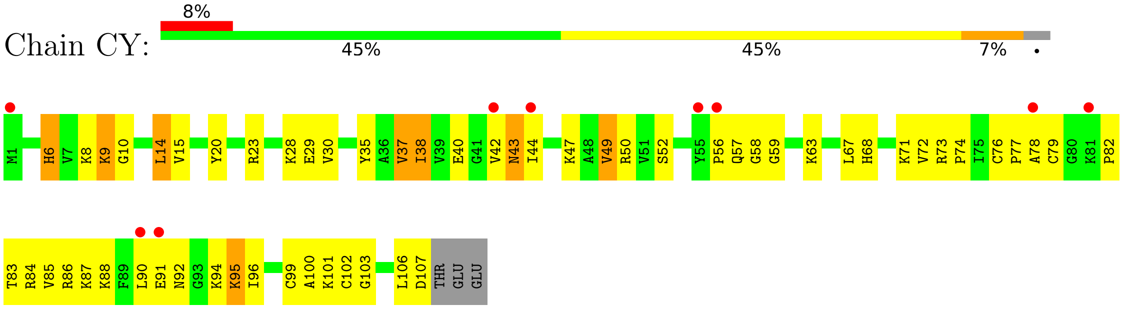
Chain CX:



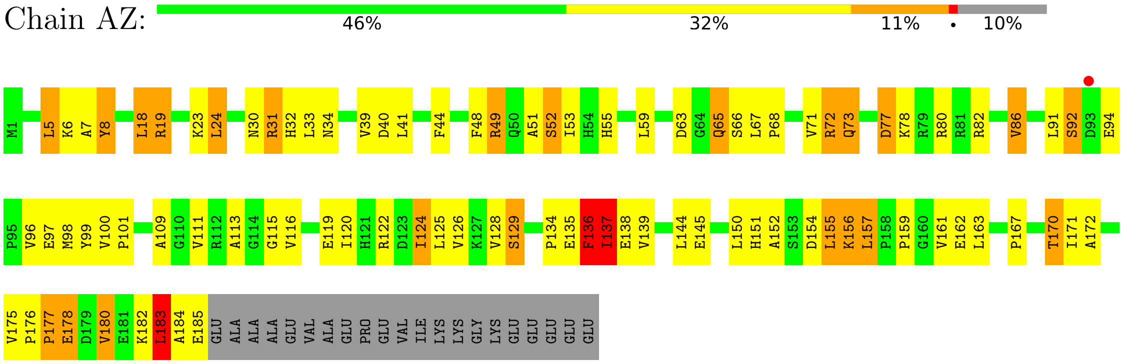
- Molecule 22: 50S ribosomal protein L24



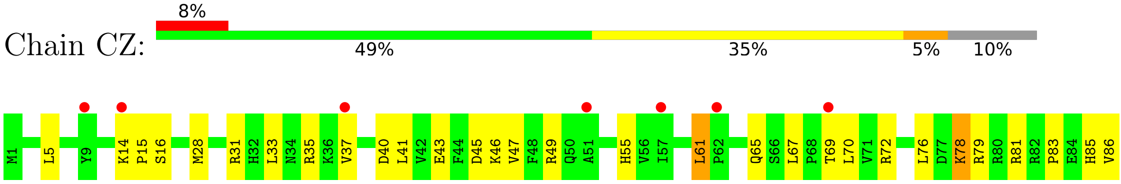
- Molecule 22: 50S ribosomal protein L24

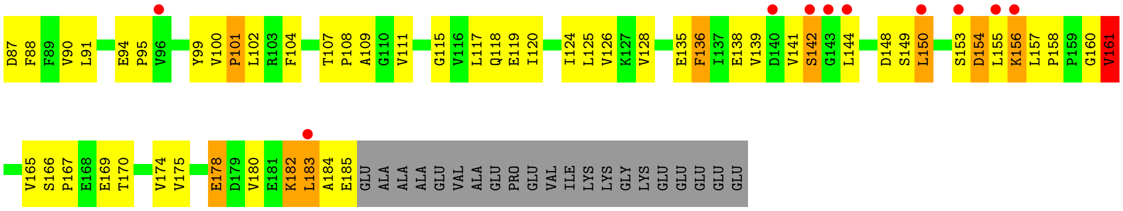


- Molecule 23: 50S ribosomal protein L25



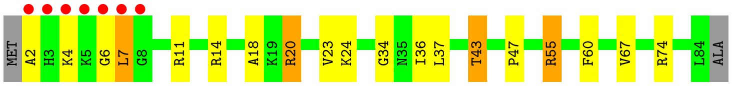
- Molecule 23: 50S ribosomal protein L25





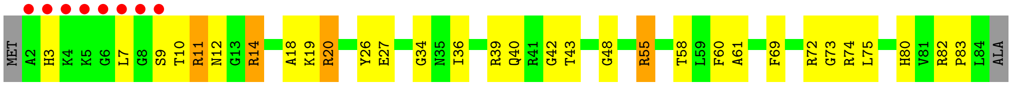
- Molecule 24: 50S ribosomal protein L27

Chain A0:



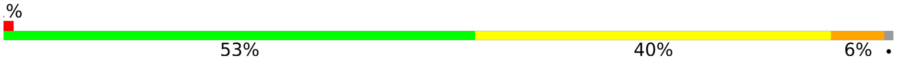
- Molecule 24: 50S ribosomal protein L27

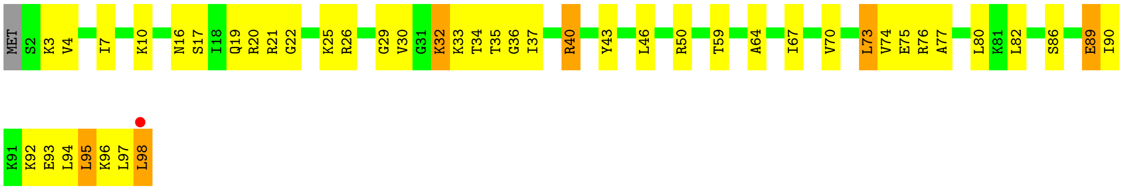
Chain C0:



- Molecule 25: 50S ribosomal protein L28

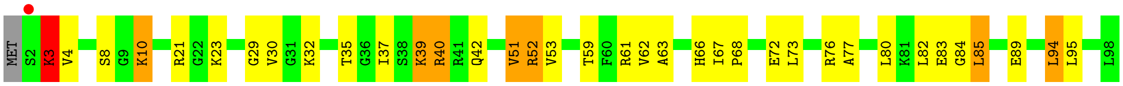
Chain A1:





- Molecule 25: 50S ribosomal protein L28

Chain C1:

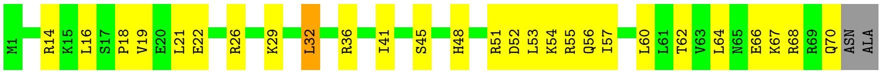


- Molecule 26: 50S ribosomal protein L29

Chain A2:

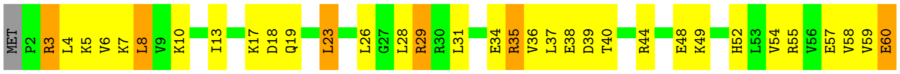
- Molecule 26: 50S ribosomal protein L29

Chain C2:



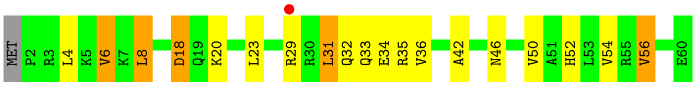
- Molecule 27: 50S ribosomal protein L30

Chain A3:

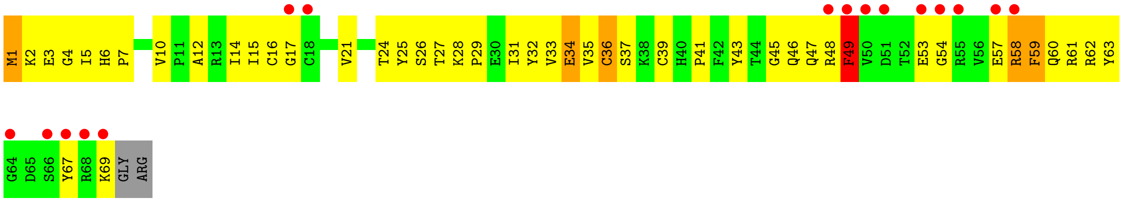
- Molecule 27: 50S ribosomal protein L30

Chain C3:

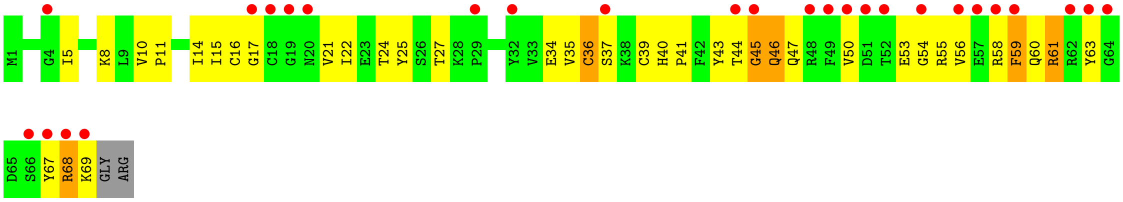
- Molecule 28: 50S ribosomal protein L31

Chain A4:

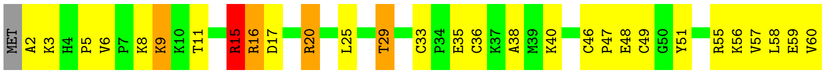
- Molecule 28: 50S ribosomal protein L31

Chain C4:

- Molecule 29: 50S ribosomal protein L32

Chain A5:

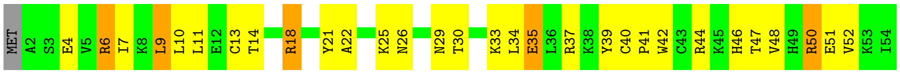



- Molecule 29: 50S ribosomal protein L32

Chain C5:

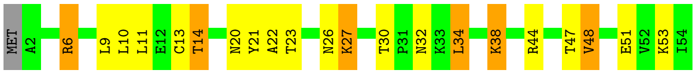

- Molecule 30: 50S ribosomal protein L33

Chain A6:



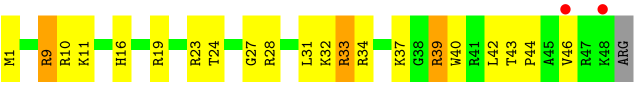
- Molecule 30: 50S ribosomal protein L33

Chain C6:



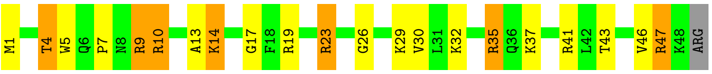
- Molecule 31: 50S ribosomal protein L34

Chain A7:



- Molecule 31: 50S ribosomal protein L34

Chain C7:



- Molecule 32: 50S ribosomal protein L35

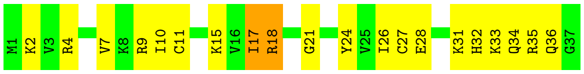
Chain A8:

- Molecule 32: 50S ribosomal protein L35

Chain C8:

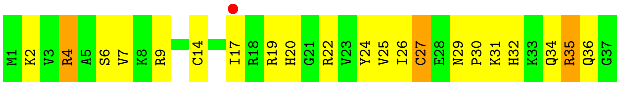
- Molecule 33: 50S ribosomal protein L36

Chain A9:



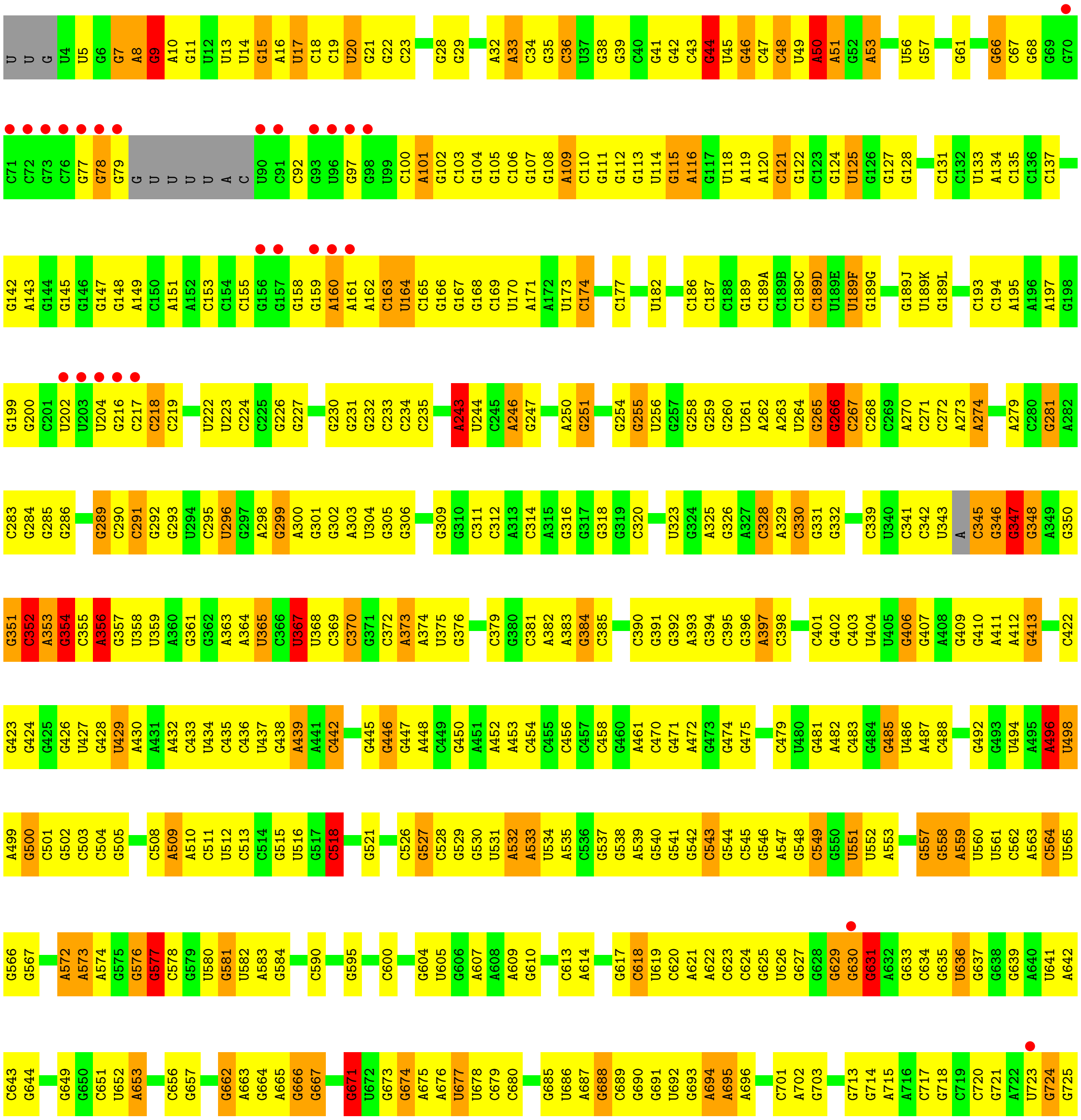
- Molecule 33: 50S ribosomal protein L36

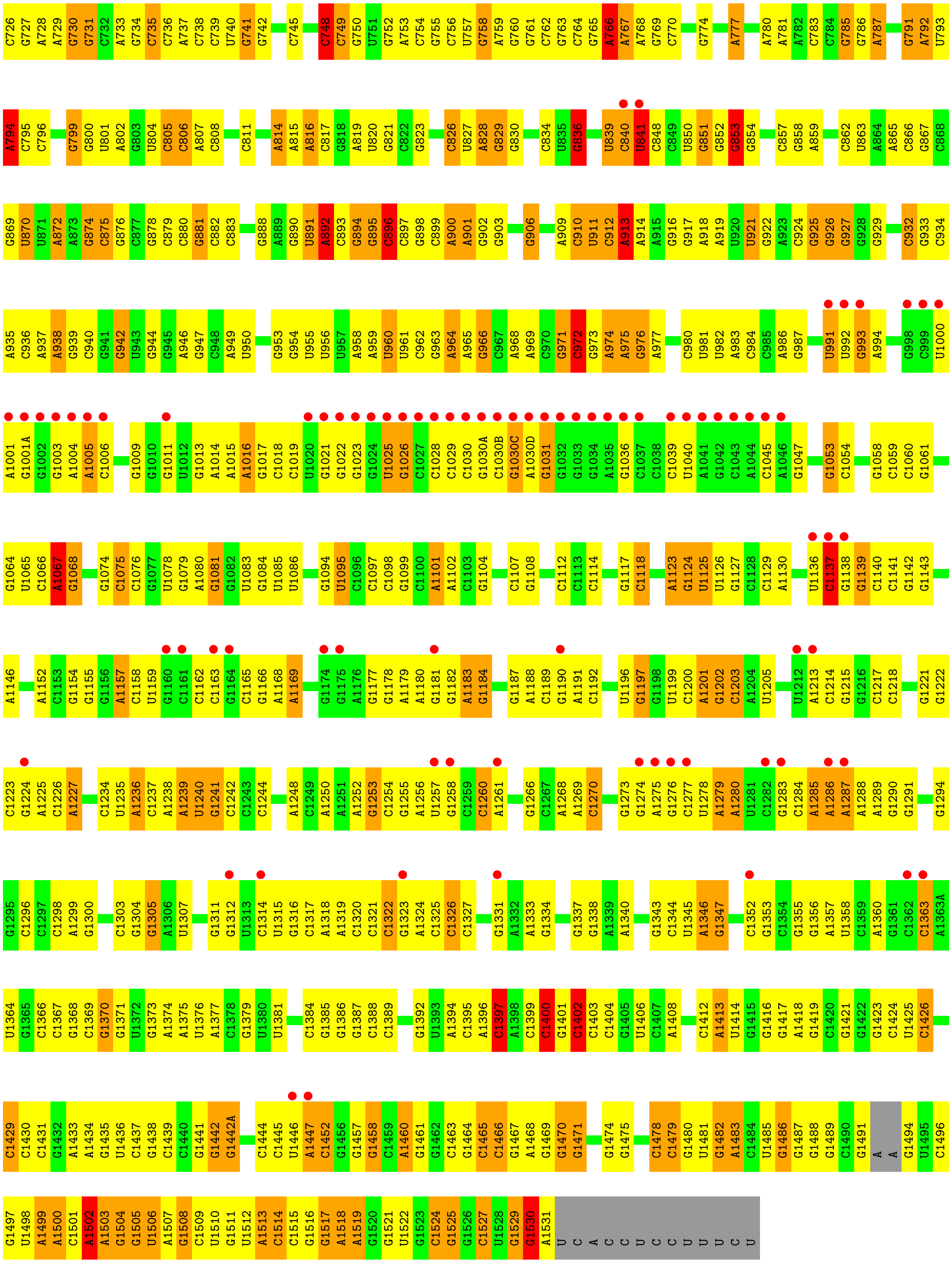
Chain C9:



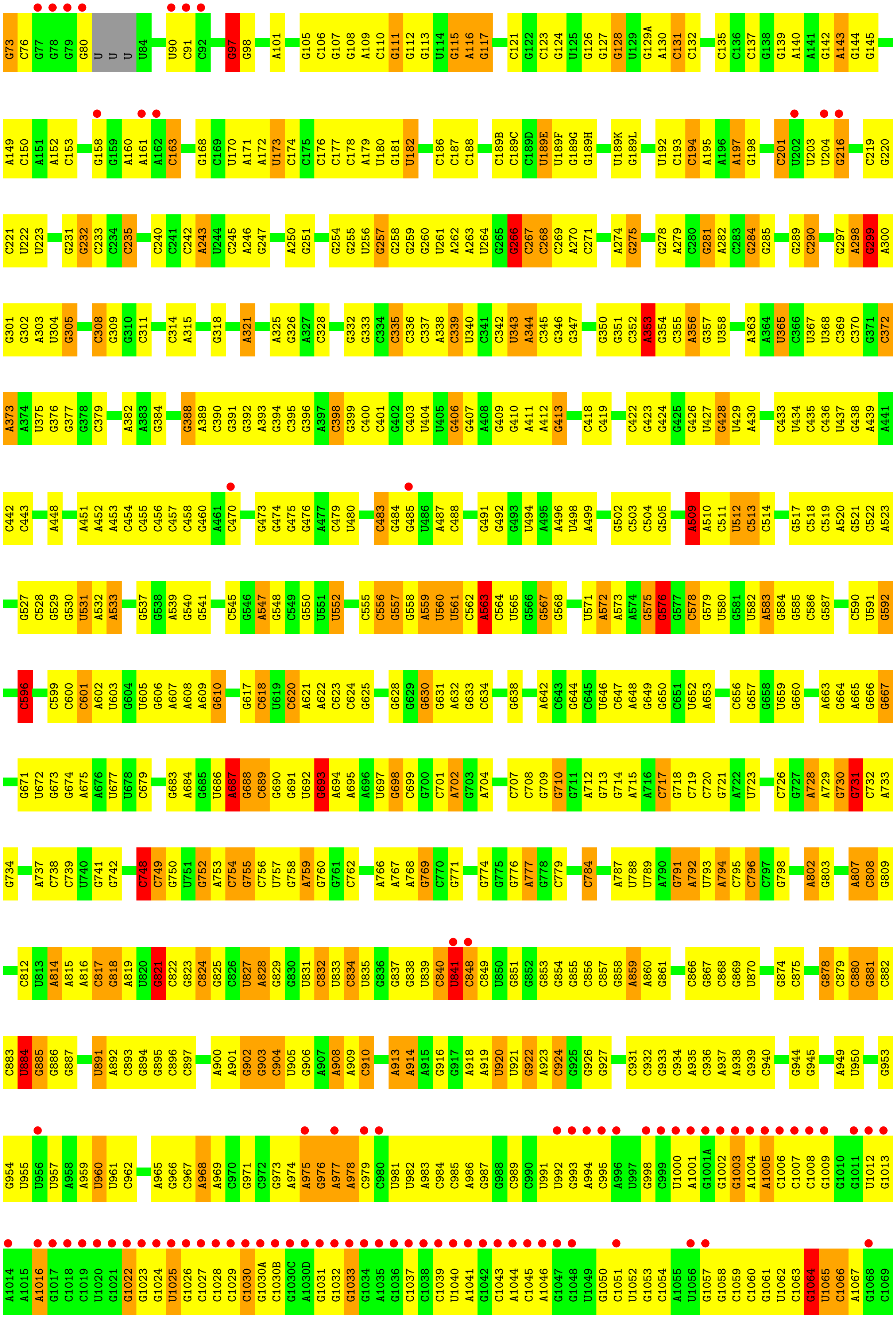
- Molecule 34: 16S Ribosomal RNA

Chain BA:





- Molecule 34: 16S Ribosomal RNA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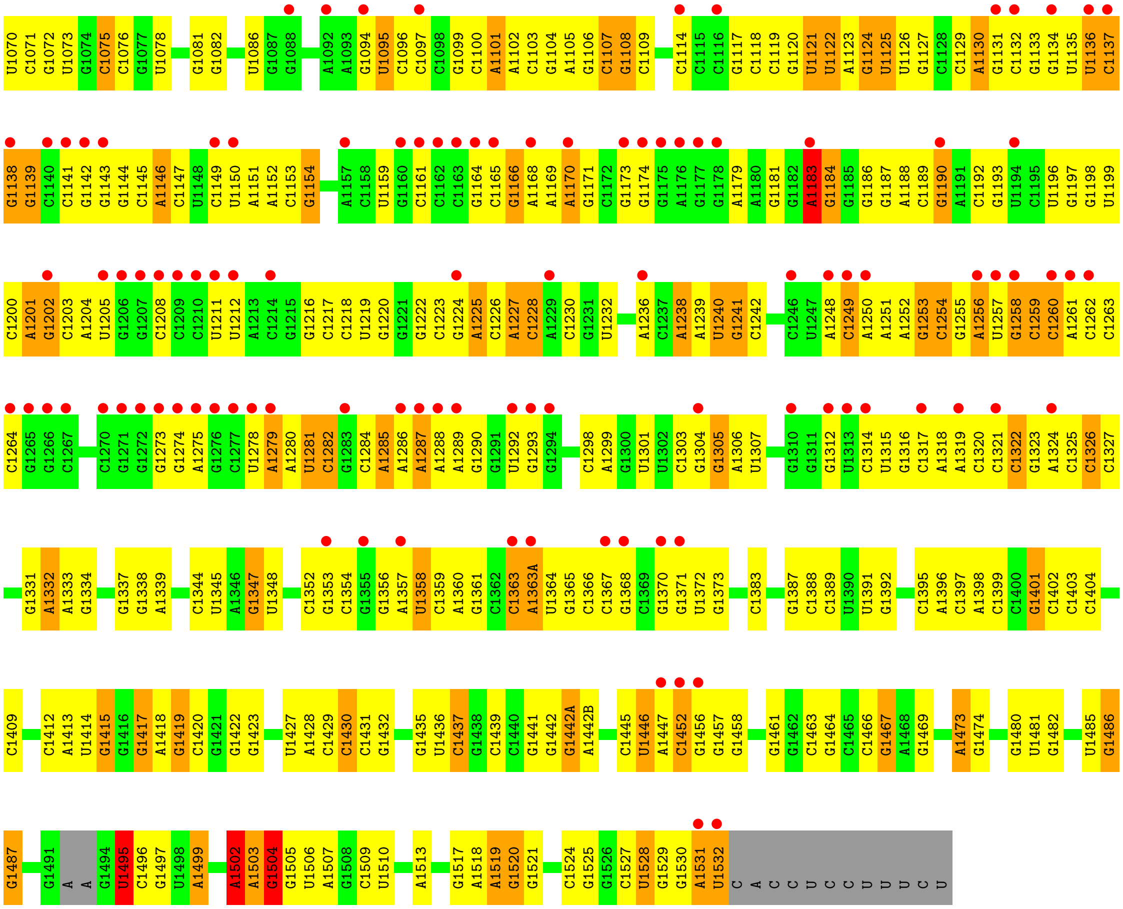
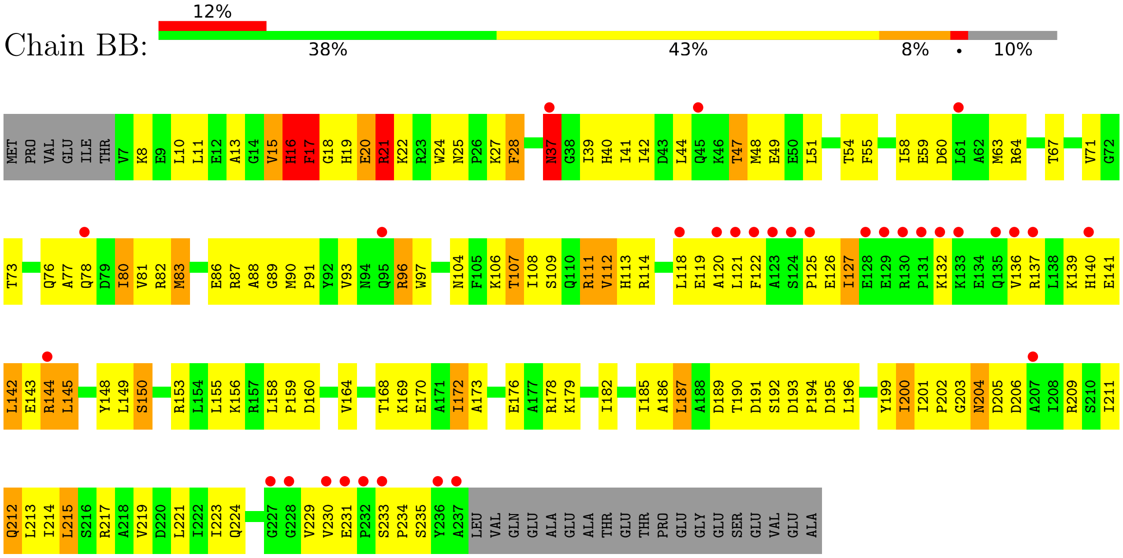
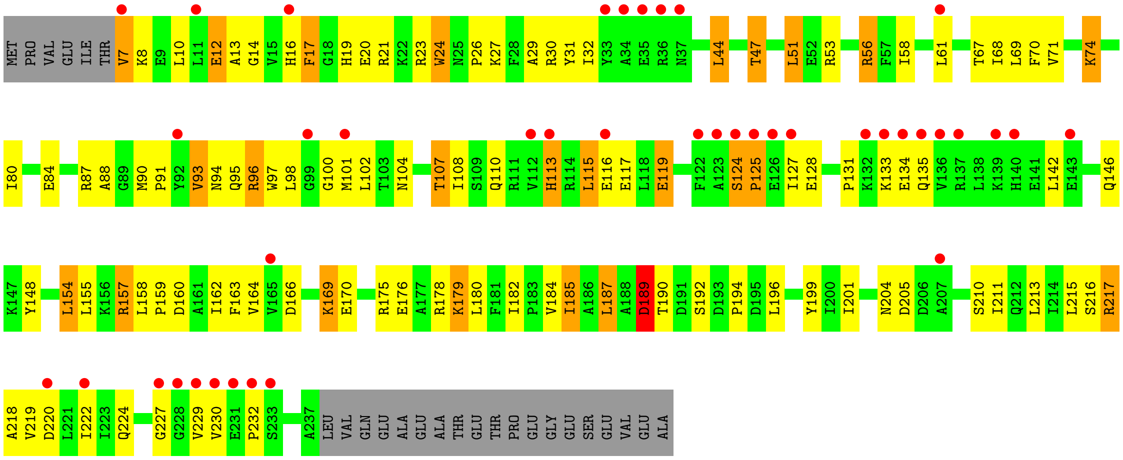


- Molecule 35: 30S ribosomal protein S2

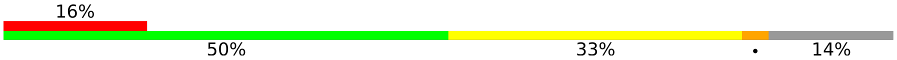


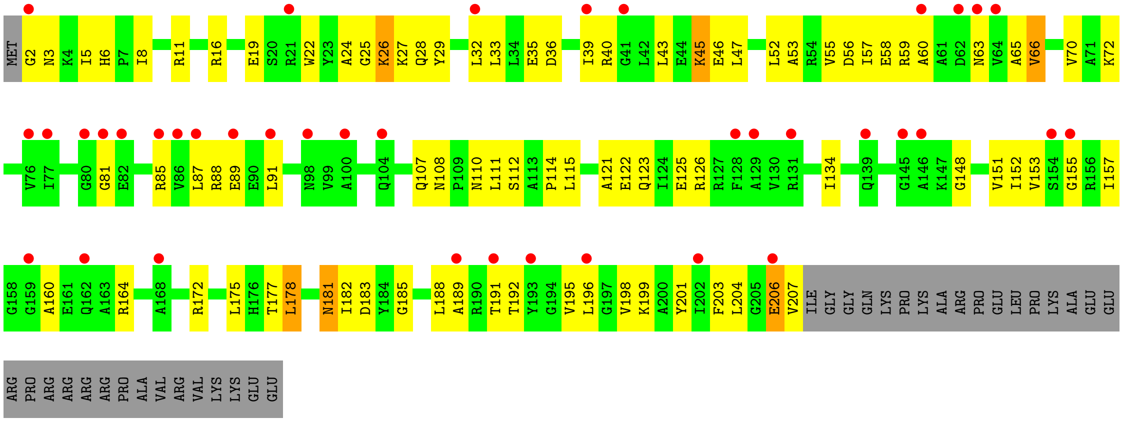
- Molecule 35: 30S ribosomal protein S2



- Molecule 36: 30S ribosomal protein S3

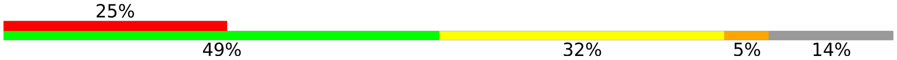
Chain BC:

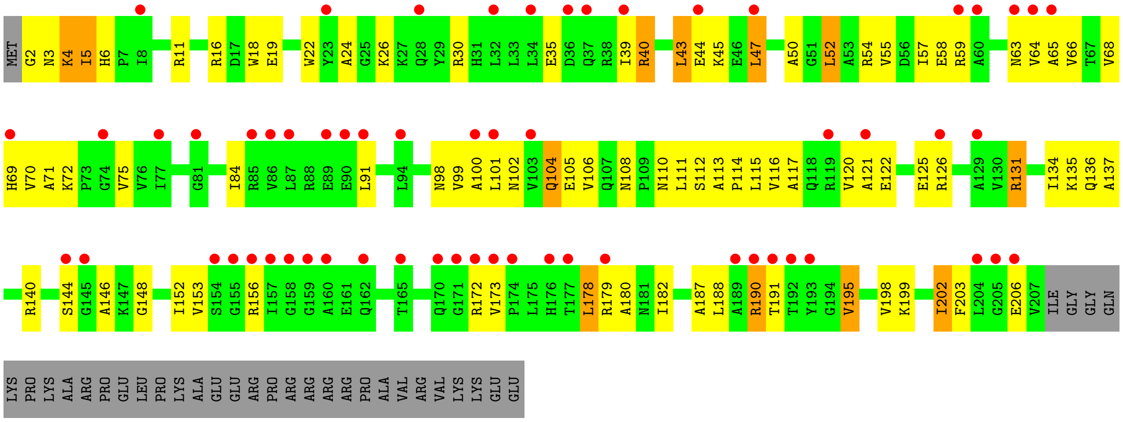




- Molecule 36: 30S ribosomal protein S3

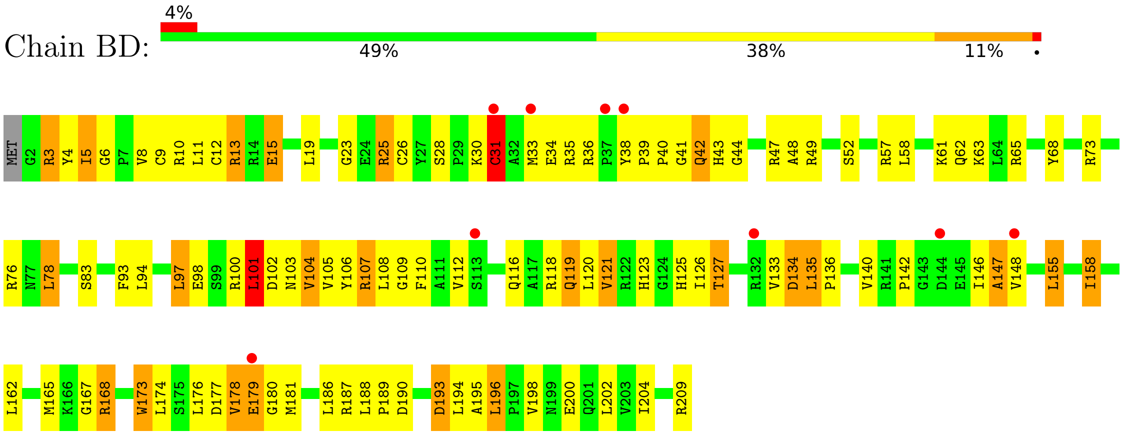
Chain DC:





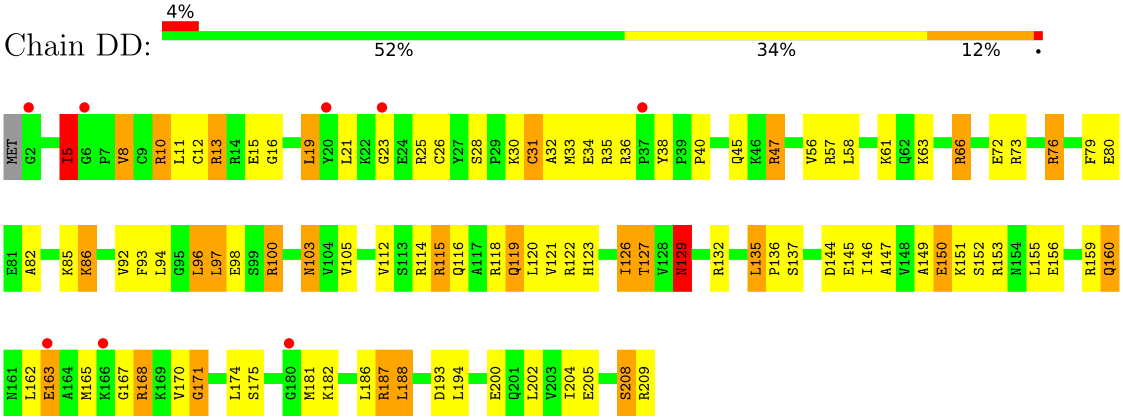
- Molecule 37: 30S ribosomal protein S4

Chain BD:



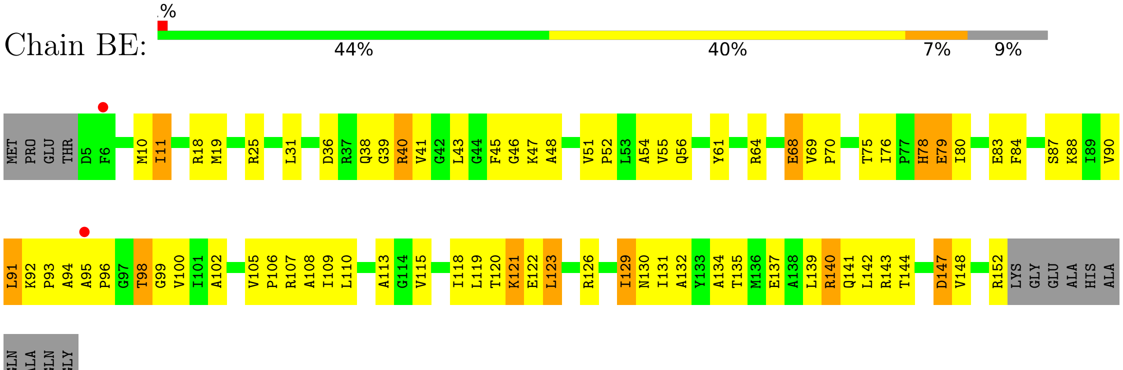
- Molecule 37: 30S ribosomal protein S4

Chain DD:



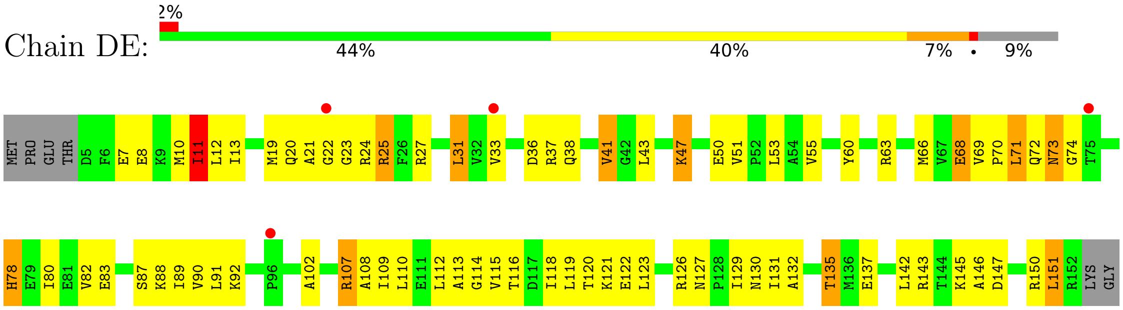
- Molecule 38: 30S ribosomal protein S5

Chain BE:



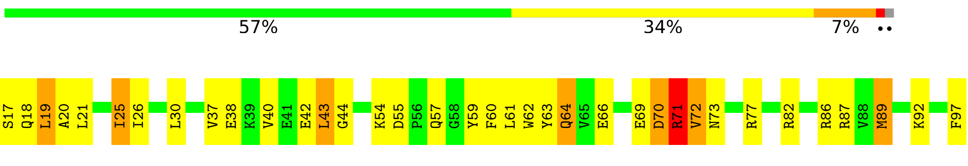
- Molecule 38: 30S ribosomal protein S5

Chain DE:



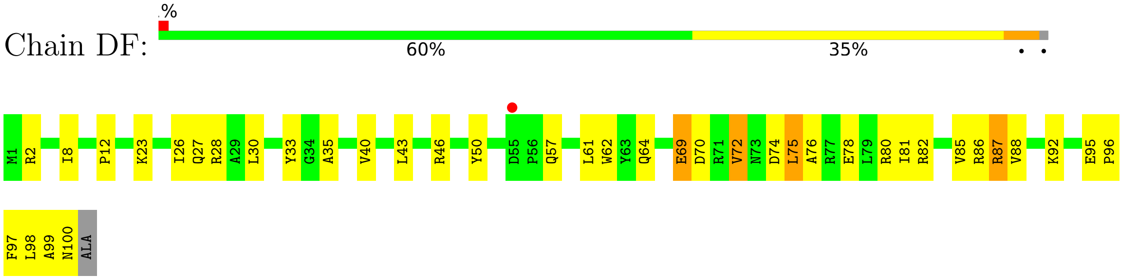
- Molecule 39: 30S ribosomal protein S6

Chain BF:



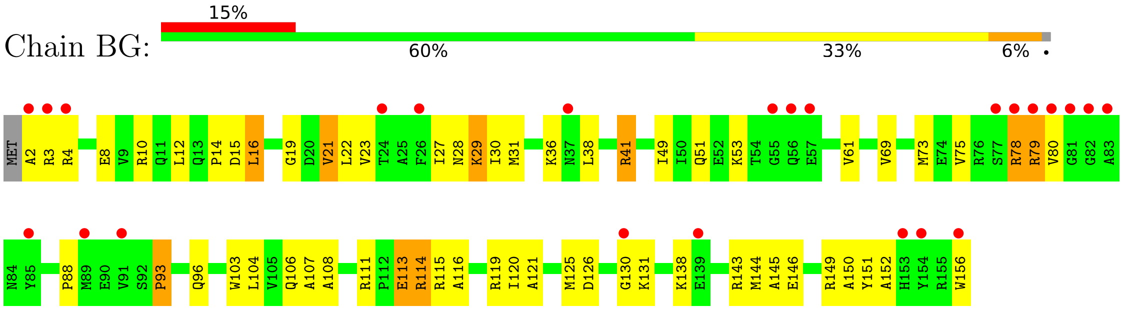
- Molecule 39: 30S ribosomal protein S6

Chain DF:



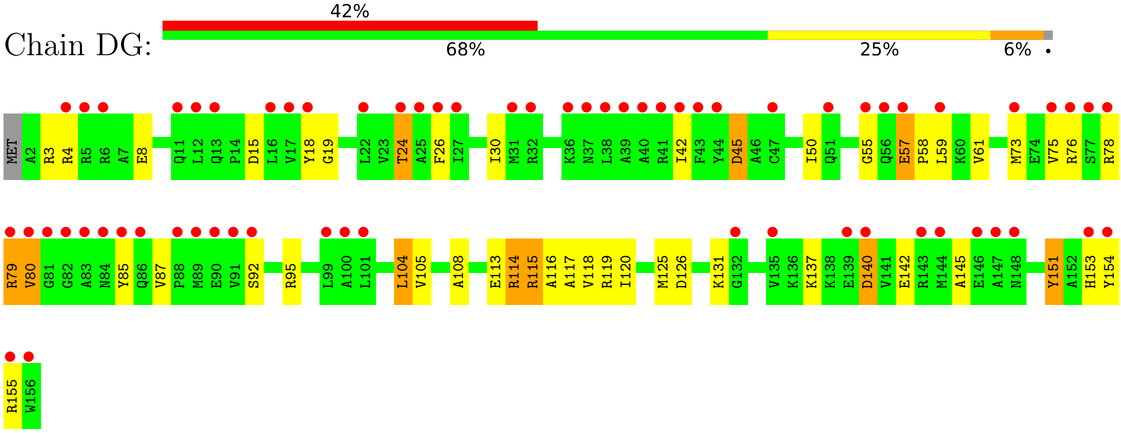
- Molecule 40: 30S ribosomal protein S7

Chain BG:

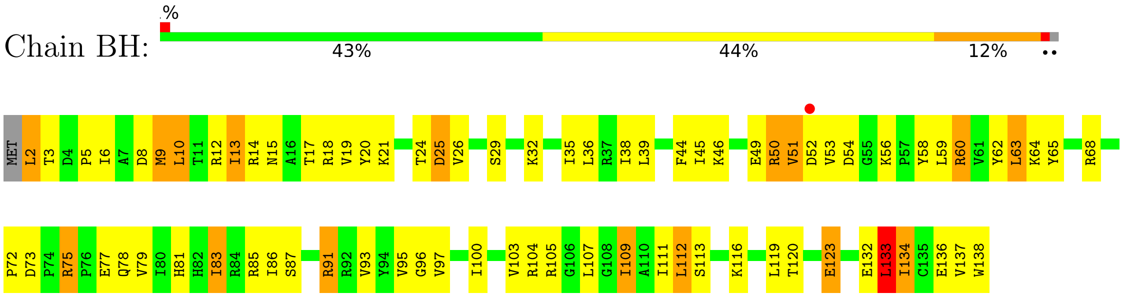


- Molecule 40: 30S ribosomal protein S7

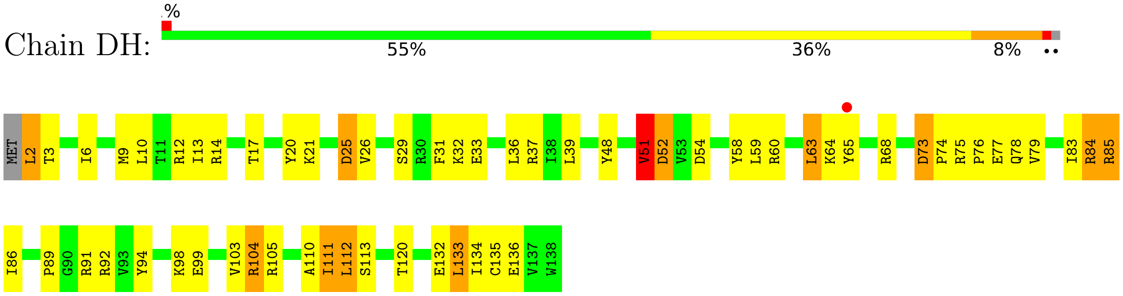
Chain DG:



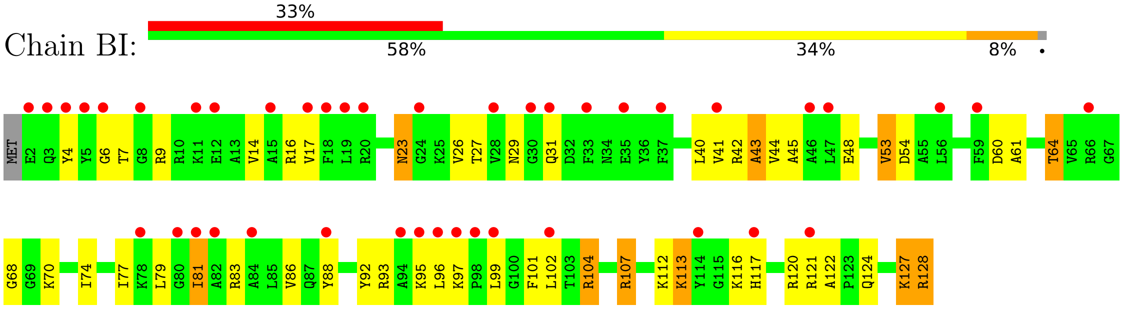
- Molecule 41: 30S ribosomal protein S8



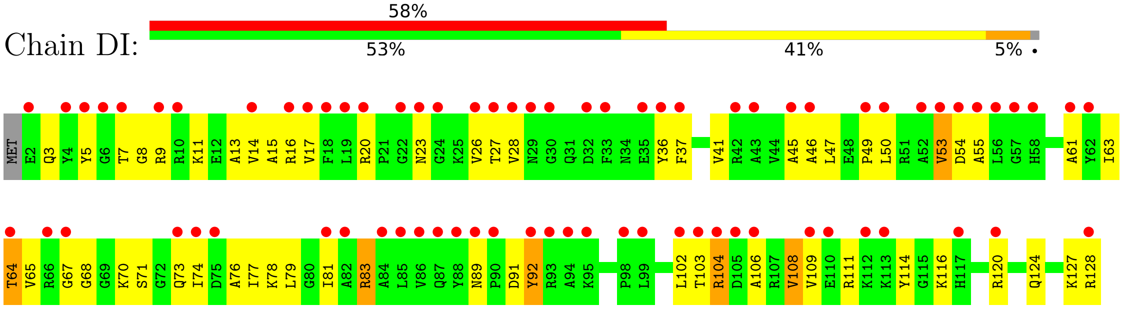
- Molecule 41: 30S ribosomal protein S8



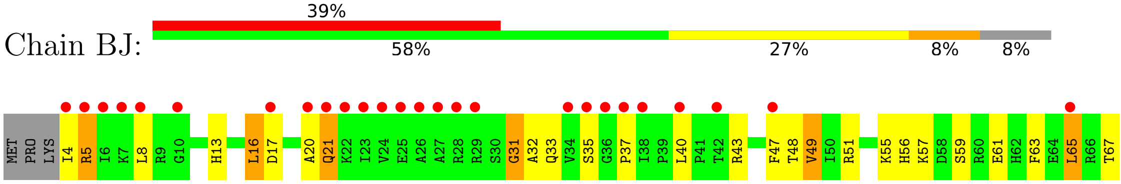
- Molecule 42: 30S ribosomal protein S9

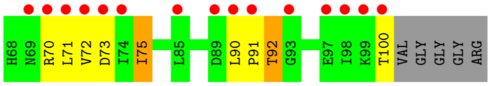


- Molecule 42: 30S ribosomal protein S9

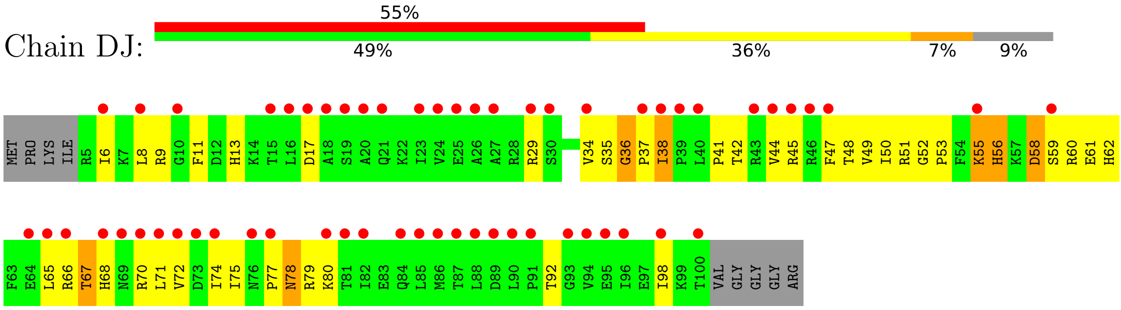


- Molecule 43: 30S ribosomal protein S10

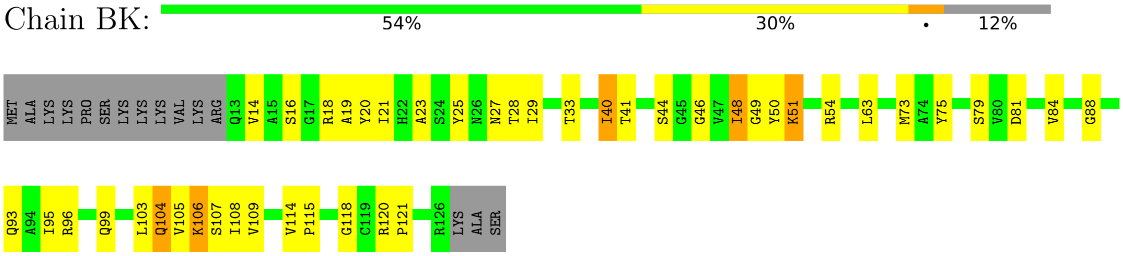




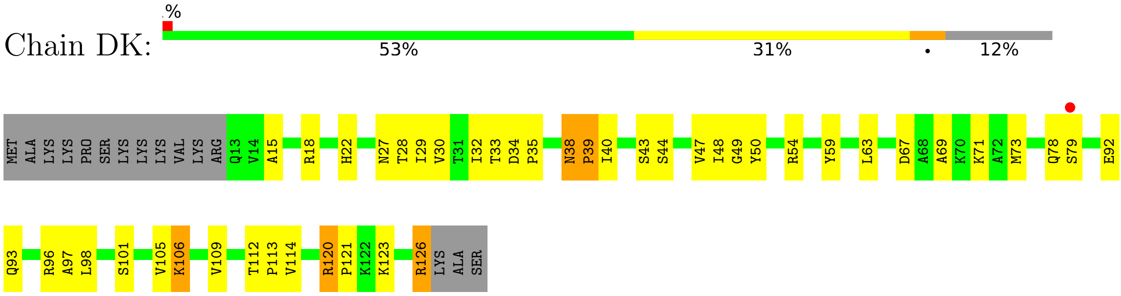
- Molecule 43: 30S ribosomal protein S10



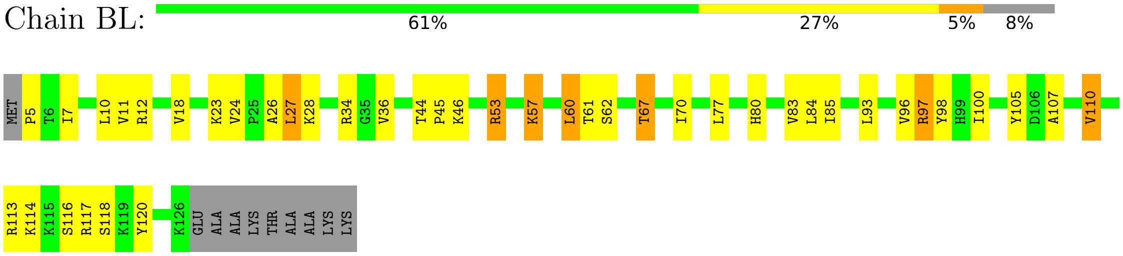
- Molecule 44: 30S ribosomal protein S11



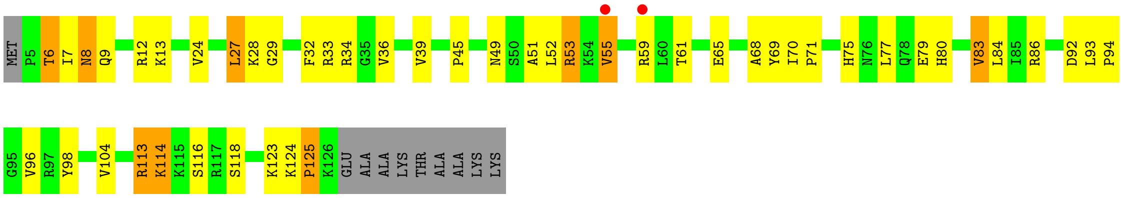
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12

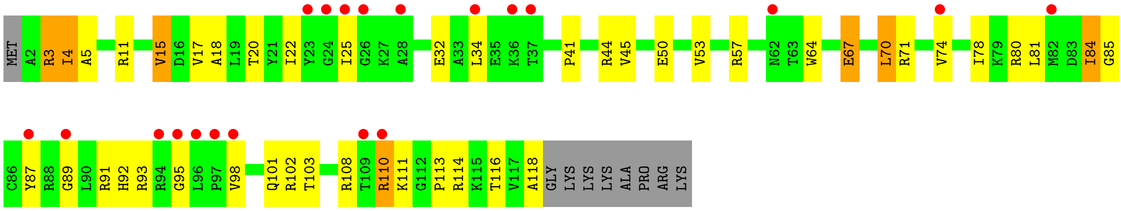


- Molecule 45: 30S ribosomal protein S12



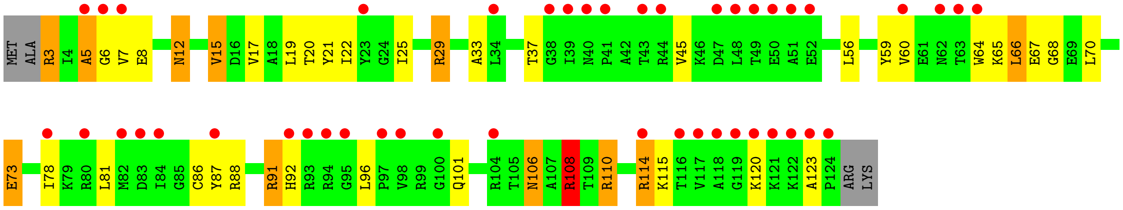
- Molecule 46: 30S ribosomal protein S13

Chain BM:



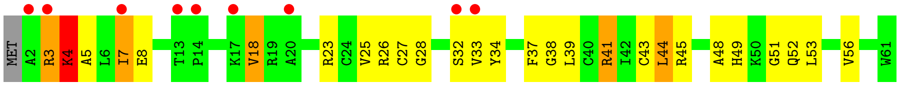
- Molecule 46: 30S ribosomal protein S13

Chain DM:



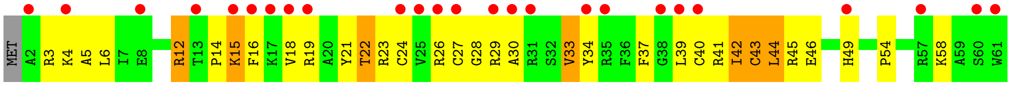
- Molecule 47: 30S ribosomal protein S14 type Z

Chain BN:



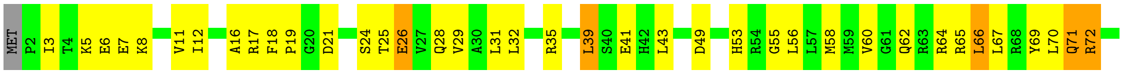
- Molecule 47: 30S ribosomal protein S14 type Z

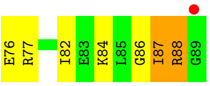
Chain DN:



- Molecule 48: 30S ribosomal protein S15

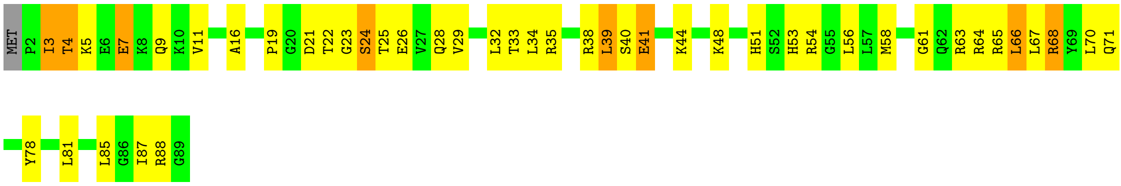
Chain BO:





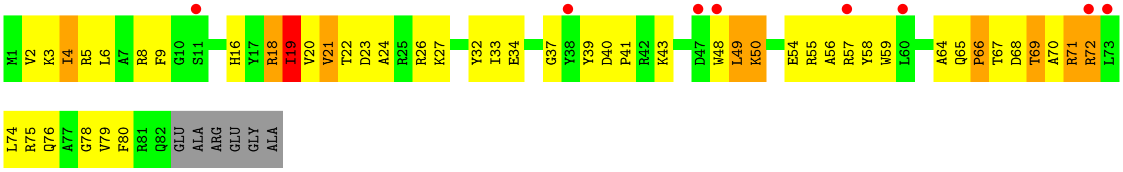
- Molecule 48: 30S ribosomal protein S15

Chain DO:



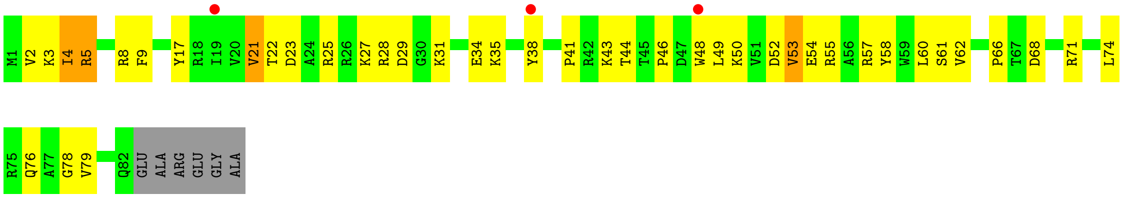
- Molecule 49: 30S ribosomal protein S16

Chain BP:



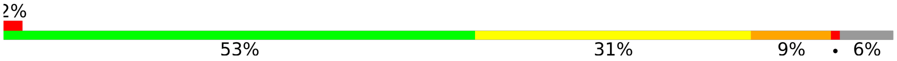
- Molecule 49: 30S ribosomal protein S16

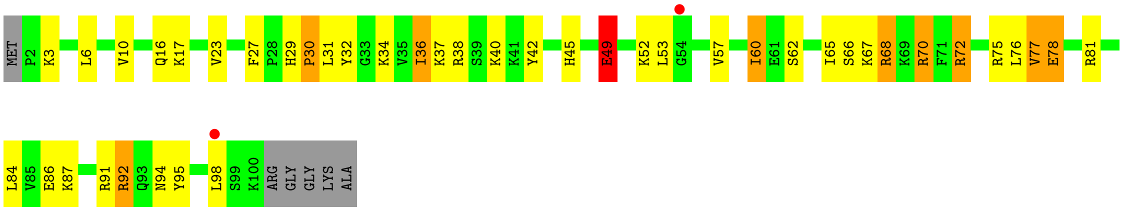
Chain DP:



- Molecule 50: 30S ribosomal protein S17

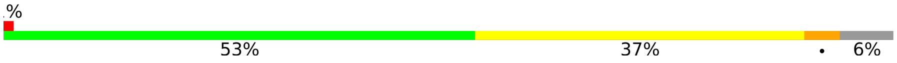
Chain BQ:





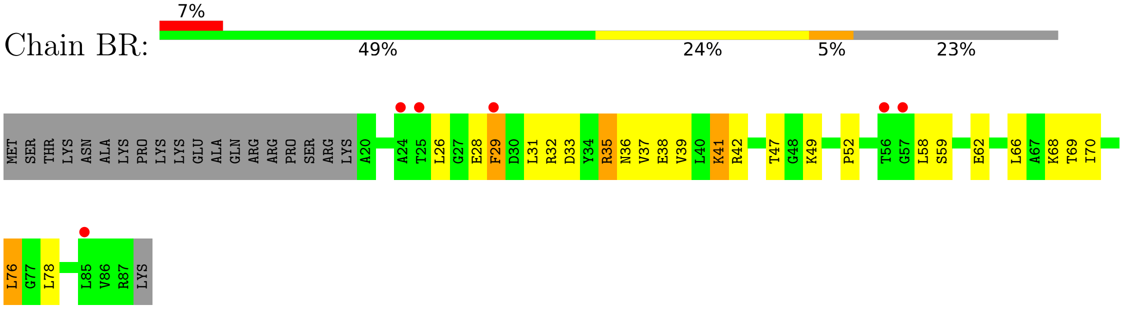
- Molecule 50: 30S ribosomal protein S17

Chain DQ:



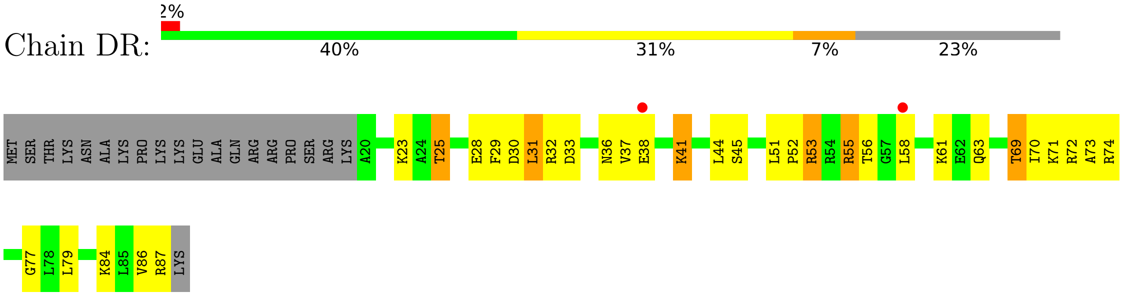
- Molecule 51: 30S ribosomal protein S18

Chain BR:



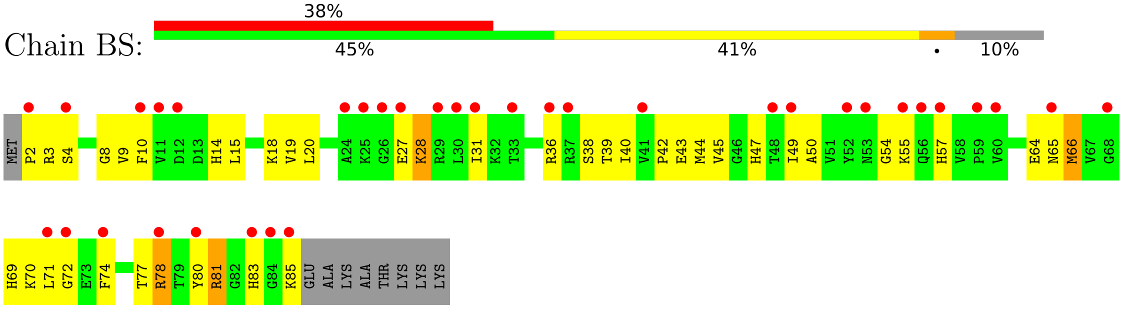
- Molecule 51: 30S ribosomal protein S18

Chain DR:



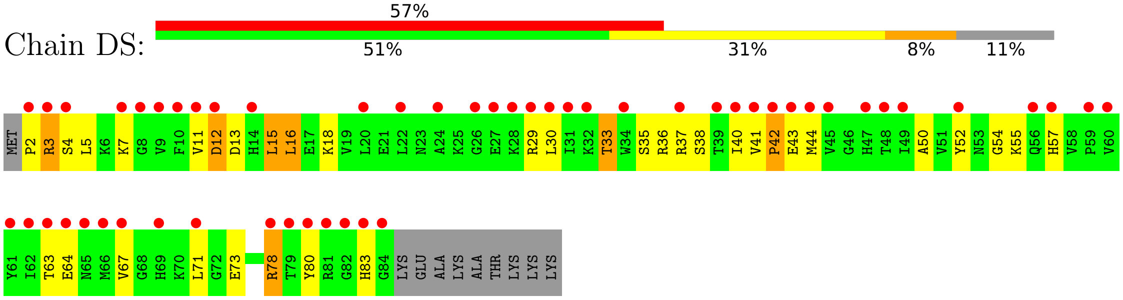
- Molecule 52: 30S ribosomal protein S19

Chain BS:

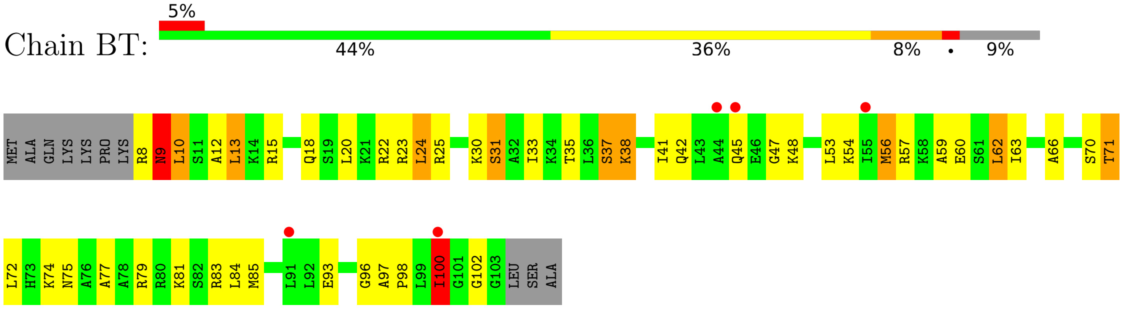


- Molecule 52: 30S ribosomal protein S19

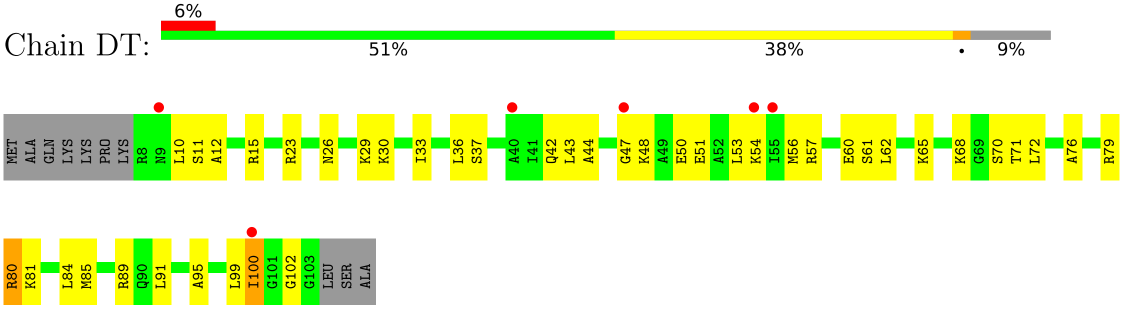
Chain DS:



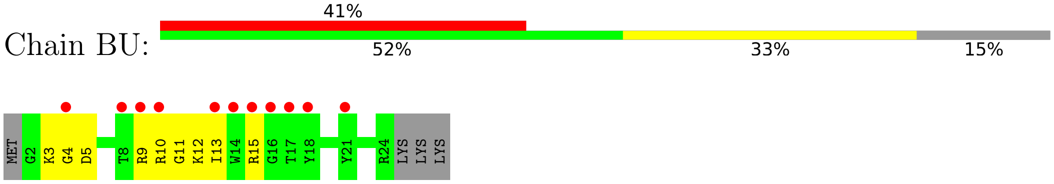
- Molecule 53: 30S ribosomal protein S20



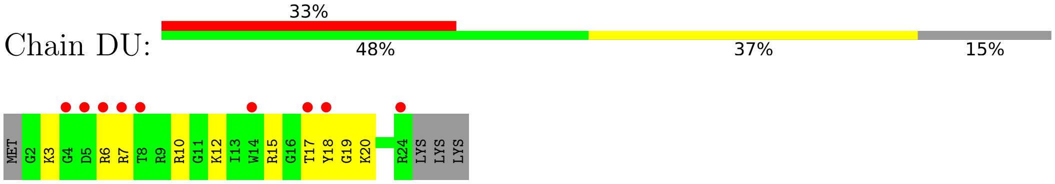
- Molecule 53: 30S ribosomal protein S20



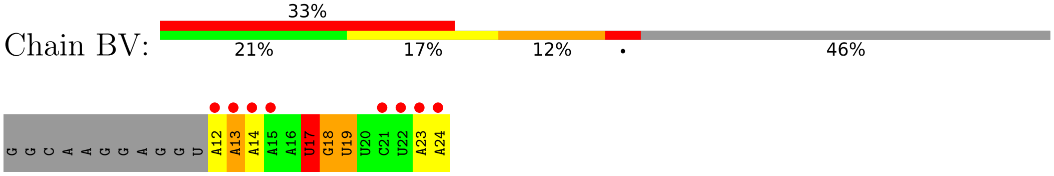
- Molecule 54: 30S ribosomal protein Thx



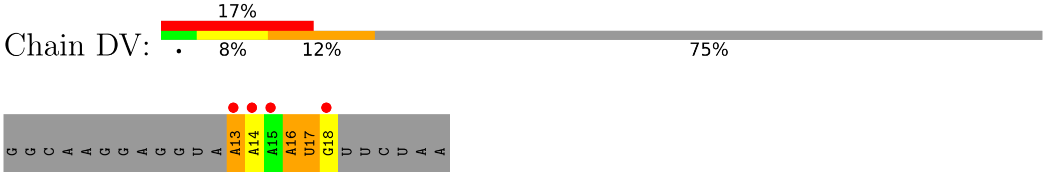
- Molecule 54: 30S ribosomal protein Thx



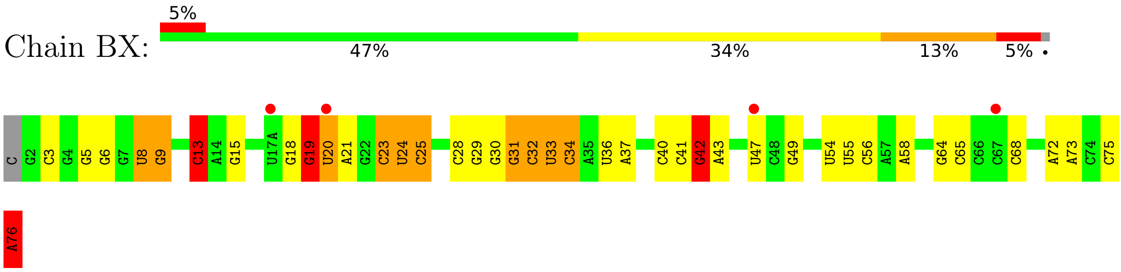
- Molecule 55: mRNA



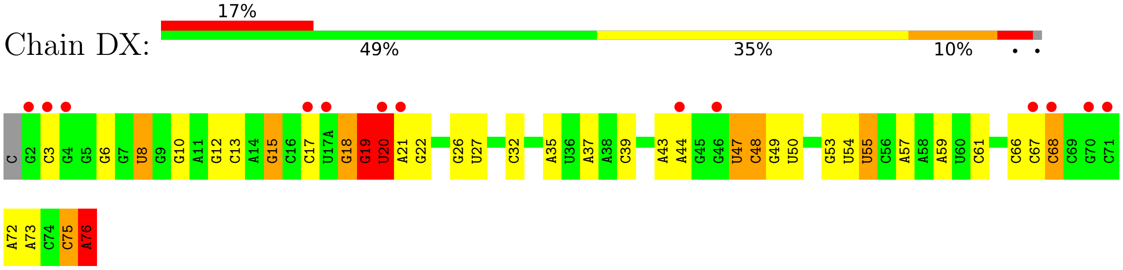
- Molecule 55: mRNA



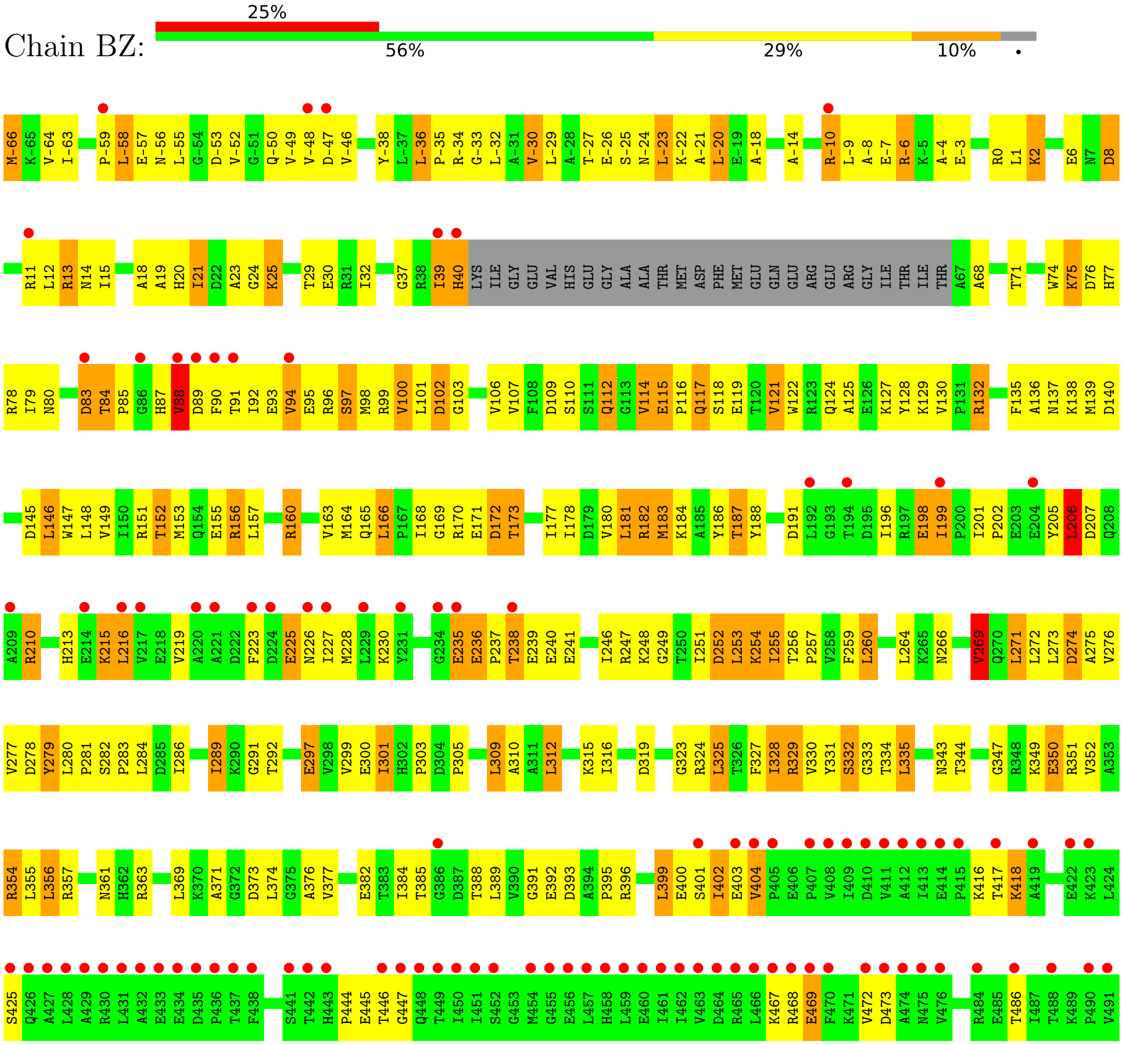
- Molecule 56: P-site tRNA

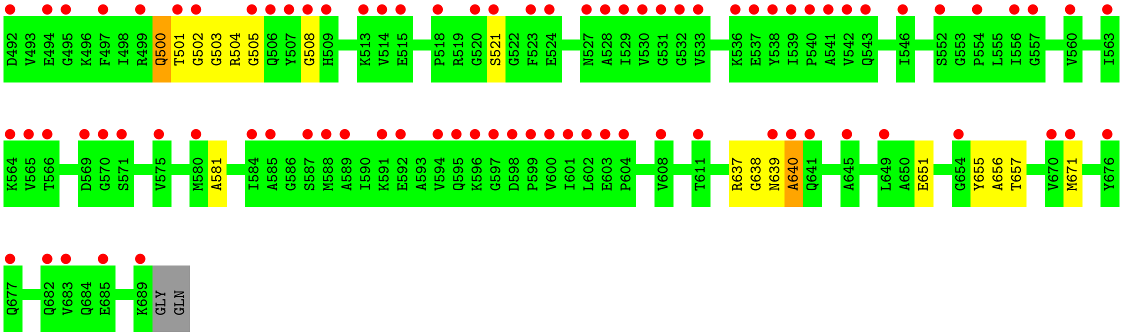


- Molecule 56: P-site tRNA



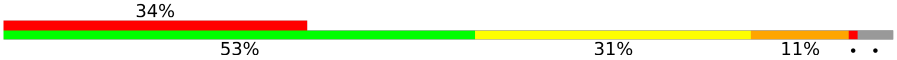
- Molecule 57: 50S ribosomal protein L9,Elongation factor G

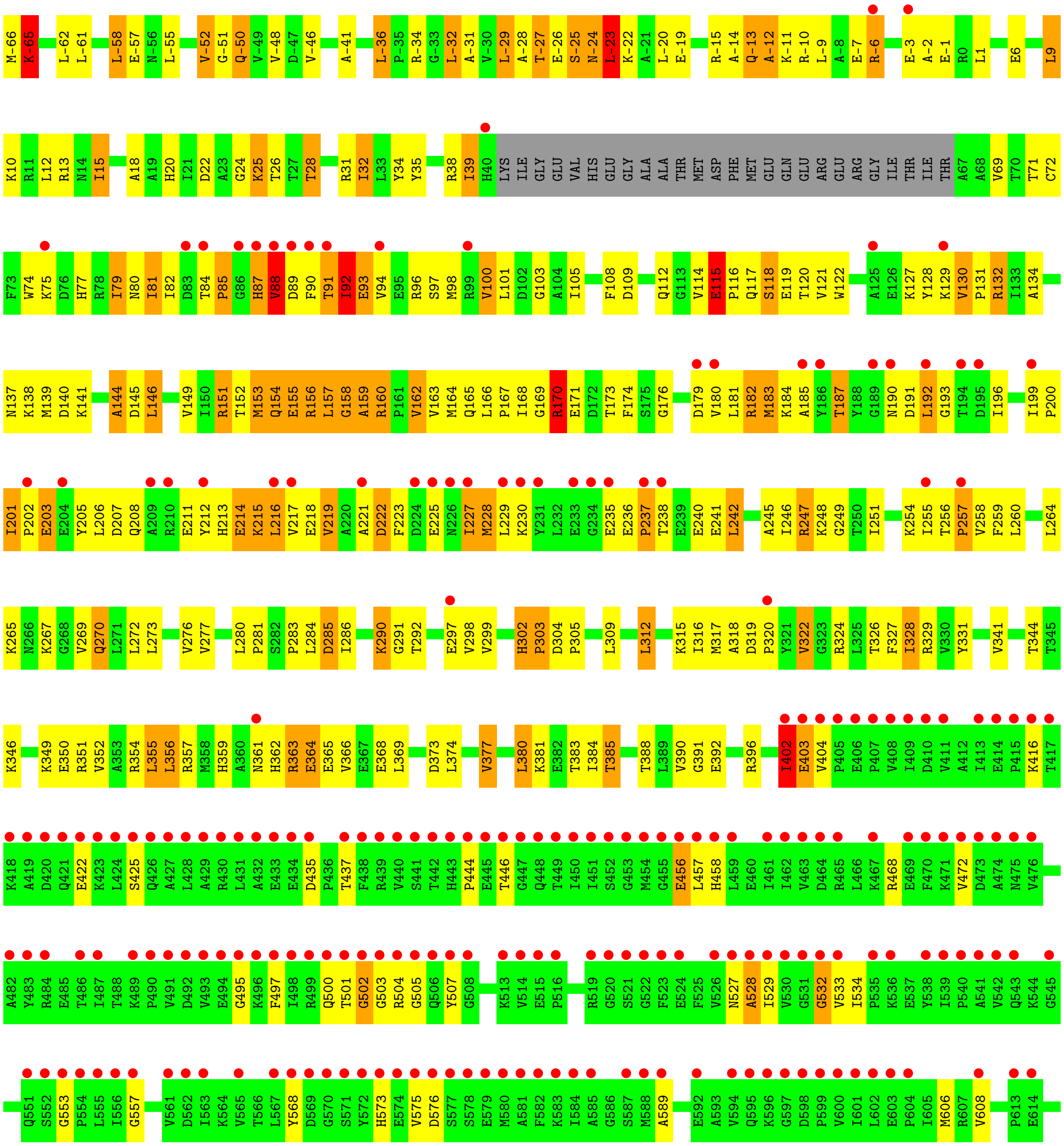


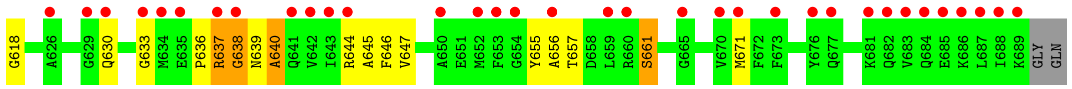


- Molecule 57: 50S ribosomal protein L9,Elongation factor G

Chain DZ:






G618
A626
G629
Q630
G633
M634
E635
P636
R637
G638
N639
A640
Q641
V642
I643
R644
A645
F646
V647
A650
E651
M652
F653
G654
Y655
A656
T657
D658
L659
R660
S661
G665
V670
M671
F672
F673
Y676
Q677
K681
Q682
V683
Q684
E685
K686
L687
I688
K689
GLY
GLN

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.48Å 448.89Å 622.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 2.80 49.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.31-2.80) 96.8 (49.71-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.221 , 0.266 0.221 , 0.266	Depositor DCC
R_{free} test set	69082 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 71.5	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.38, $< L^2 >$ = 0.20	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	305548	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PSU, GDP, MG, 5MU, 4SU, SF4, 5MC, K

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	1.44	524/68792 (0.8%)	2.20	4798/107377 (4.5%)
1	CA	1.00	54/68691 (0.1%)	1.63	1529/107219 (1.4%)
2	AB	1.20	7/2878 (0.2%)	2.00	147/4490 (3.3%)
2	CB	0.69	0/2878	1.28	12/4490 (0.3%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.91	1/2186 (0.0%)	1.09	10/2944 (0.3%)
4	CD	0.75	0/2192	0.94	2/2951 (0.1%)
5	AE	0.99	0/1592	1.10	1/2149 (0.0%)
5	CE	0.65	0/1592	0.87	1/2149 (0.0%)
6	AF	0.92	1/1619 (0.1%)	1.06	11/2193 (0.5%)
6	CF	0.67	0/1615	0.84	1/2188 (0.0%)
7	AG	0.60	0/1450	0.80	0/1959
7	CG	0.41	0/1449	0.65	0/1958
8	AH	0.82	0/1356	0.95	0/1834
8	CH	0.40	0/1356	0.61	0/1834
9	AK	0.40	0/640	0.75	0/889
9	CK	0.31	0/640	0.64	0/889
10	AL	0.38	0/1044	0.58	0/1416
10	CL	0.39	0/1044	0.59	0/1416
11	AN	1.06	0/1144	1.09	4/1543 (0.3%)
11	CN	0.54	0/1144	0.74	0/1543
12	AO	0.91	2/943 (0.2%)	1.07	3/1269 (0.2%)
12	CO	0.71	0/943	0.81	0/1269
13	AP	0.87	0/1156	1.10	4/1537 (0.3%)
13	CP	0.60	0/1152	0.85	1/1533 (0.1%)
14	AQ	0.99	0/1143	1.05	2/1527 (0.1%)
14	CQ	0.64	0/1143	0.79	0/1527
15	AR	1.00	0/982	1.14	3/1312 (0.2%)
15	CR	0.62	0/982	0.85	0/1312
16	AS	0.77	0/887	0.90	0/1180
16	CS	0.53	0/880	0.76	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AT	0.89	0/1105	1.08	3/1477 (0.2%)
17	CT	0.64	0/1097	0.88	0/1468
18	AU	1.17	1/977 (0.1%)	1.18	5/1301 (0.4%)
18	CU	0.65	0/977	0.78	0/1301
19	AV	1.13	0/782	1.15	1/1049 (0.1%)
19	CV	0.54	0/782	0.76	0/1049
20	AW	1.16	1/897 (0.1%)	1.23	8/1205 (0.7%)
20	CW	0.78	0/897	0.89	0/1205
21	AX	0.96	0/764	1.09	2/1025 (0.2%)
21	CX	0.68	0/764	0.88	1/1025 (0.1%)
22	AY	0.86	0/819	1.01	0/1095
22	CY	0.59	0/819	0.78	0/1095
23	AZ	0.74	0/1483	0.96	3/2017 (0.1%)
23	CZ	0.44	0/1483	0.71	0/2017
24	A0	0.92	0/662	1.01	0/881
24	C0	0.61	0/662	0.75	0/881
25	A1	0.84	0/762	1.00	1/1014 (0.1%)
25	C1	0.69	0/762	0.86	0/1014
26	A2	0.89	1/590 (0.2%)	0.96	0/781
26	C2	0.58	0/590	0.79	0/781
27	A3	0.97	0/474	1.17	0/635
27	C3	0.57	0/469	0.77	1/630 (0.2%)
28	A4	0.47	0/571	0.72	0/768
28	C4	0.36	0/545	0.57	0/737
29	A5	1.16	2/469 (0.4%)	1.21	3/635 (0.5%)
29	C5	0.73	0/469	0.93	2/635 (0.3%)
30	A6	0.93	0/460	1.01	2/613 (0.3%)
30	C6	0.68	0/456	0.86	0/608
31	A7	1.07	2/426 (0.5%)	1.21	3/561 (0.5%)
31	C7	0.79	0/426	0.92	2/561 (0.4%)
32	A8	0.99	0/525	1.07	1/691 (0.1%)
32	C8	0.68	0/525	0.85	0/691
33	A9	0.94	0/310	1.05	0/407
33	C9	0.59	0/310	0.78	0/407
34	BA	0.78	9/35976 (0.0%)	1.40	403/56145 (0.7%)
34	DA	0.70	5/36119 (0.0%)	1.30	246/56370 (0.4%)
35	BB	0.45	0/1881	0.72	0/2542
35	DB	0.39	0/1860	0.65	0/2518
36	BC	0.40	0/1576	0.58	0/2130
36	DC	0.37	0/1568	0.57	0/2122
37	BD	0.51	0/1689	0.74	0/2267
37	DD	0.49	0/1708	0.73	0/2289
38	BE	0.59	0/1145	0.81	1/1543 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DE	0.54	0/1149	0.79	0/1548
39	BF	0.52	0/825	0.73	1/1118 (0.1%)
39	DF	0.56	0/833	0.74	1/1128 (0.1%)
40	BG	0.44	0/1250	0.57	0/1679
40	DG	0.35	0/1254	0.55	0/1683
41	BH	0.59	0/1108	0.80	0/1494
41	DH	0.50	0/1108	0.72	0/1494
42	BI	0.41	0/1005	0.63	0/1350
42	DI	0.37	0/997	0.55	0/1343
43	BJ	0.36	0/722	0.62	0/982
43	DJ	0.37	0/727	0.59	0/988
44	BK	0.50	0/848	0.71	0/1149
44	DK	0.52	0/848	0.68	0/1149
45	BL	0.68	0/946	0.82	0/1274
45	DL	0.56	0/946	0.78	0/1274
46	BM	0.36	0/933	0.61	0/1253
46	DM	0.33	0/961	0.56	0/1291
47	BN	0.44	0/501	0.70	1/664 (0.2%)
47	DN	0.39	0/501	0.56	1/664 (0.2%)
48	BO	0.58	0/739	0.81	0/985
48	DO	0.56	0/739	0.77	0/985
49	BP	0.55	0/697	0.79	0/939
49	DP	0.47	0/693	0.70	0/935
50	BQ	0.61	0/836	0.79	0/1117
50	DQ	0.57	0/836	0.72	0/1117
51	BR	0.53	0/560	0.77	0/746
51	DR	0.56	0/560	0.65	0/746
52	BS	0.33	0/676	0.56	0/911
52	DS	0.33	0/661	0.59	0/893
53	BT	0.52	0/730	0.75	0/965
53	DT	0.48	0/733	0.74	0/969
54	BU	0.38	0/203	0.67	0/266
54	DU	0.33	0/203	0.56	0/266
55	BV	1.23	1/310 (0.3%)	1.38	3/480 (0.6%)
55	DV	0.94	0/144	1.64	5/223 (2.2%)
56	BX	0.90	2/1725 (0.1%)	1.50	30/2689 (1.1%)
56	DX	0.80	5/1719 (0.3%)	1.31	15/2677 (0.6%)
57	BZ	0.62	0/4927	0.84	2/6727 (0.0%)
57	DZ	0.54	0/4925	0.77	3/6724 (0.0%)
All	All	0.97	618/325388 (0.2%)	1.54	7279/485060 (1.5%)

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
4	AD	0	3
5	AE	0	1
8	AH	0	1
12	AO	0	2
21	CX	0	1
23	AZ	0	1
37	BD	0	1
53	BT	0	1
57	BZ	0	1
57	DZ	0	4
All	All	0	16

The worst 5 of 618 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	990	A	N9-C4	-14.73	1.29	1.37
1	AA	1188	A	N9-C4	-13.98	1.29	1.37
1	AA	2065	C	N3-C4	-12.04	1.25	1.33
1	AA	354	A	N9-C4	-11.71	1.30	1.37
1	AA	2517	G	N3-C4	-11.66	1.27	1.35

The worst 5 of 7279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	990	A	C5-N7-C8	-26.49	90.66	103.90
1	AA	990	A	N7-C8-N9	22.72	125.16	113.80
1	AA	990	A	N1-C6-N6	21.81	131.68	118.60
1	AA	991	G	O5'-P-OP1	-21.27	85.17	110.70
1	AA	990	A	C6-C5-N7	-21.06	117.56	132.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	141	VAL	Peptide
4	AD	70	TRP	Peptide
4	AD	98	VAL	Peptide
5	AE	132	HIS	Sidechain
8	AH	23	ARG	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	61426	0	30938	1072	0
1	CA	61337	0	30928	1179	0
2	AB	2573	0	1306	32	0
2	CB	2573	0	1306	43	0
3	AC	1063	0	1089	151	0
3	CC	1063	0	1091	214	0
4	AD	2136	0	2218	104	0
4	CD	2142	0	2229	84	0
5	AE	1559	0	1618	65	0
5	CE	1559	0	1618	59	0
6	AF	1584	0	1625	68	0
6	CF	1580	0	1619	78	0
7	AG	1425	0	1443	63	0
7	CG	1424	0	1434	61	0
8	AH	1330	0	1407	47	0
8	CH	1330	0	1407	48	0
9	AK	641	0	309	20	0
9	CK	641	0	309	11	0
10	AL	1025	0	1066	52	0
10	CL	1025	0	1066	46	0
11	AN	1117	0	1184	35	0
11	CN	1117	0	1184	40	0
12	AO	933	0	996	36	0
12	CO	933	0	996	26	0
13	AP	1139	0	1223	50	0
13	CP	1135	0	1212	53	0
14	AQ	1122	0	1179	57	0
14	CQ	1122	0	1179	52	0
15	AR	968	0	1033	49	0
15	CR	968	0	1033	48	0
16	AS	877	0	938	47	0
16	CS	870	0	923	36	0
17	AT	1091	0	1151	53	0
17	CT	1083	0	1136	45	0
18	AU	959	0	1019	37	0
18	CU	959	0	1018	31	0
19	AV	771	0	829	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CV	771	0	830	30	0
20	AW	886	0	940	23	0
20	CW	886	0	940	35	0
21	AX	750	0	814	31	0
21	CX	750	0	814	36	0
22	AY	806	0	881	26	0
22	CY	806	0	881	33	0
23	AZ	1451	0	1457	61	0
23	CZ	1451	0	1457	50	0
24	A0	653	0	674	21	0
24	C0	653	0	674	25	0
25	A1	755	0	826	33	0
25	C1	755	0	826	25	0
26	A2	588	0	643	14	0
26	C2	588	0	643	18	0
27	A3	469	0	518	26	0
27	C3	464	0	514	12	0
28	A4	558	0	545	28	0
28	C4	532	0	504	19	0
29	A5	455	0	466	20	0
29	C5	455	0	465	12	0
30	A6	453	0	473	20	0
30	C6	449	0	469	15	0
31	A7	418	0	467	23	0
31	C7	418	0	467	20	0
32	A8	517	0	582	28	0
32	C8	517	0	582	26	0
33	A9	307	0	335	15	0
33	C9	307	0	335	15	0
34	BA	32141	0	16222	665	0
34	DA	32268	0	16287	692	0
35	BB	1846	0	1867	96	0
35	DB	1825	0	1828	89	0
36	BC	1552	0	1546	51	0
36	DC	1544	0	1524	52	0
37	BD	1659	0	1677	95	0
37	DD	1678	0	1719	68	0
38	BE	1129	0	1185	52	0
38	DE	1133	0	1191	61	0
39	BF	812	0	804	28	0
39	DF	820	0	814	29	0
40	BG	1231	0	1238	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DG	1235	0	1249	23	0
41	BH	1088	0	1126	54	0
41	DH	1088	0	1126	46	0
42	BI	986	0	995	37	0
42	DI	978	0	966	42	0
43	BJ	709	0	650	31	0
43	DJ	714	0	672	38	0
44	BK	833	0	836	31	0
44	DK	833	0	836	25	0
45	BL	930	0	980	24	0
45	DL	930	0	980	42	0
46	BM	923	0	970	31	0
46	DM	950	0	988	31	0
47	BN	492	0	529	19	0
47	DN	492	0	531	34	0
48	BO	728	0	760	33	0
48	DO	728	0	760	32	0
49	BP	681	0	697	34	0
49	DP	677	0	686	28	0
50	BQ	823	0	891	27	0
50	DQ	823	0	891	37	0
51	BR	555	0	618	19	0
51	DR	555	0	618	25	0
52	BS	661	0	675	31	0
52	DS	646	0	644	27	0
53	BT	728	0	798	34	0
53	DT	731	0	807	29	0
54	BU	199	0	208	5	0
54	DU	199	0	208	7	0
55	BV	277	0	140	4	0
55	DV	128	0	67	5	0
56	BX	1625	0	829	24	0
56	DX	1621	0	826	21	0
57	BZ	4869	0	4164	253	0
57	DZ	4867	0	4166	237	0
58	A0	4	0	0	0	0
58	A1	1	0	0	0	0
58	A2	1	0	0	0	0
58	A4	1	0	0	0	0
58	A5	2	0	0	0	0
58	A6	2	0	0	0	0
58	A7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	A8	2	0	0	0	0
58	A9	1	0	0	0	0
58	AA	836	0	0	0	0
58	AB	23	0	0	0	0
58	AD	10	0	0	0	0
58	AE	4	0	0	0	0
58	AF	5	0	0	0	0
58	AG	2	0	0	0	0
58	AH	2	0	0	0	0
58	AN	3	0	0	0	0
58	AO	1	0	0	0	0
58	AP	2	0	0	0	0
58	AQ	2	0	0	0	0
58	AR	1	0	0	0	0
58	AU	3	0	0	0	0
58	AV	2	0	0	0	0
58	AW	4	0	0	0	0
58	AX	2	0	0	0	0
58	AZ	2	0	0	0	0
58	BA	212	0	0	0	0
58	BB	1	0	0	0	0
58	BD	1	0	0	0	0
58	BE	1	0	0	0	0
58	BF	1	0	0	0	0
58	BK	1	0	0	0	0
58	BL	4	0	0	0	0
58	BN	2	0	0	0	0
58	BT	1	0	0	0	0
58	BV	1	0	0	0	0
58	BX	10	0	0	0	0
58	BZ	1	0	0	0	0
58	C0	1	0	0	0	0
58	C1	1	0	0	0	0
58	C3	1	0	0	0	0
58	C7	1	0	0	0	0
58	C8	1	0	0	0	0
58	CA	666	0	0	0	0
58	CB	13	0	0	0	0
58	CD	3	0	0	0	0
58	CE	7	0	0	0	0
58	CF	4	0	0	0	0
58	CG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	CN	1	0	0	0	0
58	CO	2	0	0	0	0
58	CQ	4	0	0	0	0
58	CR	1	0	0	0	0
58	CU	2	0	0	0	0
58	CV	2	0	0	0	0
58	CY	1	0	0	0	0
58	DA	166	0	0	0	0
58	DD	1	0	0	0	0
58	DE	2	0	0	0	0
58	DF	1	0	0	0	0
58	DJ	1	0	0	0	0
58	DK	1	0	0	0	0
58	DL	2	0	0	0	0
58	DT	1	0	0	0	0
58	DZ	3	0	0	0	0
59	AA	1	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	0	0
61	DD	8	0	0	0	0
62	BZ	28	0	12	4	0
62	DZ	28	0	12	7	0
63	A0	9	0	0	2	0
63	A1	2	0	0	1	0
63	A2	1	0	0	0	0
63	A3	2	0	0	0	0
63	A5	4	0	0	1	0
63	A7	4	0	0	2	0
63	A8	9	0	0	3	0
63	A9	1	0	0	0	0
63	AA	1406	0	0	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	AB	37	0	0	3	0
63	AD	16	0	0	0	0
63	AE	14	0	0	3	0
63	AF	6	0	0	2	0
63	AG	3	0	0	0	0
63	AH	1	0	0	0	0
63	AN	3	0	0	0	0
63	AO	1	0	0	0	0
63	AP	18	0	0	0	0
63	AQ	5	0	0	1	0
63	AR	2	0	0	0	0
63	AS	1	0	0	0	0
63	AT	3	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	4	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	203	0	0	15	0
63	BD	3	0	0	0	0
63	BE	2	0	0	0	0
63	BG	1	0	0	0	0
63	BJ	1	0	0	0	0
63	BL	1	0	0	0	0
63	BM	1	0	0	0	0
63	BO	2	0	0	0	0
63	BP	1	0	0	0	0
63	BV	3	0	0	0	0
63	BX	5	0	0	0	0
63	BZ	2	0	0	0	0
63	C0	5	0	0	0	0
63	C1	1	0	0	0	0
63	C3	2	0	0	0	0
63	C6	1	0	0	1	0
63	C7	1	0	0	0	0
63	C8	3	0	0	0	0
63	CA	974	0	0	87	0
63	CB	9	0	0	0	0
63	CD	17	0	0	0	0
63	CE	14	0	0	3	0
63	CF	6	0	0	0	0
63	CN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	CP	12	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	1	0
63	CV	2	0	0	0	0
63	CW	1	0	0	0	0
63	CX	2	0	0	0	0
63	CY	2	0	0	1	0
63	DA	154	0	0	11	0
63	DE	3	0	0	0	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DP	1	0	0	0	0
63	DT	1	0	0	0	0
63	DV	1	0	0	0	0
63	DZ	1	0	0	0	0
All	All	305548	0	205094	7289	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7289 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:CA:2128:C:H5”	3:CC:219:MET:CE	1.49	1.42
1:CA:2132:U:O2	3:CC:6:LYS:CB	1.64	1.41
1:CA:2128:C:OP1	3:CC:219:MET:CE	1.71	1.39
1:CA:2176:A:H4’	3:CC:45:HIS:CD2	1.60	1.37
1:AA:2143:G:N2	3:AC:169:THR:OG1	1.58	1.36

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	239 (88%)	28 (10%)	6 (2%)	6	22
4	CD	273/276 (99%)	234 (86%)	35 (13%)	4 (2%)	10	33
5	AE	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	15	44
5	CE	202/206 (98%)	178 (88%)	20 (10%)	4 (2%)	7	24
6	AF	201/210 (96%)	182 (90%)	15 (8%)	4 (2%)	7	24
6	CF	201/210 (96%)	181 (90%)	14 (7%)	6 (3%)	4	15
7	AG	179/182 (98%)	152 (85%)	19 (11%)	8 (4%)	2	8
7	CG	179/182 (98%)	148 (83%)	21 (12%)	10 (6%)	2	5
8	AH	172/180 (96%)	152 (88%)	17 (10%)	3 (2%)	9	29
8	CH	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	9	29
9	AK	128/173 (74%)	66 (52%)	31 (24%)	31 (24%)	0	0
9	CK	128/173 (74%)	77 (60%)	29 (23%)	22 (17%)	0	0
10	AL	137/147 (93%)	105 (77%)	24 (18%)	8 (6%)	1	4
10	CL	137/147 (93%)	97 (71%)	35 (26%)	5 (4%)	3	11
11	AN	138/140 (99%)	127 (92%)	10 (7%)	1 (1%)	22	53
11	CN	138/140 (99%)	127 (92%)	9 (6%)	2 (1%)	11	34
12	AO	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19	49
12	CO	120/122 (98%)	108 (90%)	9 (8%)	3 (2%)	5	19
13	AP	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	5	17
13	CP	147/150 (98%)	124 (84%)	18 (12%)	5 (3%)	3	13
14	AQ	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	11	34
14	CQ	139/141 (99%)	124 (89%)	12 (9%)	3 (2%)	6	22
15	AR	116/118 (98%)	105 (90%)	9 (8%)	2 (2%)	9	29
15	CR	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	9	29
16	AS	108/112 (96%)	92 (85%)	12 (11%)	4 (4%)	3	11
16	CS	108/112 (96%)	91 (84%)	13 (12%)	4 (4%)	3	11
17	AT	129/146 (88%)	115 (89%)	13 (10%)	1 (1%)	19	49
17	CT	129/146 (88%)	118 (92%)	9 (7%)	2 (2%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AU	114/118 (97%)	106 (93%)	6 (5%)	2 (2%)	8	28
18	CU	114/118 (97%)	102 (90%)	11 (10%)	1 (1%)	17	46
19	AV	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4	15
19	CV	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	2	6
20	AW	110/113 (97%)	99 (90%)	9 (8%)	2 (2%)	8	28
20	CW	110/113 (97%)	97 (88%)	11 (10%)	2 (2%)	8	28
21	AX	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	14	41
21	CX	93/96 (97%)	75 (81%)	14 (15%)	4 (4%)	2	8
22	AY	105/110 (96%)	90 (86%)	11 (10%)	4 (4%)	3	10
22	CY	105/110 (96%)	82 (78%)	21 (20%)	2 (2%)	8	26
23	AZ	183/206 (89%)	147 (80%)	23 (13%)	13 (7%)	1	2
23	CZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	3
24	A0	81/85 (95%)	72 (89%)	7 (9%)	2 (2%)	5	19
24	C0	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	13	39
25	A1	95/98 (97%)	90 (95%)	3 (3%)	2 (2%)	7	23
25	C1	95/98 (97%)	88 (93%)	4 (4%)	3 (3%)	4	13
26	A2	68/72 (94%)	59 (87%)	9 (13%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	10	33
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	A4	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0	1
28	C4	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	2
29	A5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
29	C5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
30	A6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
30	C6	51/54 (94%)	44 (86%)	6 (12%)	1 (2%)	7	24
31	A7	46/49 (94%)	41 (89%)	5 (11%)	0	100	100
31	C7	46/49 (94%)	39 (85%)	6 (13%)	1 (2%)	6	22
32	A8	62/65 (95%)	54 (87%)	5 (8%)	3 (5%)	2	7
32	C8	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	A9	35/37 (95%)	34 (97%)	0	1 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	174 (76%)	42 (18%)	13 (6%)	1	5
35	DB	229/256 (90%)	176 (77%)	40 (18%)	13 (6%)	1	5
36	BC	204/239 (85%)	165 (81%)	32 (16%)	7 (3%)	3	13
36	DC	204/239 (85%)	172 (84%)	30 (15%)	2 (1%)	15	44
37	BD	206/209 (99%)	150 (73%)	42 (20%)	14 (7%)	1	3
37	DD	206/209 (99%)	165 (80%)	30 (15%)	11 (5%)	2	6
38	BE	146/162 (90%)	123 (84%)	17 (12%)	6 (4%)	3	9
38	DE	146/162 (90%)	122 (84%)	19 (13%)	5 (3%)	3	13
39	BF	98/101 (97%)	84 (86%)	10 (10%)	4 (4%)	3	9
39	DF	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
40	BG	153/156 (98%)	127 (83%)	20 (13%)	6 (4%)	3	10
40	DG	153/156 (98%)	127 (83%)	19 (12%)	7 (5%)	2	7
41	BH	135/138 (98%)	111 (82%)	17 (13%)	7 (5%)	2	6
41	DH	135/138 (98%)	120 (89%)	13 (10%)	2 (2%)	10	33
42	BI	125/128 (98%)	105 (84%)	14 (11%)	6 (5%)	2	7
42	DI	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	19	49
43	BJ	95/105 (90%)	80 (84%)	12 (13%)	3 (3%)	4	13
43	DJ	94/105 (90%)	76 (81%)	9 (10%)	9 (10%)	0	1
44	BK	112/129 (87%)	94 (84%)	16 (14%)	2 (2%)	8	28
44	DK	112/129 (87%)	93 (83%)	15 (13%)	4 (4%)	3	11
45	BL	120/132 (91%)	108 (90%)	12 (10%)	0	100	100
45	DL	120/132 (91%)	109 (91%)	9 (8%)	2 (2%)	9	29
46	BM	115/126 (91%)	97 (84%)	15 (13%)	3 (3%)	5	18
46	DM	120/126 (95%)	96 (80%)	18 (15%)	6 (5%)	2	6
47	BN	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	13
47	DN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
48	BO	86/89 (97%)	71 (83%)	15 (17%)	0	100	100
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	7
49	BP	80/88 (91%)	55 (69%)	19 (24%)	6 (8%)	1	2
49	DP	80/88 (91%)	67 (84%)	10 (12%)	3 (4%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BQ	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	7	23
50	DQ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	9 (14%)	0	100	100
51	DR	66/88 (75%)	56 (85%)	9 (14%)	1 (2%)	10	33
52	BS	82/93 (88%)	71 (87%)	10 (12%)	1 (1%)	13	39
52	DS	81/93 (87%)	69 (85%)	8 (10%)	4 (5%)	2	7
53	BT	94/106 (89%)	81 (86%)	5 (5%)	8 (8%)	1	1
53	DT	94/106 (89%)	80 (85%)	10 (11%)	4 (4%)	2	8
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	7
57	BZ	726/758 (96%)	561 (77%)	115 (16%)	50 (7%)	1	3
57	DZ	726/758 (96%)	558 (77%)	113 (16%)	55 (8%)	1	2
All	All	13389/14444 (93%)	11204 (84%)	1645 (12%)	540 (4%)	3	9

5 of 540 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS
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%)	178 (83%)	37 (17%)	2	6
4	CD	216/218 (99%)	183 (85%)	33 (15%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	164/166 (99%)	134 (82%)	30 (18%)	1	5
5	CE	164/166 (99%)	134 (82%)	30 (18%)	1	5
6	AF	160/166 (96%)	123 (77%)	37 (23%)	1	2
6	CF	159/166 (96%)	127 (80%)	32 (20%)	1	4
7	AG	143/156 (92%)	114 (80%)	29 (20%)	1	4
7	CG	142/156 (91%)	110 (78%)	32 (22%)	1	2
8	AH	144/148 (97%)	126 (88%)	18 (12%)	4	14
8	CH	144/148 (97%)	123 (85%)	21 (15%)	3	9
10	AL	104/111 (94%)	88 (85%)	16 (15%)	2	8
10	CL	104/111 (94%)	82 (79%)	22 (21%)	1	3
11	AN	118/119 (99%)	96 (81%)	22 (19%)	1	5
11	CN	118/119 (99%)	99 (84%)	19 (16%)	2	7
12	AO	100/100 (100%)	87 (87%)	13 (13%)	4	13
12	CO	100/100 (100%)	85 (85%)	15 (15%)	3	9
13	AP	116/116 (100%)	95 (82%)	21 (18%)	1	5
13	CP	115/116 (99%)	98 (85%)	17 (15%)	3	9
14	AQ	111/111 (100%)	92 (83%)	19 (17%)	2	6
14	CQ	111/111 (100%)	98 (88%)	13 (12%)	5	16
15	AR	101/101 (100%)	82 (81%)	19 (19%)	1	5
15	CR	101/101 (100%)	82 (81%)	19 (19%)	1	5
16	AS	87/88 (99%)	76 (87%)	11 (13%)	4	14
16	CS	85/88 (97%)	68 (80%)	17 (20%)	1	4
17	AT	115/127 (91%)	98 (85%)	17 (15%)	3	9
17	CT	113/127 (89%)	90 (80%)	23 (20%)	1	4
18	AU	93/94 (99%)	83 (89%)	10 (11%)	6	19
18	CU	93/94 (99%)	78 (84%)	15 (16%)	2	7
19	AV	80/82 (98%)	62 (78%)	18 (22%)	1	2
19	CV	80/82 (98%)	68 (85%)	12 (15%)	3	9
20	AW	90/92 (98%)	76 (84%)	14 (16%)	2	8
20	CW	90/92 (98%)	76 (84%)	14 (16%)	2	8
21	AX	77/78 (99%)	70 (91%)	7 (9%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CX	77/78 (99%)	67 (87%)	10 (13%)	4	13
22	AY	85/91 (93%)	70 (82%)	15 (18%)	2	5
22	CY	85/91 (93%)	68 (80%)	17 (20%)	1	4
23	AZ	156/179 (87%)	126 (81%)	30 (19%)	1	4
23	CZ	156/179 (87%)	135 (86%)	21 (14%)	4	11
24	A0	65/67 (97%)	60 (92%)	5 (8%)	13	35
24	C0	65/67 (97%)	58 (89%)	7 (11%)	6	19
25	A1	80/83 (96%)	69 (86%)	11 (14%)	3	11
25	C1	80/83 (96%)	69 (86%)	11 (14%)	3	11
26	A2	65/67 (97%)	54 (83%)	11 (17%)	2	6
26	C2	65/67 (97%)	59 (91%)	6 (9%)	9	27
27	A3	51/52 (98%)	39 (76%)	12 (24%)	1	2
27	C3	50/52 (96%)	42 (84%)	8 (16%)	2	7
28	A4	60/63 (95%)	49 (82%)	11 (18%)	1	5
28	C4	53/63 (84%)	40 (76%)	13 (24%)	0	2
29	A5	50/52 (96%)	42 (84%)	8 (16%)	2	7
29	C5	50/52 (96%)	38 (76%)	12 (24%)	0	2
30	A6	51/52 (98%)	40 (78%)	11 (22%)	1	3
30	C6	50/52 (96%)	40 (80%)	10 (20%)	1	4
31	A7	41/42 (98%)	37 (90%)	4 (10%)	8	24
31	C7	41/42 (98%)	31 (76%)	10 (24%)	0	2
32	A8	54/55 (98%)	45 (83%)	9 (17%)	2	6
32	C8	54/55 (98%)	47 (87%)	7 (13%)	4	13
33	A9	34/34 (100%)	31 (91%)	3 (9%)	10	29
33	C9	34/34 (100%)	30 (88%)	4 (12%)	5	16
35	BB	192/220 (87%)	153 (80%)	39 (20%)	1	4
35	DB	187/220 (85%)	152 (81%)	35 (19%)	1	5
36	BC	143/188 (76%)	131 (92%)	12 (8%)	11	31
36	DC	141/188 (75%)	117 (83%)	24 (17%)	2	6
37	BD	170/181 (94%)	139 (82%)	31 (18%)	1	5
37	DD	174/181 (96%)	139 (80%)	35 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BE	113/123 (92%)	99 (88%)	14 (12%)	4	14
38	DE	114/123 (93%)	96 (84%)	18 (16%)	2	8
39	BF	84/90 (93%)	70 (83%)	14 (17%)	2	6
39	DF	86/90 (96%)	78 (91%)	8 (9%)	9	26
40	BG	119/127 (94%)	102 (86%)	17 (14%)	3	10
40	DG	120/127 (94%)	101 (84%)	19 (16%)	2	8
41	BH	114/119 (96%)	91 (80%)	23 (20%)	1	4
41	DH	114/119 (96%)	94 (82%)	20 (18%)	2	6
42	BI	91/99 (92%)	78 (86%)	13 (14%)	3	10
42	DI	89/99 (90%)	74 (83%)	15 (17%)	2	6
43	BJ	66/92 (72%)	60 (91%)	6 (9%)	9	27
43	DJ	69/92 (75%)	64 (93%)	5 (7%)	14	38
44	BK	83/99 (84%)	72 (87%)	11 (13%)	4	12
44	DK	83/99 (84%)	74 (89%)	9 (11%)	6	19
45	BL	97/109 (89%)	85 (88%)	12 (12%)	4	14
45	DL	97/109 (89%)	83 (86%)	14 (14%)	3	10
46	BM	91/101 (90%)	79 (87%)	12 (13%)	4	12
46	DM	92/101 (91%)	78 (85%)	14 (15%)	3	8
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	2
47	DN	49/50 (98%)	41 (84%)	8 (16%)	2	7
48	BO	78/80 (98%)	66 (85%)	12 (15%)	2	8
48	DO	78/80 (98%)	66 (85%)	12 (15%)	2	8
49	BP	69/74 (93%)	57 (83%)	12 (17%)	2	6
49	DP	68/74 (92%)	58 (85%)	10 (15%)	3	9
50	BQ	94/97 (97%)	80 (85%)	14 (15%)	3	9
50	DQ	94/97 (97%)	87 (93%)	7 (7%)	13	37
51	BR	59/77 (77%)	51 (86%)	8 (14%)	3	11
51	DR	59/77 (77%)	49 (83%)	10 (17%)	2	6
52	BS	70/80 (88%)	61 (87%)	9 (13%)	4	13
52	DS	67/80 (84%)	59 (88%)	8 (12%)	5	16
53	BT	70/82 (85%)	54 (77%)	16 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	DT	71/82 (87%)	65 (92%)	6 (8%)	10	31
54	BU	18/22 (82%)	16 (89%)	2 (11%)	6	19
54	DU	18/22 (82%)	17 (94%)	1 (6%)	21	51
57	BZ	369/636 (58%)	280 (76%)	89 (24%)	0	2
57	DZ	370/636 (58%)	280 (76%)	90 (24%)	0	2
All	All	10306/11672 (88%)	8607 (84%)	1699 (16%)	2	7

5 of 1699 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CF	24	LEU
17	CT	78	LEU
52	DS	38	SER
6	CF	200	GLU
6	CF	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
18	CU	94	ASN
38	DE	130	ASN
22	CY	43	ASN
35	DB	94	ASN
45	DL	49	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2845/2915 (97%)	563 (19%)	43 (1%)
1	CA	2839/2915 (97%)	578 (20%)	33 (1%)
2	AB	119/121 (98%)	25 (21%)	1 (0%)
2	CB	119/121 (98%)	23 (19%)	0
34	BA	1491/1521 (98%)	299 (20%)	18 (1%)
34	DA	1498/1521 (98%)	296 (19%)	20 (1%)
55	BV	12/24 (50%)	7 (58%)	0
55	DV	5/24 (20%)	1 (20%)	0
56	BX	75/77 (97%)	15 (20%)	1 (1%)
56	DX	75/77 (97%)	11 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9078/9316 (97%)	1818 (20%)	116 (1%)

5 of 1818 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	17	G
1	AA	34	C
1	AA	36	G

5 of 116 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	1067	A
34	DA	1065	U
1	CA	774	A
34	DA	1064	G
34	DA	428	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	5MC	DX	32	56	18,22,23	1.10	1 (5%)	26,32,35	1.27	4 (15%)
56	5MU	DX	54	56	19,22,23	1.39	5 (26%)	28,32,35	2.16	9 (32%)
56	5MC	BX	32	56	18,22,23	1.05	2 (11%)	26,32,35	1.09	2 (7%)
56	5MU	BX	54	56,58	19,22,23	1.59	5 (26%)	28,32,35	1.95	7 (25%)
56	PSU	BX	55	56	18,21,22	1.32	1 (5%)	22,30,33	2.05	4 (18%)
56	4SU	BX	8	56	18,21,22	1.72	5 (27%)	26,30,33	2.48	7 (26%)
56	PSU	DX	55	56	18,21,22	1.39	2 (11%)	22,30,33	1.78	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
56	4SU	DX	8	56	18,21,22	1.64	4 (22%)	26,30,33	2.03	6 (23%)

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
56	5MC	DX	32	56	-	0/7/25/26	0/2/2/2
56	5MU	DX	54	56	-	0/7/25/26	0/2/2/2
56	5MC	BX	32	56	-	0/7/25/26	0/2/2/2
56	5MU	BX	54	56,58	-	0/7/25/26	0/2/2/2
56	PSU	BX	55	56	-	0/7/25/26	0/2/2/2
56	4SU	BX	8	56	-	0/7/25/26	0/2/2/2
56	PSU	DX	55	56	-	0/7/25/26	0/2/2/2
56	4SU	DX	8	56	-	0/7/25/26	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BX	8	4SU	C4-S4	-4.53	1.59	1.68
56	BX	55	PSU	C6-C5	4.27	1.40	1.35
56	DX	8	4SU	C4-S4	-4.04	1.60	1.68
56	DX	55	PSU	C6-C5	3.75	1.39	1.35
56	DX	32	5MC	C6-C5	3.47	1.40	1.34

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	BX	8	4SU	C4-N3-C2	-6.95	120.58	127.34
56	BX	8	4SU	C5-C4-N3	6.80	121.00	114.69
56	DX	8	4SU	C4-N3-C2	-6.02	121.50	127.34
56	BX	55	PSU	N1-C2-N3	5.81	121.71	115.13
56	DX	55	PSU	N1-C2-N3	5.50	121.36	115.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BX	32	5MC	4	0
56	BX	8	4SU	1	0
56	DX	55	PSU	1	0
56	DX	8	4SU	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2062 ligands modelled in this entry, 2058 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	704	58	24,30,30	1.03	2 (8%)	30,47,47	1.45	3 (10%)
62	GDP	BZ	801	58	24,30,30	0.91	1 (4%)	30,47,47	1.43	4 (13%)
61	SF4	DD	501	37	0,12,12	-	-	-		
61	SF4	BD	501	37	0,12,12	-	-	-		

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
61	SF4	DD	501	37	-	-	0/6/5/5
62	GDP	BZ	801	58	-	5/12/32/32	0/3/3/3
62	GDP	DZ	704	58	-	5/12/32/32	0/3/3/3
61	SF4	BD	501	37	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	DZ	704	GDP	C6-N1	-2.47	1.34	1.37
62	BZ	801	GDP	C6-N1	-2.03	1.34	1.37
62	DZ	704	GDP	C2'-C1'	-2.02	1.50	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	BZ	801	GDP	PA-O3A-PB	-4.54	117.26	132.83
62	DZ	704	GDP	PA-O3A-PB	-4.48	117.47	132.83
62	DZ	704	GDP	C3'-C2'-C1'	2.85	105.27	100.98
62	DZ	704	GDP	O2B-PB-O3A	2.48	112.94	104.64
62	BZ	801	GDP	O2B-PB-O3A	2.47	112.91	104.64

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	BZ	801	GDP	C5'-O5'-PA-O3A
62	DZ	704	GDP	C5'-O5'-PA-O3A
62	DZ	704	GDP	O4'-C4'-C5'-O5'
62	DZ	704	GDP	C3'-C4'-C5'-O5'
62	BZ	801	GDP	O4'-C4'-C5'-O5'

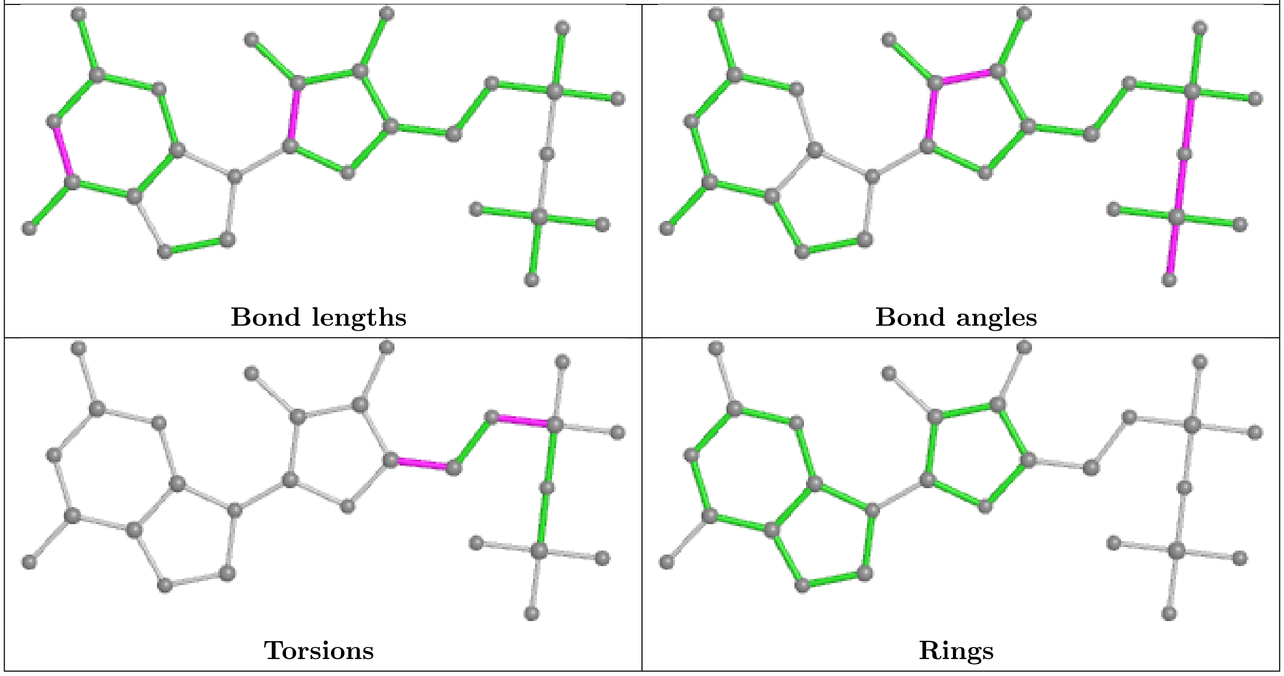
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	DZ	704	GDP	7	0
62	BZ	801	GDP	4	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 704



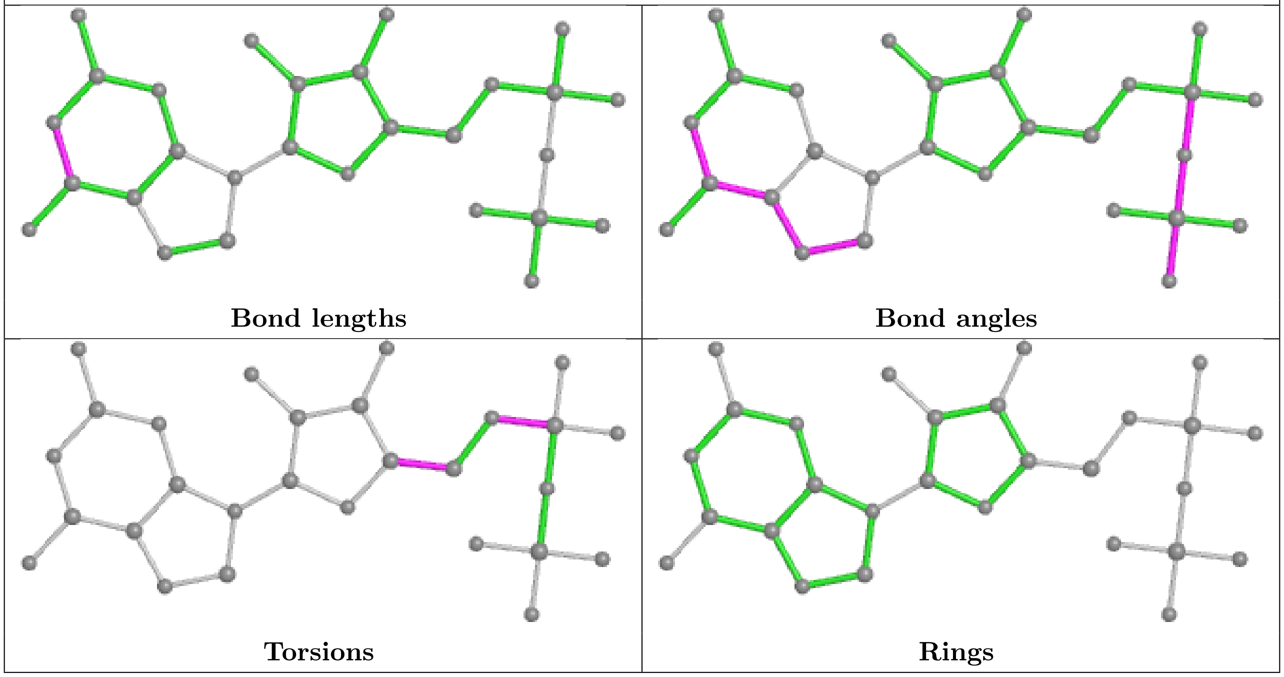
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP BZ 801



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, 95^{th} 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	2852/2915 (97%)	0.37	131 (4%)	32	22	14, 34, 142, 356	0
1	CA	2848/2915 (97%)	0.56	198 (6%)	16	9	27, 58, 179, 348	0
2	AB	120/121 (99%)	-0.01	0	100	100	23, 51, 72, 109	0
2	CB	120/121 (99%)	0.34	0	100	100	66, 92, 119, 166	0
3	AC	137/228 (60%)	8.87	133 (97%)	0	0	132, 205, 251, 280	0
3	CC	137/228 (60%)	8.97	135 (98%)	0	0	144, 214, 251, 276	0
4	AD	275/276 (99%)	-0.27	1 (0%)	92	91	12, 35, 61, 136	0
4	CD	275/276 (99%)	-0.28	1 (0%)	92	91	24, 47, 74, 128	0
5	AE	204/206 (99%)	-0.33	0	100	100	6, 34, 58, 82	0
5	CE	204/206 (99%)	0.04	2 (0%)	82	77	20, 63, 107, 135	0
6	AF	203/210 (96%)	-0.23	2 (0%)	82	77	11, 35, 78, 173	0
6	CF	203/210 (96%)	-0.18	0	100	100	21, 63, 106, 155	0
7	AG	181/182 (99%)	0.26	8 (4%)	34	24	37, 77, 134, 208	0
7	CG	181/182 (99%)	0.97	30 (16%)	1	1	72, 111, 175, 201	0
8	AH	174/180 (96%)	-0.28	1 (0%)	89	86	25, 46, 70, 111	0
8	CH	174/180 (96%)	1.19	37 (21%)	0	0	64, 113, 162, 199	0
9	AK	130/173 (75%)	1.49	38 (29%)	0	0	47, 104, 172, 222	0
9	CK	130/173 (75%)	3.08	86 (66%)	0	0	75, 160, 200, 225	0
10	AL	139/147 (94%)	4.82	118 (84%)	0	0	96, 172, 230, 251	0
10	CL	139/147 (94%)	6.28	127 (91%)	0	0	128, 195, 248, 278	0
11	AN	140/140 (100%)	-0.43	0	100	100	14, 28, 59, 95	0
11	CN	140/140 (100%)	0.11	1 (0%)	87	84	33, 71, 108, 151	0
12	AO	122/122 (100%)	-0.38	0	100	100	19, 37, 61, 78	0
12	CO	122/122 (100%)	-0.13	0	100	100	36, 58, 85, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AP	149/150 (99%)	0.14	2 (1%)	77	72	12, 44, 81, 111	0
13	CP	149/150 (99%)	0.23	3 (2%)	65	56	31, 68, 116, 136	0
14	AQ	141/141 (100%)	-0.35	0	100	100	12, 34, 55, 84	0
14	CQ	141/141 (100%)	0.02	1 (0%)	87	84	38, 69, 100, 120	0
15	AR	118/118 (100%)	-0.33	0	100	100	16, 29, 47, 55	0
15	CR	118/118 (100%)	-0.07	0	100	100	34, 56, 91, 103	0
16	AS	110/112 (98%)	0.02	1 (0%)	84	80	31, 50, 81, 94	0
16	CS	110/112 (98%)	0.50	3 (2%)	54	44	47, 86, 120, 150	0
17	AT	131/146 (89%)	-0.18	3 (2%)	60	51	24, 40, 91, 169	0
17	CT	131/146 (89%)	-0.07	1 (0%)	86	81	43, 65, 107, 142	0
18	AU	116/118 (98%)	-0.31	0	100	100	10, 22, 39, 88	0
18	CU	116/118 (98%)	-0.03	0	100	100	28, 65, 92, 106	0
19	AV	101/101 (100%)	-0.38	0	100	100	9, 28, 51, 74	0
19	CV	101/101 (100%)	0.28	2 (1%)	65	56	36, 79, 113, 165	0
20	AW	112/113 (99%)	-0.35	0	100	100	13, 25, 43, 111	0
20	CW	112/113 (99%)	-0.18	0	100	100	29, 50, 80, 117	0
21	AX	95/96 (98%)	-0.22	0	100	100	16, 35, 69, 99	0
21	CX	95/96 (98%)	0.03	0	100	100	39, 61, 85, 105	0
22	AY	107/110 (97%)	-0.17	1 (0%)	84	80	23, 45, 84, 165	0
22	CY	107/110 (97%)	0.59	9 (8%)	11	5	45, 75, 115, 172	0
23	AZ	185/206 (89%)	-0.12	1 (0%)	91	88	28, 57, 92, 145	0
23	CZ	185/206 (89%)	0.69	17 (9%)	9	5	62, 105, 150, 210	0
24	A0	83/85 (97%)	0.06	7 (8%)	11	5	13, 35, 85, 220	0
24	C0	83/85 (97%)	0.69	8 (9%)	8	4	44, 66, 120, 224	0
25	A1	97/98 (98%)	-0.12	1 (1%)	82	77	20, 44, 79, 102	0
25	C1	97/98 (98%)	-0.11	1 (1%)	82	77	30, 52, 90, 127	0
26	A2	70/72 (97%)	-0.31	0	100	100	24, 44, 71, 121	0
26	C2	70/72 (97%)	0.16	0	100	100	48, 71, 102, 116	0
27	A3	59/60 (98%)	-0.37	0	100	100	15, 30, 55, 101	0
27	C3	59/60 (98%)	0.50	1 (1%)	70	63	46, 73, 112, 147	0
28	A4	69/71 (97%)	1.03	16 (23%)	0	0	61, 118, 203, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	C4	69/71 (97%)	1.83	27 (39%) 0 0	81, 159, 204, 222	0
29	A5	59/60 (98%)	-0.34	0 100 100	9, 25, 41, 53	0
29	C5	59/60 (98%)	-0.07	1 (1%) 70 63	26, 52, 89, 105	0
30	A6	53/54 (98%)	-0.28	0 100 100	22, 41, 56, 76	0
30	C6	53/54 (98%)	0.02	0 100 100	41, 60, 80, 106	0
31	A7	48/49 (97%)	-0.10	2 (4%) 36 26	14, 25, 68, 134	0
31	C7	48/49 (97%)	-0.10	0 100 100	28, 39, 95, 119	0
32	A8	64/65 (98%)	-0.32	0 100 100	15, 28, 46, 67	0
32	C8	64/65 (98%)	-0.08	0 100 100	38, 52, 72, 87	0
33	A9	37/37 (100%)	-0.13	0 100 100	23, 36, 56, 67	0
33	C9	37/37 (100%)	0.35	1 (2%) 54 44	45, 78, 96, 127	0
34	BA	1495/1521 (98%)	0.63	106 (7%) 16 9	32, 84, 187, 330	0
34	DA	1501/1521 (98%)	0.80	189 (12%) 3 2	39, 89, 197, 334	0
35	BB	231/256 (90%)	0.77	32 (13%) 2 1	43, 105, 171, 220	0
35	DB	231/256 (90%)	1.03	41 (17%) 1 1	71, 124, 177, 210	0
36	BC	206/239 (86%)	1.17	39 (18%) 1 1	58, 118, 174, 198	0
36	DC	206/239 (86%)	1.61	60 (29%) 0 0	69, 136, 181, 210	0
37	BD	208/209 (99%)	0.40	9 (4%) 35 25	45, 87, 138, 188	0
37	DD	208/209 (99%)	0.25	8 (3%) 40 30	59, 86, 135, 200	0
38	BE	148/162 (91%)	0.09	2 (1%) 75 70	34, 73, 104, 127	0
38	DE	148/162 (91%)	0.38	4 (2%) 54 44	50, 79, 117, 179	0
39	BF	100/101 (99%)	0.12	0 100 100	56, 86, 116, 135	0
39	DF	100/101 (99%)	0.08	1 (1%) 82 77	49, 86, 117, 135	0
40	BG	155/156 (99%)	1.05	24 (15%) 2 1	68, 112, 181, 225	0
40	DG	155/156 (99%)	2.07	65 (41%) 0 0	71, 133, 192, 216	0
41	BH	137/138 (99%)	0.02	1 (0%) 87 84	47, 72, 100, 119	0
41	DH	137/138 (99%)	0.17	1 (0%) 87 84	57, 80, 110, 141	0
42	BI	127/128 (99%)	1.68	42 (33%) 0 0	64, 124, 167, 200	0
42	DI	127/128 (99%)	2.42	74 (58%) 0 0	88, 145, 191, 215	0
43	BJ	97/105 (92%)	2.05	41 (42%) 0 0	81, 130, 183, 212	0
43	DJ	96/105 (91%)	2.65	58 (60%) 0 0	90, 150, 197, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BK	114/129 (88%)	0.28	0 100 100	36, 78, 126, 148	0
44	DK	114/129 (88%)	0.36	1 (0%) 84 80	51, 89, 115, 172	0
45	BL	122/132 (92%)	-0.09	0 100 100	37, 59, 78, 112	0
45	DL	122/132 (92%)	0.14	2 (1%) 72 66	47, 70, 95, 116	0
46	BM	117/126 (92%)	1.07	20 (17%) 1 1	77, 135, 181, 203	0
46	DM	122/126 (96%)	2.08	45 (36%) 0 0	94, 151, 199, 268	0
47	BN	60/61 (98%)	1.09	9 (15%) 2 1	66, 112, 146, 172	0
47	DN	60/61 (98%)	2.12	25 (41%) 0 0	99, 139, 177, 195	0
48	BO	88/89 (98%)	0.17	1 (1%) 80 75	37, 70, 106, 120	0
48	DO	88/89 (98%)	0.25	0 100 100	46, 71, 106, 153	0
49	BP	82/88 (93%)	0.79	8 (9%) 7 4	50, 80, 119, 168	0
49	DP	82/88 (93%)	0.55	3 (3%) 41 31	54, 78, 112, 155	0
50	BQ	99/105 (94%)	0.09	2 (2%) 65 56	45, 72, 98, 125	0
50	DQ	99/105 (94%)	0.24	1 (1%) 82 77	44, 77, 104, 116	0
51	BR	68/88 (77%)	0.49	6 (8%) 10 5	41, 80, 122, 134	0
51	DR	68/88 (77%)	0.52	2 (2%) 51 41	52, 83, 128, 144	0
52	BS	84/93 (90%)	2.08	35 (41%) 0 0	96, 145, 196, 210	0
52	DS	83/93 (89%)	2.81	53 (63%) 0 0	92, 165, 213, 224	0
53	BT	96/106 (90%)	0.47	5 (5%) 27 18	61, 84, 123, 166	0
53	DT	96/106 (90%)	0.47	6 (6%) 20 12	57, 86, 134, 156	0
54	BU	23/27 (85%)	1.82	11 (47%) 0 0	64, 117, 156, 182	0
54	DU	23/27 (85%)	1.73	9 (39%) 0 0	90, 136, 172, 185	0
55	BV	13/24 (54%)	3.99	8 (61%) 0 0	49, 87, 172, 178	0
55	DV	6/24 (25%)	2.41	4 (66%) 0 0	63, 79, 171, 199	0
56	BX	72/77 (93%)	0.76	4 (5%) 24 16	34, 78, 124, 188	0
56	DX	72/77 (93%)	1.33	13 (18%) 1 1	41, 100, 148, 162	0
57	BZ	730/758 (96%)	1.17	186 (25%) 0 0	35, 78, 136, 188	0
57	DZ	730/758 (96%)	1.77	255 (34%) 0 0	37, 101, 167, 222	0
All	All	22704/23760 (95%)	0.71	2669 (11%) 4 2	6, 70, 180, 356	0

The worst 5 of 2669 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CC	166	ASN	26.5
3	CC	4	HIS	23.3
3	AC	159	ALA	23.0
3	CC	35	THR	21.6
3	AC	176	VAL	19.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	PSU	DX	55	20/21	0.85	0.20	95,95,95,95	0
56	4SU	DX	8	20/21	0.89	0.22	96,96,96,96	0
56	5MC	DX	32	21/22	0.90	0.22	86,86,86,86	0
56	5MU	DX	54	21/22	0.90	0.19	108,108,108,108	0
56	PSU	BX	55	20/21	0.90	0.27	74,74,74,74	0
56	5MU	BX	54	21/22	0.92	0.26	85,85,85,85	0
56	4SU	BX	8	20/21	0.94	0.17	70,70,70,70	1
56	5MC	BX	32	21/22	0.96	0.17	65,65,65,65	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	CA	3494	1/1	0.04	1.04	88,88,88,88	0
58	MG	DA	1753	1/1	0.04	0.87	83,83,83,83	0
58	MG	BA	3169	1/1	0.06	0.49	130,130,130,130	0
58	MG	DA	1704	1/1	0.20	0.47	128,128,128,128	0
58	MG	CA	3046	1/1	0.23	0.34	113,113,113,113	0
58	MG	CA	3141	1/1	0.26	0.54	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	AA	3784	1/1	0.26	0.64	73,73,73,73	0
58	MG	CB	3013	1/1	0.28	0.24	96,96,96,96	0
58	MG	CA	3296	1/1	0.29	0.37	80,80,80,80	0
58	MG	DA	1624	1/1	0.29	0.14	115,115,115,115	0
58	MG	CA	3074	1/1	0.30	0.79	91,91,91,91	0
58	MG	DA	1714	1/1	0.34	0.30	78,78,78,78	0
58	MG	DZ	701	1/1	0.37	0.47	112,112,112,112	0
58	MG	CA	3067	1/1	0.38	0.98	83,83,83,83	0
58	MG	BA	3112	1/1	0.42	0.51	70,70,70,70	0
58	MG	CA	3114	1/1	0.46	0.29	94,94,94,94	0
58	MG	AA	3026	1/1	0.48	0.57	83,83,83,83	0
58	MG	DA	1690	1/1	0.50	0.29	85,85,85,85	0
58	MG	DA	1725	1/1	0.51	0.15	64,64,64,64	0
58	MG	CA	3461	1/1	0.52	0.42	107,107,107,107	0
58	MG	CA	3466	1/1	0.52	0.23	65,65,65,65	0
58	MG	AA	3246	1/1	0.52	0.19	98,98,98,98	0
58	MG	CA	3553	1/1	0.52	0.38	88,88,88,88	0
58	MG	AZ	301	1/1	0.53	0.52	98,98,98,98	0
58	MG	CA	3002	1/1	0.53	0.59	112,112,112,112	0
58	MG	DE	202	1/1	0.54	0.49	93,93,93,93	0
58	MG	AA	3113	1/1	0.54	1.10	97,97,97,97	0
58	MG	BA	3110	1/1	0.55	0.23	103,103,103,103	0
58	MG	CA	3081	1/1	0.55	0.37	85,85,85,85	0
58	MG	CA	3124	1/1	0.58	1.55	87,87,87,87	0
58	MG	CA	3209	1/1	0.58	0.49	82,82,82,82	0
58	MG	AA	3109	1/1	0.60	0.49	124,124,124,124	0
58	MG	BA	3035	1/1	0.60	0.55	99,99,99,99	0
58	MG	CA	3066	1/1	0.61	0.20	50,50,50,50	0
58	MG	AA	3538	1/1	0.61	0.24	91,91,91,91	0
58	MG	CA	3094	1/1	0.61	0.78	83,83,83,83	0
58	MG	DA	1659	1/1	0.62	0.50	87,87,87,87	0
58	MG	BA	3119	1/1	0.62	0.27	79,79,79,79	0
58	MG	CA	3523	1/1	0.63	0.19	62,62,62,62	0
58	MG	CA	3166	1/1	0.63	0.20	61,61,61,61	0
58	MG	AA	3193	1/1	0.63	0.57	72,72,72,72	0
58	MG	AB	3006	1/1	0.63	0.42	70,70,70,70	0
58	MG	CA	3070	1/1	0.64	0.32	82,82,82,82	0
58	MG	CA	3537	1/1	0.65	0.28	67,67,67,67	0
58	MG	DA	1634	1/1	0.65	0.32	71,71,71,71	0
58	MG	BA	3106	1/1	0.66	0.52	93,93,93,93	0
58	MG	AD	306	1/1	0.66	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	AN	3001	1/1	0.66	0.38	83,83,83,83	0
58	MG	AA	3752	1/1	0.66	0.41	64,64,64,64	1
58	MG	CA	3181	1/1	0.66	0.64	108,108,108,108	0
58	MG	BA	3140	1/1	0.66	0.14	91,91,91,91	0
58	MG	AA	3756	1/1	0.66	0.21	61,61,61,61	0
58	MG	DK	5001	1/1	0.66	0.34	101,101,101,101	0
58	MG	BA	3072	1/1	0.66	0.26	75,75,75,75	0
58	MG	CA	3238	1/1	0.67	0.47	85,85,85,85	0
58	MG	BA	3209	1/1	0.67	0.20	79,79,79,79	0
58	MG	BA	3179	1/1	0.67	0.27	78,78,78,78	0
58	MG	CA	3153	1/1	0.67	0.34	55,55,55,55	0
58	MG	BA	3090	1/1	0.68	0.38	90,90,90,90	0
58	MG	BL	3001	1/1	0.68	0.23	80,80,80,80	0
58	MG	CA	3106	1/1	0.68	0.14	79,79,79,79	0
58	MG	BA	3069	1/1	0.68	0.32	82,82,82,82	0
58	MG	CA	3195	1/1	0.68	0.45	69,69,69,69	0
58	MG	BA	3107	1/1	0.68	0.29	59,59,59,59	0
58	MG	CA	3529	1/1	0.68	0.11	79,79,79,79	0
58	MG	AA	3745	1/1	0.69	0.33	84,84,84,84	0
58	MG	CA	3060	1/1	0.69	0.36	60,60,60,60	0
58	MG	AA	3122	1/1	0.69	0.53	67,67,67,67	0
58	MG	CA	3156	1/1	0.69	0.29	84,84,84,84	0
58	MG	AA	3736	1/1	0.69	0.19	35,35,35,35	0
58	MG	AA	3767	1/1	0.69	0.28	66,66,66,66	0
58	MG	DA	1635	1/1	0.69	0.43	89,89,89,89	0
58	MG	CA	3119	1/1	0.69	0.23	55,55,55,55	0
58	MG	BA	3103	1/1	0.70	0.26	85,85,85,85	0
58	MG	CA	3078	1/1	0.70	0.28	66,66,66,66	0
58	MG	CA	3140	1/1	0.70	0.23	122,122,122,122	0
58	MG	BA	3163	1/1	0.70	0.18	52,52,52,52	0
58	MG	CA	3130	1/1	0.71	0.41	68,68,68,68	0
58	MG	CA	3275	1/1	0.71	0.32	67,67,67,67	0
58	MG	CA	3090	1/1	0.71	0.37	79,79,79,79	0
58	MG	BA	3056	1/1	0.71	0.29	67,67,67,67	0
58	MG	CA	3149	1/1	0.71	0.36	63,63,63,63	0
58	MG	CA	3008	1/1	0.71	0.37	98,98,98,98	0
58	MG	CA	3108	1/1	0.71	0.22	106,106,106,106	0
58	MG	CA	3527	1/1	0.71	0.17	81,81,81,81	0
58	MG	AA	3353	1/1	0.71	0.14	75,75,75,75	0
58	MG	CA	3118	1/1	0.71	0.19	67,67,67,67	0
58	MG	A4	502	1/1	0.71	0.21	120,120,120,120	0
58	MG	AB	3020	1/1	0.71	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	DA	1603	1/1	0.72	0.17	81,81,81,81	0
58	MG	DA	1620	1/1	0.72	0.27	69,69,69,69	0
58	MG	CA	3098	1/1	0.72	0.31	79,79,79,79	0
58	MG	BA	3088	1/1	0.72	0.45	68,68,68,68	0
58	MG	CA	3351	1/1	0.72	0.11	83,83,83,83	0
58	MG	CA	3611	1/1	0.72	0.35	58,58,58,58	0
58	MG	AA	3704	1/1	0.72	0.12	76,76,76,76	0
58	MG	CA	3216	1/1	0.73	0.09	74,74,74,74	0
58	MG	AA	3639	1/1	0.73	0.27	71,71,71,71	0
58	MG	BA	3092	1/1	0.73	0.48	86,86,86,86	0
58	MG	CA	3545	1/1	0.73	0.27	61,61,61,61	0
58	MG	AB	3004	1/1	0.73	0.37	87,87,87,87	0
58	MG	AA	3641	1/1	0.73	0.60	76,76,76,76	0
58	MG	BN	503	1/1	0.73	0.28	66,66,66,66	0
58	MG	CE	304	1/1	0.73	0.55	65,65,65,65	0
58	MG	CA	3184	1/1	0.73	0.64	85,85,85,85	0
58	MG	BX	104	1/1	0.73	0.28	69,69,69,69	0
58	MG	BA	3055	1/1	0.73	0.14	54,54,54,54	0
58	MG	CA	3173	1/1	0.74	0.33	81,81,81,81	0
58	MG	CA	3635	1/1	0.74	0.18	79,79,79,79	0
58	MG	CA	3031	1/1	0.74	0.11	74,74,74,74	0
58	MG	BX	101	1/1	0.74	0.23	78,78,78,78	0
58	MG	CA	3297	1/1	0.74	0.13	83,83,83,83	0
58	MG	DA	1740	1/1	0.74	0.36	79,79,79,79	0
58	MG	DA	1752	1/1	0.74	0.20	79,79,79,79	0
58	MG	AA	3806	1/1	0.74	0.21	60,60,60,60	0
58	MG	AA	3711	1/1	0.74	0.33	74,74,74,74	0
58	MG	BA	3205	1/1	0.74	0.14	68,68,68,68	0
58	MG	CA	3587	1/1	0.74	0.31	81,81,81,81	0
58	MG	AA	3598	1/1	0.75	0.13	61,61,61,61	0
58	MG	CA	3582	1/1	0.75	0.12	96,96,96,96	0
58	MG	CA	3059	1/1	0.75	0.32	76,76,76,76	0
58	MG	AA	3018	1/1	0.75	0.86	75,75,75,75	0
58	MG	CA	3225	1/1	0.75	0.66	79,79,79,79	0
58	MG	CA	3656	1/1	0.75	0.33	96,96,96,96	0
58	MG	CA	3232	1/1	0.75	0.68	65,65,65,65	0
58	MG	AG	202	1/1	0.75	0.09	73,73,73,73	0
58	MG	CA	3577	1/1	0.76	0.29	43,43,43,43	1
58	MG	CA	3042	1/1	0.76	0.71	96,96,96,96	0
58	MG	AA	3675	1/1	0.76	0.10	40,40,40,40	0
58	MG	CA	3604	1/1	0.76	0.10	74,74,74,74	0
58	MG	CA	3501	1/1	0.76	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	AA	3195	1/1	0.76	0.26	43,43,43,43	0
58	MG	CA	3646	1/1	0.76	0.10	75,75,75,75	0
58	MG	BA	3068	1/1	0.76	0.28	87,87,87,87	0
58	MG	AA	3821	1/1	0.76	0.33	46,46,46,46	0
58	MG	BA	3052	1/1	0.76	0.25	102,102,102,102	0
58	MG	BA	3144	1/1	0.76	0.22	53,53,53,53	0
58	MG	CA	3035	1/1	0.76	0.36	58,58,58,58	0
58	MG	CA	3572	1/1	0.76	0.29	76,76,76,76	0
58	MG	AA	3277	1/1	0.77	0.30	78,78,78,78	0
58	MG	BA	3108	1/1	0.77	0.26	49,49,49,49	0
58	MG	CA	3580	1/1	0.77	0.30	79,79,79,79	0
58	MG	AA	3689	1/1	0.77	0.17	55,55,55,55	0
58	MG	AA	3762	1/1	0.77	0.29	58,58,58,58	0
58	MG	AA	3765	1/1	0.77	0.33	61,61,61,61	0
58	MG	CA	3606	1/1	0.77	0.20	51,51,51,51	0
58	MG	BA	3061	1/1	0.77	0.24	67,67,67,67	0
58	MG	CA	3530	1/1	0.77	0.32	78,78,78,78	0
58	MG	CA	3057	1/1	0.77	0.15	84,84,84,84	0
58	MG	CA	3650	1/1	0.77	0.11	67,67,67,67	0
58	MG	DA	1749	1/1	0.77	0.16	80,80,80,80	0
58	MG	BA	3067	1/1	0.77	0.35	73,73,73,73	0
58	MG	CB	3012	1/1	0.77	0.30	74,74,74,74	0
58	MG	BA	3025	1/1	0.77	0.18	88,88,88,88	0
58	MG	CA	3565	1/1	0.77	0.09	90,90,90,90	0
58	MG	DA	1602	1/1	0.77	0.28	95,95,95,95	0
58	MG	CA	3509	1/1	0.78	0.17	96,96,96,96	0
58	MG	BA	3203	1/1	0.78	0.26	83,83,83,83	0
58	MG	DA	1631	1/1	0.78	0.22	59,59,59,59	0
58	MG	CA	3013	1/1	0.78	0.22	61,61,61,61	0
58	MG	AA	3088	1/1	0.78	0.47	73,73,73,73	0
58	MG	AA	3444	1/1	0.78	0.20	73,73,73,73	0
58	MG	DA	1677	1/1	0.78	0.45	80,80,80,80	0
58	MG	BA	3015	1/1	0.78	0.25	87,87,87,87	0
58	MG	CA	3647	1/1	0.78	0.32	82,82,82,82	0
58	MG	BA	3152	1/1	0.78	0.11	58,58,58,58	0
58	MG	CA	3379	1/1	0.78	0.17	86,86,86,86	0
58	MG	CA	3407	1/1	0.78	0.14	70,70,70,70	0
58	MG	DA	1742	1/1	0.78	0.10	77,77,77,77	0
58	MG	CA	3082	1/1	0.78	0.27	66,66,66,66	0
58	MG	AA	3461	1/1	0.78	0.34	64,64,64,64	0
58	MG	CG	3001	1/1	0.78	0.23	81,81,81,81	0
58	MG	DA	1764	1/1	0.78	0.35	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	BA	3094	1/1	0.78	0.12	78,78,78,78	0
58	MG	BA	3098	1/1	0.78	0.35	78,78,78,78	0
58	MG	DA	1605	1/1	0.78	0.43	75,75,75,75	0
58	MG	CA	3015	1/1	0.79	0.38	82,82,82,82	0
58	MG	CA	3377	1/1	0.79	0.12	64,64,64,64	0
58	MG	AA	3423	1/1	0.79	0.14	65,65,65,65	0
58	MG	DA	1622	1/1	0.79	0.15	42,42,42,42	0
58	MG	AA	3614	1/1	0.79	0.14	103,103,103,103	0
58	MG	DA	1628	1/1	0.79	0.15	69,69,69,69	0
58	MG	CA	3583	1/1	0.79	0.17	78,78,78,78	0
58	MG	AA	3622	1/1	0.79	0.19	46,46,46,46	0
58	MG	CA	3596	1/1	0.79	0.19	77,77,77,77	0
58	MG	AA	3441	1/1	0.79	0.20	46,46,46,46	0
58	MG	DA	1672	1/1	0.79	0.38	100,100,100,100	0
58	MG	AA	3640	1/1	0.79	0.19	74,74,74,74	0
58	MG	DA	1686	1/1	0.79	0.15	101,101,101,101	0
58	MG	CA	3500	1/1	0.79	0.16	82,82,82,82	0
58	MG	AA	3442	1/1	0.79	0.19	64,64,64,64	0
58	MG	CA	3644	1/1	0.79	0.24	66,66,66,66	0
58	MG	AA	3269	1/1	0.79	0.18	84,84,84,84	0
58	MG	DA	1738	1/1	0.79	0.19	78,78,78,78	0
58	MG	BV	101	1/1	0.79	0.30	110,110,110,110	0
58	MG	AA	3681	1/1	0.79	0.33	63,63,63,63	0
58	MG	AA	3201	1/1	0.79	0.24	91,91,91,91	0
58	MG	CA	3135	1/1	0.79	0.96	84,84,84,84	0
58	MG	AA	3266	1/1	0.79	0.31	74,74,74,74	0
58	MG	CA	3292	1/1	0.79	0.45	75,75,75,75	0
58	MG	BA	3093	1/1	0.79	0.19	65,65,65,65	0
58	MG	CO	201	1/1	0.79	0.17	61,61,61,61	0
58	MG	AA	3580	1/1	0.79	0.10	39,39,39,39	0
58	MG	CA	3663	1/1	0.80	0.15	73,73,73,73	0
58	MG	CA	3484	1/1	0.80	0.34	67,67,67,67	0
58	MG	CA	3174	1/1	0.80	0.27	65,65,65,65	0
58	MG	AA	3100	1/1	0.80	0.10	60,60,60,60	0
58	MG	BA	3188	1/1	0.80	0.18	86,86,86,86	0
58	MG	CA	3505	1/1	0.80	0.09	60,60,60,60	0
58	MG	CA	3185	1/1	0.80	0.23	66,66,66,66	0
58	MG	CA	3193	1/1	0.80	0.14	57,57,57,57	0
58	MG	BA	3018	1/1	0.80	0.19	72,72,72,72	0
58	MG	CA	3200	1/1	0.80	0.37	72,72,72,72	0
58	MG	AA	3071	1/1	0.80	0.27	59,59,59,59	0
58	MG	AA	3546	1/1	0.80	0.12	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	BA	3047	1/1	0.80	0.66	71,71,71,71	0
58	MG	AA	3579	1/1	0.80	0.34	53,53,53,53	0
58	MG	CA	3555	1/1	0.80	0.17	80,80,80,80	0
58	MG	AA	3096	1/1	0.80	0.51	81,81,81,81	0
58	MG	DA	1656	1/1	0.80	0.15	91,91,91,91	0
58	MG	CA	3248	1/1	0.80	0.21	58,58,58,58	0
58	MG	AA	3801	1/1	0.80	0.07	89,89,89,89	0
58	MG	CA	3286	1/1	0.80	0.42	90,90,90,90	0
58	MG	AA	3665	1/1	0.80	0.24	83,83,83,83	0
58	MG	BX	106	1/1	0.80	0.11	55,55,55,55	0
58	MG	BA	3155	1/1	0.80	0.27	96,96,96,96	0
58	MG	CA	3349	1/1	0.80	0.20	54,54,54,54	0
58	MG	BA	3100	1/1	0.80	0.21	74,74,74,74	0
58	MG	BA	3167	1/1	0.80	0.20	85,85,85,85	0
58	MG	CA	3154	1/1	0.80	0.14	77,77,77,77	0
58	MG	CA	3628	1/1	0.80	0.66	76,76,76,76	0
58	MG	CA	3406	1/1	0.80	0.20	89,89,89,89	0
58	MG	CA	3638	1/1	0.80	0.25	78,78,78,78	0
58	MG	CA	3086	1/1	0.80	0.32	63,63,63,63	0
58	MG	CA	3412	1/1	0.80	0.27	58,58,58,58	0
58	MG	CA	3413	1/1	0.80	0.21	79,79,79,79	0
58	MG	CA	3088	1/1	0.80	0.24	65,65,65,65	0
58	MG	AA	3099	1/1	0.80	0.23	57,57,57,57	0
58	MG	AA	3695	1/1	0.81	0.21	44,44,44,44	0
58	MG	AA	3119	1/1	0.81	0.36	62,62,62,62	0
58	MG	CA	3571	1/1	0.81	0.32	77,77,77,77	0
58	MG	AA	3057	1/1	0.81	0.24	56,56,56,56	0
58	MG	CA	3389	1/1	0.81	0.28	81,81,81,81	0
58	MG	CA	3390	1/1	0.81	0.28	74,74,74,74	0
58	MG	BX	103	1/1	0.81	0.23	87,87,87,87	0
58	MG	BA	3017	1/1	0.81	0.68	133,133,133,133	0
58	MG	CA	3585	1/1	0.81	0.23	80,80,80,80	0
58	MG	CA	3203	1/1	0.81	0.70	76,76,76,76	0
58	MG	CA	3590	1/1	0.81	0.30	62,62,62,62	0
58	MG	DA	1651	1/1	0.81	0.17	70,70,70,70	0
58	MG	BA	3099	1/1	0.81	0.23	70,70,70,70	0
58	MG	CA	3077	1/1	0.81	0.31	81,81,81,81	0
58	MG	DA	1662	1/1	0.81	0.22	70,70,70,70	0
58	MG	DA	1665	1/1	0.81	0.16	64,64,64,64	0
58	MG	AF	301	1/1	0.81	0.15	41,41,41,41	0
58	MG	AA	3148	1/1	0.81	0.36	68,68,68,68	0
58	MG	CA	3623	1/1	0.81	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	BA	3028	1/1	0.81	0.47	90,90,90,90	0
58	MG	CA	3243	1/1	0.81	0.41	110,110,110,110	0
58	MG	DA	1711	1/1	0.81	0.21	70,70,70,70	0
58	MG	BA	3186	1/1	0.81	0.15	67,67,67,67	0
58	MG	CA	3255	1/1	0.81	0.09	95,95,95,95	0
58	MG	DA	1734	1/1	0.81	0.12	78,78,78,78	0
58	MG	CA	3645	1/1	0.81	0.80	79,79,79,79	0
58	MG	BA	3033	1/1	0.81	0.19	52,52,52,52	0
58	MG	CA	3516	1/1	0.81	0.41	105,105,105,105	0
58	MG	BA	3074	1/1	0.81	0.15	66,66,66,66	0
58	MG	BA	3081	1/1	0.81	0.95	82,82,82,82	0
58	MG	AA	3206	1/1	0.81	0.24	62,62,62,62	0
58	MG	CA	3100	1/1	0.81	0.17	90,90,90,90	0
58	MG	CA	3311	1/1	0.81	0.14	48,48,48,48	0
58	MG	CA	3337	1/1	0.81	0.21	68,68,68,68	0
58	MG	AP	202	1/1	0.81	0.22	41,41,41,41	0
58	MG	DA	1613	1/1	0.82	0.33	70,70,70,70	0
58	MG	CA	3428	1/1	0.82	0.09	55,55,55,55	0
58	MG	AA	3002	1/1	0.82	0.18	54,54,54,54	0
58	MG	CA	3139	1/1	0.82	0.10	63,63,63,63	0
58	MG	DA	1626	1/1	0.82	0.42	72,72,72,72	0
58	MG	CA	3592	1/1	0.82	0.29	93,93,93,93	0
58	MG	CA	3072	1/1	0.82	0.33	93,93,93,93	0
58	MG	AA	3285	1/1	0.82	0.26	44,44,44,44	0
58	MG	CA	3250	1/1	0.82	0.38	76,76,76,76	0
58	MG	DA	1642	1/1	0.82	0.23	76,76,76,76	0
58	MG	AA	3431	1/1	0.82	0.30	56,56,56,56	0
58	MG	BX	109	1/1	0.82	0.12	78,78,78,78	0
58	MG	BA	3023	1/1	0.82	0.96	75,75,75,75	0
58	MG	DA	1660	1/1	0.82	0.23	70,70,70,70	0
58	MG	AA	3616	1/1	0.82	0.20	37,37,37,37	1
58	MG	CA	3637	1/1	0.82	0.28	79,79,79,79	0
58	MG	AA	3760	1/1	0.82	0.12	27,27,27,27	0
58	MG	AA	3452	1/1	0.82	0.18	67,67,67,67	0
58	MG	AA	3713	1/1	0.82	0.26	47,47,47,47	0
58	MG	BA	3078	1/1	0.82	0.24	66,66,66,66	0
58	MG	BA	3042	1/1	0.82	0.20	69,69,69,69	0
58	MG	DA	1710	1/1	0.82	0.18	79,79,79,79	0
58	MG	CA	3541	1/1	0.82	0.35	71,71,71,71	0
58	MG	CA	3043	1/1	0.82	0.69	101,101,101,101	0
58	MG	BA	3210	1/1	0.82	0.20	68,68,68,68	0
58	MG	CB	3006	1/1	0.82	0.12	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DA	1737	1/1	0.82	0.29	78,78,78,78	0
58	MG	BB	3001	1/1	0.82	0.26	76,76,76,76	0
58	MG	BA	3046	1/1	0.82	0.81	60,60,60,60	0
58	MG	CD	302	1/1	0.82	0.13	76,76,76,76	0
58	MG	AB	3014	1/1	0.82	0.15	67,67,67,67	0
58	MG	CA	3397	1/1	0.82	0.22	59,59,59,59	0
58	MG	BA	3051	1/1	0.82	0.39	71,71,71,71	0
58	MG	CQ	203	1/1	0.82	0.31	59,59,59,59	0
58	MG	CA	3210	1/1	0.82	0.44	93,93,93,93	0
58	MG	A8	5001	1/1	0.82	0.27	57,57,57,57	0
58	MG	CA	3069	1/1	0.82	0.23	56,56,56,56	0
58	MG	BA	3154	1/1	0.83	0.13	94,94,94,94	0
58	MG	DA	1607	1/1	0.83	1.19	82,82,82,82	0
58	MG	BA	3029	1/1	0.83	0.30	54,54,54,54	0
58	MG	CA	3175	1/1	0.83	0.54	60,60,60,60	0
58	MG	BA	3158	1/1	0.83	0.15	63,63,63,63	0
58	MG	AA	3625	1/1	0.83	0.27	63,63,63,63	0
58	MG	AA	3634	1/1	0.83	0.27	57,57,57,57	1
58	MG	CA	3190	1/1	0.83	0.19	68,68,68,68	0
58	MG	AA	3483	1/1	0.83	0.11	44,44,44,44	0
58	MG	AA	3060	1/1	0.83	0.48	64,64,64,64	0
58	MG	CA	3197	1/1	0.83	0.56	63,63,63,63	0
58	MG	CA	3034	1/1	0.83	0.42	100,100,100,100	0
58	MG	BA	3185	1/1	0.83	0.52	111,111,111,111	0
58	MG	DA	1654	1/1	0.83	0.32	57,57,57,57	0
58	MG	CA	3450	1/1	0.83	0.08	66,66,66,66	0
58	MG	CA	3206	1/1	0.83	0.65	104,104,104,104	0
58	MG	CA	3617	1/1	0.83	0.37	52,52,52,52	0
58	MG	AA	3239	1/1	0.83	0.15	69,69,69,69	0
58	MG	CA	3473	1/1	0.83	0.40	70,70,70,70	0
58	MG	AA	3649	1/1	0.83	0.29	90,90,90,90	0
58	MG	CA	3486	1/1	0.83	0.33	81,81,81,81	0
58	MG	CA	3214	1/1	0.83	0.24	43,43,43,43	0
58	MG	DA	1687	1/1	0.83	0.17	66,66,66,66	0
58	MG	BA	3190	1/1	0.83	0.28	89,89,89,89	0
58	MG	CA	3056	1/1	0.83	0.43	61,61,61,61	0
58	MG	AA	3651	1/1	0.83	0.27	49,49,49,49	0
58	MG	CA	3125	1/1	0.83	0.14	47,47,47,47	0
58	MG	CA	3649	1/1	0.83	0.18	94,94,94,94	0
58	MG	CA	3511	1/1	0.83	0.15	74,74,74,74	0
58	MG	AA	3440	1/1	0.83	0.21	51,51,51,51	0
58	MG	AA	3086	1/1	0.83	0.40	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	CA	3136	1/1	0.83	0.29	64,64,64,64	0
58	MG	AA	3769	1/1	0.83	0.36	56,56,56,56	0
58	MG	BA	3013	1/1	0.83	0.20	75,75,75,75	0
58	MG	AA	3247	1/1	0.83	0.78	68,68,68,68	0
58	MG	AA	3609	1/1	0.83	0.12	71,71,71,71	0
58	MG	AA	3690	1/1	0.83	0.19	69,69,69,69	0
58	MG	DA	1761	1/1	0.83	0.13	75,75,75,75	0
58	MG	CA	3548	1/1	0.83	0.12	116,116,116,116	0
58	MG	AA	3264	1/1	0.83	0.51	77,77,77,77	0
58	MG	AA	3354	1/1	0.83	0.23	58,58,58,58	0
58	MG	AA	3410	1/1	0.83	0.21	46,46,46,46	0
59	K	AA	3818	1/1	0.83	0.36	87,87,87,87	0
58	MG	AA	3737	1/1	0.84	0.46	75,75,75,75	0
58	MG	AA	3017	1/1	0.84	0.17	78,78,78,78	0
58	MG	A6	101	1/1	0.84	0.28	58,58,58,58	0
58	MG	CA	3633	1/1	0.84	0.12	61,61,61,61	0
58	MG	AA	3807	1/1	0.84	0.26	65,65,65,65	0
58	MG	BA	3004	1/1	0.84	0.16	64,64,64,64	0
58	MG	BA	3160	1/1	0.84	0.22	61,61,61,61	0
58	MG	CA	3526	1/1	0.84	0.20	75,75,75,75	0
58	MG	AA	3278	1/1	0.84	0.18	35,35,35,35	0
58	MG	CA	3191	1/1	0.84	0.17	84,84,84,84	0
58	MG	AA	3591	1/1	0.84	0.21	66,66,66,66	0
58	MG	AA	3759	1/1	0.84	0.28	63,63,63,63	0
58	MG	BA	3063	1/1	0.84	0.19	51,51,51,51	0
58	MG	DA	1683	1/1	0.84	0.45	70,70,70,70	0
58	MG	CA	3071	1/1	0.84	0.94	84,84,84,84	0
58	MG	AA	3652	1/1	0.84	0.20	74,74,74,74	0
58	MG	DA	1688	1/1	0.84	0.14	57,57,57,57	0
58	MG	CA	3205	1/1	0.84	0.25	71,71,71,71	0
58	MG	CA	3394	1/1	0.84	0.13	84,84,84,84	0
58	MG	AA	3186	1/1	0.84	0.24	41,41,41,41	0
58	MG	AA	3443	1/1	0.84	0.12	61,61,61,61	0
58	MG	AA	3766	1/1	0.84	0.20	70,70,70,70	0
58	MG	DA	1723	1/1	0.84	0.08	68,68,68,68	0
58	MG	CE	306	1/1	0.84	0.51	99,99,99,99	0
58	MG	DA	1729	1/1	0.84	0.60	79,79,79,79	0
58	MG	CA	3576	1/1	0.84	0.29	71,71,71,71	0
58	MG	CA	3211	1/1	0.84	0.37	72,72,72,72	0
58	MG	BA	3199	1/1	0.84	0.18	68,68,68,68	0
58	MG	AA	3728	1/1	0.84	0.14	48,48,48,48	0
58	MG	CA	3224	1/1	0.84	0.45	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	CA	3151	1/1	0.84	0.15	54,54,54,54	0
58	MG	CA	3227	1/1	0.84	0.37	68,68,68,68	0
58	MG	CA	3084	1/1	0.84	0.47	86,86,86,86	0
58	MG	CA	3479	1/1	0.84	0.12	56,56,56,56	0
58	MG	AA	3729	1/1	0.84	0.27	58,58,58,58	0
58	MG	CA	3039	1/1	0.84	0.58	69,69,69,69	0
58	MG	CA	3160	1/1	0.84	0.62	74,74,74,74	0
58	MG	AA	3116	1/1	0.84	0.43	75,75,75,75	0
58	MG	DA	1629	1/1	0.84	0.21	73,73,73,73	0
58	MG	AA	3137	1/1	0.85	0.10	49,49,49,49	0
58	MG	CA	3464	1/1	0.85	0.23	47,47,47,47	0
58	MG	AA	3087	1/1	0.85	0.38	49,49,49,49	0
58	MG	CA	3148	1/1	0.85	0.37	77,77,77,77	0
58	MG	AA	3364	1/1	0.85	0.33	79,79,79,79	0
58	MG	AA	3562	1/1	0.85	0.18	57,57,57,57	0
58	MG	CA	3616	1/1	0.85	0.34	71,71,71,71	0
58	MG	AB	3018	1/1	0.85	0.18	81,81,81,81	0
58	MG	CA	3619	1/1	0.85	0.58	79,79,79,79	0
58	MG	AA	3158	1/1	0.85	0.17	35,35,35,35	0
58	MG	DA	1655	1/1	0.85	0.29	73,73,73,73	0
58	MG	CA	3624	1/1	0.85	0.33	72,72,72,72	0
58	MG	CA	3083	1/1	0.85	0.26	70,70,70,70	0
58	MG	AA	3167	1/1	0.85	0.26	29,29,29,29	0
58	MG	AA	3179	1/1	0.85	0.35	78,78,78,78	0
58	MG	AA	3597	1/1	0.85	0.20	40,40,40,40	0
58	MG	AA	3761	1/1	0.85	0.25	48,48,48,48	0
58	MG	DA	1675	1/1	0.85	0.15	77,77,77,77	0
58	MG	AA	3082	1/1	0.85	0.20	38,38,38,38	0
58	MG	AA	3268	1/1	0.85	0.51	61,61,61,61	0
58	MG	CA	3099	1/1	0.85	0.28	82,82,82,82	0
58	MG	BA	3101	1/1	0.85	0.20	60,60,60,60	0
58	MG	CA	3102	1/1	0.85	0.16	76,76,76,76	0
58	MG	AA	3611	1/1	0.85	0.13	55,55,55,55	0
58	MG	CA	3535	1/1	0.85	0.13	79,79,79,79	0
58	MG	CA	3374	1/1	0.85	0.28	56,56,56,56	0
58	MG	CA	3666	1/1	0.85	0.34	62,62,62,62	0
58	MG	CA	3538	1/1	0.85	0.10	69,69,69,69	0
58	MG	CA	3107	1/1	0.85	0.37	54,54,54,54	0
58	MG	CA	3378	1/1	0.85	0.14	78,78,78,78	0
58	MG	AA	3004	1/1	0.85	0.21	24,24,24,24	0
58	MG	BA	3058	1/1	0.85	0.41	69,69,69,69	0
58	MG	CA	3116	1/1	0.85	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3112	1/1	0.85	0.29	46,46,46,46	0
58	MG	CN	5001	1/1	0.85	0.14	76,76,76,76	0
58	MG	AA	3198	1/1	0.85	0.25	36,36,36,36	0
58	MG	AA	3126	1/1	0.85	0.36	26,26,26,26	0
58	MG	AA	3727	1/1	0.85	0.18	66,66,66,66	0
58	MG	BA	3126	1/1	0.85	0.17	59,59,59,59	0
58	MG	BA	3131	1/1	0.85	0.13	76,76,76,76	0
58	MG	BA	3133	1/1	0.85	0.12	68,68,68,68	0
58	MG	DD	502	1/1	0.85	0.40	61,61,61,61	0
58	MG	CA	3429	1/1	0.85	0.34	62,62,62,62	1
58	MG	DA	1615	1/1	0.85	0.63	85,85,85,85	0
58	MG	DT	3001	1/1	0.85	0.34	66,66,66,66	0
58	MG	AA	3345	1/1	0.85	0.18	67,67,67,67	0
58	MG	CA	3455	1/1	0.85	0.18	78,78,78,78	0
58	MG	AA	3836	1/1	0.86	0.32	48,48,48,48	0
58	MG	AA	3626	1/1	0.86	0.18	58,58,58,58	0
58	MG	DA	1648	1/1	0.86	0.54	90,90,90,90	0
58	MG	BA	3014	1/1	0.86	0.12	97,97,97,97	0
58	MG	AA	3014	1/1	0.86	0.15	44,44,44,44	0
58	MG	AA	3036	1/1	0.86	0.20	49,49,49,49	0
58	MG	CA	3014	1/1	0.86	0.31	62,62,62,62	0
58	MG	CA	3539	1/1	0.86	0.45	77,77,77,77	0
58	MG	BA	3062	1/1	0.86	1.07	81,81,81,81	0
58	MG	AA	3238	1/1	0.86	0.26	55,55,55,55	0
58	MG	AA	3024	1/1	0.86	0.19	55,55,55,55	0
58	MG	CA	3657	1/1	0.86	0.29	62,62,62,62	0
58	MG	AA	3162	1/1	0.86	0.38	58,58,58,58	0
58	MG	AA	3115	1/1	0.86	0.17	15,15,15,15	0
58	MG	AA	3519	1/1	0.86	0.19	32,32,32,32	0
58	MG	CA	3241	1/1	0.86	0.23	74,74,74,74	0
58	MG	BA	3030	1/1	0.86	0.29	62,62,62,62	0
58	MG	CA	3575	1/1	0.86	0.19	78,78,78,78	0
58	MG	CE	303	1/1	0.86	0.39	53,53,53,53	0
58	MG	CA	3245	1/1	0.86	0.32	77,77,77,77	0
58	MG	DA	1709	1/1	0.86	0.14	44,44,44,44	0
58	MG	BA	3031	1/1	0.86	0.12	61,61,61,61	0
58	MG	CF	303	1/1	0.86	0.20	50,50,50,50	0
58	MG	CA	3048	1/1	0.86	0.49	85,85,85,85	0
58	MG	DA	1717	1/1	0.86	0.15	74,74,74,74	0
58	MG	DA	1720	1/1	0.86	0.21	64,64,64,64	0
58	MG	CA	3472	1/1	0.86	0.15	45,45,45,45	0
58	MG	AA	3249	1/1	0.86	0.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	BA	3135	1/1	0.86	0.41	80,80,80,80	0
58	MG	AA	3304	1/1	0.86	0.23	30,30,30,30	0
58	MG	CA	3485	1/1	0.86	0.18	74,74,74,74	0
58	MG	AA	3680	1/1	0.86	0.20	58,58,58,58	0
58	MG	BA	3148	1/1	0.86	0.33	67,67,67,67	0
58	MG	DA	1611	1/1	0.86	0.14	74,74,74,74	0
58	MG	DA	1744	1/1	0.86	0.41	90,90,90,90	0
58	MG	BT	3001	1/1	0.86	0.50	60,60,60,60	0
58	MG	AA	3330	1/1	0.86	0.14	66,66,66,66	0
58	MG	CA	3194	1/1	0.86	0.19	61,61,61,61	0
58	MG	DA	1621	1/1	0.86	0.17	58,58,58,58	0
58	MG	CA	3339	1/1	0.86	0.17	62,62,62,62	0
58	MG	CA	3510	1/1	0.86	0.24	93,93,93,93	0
58	MG	DE	201	1/1	0.86	0.24	82,82,82,82	0
58	MG	AA	3813	1/1	0.86	0.23	57,57,57,57	0
58	MG	CA	3514	1/1	0.86	0.39	63,63,63,63	0
58	MG	AA	3577	1/1	0.86	0.21	36,36,36,36	0
58	MG	CA	3127	1/1	0.86	0.25	94,94,94,94	0
58	MG	BA	3157	1/1	0.86	0.32	67,67,67,67	0
60	ZN	C4	501	1/1	0.86	0.07	192,192,192,192	0
58	MG	BD	502	1/1	0.87	0.45	80,80,80,80	0
58	MG	AA	3783	1/1	0.87	0.15	52,52,52,52	0
58	MG	CA	3237	1/1	0.87	0.57	75,75,75,75	0
58	MG	AA	3042	1/1	0.87	0.27	36,36,36,36	0
58	MG	CA	3613	1/1	0.87	0.22	96,96,96,96	0
58	MG	DA	1646	1/1	0.87	0.27	57,57,57,57	0
58	MG	CA	3239	1/1	0.87	0.23	74,74,74,74	0
58	MG	CA	3481	1/1	0.87	0.29	55,55,55,55	0
58	MG	AA	3794	1/1	0.87	0.23	68,68,68,68	0
58	MG	AA	3437	1/1	0.87	0.15	55,55,55,55	0
58	MG	CA	3076	1/1	0.87	0.68	69,69,69,69	0
58	MG	AA	3802	1/1	0.87	0.25	54,54,54,54	0
58	MG	AA	3232	1/1	0.87	0.45	79,79,79,79	0
58	MG	BA	3016	1/1	0.87	0.26	73,73,73,73	0
58	MG	CA	3260	1/1	0.87	0.30	69,69,69,69	0
58	MG	CA	3274	1/1	0.87	0.41	73,73,73,73	0
58	MG	BA	3070	1/1	0.87	0.17	72,72,72,72	0
58	MG	CA	3278	1/1	0.87	0.18	48,48,48,48	0
58	MG	BX	108	1/1	0.87	0.10	78,78,78,78	0
58	MG	BA	3071	1/1	0.87	0.29	93,93,93,93	0
58	MG	AA	3572	1/1	0.87	0.13	49,49,49,49	0
58	MG	AA	3192	1/1	0.87	0.16	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3651	1/1	0.87	0.34	51,51,51,51	0
58	MG	DA	1695	1/1	0.87	0.40	88,88,88,88	0
58	MG	CA	3010	1/1	0.87	0.15	40,40,40,40	0
58	MG	AA	3132	1/1	0.87	0.39	53,53,53,53	0
58	MG	CA	3095	1/1	0.87	0.35	86,86,86,86	0
58	MG	AA	3273	1/1	0.87	0.24	52,52,52,52	0
58	MG	AA	3650	1/1	0.87	0.08	59,59,59,59	0
58	MG	AA	3589	1/1	0.87	0.16	38,38,38,38	0
58	MG	AA	3165	1/1	0.87	0.16	56,56,56,56	0
58	MG	AA	3373	1/1	0.87	0.19	57,57,57,57	0
58	MG	CA	3543	1/1	0.87	0.21	70,70,70,70	0
58	MG	AA	3382	1/1	0.87	0.13	38,38,38,38	1
58	MG	DA	1733	1/1	0.87	0.53	81,81,81,81	0
58	MG	AA	3027	1/1	0.87	0.40	77,77,77,77	0
58	MG	CA	3552	1/1	0.87	0.13	34,34,34,34	0
58	MG	AE	301	1/1	0.87	0.40	68,68,68,68	0
58	MG	BA	3045	1/1	0.87	0.29	75,75,75,75	0
58	MG	CA	3559	1/1	0.87	0.12	75,75,75,75	0
58	MG	AA	3491	1/1	0.87	0.28	33,33,33,33	0
58	MG	AA	3683	1/1	0.87	0.38	65,65,65,65	0
58	MG	AA	3492	1/1	0.87	0.37	61,61,61,61	0
58	MG	AA	3006	1/1	0.87	0.42	52,52,52,52	0
58	MG	AA	3531	1/1	0.87	0.11	52,52,52,52	0
58	MG	CA	3414	1/1	0.87	0.17	39,39,39,39	0
58	MG	AA	3703	1/1	0.87	0.28	41,41,41,41	1
58	MG	CA	3131	1/1	0.87	0.63	70,70,70,70	0
58	MG	CA	3445	1/1	0.87	0.23	91,91,91,91	0
58	MG	CA	3448	1/1	0.87	0.30	78,78,78,78	0
58	MG	DL	3001	1/1	0.87	0.43	57,57,57,57	0
58	MG	CA	3223	1/1	0.87	0.45	75,75,75,75	0
58	MG	CA	3134	1/1	0.87	0.28	69,69,69,69	0
58	MG	CA	3591	1/1	0.87	0.17	77,77,77,77	0
58	MG	BA	3057	1/1	0.87	0.11	89,89,89,89	0
58	MG	CA	3459	1/1	0.88	0.20	48,48,48,48	0
58	MG	AB	3001	1/1	0.88	0.63	85,85,85,85	0
58	MG	CA	3463	1/1	0.88	0.09	50,50,50,50	0
58	MG	DA	1630	1/1	0.88	0.30	56,56,56,56	0
58	MG	CA	3235	1/1	0.88	0.41	70,70,70,70	0
58	MG	CA	3138	1/1	0.88	0.35	70,70,70,70	0
58	MG	AA	3052	1/1	0.88	0.49	63,63,63,63	0
58	MG	DA	1640	1/1	0.88	0.15	74,74,74,74	0
58	MG	BA	3117	1/1	0.88	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3476	1/1	0.88	0.25	54,54,54,54	0
58	MG	AA	3379	1/1	0.88	0.14	30,30,30,30	0
58	MG	AA	3633	1/1	0.88	0.27	75,75,75,75	0
58	MG	BA	3019	1/1	0.88	0.34	55,55,55,55	0
58	MG	AA	3696	1/1	0.88	0.69	76,76,76,76	0
58	MG	AA	3019	1/1	0.88	0.30	57,57,57,57	0
58	MG	AA	3034	1/1	0.88	0.29	56,56,56,56	0
58	MG	AD	307	1/1	0.88	0.34	37,37,37,37	0
58	MG	DA	1661	1/1	0.88	0.13	62,62,62,62	0
58	MG	CA	3634	1/1	0.88	0.16	75,75,75,75	0
58	MG	AA	3587	1/1	0.88	0.15	59,59,59,59	0
58	MG	CA	3636	1/1	0.88	0.25	65,65,65,65	0
58	MG	BA	3077	1/1	0.88	0.43	86,86,86,86	0
58	MG	AA	3781	1/1	0.88	0.23	52,52,52,52	1
58	MG	AF	304	1/1	0.88	0.29	61,61,61,61	0
58	MG	AA	3490	1/1	0.88	0.11	50,50,50,50	0
58	MG	BA	3089	1/1	0.88	0.64	89,89,89,89	0
58	MG	AA	3170	1/1	0.88	0.23	39,39,39,39	0
58	MG	DA	1689	1/1	0.88	0.39	80,80,80,80	0
58	MG	CA	3300	1/1	0.88	0.28	66,66,66,66	0
58	MG	BA	3162	1/1	0.88	0.09	54,54,54,54	0
58	MG	DA	1699	1/1	0.88	0.36	123,123,123,123	0
58	MG	CA	3329	1/1	0.88	0.17	57,57,57,57	0
58	MG	DA	1705	1/1	0.88	0.32	86,86,86,86	0
58	MG	CA	3187	1/1	0.88	0.43	67,67,67,67	0
58	MG	CA	3189	1/1	0.88	0.59	58,58,58,58	0
58	MG	CA	3659	1/1	0.88	0.33	104,104,104,104	0
58	MG	BA	3043	1/1	0.88	0.22	65,65,65,65	0
58	MG	CA	3017	1/1	0.88	0.39	45,45,45,45	0
58	MG	CA	3018	1/1	0.88	0.25	62,62,62,62	0
58	MG	CA	3376	1/1	0.88	0.46	70,70,70,70	0
58	MG	AA	3253	1/1	0.88	0.37	65,65,65,65	0
58	MG	AA	3013	1/1	0.88	0.28	34,34,34,34	0
58	MG	CA	3196	1/1	0.88	0.21	58,58,58,58	0
58	MG	CA	3546	1/1	0.88	0.09	79,79,79,79	0
58	MG	BA	3173	1/1	0.88	0.62	113,113,113,113	0
58	MG	CA	3038	1/1	0.88	0.20	46,46,46,46	0
58	MG	DA	1739	1/1	0.88	0.21	76,76,76,76	0
58	MG	BA	3177	1/1	0.88	0.17	73,73,73,73	0
58	MG	AA	3606	1/1	0.88	0.14	64,64,64,64	0
58	MG	AA	3079	1/1	0.88	0.28	63,63,63,63	0
58	MG	CA	3044	1/1	0.88	0.30	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	C7	101	1/1	0.88	0.25	47,47,47,47	0
58	MG	AA	3235	1/1	0.88	0.27	54,54,54,54	0
58	MG	AA	3001	1/1	0.88	0.14	36,36,36,36	0
58	MG	CA	3212	1/1	0.88	0.12	37,37,37,37	0
58	MG	BA	3007	1/1	0.88	0.17	75,75,75,75	0
58	MG	CA	3128	1/1	0.88	0.32	60,60,60,60	0
58	MG	CA	3579	1/1	0.88	0.20	83,83,83,83	0
58	MG	CA	3437	1/1	0.88	0.14	74,74,74,74	0
58	MG	DA	1617	1/1	0.88	0.15	63,63,63,63	0
58	MG	BA	3104	1/1	0.88	0.41	76,76,76,76	0
58	MG	AA	3271	1/1	0.88	0.15	55,55,55,55	0
58	MG	AA	3563	1/1	0.88	0.19	49,49,49,49	1
60	ZN	A4	501	1/1	0.88	0.07	133,133,133,133	0
58	MG	BA	3059	1/1	0.88	0.56	76,76,76,76	0
58	MG	AA	3130	1/1	0.89	0.38	70,70,70,70	0
58	MG	AA	3645	1/1	0.89	0.56	78,78,78,78	0
58	MG	AA	3056	1/1	0.89	0.24	61,61,61,61	0
58	MG	AA	3274	1/1	0.89	0.50	88,88,88,88	0
58	MG	BA	3073	1/1	0.89	0.83	74,74,74,74	0
58	MG	CA	3221	1/1	0.89	0.18	76,76,76,76	0
58	MG	CA	3222	1/1	0.89	0.31	53,53,53,53	0
58	MG	BA	3195	1/1	0.89	0.33	73,73,73,73	0
58	MG	AA	3184	1/1	0.89	0.20	36,36,36,36	0
58	MG	CQ	202	1/1	0.89	0.15	66,66,66,66	0
58	MG	BA	3003	1/1	0.89	0.13	51,51,51,51	0
58	MG	CQ	204	1/1	0.89	0.61	79,79,79,79	0
58	MG	CV	202	1/1	0.89	0.35	85,85,85,85	0
58	MG	AA	3574	1/1	0.89	0.12	47,47,47,47	0
58	MG	BA	3006	1/1	0.89	0.14	71,71,71,71	0
58	MG	CA	3512	1/1	0.89	0.11	64,64,64,64	0
58	MG	CA	3513	1/1	0.89	0.19	66,66,66,66	0
58	MG	DA	1606	1/1	0.89	0.11	72,72,72,72	0
58	MG	CA	3233	1/1	0.89	0.15	56,56,56,56	0
58	MG	BA	3082	1/1	0.89	0.08	69,69,69,69	0
58	MG	BA	3083	1/1	0.89	0.34	68,68,68,68	0
58	MG	CA	3103	1/1	0.89	0.26	55,55,55,55	0
58	MG	AA	3062	1/1	0.89	0.53	66,66,66,66	0
58	MG	CA	3240	1/1	0.89	0.27	58,58,58,58	0
58	MG	BF	3001	1/1	0.89	0.42	71,71,71,71	0
58	MG	CA	3242	1/1	0.89	0.21	63,63,63,63	0
58	MG	DA	1623	1/1	0.89	0.49	77,77,77,77	0
58	MG	BA	3010	1/1	0.89	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	BL	3002	1/1	0.89	0.17	49,49,49,49	0
58	MG	AA	3144	1/1	0.89	0.38	47,47,47,47	0
58	MG	AA	3677	1/1	0.89	0.20	40,40,40,40	0
58	MG	CA	3254	1/1	0.89	0.26	63,63,63,63	0
58	MG	AA	3292	1/1	0.89	0.20	71,71,71,71	0
58	MG	AA	3302	1/1	0.89	0.23	56,56,56,56	0
58	MG	CA	3271	1/1	0.89	0.22	84,84,84,84	0
58	MG	CA	3549	1/1	0.89	0.17	61,61,61,61	0
58	MG	DA	1641	1/1	0.89	0.17	79,79,79,79	0
58	MG	BA	3097	1/1	0.89	0.40	66,66,66,66	0
58	MG	AA	3789	1/1	0.89	0.22	52,52,52,52	0
58	MG	AA	3792	1/1	0.89	0.22	27,27,27,27	0
58	MG	CA	3279	1/1	0.89	0.11	89,89,89,89	0
58	MG	AA	3106	1/1	0.89	0.12	80,80,80,80	0
58	MG	CA	3570	1/1	0.89	0.07	41,41,41,41	0
58	MG	AA	3590	1/1	0.89	0.26	23,23,23,23	1
58	MG	AA	3248	1/1	0.89	0.49	72,72,72,72	0
58	MG	AA	3805	1/1	0.89	0.24	40,40,40,40	1
58	MG	AA	3458	1/1	0.89	0.14	70,70,70,70	0
58	MG	CA	3308	1/1	0.89	0.23	50,50,50,50	0
58	MG	AA	3107	1/1	0.89	0.32	48,48,48,48	0
58	MG	DA	1668	1/1	0.89	0.34	82,82,82,82	0
58	MG	DA	1670	1/1	0.89	0.33	81,81,81,81	0
58	MG	AA	3808	1/1	0.89	0.24	33,33,33,33	1
58	MG	BA	3032	1/1	0.89	0.18	47,47,47,47	0
58	MG	AA	3477	1/1	0.89	0.20	57,57,57,57	0
58	MG	CA	3142	1/1	0.89	0.32	54,54,54,54	0
58	MG	DA	1685	1/1	0.89	0.19	52,52,52,52	0
58	MG	AA	3816	1/1	0.89	0.25	91,91,91,91	0
58	MG	AA	3480	1/1	0.89	0.18	54,54,54,54	0
58	MG	BA	3121	1/1	0.89	0.15	59,59,59,59	0
58	MG	BA	3125	1/1	0.89	0.26	63,63,63,63	0
58	MG	CA	3593	1/1	0.89	0.15	82,82,82,82	0
58	MG	AA	3197	1/1	0.89	0.37	49,49,49,49	0
58	MG	CA	3598	1/1	0.89	0.25	66,66,66,66	0
58	MG	CA	3603	1/1	0.89	0.16	48,48,48,48	0
58	MG	CA	3155	1/1	0.89	0.29	69,69,69,69	0
58	MG	DA	1706	1/1	0.89	0.10	85,85,85,85	0
58	MG	AA	3092	1/1	0.89	0.40	43,43,43,43	0
58	MG	AA	3715	1/1	0.89	0.22	54,54,54,54	0
58	MG	AA	3029	1/1	0.89	0.32	50,50,50,50	0
58	MG	BA	3136	1/1	0.89	0.25	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3400	1/1	0.89	0.12	73,73,73,73	0
58	MG	CA	3404	1/1	0.89	0.06	86,86,86,86	0
58	MG	BA	3048	1/1	0.89	0.15	75,75,75,75	0
58	MG	AA	3267	1/1	0.89	0.31	49,49,49,49	0
58	MG	DA	1728	1/1	0.89	0.13	85,85,85,85	0
58	MG	CA	3627	1/1	0.89	0.19	101,101,101,101	0
58	MG	AA	3498	1/1	0.89	0.07	45,45,45,45	0
58	MG	AA	3730	1/1	0.89	0.08	38,38,38,38	0
58	MG	AB	3023	1/1	0.89	0.30	74,74,74,74	0
58	MG	CA	3422	1/1	0.89	0.24	74,74,74,74	0
58	MG	CA	3424	1/1	0.89	0.24	51,51,51,51	0
58	MG	AA	3129	1/1	0.89	0.36	57,57,57,57	0
58	MG	AA	3229	1/1	0.89	0.26	54,54,54,54	0
58	MG	AA	3743	1/1	0.89	0.18	80,80,80,80	0
58	MG	CA	3068	1/1	0.89	0.33	72,72,72,72	0
58	MG	DA	1751	1/1	0.89	0.21	69,69,69,69	0
58	MG	AA	3391	1/1	0.89	0.13	42,42,42,42	0
58	MG	AF	303	1/1	0.89	0.45	48,48,48,48	0
58	MG	DA	1758	1/1	0.89	0.17	64,64,64,64	0
58	MG	AA	3539	1/1	0.89	0.37	63,63,63,63	0
58	MG	CA	3458	1/1	0.89	0.26	46,46,46,46	0
58	MG	BA	3065	1/1	0.89	0.28	57,57,57,57	0
58	MG	BA	3066	1/1	0.89	0.38	53,53,53,53	0
58	MG	BA	3170	1/1	0.89	0.09	71,71,71,71	0
58	MG	DJ	5001	1/1	0.89	0.26	105,105,105,105	0
58	MG	AA	3754	1/1	0.89	0.12	40,40,40,40	0
58	MG	CA	3204	1/1	0.89	0.12	58,58,58,58	0
58	MG	BA	3176	1/1	0.89	0.22	61,61,61,61	0
58	MG	CA	3080	1/1	0.89	0.20	56,56,56,56	0
58	MG	CB	3008	1/1	0.89	0.14	58,58,58,58	0
58	MG	CB	3010	1/1	0.89	0.14	53,53,53,53	0
58	MG	AA	3544	1/1	0.89	0.17	52,52,52,52	0
58	MG	BA	3168	1/1	0.90	0.06	57,57,57,57	0
58	MG	AA	3303	1/1	0.90	0.29	53,53,53,53	0
58	MG	AA	3714	1/1	0.90	0.29	55,55,55,55	1
58	MG	CA	3342	1/1	0.90	0.20	69,69,69,69	0
58	MG	AA	3073	1/1	0.90	0.11	25,25,25,25	0
58	MG	CA	3061	1/1	0.90	0.53	74,74,74,74	0
58	MG	CA	3363	1/1	0.90	0.19	42,42,42,42	0
58	MG	CA	3063	1/1	0.90	0.28	66,66,66,66	0
58	MG	CA	3064	1/1	0.90	0.27	51,51,51,51	0
58	MG	AA	3721	1/1	0.90	0.54	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	DA	1627	1/1	0.90	0.52	48,48,48,48	0
58	MG	AA	3481	1/1	0.90	0.11	50,50,50,50	0
58	MG	AA	3039	1/1	0.90	0.20	44,44,44,44	0
58	MG	AA	3488	1/1	0.90	0.17	23,23,23,23	0
58	MG	BA	3091	1/1	0.90	0.41	72,72,72,72	0
58	MG	AA	3163	1/1	0.90	0.22	45,45,45,45	0
58	MG	AA	3089	1/1	0.90	0.29	33,33,33,33	0
58	MG	DA	1637	1/1	0.90	0.38	67,67,67,67	0
58	MG	BA	3191	1/1	0.90	0.17	74,74,74,74	0
58	MG	BA	3194	1/1	0.90	0.15	60,60,60,60	0
58	MG	AB	3010	1/1	0.90	0.20	51,51,51,51	1
58	MG	DA	1645	1/1	0.90	0.20	61,61,61,61	0
58	MG	AA	3257	1/1	0.90	0.25	26,26,26,26	0
58	MG	CA	3410	1/1	0.90	0.20	40,40,40,40	0
58	MG	CA	3199	1/1	0.90	0.16	36,36,36,36	0
58	MG	AB	3017	1/1	0.90	0.21	76,76,76,76	0
58	MG	AA	3362	1/1	0.90	0.36	67,67,67,67	0
58	MG	CA	3420	1/1	0.90	0.25	58,58,58,58	0
58	MG	CA	3602	1/1	0.90	0.13	78,78,78,78	0
58	MG	AA	3064	1/1	0.90	0.19	35,35,35,35	0
58	MG	AA	3200	1/1	0.90	0.07	52,52,52,52	0
58	MG	AA	3138	1/1	0.90	0.22	54,54,54,54	0
58	MG	AA	3381	1/1	0.90	0.14	26,26,26,26	0
58	MG	CA	3431	1/1	0.90	0.33	51,51,51,51	0
58	MG	CA	3432	1/1	0.90	0.31	96,96,96,96	0
58	MG	DA	1671	1/1	0.90	0.41	72,72,72,72	0
58	MG	AD	309	1/1	0.90	0.22	55,55,55,55	0
58	MG	AA	3757	1/1	0.90	0.17	43,43,43,43	0
58	MG	DA	1676	1/1	0.90	0.18	75,75,75,75	0
58	MG	BA	3049	1/1	0.90	0.18	36,36,36,36	0
58	MG	DA	1682	1/1	0.90	0.28	52,52,52,52	0
58	MG	BL	3004	1/1	0.90	0.25	67,67,67,67	0
58	MG	AA	3172	1/1	0.90	0.64	32,32,32,32	0
58	MG	AA	3142	1/1	0.90	0.17	41,41,41,41	0
58	MG	BA	3115	1/1	0.90	0.45	86,86,86,86	0
58	MG	BA	3116	1/1	0.90	0.28	82,82,82,82	0
58	MG	BX	102	1/1	0.90	0.20	67,67,67,67	0
58	MG	BA	3054	1/1	0.90	0.29	77,77,77,77	0
58	MG	AA	3547	1/1	0.90	0.21	30,30,30,30	0
58	MG	AA	3270	1/1	0.90	0.20	80,80,80,80	0
58	MG	DA	1703	1/1	0.90	0.09	68,68,68,68	0
58	MG	AH	3002	1/1	0.90	0.31	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3422	1/1	0.90	0.10	23,23,23,23	0
58	MG	CA	3477	1/1	0.90	0.22	54,54,54,54	0
58	MG	BA	3128	1/1	0.90	0.13	47,47,47,47	0
58	MG	AA	3231	1/1	0.90	0.29	41,41,41,41	0
58	MG	CA	3122	1/1	0.90	0.15	43,43,43,43	0
58	MG	BA	3060	1/1	0.90	0.25	82,82,82,82	0
58	MG	DA	1716	1/1	0.90	0.26	75,75,75,75	0
58	MG	CA	3654	1/1	0.90	0.12	29,29,29,29	0
58	MG	DA	1718	1/1	0.90	0.23	72,72,72,72	0
58	MG	AA	3272	1/1	0.90	0.23	69,69,69,69	0
58	MG	CA	3491	1/1	0.90	0.18	65,65,65,65	0
58	MG	CA	3493	1/1	0.90	0.74	105,105,105,105	0
58	MG	AA	3181	1/1	0.90	0.31	94,94,94,94	0
58	MG	A5	103	1/1	0.90	0.33	60,60,60,60	0
58	MG	CB	3002	1/1	0.90	0.18	64,64,64,64	0
58	MG	CA	3129	1/1	0.90	0.27	69,69,69,69	0
58	MG	DA	1736	1/1	0.90	0.71	78,78,78,78	0
58	MG	CA	3246	1/1	0.90	0.49	77,77,77,77	0
58	MG	AA	3044	1/1	0.90	0.23	34,34,34,34	0
58	MG	BA	3146	1/1	0.90	0.28	65,65,65,65	0
58	MG	AA	3275	1/1	0.90	0.25	56,56,56,56	0
58	MG	CA	3033	1/1	0.90	0.60	88,88,88,88	0
58	MG	AA	3237	1/1	0.90	0.20	63,63,63,63	0
58	MG	DA	1746	1/1	0.90	0.16	77,77,77,77	0
58	MG	CA	3262	1/1	0.90	0.20	64,64,64,64	0
58	MG	CE	305	1/1	0.90	0.26	41,41,41,41	0
58	MG	CA	3266	1/1	0.90	0.27	58,58,58,58	0
58	MG	CF	301	1/1	0.90	0.28	62,62,62,62	0
58	MG	DA	1755	1/1	0.90	0.25	71,71,71,71	0
58	MG	AA	3097	1/1	0.90	0.16	61,61,61,61	0
58	MG	DA	1760	1/1	0.90	0.05	71,71,71,71	0
58	MG	AA	3283	1/1	0.90	0.42	59,59,59,59	0
58	MG	DA	1763	1/1	0.90	0.31	94,94,94,94	0
58	MG	AA	3187	1/1	0.90	0.08	36,36,36,36	0
58	MG	AA	3593	1/1	0.90	0.21	51,51,51,51	0
58	MG	BA	3012	1/1	0.90	0.14	29,29,29,29	0
58	MG	CA	3147	1/1	0.90	0.29	58,58,58,58	0
58	MG	CA	3536	1/1	0.90	0.15	75,75,75,75	0
58	MG	AA	3243	1/1	0.90	0.20	66,66,66,66	0
58	MG	AA	3188	1/1	0.90	0.14	31,31,31,31	0
58	MG	AA	3605	1/1	0.90	0.21	40,40,40,40	1
58	MG	CA	3050	1/1	0.90	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DZ	702	1/1	0.90	0.27	61,61,61,61	0
58	MG	CA	3052	1/1	0.90	0.39	69,69,69,69	0
58	MG	CA	3054	1/1	0.90	0.24	68,68,68,68	0
58	MG	CA	3315	1/1	0.90	0.60	76,76,76,76	0
58	MG	AW	3001	1/1	0.91	0.28	50,50,50,50	0
58	MG	BA	3204	1/1	0.91	0.35	68,68,68,68	0
58	MG	AW	3004	1/1	0.91	0.27	64,64,64,64	0
58	MG	DA	1608	1/1	0.91	0.14	58,58,58,58	0
58	MG	BA	3208	1/1	0.91	0.12	81,81,81,81	0
58	MG	CA	3247	1/1	0.91	0.24	55,55,55,55	0
58	MG	AA	3455	1/1	0.91	0.19	56,56,56,56	0
58	MG	A1	101	1/1	0.91	0.11	54,54,54,54	0
58	MG	DA	1618	1/1	0.91	0.09	47,47,47,47	0
58	MG	BA	3211	1/1	0.91	0.20	59,59,59,59	0
58	MG	AA	3090	1/1	0.91	0.24	50,50,50,50	0
58	MG	AA	3319	1/1	0.91	0.19	66,66,66,66	0
58	MG	CA	3117	1/1	0.91	0.61	73,73,73,73	0
58	MG	AA	3618	1/1	0.91	0.12	49,49,49,49	0
58	MG	A6	102	1/1	0.91	0.31	64,64,64,64	0
58	MG	CA	3542	1/1	0.91	0.37	82,82,82,82	0
58	MG	AA	3325	1/1	0.91	0.07	65,65,65,65	0
58	MG	AA	3252	1/1	0.91	0.23	46,46,46,46	0
58	MG	BN	502	1/1	0.91	0.23	64,64,64,64	0
58	MG	AA	3758	1/1	0.91	0.43	81,81,81,81	0
58	MG	CA	3282	1/1	0.91	0.11	31,31,31,31	0
58	MG	AA	3333	1/1	0.91	0.12	66,66,66,66	0
58	MG	CA	3289	1/1	0.91	0.22	51,51,51,51	0
58	MG	CA	3290	1/1	0.91	0.22	53,53,53,53	0
58	MG	AA	3627	1/1	0.91	0.29	72,72,72,72	0
58	MG	BA	3008	1/1	0.91	0.13	61,61,61,61	0
58	MG	DA	1643	1/1	0.91	0.11	55,55,55,55	0
58	MG	BA	3009	1/1	0.91	0.52	58,58,58,58	0
58	MG	AA	3335	1/1	0.91	0.16	40,40,40,40	0
58	MG	CA	3305	1/1	0.91	0.10	90,90,90,90	0
58	MG	CA	3573	1/1	0.91	0.19	64,64,64,64	0
58	MG	AA	3336	1/1	0.91	0.14	53,53,53,53	0
58	MG	AA	3637	1/1	0.91	0.27	64,64,64,64	0
58	MG	AA	3091	1/1	0.91	0.34	34,34,34,34	0
58	MG	AA	3350	1/1	0.91	0.22	32,32,32,32	0
58	MG	CA	3001	1/1	0.91	0.33	71,71,71,71	0
58	MG	AA	3012	1/1	0.91	0.27	34,34,34,34	0
58	MG	CA	3006	1/1	0.91	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3143	1/1	0.91	0.23	69,69,69,69	0
58	MG	CA	3145	1/1	0.91	0.32	66,66,66,66	0
58	MG	CA	3356	1/1	0.91	0.08	41,41,41,41	0
58	MG	AA	3778	1/1	0.91	0.43	55,55,55,55	0
58	MG	BA	3109	1/1	0.91	0.12	79,79,79,79	0
58	MG	DA	1673	1/1	0.91	0.34	61,61,61,61	0
58	MG	AA	3095	1/1	0.91	0.81	110,110,110,110	0
58	MG	AA	3360	1/1	0.91	0.17	111,111,111,111	0
58	MG	BA	3021	1/1	0.91	0.09	37,37,37,37	0
58	MG	AA	3203	1/1	0.91	0.22	46,46,46,46	0
58	MG	CA	3380	1/1	0.91	0.27	63,63,63,63	0
58	MG	AA	3204	1/1	0.91	0.23	55,55,55,55	0
58	MG	AA	3205	1/1	0.91	0.33	56,56,56,56	0
58	MG	CA	3158	1/1	0.91	0.19	54,54,54,54	0
58	MG	CA	3159	1/1	0.91	0.40	68,68,68,68	0
58	MG	AA	3653	1/1	0.91	0.08	67,67,67,67	0
58	MG	AA	3795	1/1	0.91	0.20	49,49,49,49	0
58	MG	CA	3169	1/1	0.91	0.45	55,55,55,55	0
58	MG	AA	3656	1/1	0.91	0.15	55,55,55,55	0
58	MG	DA	1700	1/1	0.91	0.20	62,62,62,62	0
58	MG	AA	3662	1/1	0.91	0.20	58,58,58,58	0
58	MG	CA	3626	1/1	0.91	0.14	62,62,62,62	0
58	MG	AA	3543	1/1	0.91	0.17	62,62,62,62	0
58	MG	AA	3173	1/1	0.91	0.37	71,71,71,71	0
58	MG	AA	3222	1/1	0.91	0.26	61,61,61,61	0
58	MG	AA	3679	1/1	0.91	0.18	64,64,64,64	0
58	MG	BA	3139	1/1	0.91	0.18	54,54,54,54	0
58	MG	CA	3047	1/1	0.91	0.16	60,60,60,60	0
58	MG	BA	3044	1/1	0.91	0.10	56,56,56,56	0
58	MG	AA	3811	1/1	0.91	0.22	53,53,53,53	0
58	MG	CA	3192	1/1	0.91	0.23	65,65,65,65	0
58	MG	AA	3083	1/1	0.91	0.17	27,27,27,27	1
58	MG	AA	3025	1/1	0.91	0.45	41,41,41,41	0
58	MG	CA	3439	1/1	0.91	0.09	46,46,46,46	0
58	MG	DA	1726	1/1	0.91	0.08	61,61,61,61	0
58	MG	AA	3402	1/1	0.91	0.11	27,27,27,27	0
58	MG	AA	3825	1/1	0.91	0.28	43,43,43,43	0
58	MG	AA	3685	1/1	0.91	0.19	47,47,47,47	0
58	MG	AA	3564	1/1	0.91	0.10	48,48,48,48	0
58	MG	AA	3183	1/1	0.91	0.16	75,75,75,75	0
58	MG	BA	3159	1/1	0.91	0.07	55,55,55,55	0
58	MG	AA	3691	1/1	0.91	0.18	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	BA	3161	1/1	0.91	0.28	87,87,87,87	0
58	MG	AA	3411	1/1	0.91	0.21	41,41,41,41	0
58	MG	AA	3414	1/1	0.91	0.12	55,55,55,55	0
58	MG	CB	3004	1/1	0.91	0.12	67,67,67,67	0
58	MG	AA	3234	1/1	0.91	0.40	77,77,77,77	0
58	MG	AA	3041	1/1	0.91	0.30	75,75,75,75	0
58	MG	CB	3009	1/1	0.91	0.18	64,64,64,64	0
58	MG	AA	3428	1/1	0.91	0.23	41,41,41,41	0
58	MG	AB	3021	1/1	0.91	0.23	60,60,60,60	0
58	MG	DA	1754	1/1	0.91	0.20	66,66,66,66	0
58	MG	AA	3147	1/1	0.91	0.37	37,37,37,37	0
58	MG	AA	3121	1/1	0.91	0.24	46,46,46,46	0
58	MG	CA	3482	1/1	0.91	0.15	89,89,89,89	0
58	MG	CA	3483	1/1	0.91	0.25	68,68,68,68	0
58	MG	AA	3279	1/1	0.91	0.21	51,51,51,51	0
58	MG	AA	3718	1/1	0.91	0.24	47,47,47,47	0
58	MG	DA	1766	1/1	0.91	0.19	53,53,53,53	0
58	MG	BA	3181	1/1	0.91	0.14	47,47,47,47	0
58	MG	AA	3007	1/1	0.91	0.17	20,20,20,20	0
58	MG	CA	3226	1/1	0.91	0.44	64,64,64,64	0
58	MG	AA	3159	1/1	0.91	0.30	97,97,97,97	0
58	MG	AA	3125	1/1	0.91	0.23	63,63,63,63	0
58	MG	AA	3601	1/1	0.91	0.31	59,59,59,59	0
58	MG	AA	3043	1/1	0.91	0.28	32,32,32,32	0
58	MG	BA	3192	1/1	0.91	0.16	65,65,65,65	0
58	MG	AA	3733	1/1	0.91	0.20	66,66,66,66	0
58	MG	AA	3449	1/1	0.91	0.22	53,53,53,53	0
58	MG	BA	3196	1/1	0.91	0.51	84,84,84,84	0
58	MG	AA	3196	1/1	0.91	0.14	50,50,50,50	0
60	ZN	DN	501	1/1	0.91	0.07	127,127,127,127	0
58	MG	CA	3531	1/1	0.92	0.09	58,58,58,58	0
58	MG	CA	3302	1/1	0.92	0.25	84,84,84,84	0
58	MG	AA	3294	1/1	0.92	0.06	65,65,65,65	0
58	MG	DA	1609	1/1	0.92	0.14	45,45,45,45	0
58	MG	AA	3819	1/1	0.92	0.12	44,44,44,44	0
58	MG	AA	3716	1/1	0.92	0.13	63,63,63,63	0
58	MG	BA	3096	1/1	0.92	0.13	64,64,64,64	0
58	MG	CA	3317	1/1	0.92	0.11	51,51,51,51	0
58	MG	CA	3318	1/1	0.92	0.08	45,45,45,45	0
58	MG	DA	1619	1/1	0.92	0.35	62,62,62,62	0
58	MG	CA	3320	1/1	0.92	0.14	66,66,66,66	0
58	MG	CA	3179	1/1	0.92	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	AA	3108	1/1	0.92	0.24	74,74,74,74	0
58	MG	BA	3022	1/1	0.92	0.28	46,46,46,46	0
58	MG	BA	3200	1/1	0.92	0.13	63,63,63,63	0
58	MG	CA	3343	1/1	0.92	0.15	46,46,46,46	0
58	MG	CA	3344	1/1	0.92	0.11	36,36,36,36	0
58	MG	AA	3827	1/1	0.92	0.56	51,51,51,51	0
58	MG	CA	3557	1/1	0.92	0.21	82,82,82,82	0
58	MG	CA	3188	1/1	0.92	0.17	36,36,36,36	0
58	MG	AA	3828	1/1	0.92	0.35	44,44,44,44	0
58	MG	CA	3357	1/1	0.92	0.21	57,57,57,57	0
58	MG	AA	3493	1/1	0.92	0.35	44,44,44,44	0
58	MG	CA	3370	1/1	0.92	0.14	56,56,56,56	0
58	MG	DA	1639	1/1	0.92	0.35	83,83,83,83	0
58	MG	AA	3495	1/1	0.92	0.24	50,50,50,50	0
58	MG	AA	3399	1/1	0.92	0.34	39,39,39,39	0
58	MG	AA	3502	1/1	0.92	0.08	24,24,24,24	0
58	MG	AA	3510	1/1	0.92	0.17	47,47,47,47	0
58	MG	AA	3059	1/1	0.92	0.27	49,49,49,49	0
58	MG	BA	3034	1/1	0.92	0.19	61,61,61,61	0
58	MG	AA	3045	1/1	0.92	0.60	43,43,43,43	0
58	MG	BK	201	1/1	0.92	0.19	56,56,56,56	0
58	MG	CA	3392	1/1	0.92	0.08	63,63,63,63	0
58	MG	CA	3393	1/1	0.92	0.22	35,35,35,35	0
58	MG	BA	3037	1/1	0.92	0.22	64,64,64,64	0
58	MG	CA	3396	1/1	0.92	0.38	64,64,64,64	0
58	MG	AA	3310	1/1	0.92	0.15	57,57,57,57	0
58	MG	BL	3003	1/1	0.92	0.18	79,79,79,79	0
58	MG	CA	3595	1/1	0.92	0.11	69,69,69,69	0
58	MG	DA	1664	1/1	0.92	0.34	59,59,59,59	0
58	MG	CA	3402	1/1	0.92	0.30	67,67,67,67	0
58	MG	AA	3740	1/1	0.92	0.33	92,92,92,92	0
58	MG	DA	1669	1/1	0.92	0.12	73,73,73,73	0
58	MG	AA	3742	1/1	0.92	0.22	39,39,39,39	1
58	MG	AA	3317	1/1	0.92	0.21	57,57,57,57	0
58	MG	CA	3408	1/1	0.92	0.17	54,54,54,54	0
58	MG	AA	3744	1/1	0.92	0.24	77,77,77,77	0
58	MG	CA	3608	1/1	0.92	0.18	70,70,70,70	0
58	MG	CA	3609	1/1	0.92	0.24	64,64,64,64	0
58	MG	AA	3160	1/1	0.92	0.30	50,50,50,50	0
58	MG	AA	3048	1/1	0.92	0.33	33,33,33,33	0
58	MG	AD	310	1/1	0.92	0.55	58,58,58,58	0
58	MG	CA	3215	1/1	0.92	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3647	1/1	0.92	0.21	71,71,71,71	0
58	MG	AA	3021	1/1	0.92	0.20	39,39,39,39	0
58	MG	AA	3070	1/1	0.92	0.21	33,33,33,33	0
58	MG	AA	3560	1/1	0.92	0.20	39,39,39,39	0
58	MG	BA	3138	1/1	0.92	0.28	62,62,62,62	0
58	MG	DA	1691	1/1	0.92	0.12	74,74,74,74	0
58	MG	AA	3334	1/1	0.92	0.21	58,58,58,58	0
58	MG	AA	3244	1/1	0.92	0.10	69,69,69,69	0
58	MG	CA	3438	1/1	0.92	0.14	49,49,49,49	0
58	MG	DA	1701	1/1	0.92	0.33	64,64,64,64	0
58	MG	BA	3143	1/1	0.92	0.14	79,79,79,79	0
58	MG	CA	3444	1/1	0.92	0.11	37,37,37,37	0
58	MG	CA	3228	1/1	0.92	0.17	51,51,51,51	0
58	MG	CA	3229	1/1	0.92	0.40	61,61,61,61	0
58	MG	AA	3117	1/1	0.92	0.23	50,50,50,50	0
58	MG	CA	3451	1/1	0.92	0.12	47,47,47,47	0
58	MG	AA	3344	1/1	0.92	0.12	85,85,85,85	0
58	MG	CA	3234	1/1	0.92	0.13	58,58,58,58	0
58	MG	AA	3210	1/1	0.92	0.20	63,63,63,63	0
58	MG	AA	3347	1/1	0.92	0.10	40,40,40,40	0
58	MG	AA	3349	1/1	0.92	0.19	39,39,39,39	0
58	MG	DA	1719	1/1	0.92	0.14	66,66,66,66	0
58	MG	A0	103	1/1	0.92	0.18	41,41,41,41	0
58	MG	AA	3215	1/1	0.92	0.21	56,56,56,56	0
58	MG	CA	3471	1/1	0.92	0.24	69,69,69,69	0
58	MG	CA	3020	1/1	0.92	0.16	61,61,61,61	0
58	MG	CA	3132	1/1	0.92	0.25	61,61,61,61	0
58	MG	CA	3665	1/1	0.92	0.18	55,55,55,55	0
58	MG	CA	3025	1/1	0.92	0.42	75,75,75,75	0
58	MG	CB	3001	1/1	0.92	0.24	96,96,96,96	0
58	MG	AA	3055	1/1	0.92	0.22	34,34,34,34	0
58	MG	CA	3032	1/1	0.92	0.65	67,67,67,67	0
58	MG	CA	3137	1/1	0.92	0.12	51,51,51,51	0
58	MG	CB	3007	1/1	0.92	0.27	64,64,64,64	0
58	MG	AA	3251	1/1	0.92	0.45	33,33,33,33	1
58	MG	AA	3460	1/1	0.92	0.19	71,71,71,71	0
58	MG	AA	3225	1/1	0.92	0.43	34,34,34,34	0
58	MG	AA	3462	1/1	0.92	0.30	70,70,70,70	0
58	MG	CA	3259	1/1	0.92	0.42	56,56,56,56	0
58	MG	CD	301	1/1	0.92	0.28	79,79,79,79	0
58	MG	BA	3002	1/1	0.92	0.19	91,91,91,91	0
58	MG	CD	303	1/1	0.92	0.28	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3466	1/1	0.92	0.10	59,59,59,59	0
58	MG	AA	3470	1/1	0.92	0.12	28,28,28,28	0
58	MG	AA	3282	1/1	0.92	0.31	39,39,39,39	0
58	MG	BA	3075	1/1	0.92	0.18	56,56,56,56	0
58	MG	CE	307	1/1	0.92	0.10	65,65,65,65	0
58	MG	AA	3028	1/1	0.92	0.30	55,55,55,55	0
58	MG	CF	302	1/1	0.92	0.51	63,63,63,63	0
58	MG	BA	3174	1/1	0.92	0.13	69,69,69,69	0
58	MG	AA	3700	1/1	0.92	0.25	48,48,48,48	0
58	MG	AA	3701	1/1	0.92	0.23	33,33,33,33	0
58	MG	CA	3285	1/1	0.92	0.21	59,59,59,59	0
58	MG	AA	3372	1/1	0.92	0.34	61,61,61,61	0
58	MG	AA	3035	1/1	0.92	0.35	59,59,59,59	0
58	MG	AA	3610	1/1	0.92	0.13	51,51,51,51	0
58	MG	CU	3001	1/1	0.92	0.37	91,91,91,91	0
58	MG	AA	3291	1/1	0.92	0.18	44,44,44,44	0
58	MG	CA	3294	1/1	0.92	0.12	71,71,71,71	0
58	MG	DA	1601	1/1	0.92	0.20	59,59,59,59	0
58	MG	AA	3258	1/1	0.92	0.24	13,13,13,13	0
60	ZN	BN	501	1/1	0.92	0.06	121,121,121,121	0
58	MG	AA	3815	1/1	0.92	0.54	53,53,53,53	0
58	MG	CA	3168	1/1	0.92	0.12	58,58,58,58	0
58	MG	CA	3452	1/1	0.93	0.12	62,62,62,62	0
58	MG	BA	3156	1/1	0.93	0.14	36,36,36,36	0
58	MG	AA	3586	1/1	0.93	0.15	65,65,65,65	0
58	MG	AA	3698	1/1	0.93	0.16	62,62,62,62	0
58	MG	AA	3080	1/1	0.93	0.20	33,33,33,33	0
58	MG	AA	3191	1/1	0.93	0.17	44,44,44,44	0
58	MG	AA	3832	1/1	0.93	0.23	43,43,43,43	1
58	MG	AA	3030	1/1	0.93	0.22	31,31,31,31	1
58	MG	CA	3467	1/1	0.93	0.35	54,54,54,54	0
58	MG	CA	3469	1/1	0.93	0.13	61,61,61,61	0
58	MG	AA	3161	1/1	0.93	0.11	54,54,54,54	0
58	MG	BA	3164	1/1	0.93	0.10	60,60,60,60	0
58	MG	BA	3166	1/1	0.93	0.10	58,58,58,58	0
58	MG	CQ	201	1/1	0.93	0.51	63,63,63,63	0
58	MG	CA	3073	1/1	0.93	0.32	53,53,53,53	0
58	MG	AA	3705	1/1	0.93	0.18	57,57,57,57	0
58	MG	CA	3478	1/1	0.93	0.12	73,73,73,73	0
58	MG	AA	3709	1/1	0.93	0.19	53,53,53,53	0
58	MG	AA	3453	1/1	0.93	0.22	54,54,54,54	0
58	MG	AA	3093	1/1	0.93	0.25	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	C8	5001	1/1	0.93	0.53	48,48,48,48	0
58	MG	AA	3456	1/1	0.93	0.11	32,32,32,32	0
58	MG	AA	3094	1/1	0.93	0.26	29,29,29,29	0
58	MG	AA	3063	1/1	0.93	0.46	66,66,66,66	0
58	MG	DA	1604	1/1	0.93	0.15	72,72,72,72	0
58	MG	AA	3717	1/1	0.93	0.16	56,56,56,56	0
58	MG	CA	3488	1/1	0.93	0.10	69,69,69,69	0
58	MG	CA	3490	1/1	0.93	0.32	78,78,78,78	0
58	MG	AA	3240	1/1	0.93	0.38	60,60,60,60	0
58	MG	AD	303	1/1	0.93	0.27	64,64,64,64	0
58	MG	BA	3182	1/1	0.93	0.14	80,80,80,80	0
58	MG	CA	3498	1/1	0.93	0.30	71,71,71,71	0
58	MG	AA	3241	1/1	0.93	0.35	64,64,64,64	0
58	MG	AA	3359	1/1	0.93	0.14	49,49,49,49	0
58	MG	CA	3502	1/1	0.93	0.36	69,69,69,69	0
58	MG	BA	3187	1/1	0.93	0.08	59,59,59,59	0
58	MG	AA	3166	1/1	0.93	0.30	57,57,57,57	0
58	MG	CA	3249	1/1	0.93	0.48	64,64,64,64	0
58	MG	AA	3280	1/1	0.93	0.28	46,46,46,46	0
58	MG	CA	3252	1/1	0.93	0.13	51,51,51,51	0
58	MG	AA	3615	1/1	0.93	0.12	55,55,55,55	0
58	MG	AE	304	1/1	0.93	0.16	29,29,29,29	0
58	MG	CA	3258	1/1	0.93	0.14	40,40,40,40	0
58	MG	CA	3520	1/1	0.93	0.34	83,83,83,83	0
58	MG	AA	3133	1/1	0.93	0.30	30,30,30,30	0
58	MG	AA	3365	1/1	0.93	0.18	54,54,54,54	0
58	MG	AA	3620	1/1	0.93	0.14	42,42,42,42	0
58	MG	DA	1632	1/1	0.93	0.19	69,69,69,69	0
58	MG	DA	1633	1/1	0.93	0.38	60,60,60,60	0
58	MG	CA	3264	1/1	0.93	0.12	60,60,60,60	0
58	MG	BA	3198	1/1	0.93	0.36	68,68,68,68	0
58	MG	AA	3046	1/1	0.93	0.15	35,35,35,35	0
58	MG	DA	1638	1/1	0.93	0.16	74,74,74,74	0
58	MG	CA	3532	1/1	0.93	0.12	58,58,58,58	0
58	MG	CA	3534	1/1	0.93	0.20	79,79,79,79	0
58	MG	AA	3741	1/1	0.93	0.22	45,45,45,45	0
58	MG	BA	3201	1/1	0.93	0.10	68,68,68,68	0
58	MG	BA	3202	1/1	0.93	0.12	62,62,62,62	0
58	MG	AA	3202	1/1	0.93	0.15	63,63,63,63	0
58	MG	CA	3280	1/1	0.93	0.22	38,38,38,38	0
58	MG	CA	3281	1/1	0.93	0.14	34,34,34,34	0
58	MG	DA	1650	1/1	0.93	0.29	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	AO	5001	1/1	0.93	0.20	53,53,53,53	0
58	MG	AA	3375	1/1	0.93	0.21	57,57,57,57	0
58	MG	CA	3544	1/1	0.93	0.26	66,66,66,66	0
58	MG	AU	202	1/1	0.93	0.34	56,56,56,56	0
58	MG	DA	1657	1/1	0.93	0.15	72,72,72,72	0
58	MG	CA	3287	1/1	0.93	0.19	55,55,55,55	0
58	MG	CA	3126	1/1	0.93	0.36	71,71,71,71	0
58	MG	AV	202	1/1	0.93	0.23	37,37,37,37	0
58	MG	CA	3551	1/1	0.93	0.05	57,57,57,57	0
58	MG	BA	3079	1/1	0.93	0.12	35,35,35,35	0
58	MG	AA	3020	1/1	0.93	0.15	23,23,23,23	0
58	MG	AW	3002	1/1	0.93	0.20	52,52,52,52	0
58	MG	CA	3556	1/1	0.93	0.24	66,66,66,66	0
58	MG	AA	3139	1/1	0.93	0.29	49,49,49,49	0
58	MG	BA	3084	1/1	0.93	0.10	80,80,80,80	0
58	MG	AA	3049	1/1	0.93	0.20	51,51,51,51	0
58	MG	CA	3569	1/1	0.93	0.16	54,54,54,54	0
58	MG	AZ	302	1/1	0.93	0.23	66,66,66,66	0
58	MG	A0	102	1/1	0.93	0.09	54,54,54,54	0
58	MG	CA	3309	1/1	0.93	0.11	40,40,40,40	0
58	MG	AA	3753	1/1	0.93	0.51	72,72,72,72	0
58	MG	AA	3635	1/1	0.93	0.45	60,60,60,60	0
58	MG	DA	1684	1/1	0.93	0.19	63,63,63,63	0
58	MG	A2	3001	1/1	0.93	0.24	50,50,50,50	0
58	MG	AA	3010	1/1	0.93	0.39	66,66,66,66	0
58	MG	AA	3638	1/1	0.93	0.21	45,45,45,45	0
58	MG	CA	3324	1/1	0.93	0.12	66,66,66,66	0
58	MG	AA	3209	1/1	0.93	0.38	59,59,59,59	0
58	MG	CA	3332	1/1	0.93	0.23	50,50,50,50	0
58	MG	AA	3401	1/1	0.93	0.24	33,33,33,33	0
58	MG	DA	1693	1/1	0.93	0.25	60,60,60,60	0
58	MG	AA	3505	1/1	0.93	0.14	55,55,55,55	0
58	MG	DA	1698	1/1	0.93	0.12	76,76,76,76	0
58	MG	A8	5002	1/1	0.93	0.20	30,30,30,30	0
58	MG	AA	3102	1/1	0.93	0.34	50,50,50,50	0
58	MG	BA	3102	1/1	0.93	0.35	56,56,56,56	0
58	MG	DA	1702	1/1	0.93	0.42	73,73,73,73	0
58	MG	CA	3347	1/1	0.93	0.12	33,33,33,33	0
58	MG	CA	3348	1/1	0.93	0.14	58,58,58,58	0
58	MG	BX	107	1/1	0.93	0.49	67,67,67,67	0
58	MG	AA	3404	1/1	0.93	0.37	43,43,43,43	0
58	MG	AA	3764	1/1	0.93	0.19	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	BA	3105	1/1	0.93	0.36	60,60,60,60	0
58	MG	CA	3362	1/1	0.93	0.25	57,57,57,57	0
58	MG	BA	3005	1/1	0.93	0.22	64,64,64,64	0
58	MG	CA	3607	1/1	0.93	0.10	67,67,67,67	0
58	MG	AA	3407	1/1	0.93	0.11	19,19,19,19	0
58	MG	AA	3306	1/1	0.93	0.13	47,47,47,47	0
58	MG	AA	3061	1/1	0.93	0.20	26,26,26,26	0
58	MG	AA	3261	1/1	0.93	0.39	69,69,69,69	0
58	MG	AA	3774	1/1	0.93	0.45	78,78,78,78	0
58	MG	DA	1724	1/1	0.93	0.11	77,77,77,77	0
58	MG	BA	3113	1/1	0.93	0.11	60,60,60,60	0
58	MG	BA	3011	1/1	0.93	0.10	76,76,76,76	0
58	MG	CA	3620	1/1	0.93	0.12	34,34,34,34	0
58	MG	CA	3385	1/1	0.93	0.26	70,70,70,70	0
58	MG	DA	1730	1/1	0.93	0.27	75,75,75,75	0
58	MG	DA	1732	1/1	0.93	0.09	80,80,80,80	0
58	MG	CA	3386	1/1	0.93	0.30	63,63,63,63	0
58	MG	CA	3387	1/1	0.93	0.25	62,62,62,62	0
58	MG	DA	1735	1/1	0.93	0.08	70,70,70,70	0
58	MG	AA	3415	1/1	0.93	0.17	30,30,30,30	0
58	MG	AA	3421	1/1	0.93	0.06	70,70,70,70	0
58	MG	CA	3178	1/1	0.93	0.16	34,34,34,34	0
58	MG	AA	3658	1/1	0.93	0.11	60,60,60,60	0
58	MG	CA	3026	1/1	0.93	0.24	79,79,79,79	0
58	MG	CA	3395	1/1	0.93	0.09	53,53,53,53	0
58	MG	AA	3262	1/1	0.93	0.24	49,49,49,49	0
58	MG	BA	3124	1/1	0.93	0.22	71,71,71,71	0
58	MG	AA	3663	1/1	0.93	0.65	60,60,60,60	0
58	MG	AA	3548	1/1	0.93	0.08	29,29,29,29	0
58	MG	AA	3670	1/1	0.93	0.16	31,31,31,31	0
58	MG	CA	3036	1/1	0.93	0.12	42,42,42,42	0
58	MG	CA	3648	1/1	0.93	0.11	77,77,77,77	0
58	MG	BA	3129	1/1	0.93	0.17	52,52,52,52	0
58	MG	DA	1757	1/1	0.93	0.39	73,73,73,73	0
58	MG	AA	3674	1/1	0.93	0.20	74,74,74,74	0
58	MG	DA	1759	1/1	0.93	0.20	64,64,64,64	0
58	MG	AA	3321	1/1	0.93	0.22	69,69,69,69	0
58	MG	AA	3323	1/1	0.93	0.16	21,21,21,21	0
58	MG	DA	1762	1/1	0.93	0.10	53,53,53,53	0
58	MG	AA	3804	1/1	0.93	0.21	65,65,65,65	0
58	MG	AA	3324	1/1	0.93	0.09	32,32,32,32	0
58	MG	AA	3435	1/1	0.93	0.24	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3198	1/1	0.93	0.35	62,62,62,62	0
58	MG	AA	3566	1/1	0.93	0.24	28,28,28,28	0
58	MG	AA	3436	1/1	0.93	0.20	52,52,52,52	0
58	MG	CA	3201	1/1	0.93	0.45	52,52,52,52	0
58	MG	AA	3573	1/1	0.93	0.13	31,31,31,31	0
58	MG	CA	3053	1/1	0.93	0.56	57,57,57,57	0
58	MG	DL	3002	1/1	0.93	0.33	74,74,74,74	0
58	MG	AA	3185	1/1	0.93	0.22	65,65,65,65	0
58	MG	CA	3055	1/1	0.93	0.51	37,37,37,37	0
58	MG	CA	3207	1/1	0.93	0.47	55,55,55,55	0
58	MG	AA	3153	1/1	0.93	0.20	67,67,67,67	0
58	MG	AA	3226	1/1	0.93	0.29	73,73,73,73	0
58	MG	CA	3058	1/1	0.93	0.12	48,48,48,48	0
58	MG	AA	3817	1/1	0.93	0.46	57,57,57,57	0
58	MG	AA	3124	1/1	0.93	0.47	43,43,43,43	0
58	MG	AA	3223	1/1	0.94	0.45	54,54,54,54	0
58	MG	CA	3009	1/1	0.94	0.57	67,67,67,67	0
58	MG	BA	3137	1/1	0.94	0.10	73,73,73,73	0
58	MG	CA	3495	1/1	0.94	0.33	62,62,62,62	0
58	MG	CA	3496	1/1	0.94	0.19	64,64,64,64	0
58	MG	CA	3012	1/1	0.94	0.13	58,58,58,58	0
58	MG	C0	101	1/1	0.94	0.19	64,64,64,64	0
58	MG	C1	101	1/1	0.94	0.19	67,67,67,67	0
58	MG	CA	3499	1/1	0.94	0.46	65,65,65,65	0
58	MG	AA	3224	1/1	0.94	0.27	26,26,26,26	0
58	MG	AA	3567	1/1	0.94	0.20	26,26,26,26	0
58	MG	AD	301	1/1	0.94	0.46	70,70,70,70	0
58	MG	CA	3503	1/1	0.94	0.26	49,49,49,49	1
58	MG	CA	3283	1/1	0.94	0.18	49,49,49,49	0
58	MG	CA	3506	1/1	0.94	0.12	61,61,61,61	0
58	MG	CA	3508	1/1	0.94	0.13	57,57,57,57	0
58	MG	CA	3284	1/1	0.94	0.14	48,48,48,48	0
58	MG	AA	3473	1/1	0.94	0.17	17,17,17,17	0
58	MG	AA	3016	1/1	0.94	0.43	57,57,57,57	0
58	MG	AA	3478	1/1	0.94	0.15	40,40,40,40	0
58	MG	CA	3024	1/1	0.94	0.52	87,87,87,87	0
58	MG	BA	3050	1/1	0.94	0.29	67,67,67,67	0
58	MG	CA	3515	1/1	0.94	0.34	73,73,73,73	0
58	MG	BA	3149	1/1	0.94	0.37	82,82,82,82	0
58	MG	CA	3517	1/1	0.94	0.15	77,77,77,77	0
58	MG	CA	3293	1/1	0.94	0.15	26,26,26,26	0
58	MG	CA	3521	1/1	0.94	0.27	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3522	1/1	0.94	0.11	59,59,59,59	0
58	MG	BA	3151	1/1	0.94	0.35	63,63,63,63	0
58	MG	CA	3295	1/1	0.94	0.13	69,69,69,69	0
58	MG	AA	3748	1/1	0.94	0.38	56,56,56,56	0
58	MG	CA	3528	1/1	0.94	0.10	38,38,38,38	0
58	MG	CA	3152	1/1	0.94	0.21	49,49,49,49	0
58	MG	CA	3299	1/1	0.94	0.30	54,54,54,54	0
58	MG	AA	3749	1/1	0.94	0.17	55,55,55,55	0
58	MG	BA	3053	1/1	0.94	0.16	69,69,69,69	0
58	MG	AA	3297	1/1	0.94	0.20	20,20,20,20	0
58	MG	AA	3078	1/1	0.94	0.27	49,49,49,49	0
58	MG	CA	3037	1/1	0.94	0.12	57,57,57,57	0
58	MG	AA	3657	1/1	0.94	0.19	51,51,51,51	1
58	MG	CA	3313	1/1	0.94	0.13	51,51,51,51	0
58	MG	AA	3169	1/1	0.94	0.27	61,61,61,61	0
58	MG	CA	3163	1/1	0.94	0.24	45,45,45,45	0
58	MG	AA	3582	1/1	0.94	0.17	37,37,37,37	0
58	MG	AA	3584	1/1	0.94	0.14	14,14,14,14	0
58	MG	CA	3322	1/1	0.94	0.06	32,32,32,32	0
58	MG	AH	3001	1/1	0.94	0.34	50,50,50,50	0
58	MG	DA	1644	1/1	0.94	0.13	64,64,64,64	0
58	MG	CA	3328	1/1	0.94	0.27	52,52,52,52	0
58	MG	CA	3171	1/1	0.94	0.23	45,45,45,45	0
58	MG	CA	3045	1/1	0.94	0.65	65,65,65,65	0
58	MG	AA	3156	1/1	0.94	0.29	63,63,63,63	0
58	MG	AA	3667	1/1	0.94	0.24	29,29,29,29	0
58	MG	DA	1652	1/1	0.94	0.14	58,58,58,58	0
58	MG	DA	1653	1/1	0.94	0.12	29,29,29,29	0
58	MG	CA	3177	1/1	0.94	0.37	50,50,50,50	0
58	MG	BA	3165	1/1	0.94	0.23	61,61,61,61	0
58	MG	CA	3049	1/1	0.94	0.39	78,78,78,78	0
58	MG	CA	3345	1/1	0.94	0.12	87,87,87,87	0
58	MG	DA	1658	1/1	0.94	0.09	63,63,63,63	0
58	MG	AA	3171	1/1	0.94	0.34	53,53,53,53	0
58	MG	CA	3182	1/1	0.94	0.08	47,47,47,47	0
58	MG	CA	3183	1/1	0.94	0.28	25,25,25,25	0
58	MG	AA	3671	1/1	0.94	0.11	57,57,57,57	0
58	MG	DA	1663	1/1	0.94	0.14	63,63,63,63	0
58	MG	CA	3354	1/1	0.94	0.15	46,46,46,46	0
58	MG	CA	3355	1/1	0.94	0.21	59,59,59,59	0
58	MG	DA	1666	1/1	0.94	0.38	47,47,47,47	0
58	MG	AA	3672	1/1	0.94	0.35	32,32,32,32	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3574	1/1	0.94	0.13	53,53,53,53	0
58	MG	CA	3186	1/1	0.94	0.38	58,58,58,58	0
58	MG	CA	3359	1/1	0.94	0.25	44,44,44,44	0
58	MG	AA	3309	1/1	0.94	0.21	44,44,44,44	0
58	MG	AA	3207	1/1	0.94	0.33	37,37,37,37	0
58	MG	DA	1674	1/1	0.94	0.19	72,72,72,72	0
58	MG	AA	3311	1/1	0.94	0.12	34,34,34,34	0
58	MG	AW	3003	1/1	0.94	0.26	55,55,55,55	0
58	MG	CA	3375	1/1	0.94	0.36	74,74,74,74	0
58	MG	CA	3584	1/1	0.94	0.17	43,43,43,43	0
58	MG	AA	3314	1/1	0.94	0.15	28,28,28,28	0
58	MG	AX	102	1/1	0.94	0.29	72,72,72,72	0
58	MG	CA	3588	1/1	0.94	0.17	68,68,68,68	0
58	MG	AA	3596	1/1	0.94	0.13	54,54,54,54	0
58	MG	AA	3775	1/1	0.94	0.14	45,45,45,45	0
58	MG	CA	3062	1/1	0.94	0.45	65,65,65,65	0
58	MG	A0	101	1/1	0.94	0.05	43,43,43,43	0
58	MG	AA	3367	1/1	0.94	0.21	50,50,50,50	0
58	MG	AA	3780	1/1	0.94	0.22	41,41,41,41	0
58	MG	DA	1692	1/1	0.94	0.20	53,53,53,53	0
58	MG	AA	3682	1/1	0.94	0.16	51,51,51,51	0
58	MG	CA	3599	1/1	0.94	0.14	69,69,69,69	0
58	MG	AA	3371	1/1	0.94	0.28	59,59,59,59	0
58	MG	CA	3391	1/1	0.94	0.14	61,61,61,61	0
58	MG	AA	3069	1/1	0.94	0.20	63,63,63,63	0
58	MG	AA	3786	1/1	0.94	0.23	57,57,57,57	0
58	MG	AA	3686	1/1	0.94	0.14	70,70,70,70	0
58	MG	AA	3688	1/1	0.94	0.11	29,29,29,29	0
58	MG	AA	3793	1/1	0.94	0.12	60,60,60,60	0
58	MG	AA	3509	1/1	0.94	0.19	48,48,48,48	0
58	MG	CA	3612	1/1	0.94	0.23	74,74,74,74	0
58	MG	CA	3075	1/1	0.94	0.36	52,52,52,52	0
58	MG	AA	3276	1/1	0.94	0.23	50,50,50,50	0
58	MG	AA	3796	1/1	0.94	0.25	19,19,19,19	1
58	MG	DA	1713	1/1	0.94	0.38	74,74,74,74	0
58	MG	CA	3405	1/1	0.94	0.14	53,53,53,53	0
58	MG	AA	3798	1/1	0.94	0.24	32,32,32,32	0
58	MG	AA	3515	1/1	0.94	0.18	18,18,18,18	0
58	MG	AA	3693	1/1	0.94	0.20	60,60,60,60	0
58	MG	AA	3803	1/1	0.94	0.26	62,62,62,62	0
58	MG	CA	3217	1/1	0.94	0.30	66,66,66,66	0
58	MG	DA	1722	1/1	0.94	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3218	1/1	0.94	0.19	50,50,50,50	0
58	MG	AA	3098	1/1	0.94	0.28	24,24,24,24	0
58	MG	AA	3520	1/1	0.94	0.17	23,23,23,23	0
58	MG	AA	3613	1/1	0.94	0.15	54,54,54,54	0
58	MG	AA	3529	1/1	0.94	0.14	28,28,28,28	0
58	MG	CA	3089	1/1	0.94	0.26	73,73,73,73	0
58	MG	AA	3213	1/1	0.94	0.48	50,50,50,50	1
58	MG	CA	3643	1/1	0.94	0.16	57,57,57,57	0
58	MG	CA	3091	1/1	0.94	0.36	63,63,63,63	0
58	MG	AA	3536	1/1	0.94	0.13	15,15,15,15	0
58	MG	CA	3433	1/1	0.94	0.25	61,61,61,61	0
58	MG	AA	3259	1/1	0.94	0.33	20,20,20,20	0
58	MG	CA	3231	1/1	0.94	0.28	50,50,50,50	0
58	MG	CA	3096	1/1	0.94	0.30	63,63,63,63	0
58	MG	AA	3619	1/1	0.94	0.15	37,37,37,37	0
58	MG	AA	3451	1/1	0.94	0.17	53,53,53,53	1
58	MG	CA	3652	1/1	0.94	0.19	84,84,84,84	0
58	MG	AA	3621	1/1	0.94	0.20	39,39,39,39	0
58	MG	DA	1745	1/1	0.94	0.12	69,69,69,69	0
58	MG	AA	3176	1/1	0.94	0.23	49,49,49,49	0
58	MG	DA	1747	1/1	0.94	0.38	78,78,78,78	0
58	MG	AA	3383	1/1	0.94	0.07	34,34,34,34	0
58	MG	CA	3105	1/1	0.94	0.16	45,45,45,45	0
58	MG	AA	3387	1/1	0.94	0.22	24,24,24,24	0
58	MG	CA	3664	1/1	0.94	0.29	55,55,55,55	0
58	MG	AA	3281	1/1	0.94	0.32	60,60,60,60	0
58	MG	AA	3629	1/1	0.94	0.25	74,74,74,74	0
58	MG	CA	3109	1/1	0.94	0.14	59,59,59,59	0
58	MG	AA	3630	1/1	0.94	0.12	58,58,58,58	0
58	MG	AA	3833	1/1	0.94	0.24	47,47,47,47	0
58	MG	CA	3465	1/1	0.94	0.15	46,46,46,46	0
58	MG	AA	3218	1/1	0.94	0.30	49,49,49,49	0
58	MG	AA	3550	1/1	0.94	0.07	52,52,52,52	0
58	MG	CA	3468	1/1	0.94	0.54	80,80,80,80	0
58	MG	AA	3553	1/1	0.94	0.22	60,60,60,60	0
58	MG	CA	3121	1/1	0.94	0.36	60,60,60,60	0
58	MG	CA	3251	1/1	0.94	0.15	47,47,47,47	0
58	MG	AA	3554	1/1	0.94	0.22	40,40,40,40	0
58	MG	AB	3008	1/1	0.94	0.41	51,51,51,51	0
58	MG	AA	3555	1/1	0.94	0.08	49,49,49,49	0
58	MG	CA	3257	1/1	0.94	0.40	65,65,65,65	0
58	MG	AA	3190	1/1	0.94	0.31	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	BA	3036	1/1	0.94	0.17	72,72,72,72	0
58	MG	AA	3242	1/1	0.94	0.21	28,28,28,28	0
58	MG	BA	3132	1/1	0.94	0.07	61,61,61,61	0
58	MG	BA	3041	1/1	0.94	0.18	53,53,53,53	0
58	MG	CA	3003	1/1	0.94	0.25	44,44,44,44	0
58	MG	CA	3269	1/1	0.94	0.12	54,54,54,54	0
58	MG	AA	3289	1/1	0.94	0.12	26,26,26,26	0
58	MG	CA	3489	1/1	0.94	0.15	53,53,53,53	0
58	MG	CA	3273	1/1	0.94	0.26	54,54,54,54	0
58	MG	AA	3476	1/1	0.95	0.20	68,68,68,68	0
58	MG	BA	3175	1/1	0.95	0.22	78,78,78,78	0
58	MG	AA	3592	1/1	0.95	0.09	63,63,63,63	0
58	MG	AA	3834	1/1	0.95	0.26	64,64,64,64	0
58	MG	CA	3244	1/1	0.95	0.17	40,40,40,40	0
58	MG	CA	3085	1/1	0.95	0.28	62,62,62,62	0
58	MG	AA	3164	1/1	0.95	0.41	37,37,37,37	0
58	MG	CA	3087	1/1	0.95	0.33	35,35,35,35	0
58	MG	AA	3837	1/1	0.95	0.23	44,44,44,44	1
58	MG	AA	3595	1/1	0.95	0.22	42,42,42,42	0
58	MG	AB	3003	1/1	0.95	0.26	50,50,50,50	0
58	MG	AA	3389	1/1	0.95	0.22	34,34,34,34	0
58	MG	AA	3479	1/1	0.95	0.28	53,53,53,53	0
58	MG	CR	201	1/1	0.95	0.32	51,51,51,51	0
58	MG	AA	3068	1/1	0.95	0.36	53,53,53,53	0
58	MG	CU	3002	1/1	0.95	0.33	63,63,63,63	0
58	MG	CA	3487	1/1	0.95	0.27	68,68,68,68	0
58	MG	CY	502	1/1	0.95	0.15	54,54,54,54	0
58	MG	BA	3189	1/1	0.95	0.18	66,66,66,66	0
58	MG	AB	3009	1/1	0.95	0.16	55,55,55,55	0
58	MG	AA	3712	1/1	0.95	0.22	36,36,36,36	1
58	MG	AA	3396	1/1	0.95	0.16	16,16,16,16	0
58	MG	CA	3101	1/1	0.95	0.55	77,77,77,77	0
58	MG	CA	3261	1/1	0.95	0.19	47,47,47,47	0
58	MG	AA	3482	1/1	0.95	0.10	64,64,64,64	0
58	MG	AA	3397	1/1	0.95	0.15	15,15,15,15	0
58	MG	AA	3608	1/1	0.95	0.08	29,29,29,29	0
58	MG	CA	3268	1/1	0.95	0.18	69,69,69,69	0
58	MG	BA	3197	1/1	0.95	0.11	75,75,75,75	0
58	MG	AA	3194	1/1	0.95	0.22	60,60,60,60	0
58	MG	AA	3400	1/1	0.95	0.21	33,33,33,33	0
58	MG	AA	3720	1/1	0.95	0.14	59,59,59,59	0
58	MG	CA	3110	1/1	0.95	0.19	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3112	1/1	0.95	0.13	70,70,70,70	0
58	MG	DA	1616	1/1	0.95	0.38	51,51,51,51	0
58	MG	AA	3081	1/1	0.95	0.19	56,56,56,56	0
58	MG	AD	305	1/1	0.95	0.24	56,56,56,56	0
58	MG	AA	3612	1/1	0.95	0.30	49,49,49,49	0
58	MG	AA	3118	1/1	0.95	0.24	36,36,36,36	1
58	MG	AD	308	1/1	0.95	0.39	44,44,44,44	0
58	MG	BA	3206	1/1	0.95	0.24	62,62,62,62	0
58	MG	AA	3141	1/1	0.95	0.27	51,51,51,51	0
58	MG	CA	3123	1/1	0.95	0.22	66,66,66,66	0
58	MG	DA	1625	1/1	0.95	0.09	42,42,42,42	0
58	MG	AA	3105	1/1	0.95	0.16	31,31,31,31	0
58	MG	AA	3408	1/1	0.95	0.15	44,44,44,44	0
58	MG	AA	3501	1/1	0.95	0.12	48,48,48,48	0
58	MG	AA	3040	1/1	0.95	0.27	45,45,45,45	0
58	MG	AA	3503	1/1	0.95	0.13	52,52,52,52	0
58	MG	AA	3145	1/1	0.95	0.11	38,38,38,38	0
58	MG	CA	3525	1/1	0.95	0.30	40,40,40,40	0
58	MG	AF	305	1/1	0.95	0.19	55,55,55,55	0
58	MG	AG	201	1/1	0.95	0.12	49,49,49,49	0
58	MG	AA	3058	1/1	0.95	0.15	35,35,35,35	0
58	MG	CA	3133	1/1	0.95	0.20	29,29,29,29	0
58	MG	AA	3624	1/1	0.95	0.22	70,70,70,70	0
58	MG	BA	3087	1/1	0.95	0.41	70,70,70,70	0
58	MG	AA	3174	1/1	0.95	0.29	62,62,62,62	0
58	MG	CA	3533	1/1	0.95	0.19	52,52,52,52	0
58	MG	AA	3513	1/1	0.95	0.28	58,58,58,58	0
58	MG	AA	3746	1/1	0.95	0.12	28,28,28,28	0
58	MG	AA	3514	1/1	0.95	0.15	35,35,35,35	0
58	MG	AR	5001	1/1	0.95	0.19	32,32,32,32	0
58	MG	CA	3314	1/1	0.95	0.24	50,50,50,50	0
58	MG	AA	3015	1/1	0.95	0.33	62,62,62,62	0
58	MG	CA	3540	1/1	0.95	0.09	70,70,70,70	0
58	MG	CA	3316	1/1	0.95	0.09	60,60,60,60	0
58	MG	AA	3751	1/1	0.95	0.12	26,26,26,26	0
58	MG	AA	3518	1/1	0.95	0.12	19,19,19,19	0
58	MG	CA	3144	1/1	0.95	0.57	56,56,56,56	0
58	MG	BX	105	1/1	0.95	0.14	78,78,78,78	0
58	MG	AA	3341	1/1	0.95	0.20	15,15,15,15	0
58	MG	AA	3342	1/1	0.95	0.15	4,4,4,4	0
58	MG	AA	3523	1/1	0.95	0.15	27,27,27,27	0
58	MG	CA	3550	1/1	0.95	0.10	54,54,54,54	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3330	1/1	0.95	0.15	29,29,29,29	0
58	MG	CA	3150	1/1	0.95	0.14	63,63,63,63	0
58	MG	AA	3527	1/1	0.95	0.12	21,21,21,21	0
58	MG	AA	3424	1/1	0.95	0.18	17,17,17,17	0
58	MG	CA	3340	1/1	0.95	0.12	35,35,35,35	0
58	MG	AA	3425	1/1	0.95	0.16	49,49,49,49	0
58	MG	AA	3177	1/1	0.95	0.36	51,51,51,51	0
58	MG	CA	3563	1/1	0.95	0.09	92,92,92,92	0
58	MG	CA	3004	1/1	0.95	0.45	64,64,64,64	0
58	MG	CA	3566	1/1	0.95	0.19	41,41,41,41	1
58	MG	CA	3005	1/1	0.95	0.33	56,56,56,56	0
58	MG	CA	3157	1/1	0.95	0.25	68,68,68,68	0
58	MG	AA	3178	1/1	0.95	0.26	61,61,61,61	0
58	MG	AA	3149	1/1	0.95	0.38	67,67,67,67	0
58	MG	AA	3005	1/1	0.95	0.17	61,61,61,61	0
58	MG	CA	3352	1/1	0.95	0.14	46,46,46,46	0
58	MG	AA	3154	1/1	0.95	0.33	56,56,56,56	0
58	MG	CA	3164	1/1	0.95	0.25	38,38,38,38	0
58	MG	CA	3011	1/1	0.95	0.11	46,46,46,46	0
58	MG	AA	3284	1/1	0.95	0.31	43,43,43,43	0
58	MG	AA	3250	1/1	0.95	0.26	62,62,62,62	0
58	MG	CA	3361	1/1	0.95	0.18	48,48,48,48	0
58	MG	AA	3768	1/1	0.95	0.35	96,96,96,96	0
58	MG	BA	3111	1/1	0.95	0.53	72,72,72,72	0
58	MG	CA	3364	1/1	0.95	0.17	65,65,65,65	0
58	MG	CA	3366	1/1	0.95	0.12	47,47,47,47	0
58	MG	AA	3355	1/1	0.95	0.13	57,57,57,57	0
58	MG	AA	3211	1/1	0.95	0.33	86,86,86,86	0
58	MG	CA	3019	1/1	0.95	0.18	27,27,27,27	0
58	MG	AA	3212	1/1	0.95	0.27	31,31,31,31	1
58	MG	BA	3001	1/1	0.95	0.15	55,55,55,55	0
58	MG	CA	3180	1/1	0.95	0.42	74,74,74,74	0
58	MG	AA	3776	1/1	0.95	0.09	40,40,40,40	0
58	MG	CA	3597	1/1	0.95	0.17	51,51,51,51	0
58	MG	AA	3445	1/1	0.95	0.18	59,59,59,59	0
58	MG	CA	3381	1/1	0.95	0.18	68,68,68,68	0
58	MG	CA	3600	1/1	0.95	0.10	39,39,39,39	0
58	MG	CA	3601	1/1	0.95	0.09	73,73,73,73	0
58	MG	CA	3027	1/1	0.95	0.19	47,47,47,47	0
58	MG	DA	1707	1/1	0.95	0.17	69,69,69,69	0
58	MG	CA	3029	1/1	0.95	0.12	32,32,32,32	0
58	MG	CA	3030	1/1	0.95	0.29	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	BA	3120	1/1	0.95	0.28	78,78,78,78	0
58	MG	AA	3447	1/1	0.95	0.08	75,75,75,75	0
58	MG	BA	3122	1/1	0.95	0.22	58,58,58,58	0
58	MG	DA	1715	1/1	0.95	0.21	49,49,49,49	0
58	MG	AA	3660	1/1	0.95	0.23	68,68,68,68	0
58	MG	AA	3556	1/1	0.95	0.13	37,37,37,37	0
58	MG	AA	3559	1/1	0.95	0.10	50,50,50,50	0
58	MG	AA	3785	1/1	0.95	0.15	70,70,70,70	0
58	MG	AA	3448	1/1	0.95	0.14	17,17,17,17	0
58	MG	BA	3130	1/1	0.95	0.15	49,49,49,49	0
58	MG	CA	3399	1/1	0.95	0.12	63,63,63,63	0
58	MG	CA	3041	1/1	0.95	0.28	31,31,31,31	0
58	MG	CA	3622	1/1	0.95	0.30	51,51,51,51	0
58	MG	CA	3401	1/1	0.95	0.29	60,60,60,60	0
58	MG	AA	3787	1/1	0.95	0.20	50,50,50,50	0
58	MG	CA	3625	1/1	0.95	0.28	53,53,53,53	0
58	MG	AA	3110	1/1	0.95	0.20	50,50,50,50	0
58	MG	DA	1731	1/1	0.95	0.11	82,82,82,82	0
58	MG	AA	3668	1/1	0.95	0.20	38,38,38,38	0
58	MG	AA	3450	1/1	0.95	0.21	48,48,48,48	0
58	MG	CA	3632	1/1	0.95	0.15	54,54,54,54	0
58	MG	AA	3254	1/1	0.95	0.21	35,35,35,35	0
58	MG	AA	3295	1/1	0.95	0.28	46,46,46,46	0
58	MG	AA	3127	1/1	0.95	0.30	52,52,52,52	0
58	MG	AA	3569	1/1	0.95	0.15	15,15,15,15	0
58	MG	AA	3799	1/1	0.95	0.21	48,48,48,48	0
58	MG	BA	3141	1/1	0.95	0.19	49,49,49,49	0
58	MG	CA	3641	1/1	0.95	0.22	54,54,54,54	0
58	MG	AA	3676	1/1	0.95	0.22	64,64,64,64	0
58	MG	BA	3020	1/1	0.95	0.13	51,51,51,51	0
58	MG	AA	3111	1/1	0.95	0.34	79,79,79,79	0
58	MG	CA	3427	1/1	0.95	0.23	53,53,53,53	0
58	MG	BA	3147	1/1	0.95	0.08	84,84,84,84	0
58	MG	AA	3076	1/1	0.95	0.12	8,8,8,8	0
58	MG	CA	3430	1/1	0.95	0.38	71,71,71,71	0
58	MG	AA	3066	1/1	0.95	0.29	48,48,48,48	0
58	MG	AA	3576	1/1	0.95	0.23	69,69,69,69	0
58	MG	BA	3027	1/1	0.95	0.21	75,75,75,75	0
58	MG	CA	3435	1/1	0.95	0.14	28,28,28,28	0
58	MG	CA	3436	1/1	0.95	0.11	53,53,53,53	0
58	MG	AA	3189	1/1	0.95	0.17	11,11,11,11	0
58	MG	AA	3578	1/1	0.95	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3308	1/1	0.95	0.14	28,28,28,28	0
58	MG	CA	3443	1/1	0.95	0.48	66,66,66,66	0
58	MG	AA	3809	1/1	0.95	0.35	60,60,60,60	0
58	MG	AA	3263	1/1	0.95	0.44	71,71,71,71	0
58	MG	DA	1765	1/1	0.95	0.16	64,64,64,64	0
58	MG	AA	3687	1/1	0.95	0.20	46,46,46,46	0
58	MG	AA	3581	1/1	0.95	0.13	27,27,27,27	0
58	MG	AA	3067	1/1	0.95	0.08	50,50,50,50	0
58	MG	CB	3005	1/1	0.95	0.33	61,61,61,61	0
58	MG	AA	3134	1/1	0.95	0.32	67,67,67,67	0
58	MG	AA	3472	1/1	0.95	0.16	25,25,25,25	0
58	MG	CA	3457	1/1	0.95	0.15	58,58,58,58	0
58	MG	BA	3038	1/1	0.95	0.36	65,65,65,65	0
58	MG	BA	3040	1/1	0.95	0.27	48,48,48,48	0
58	MG	AA	3385	1/1	0.95	0.16	28,28,28,28	0
58	MG	AA	3822	1/1	0.95	0.17	19,19,19,19	0
58	MG	AA	3824	1/1	0.95	0.22	31,31,31,31	1
58	MG	AA	3588	1/1	0.95	0.35	54,54,54,54	0
58	MG	AA	3474	1/1	0.95	0.22	50,50,50,50	0
58	MG	CA	3079	1/1	0.95	0.16	46,46,46,46	0
58	MG	AA	3475	1/1	0.95	0.12	60,60,60,60	0
62	GDP	DZ	704	28/28	0.95	0.14	80,80,80,80	0
58	MG	CA	3051	1/1	0.96	0.51	64,64,64,64	0
58	MG	CA	3326	1/1	0.96	0.13	39,39,39,39	0
58	MG	AA	3755	1/1	0.96	0.18	29,29,29,29	0
58	MG	AA	3583	1/1	0.96	0.30	64,64,64,64	0
58	MG	AA	3500	1/1	0.96	0.19	55,55,55,55	0
58	MG	CA	3331	1/1	0.96	0.24	43,43,43,43	0
58	MG	AA	3664	1/1	0.96	0.17	55,55,55,55	0
58	MG	CA	3333	1/1	0.96	0.21	41,41,41,41	0
58	MG	CA	3334	1/1	0.96	0.40	72,72,72,72	0
58	MG	CA	3336	1/1	0.96	0.11	60,60,60,60	0
58	MG	AA	3585	1/1	0.96	0.12	63,63,63,63	0
58	MG	CA	3524	1/1	0.96	0.23	54,54,54,54	0
58	MG	CA	3338	1/1	0.96	0.14	41,41,41,41	0
58	MG	AA	3233	1/1	0.96	0.24	51,51,51,51	0
58	MG	AA	3298	1/1	0.96	0.08	57,57,57,57	0
58	MG	AA	3669	1/1	0.96	0.12	34,34,34,34	0
58	MG	AE	303	1/1	0.96	0.14	40,40,40,40	0
58	MG	AA	3300	1/1	0.96	0.12	51,51,51,51	0
58	MG	AA	3221	1/1	0.96	0.24	55,55,55,55	0
58	MG	DA	1612	1/1	0.96	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3346	1/1	0.96	0.12	40,40,40,40	0
58	MG	DA	1614	1/1	0.96	0.24	70,70,70,70	0
58	MG	AA	3386	1/1	0.96	0.15	18,18,18,18	0
58	MG	AA	3340	1/1	0.96	0.15	58,58,58,58	0
58	MG	BA	3184	1/1	0.96	0.07	49,49,49,49	0
58	MG	AA	3265	1/1	0.96	0.13	60,60,60,60	0
58	MG	AA	3390	1/1	0.96	0.18	47,47,47,47	0
58	MG	AA	3770	1/1	0.96	0.31	39,39,39,39	0
58	MG	AA	3771	1/1	0.96	0.24	38,38,38,38	1
58	MG	AA	3772	1/1	0.96	0.18	22,22,22,22	1
58	MG	AA	3773	1/1	0.96	0.33	36,36,36,36	0
58	MG	AA	3123	1/1	0.96	0.20	53,53,53,53	0
58	MG	CA	3360	1/1	0.96	0.22	43,43,43,43	0
58	MG	AA	3394	1/1	0.96	0.13	18,18,18,18	0
58	MG	BA	3193	1/1	0.96	0.09	70,70,70,70	0
58	MG	CA	3202	1/1	0.96	0.27	58,58,58,58	0
58	MG	CA	3547	1/1	0.96	0.13	66,66,66,66	0
58	MG	AQ	201	1/1	0.96	0.14	29,29,29,29	0
58	MG	BA	3076	1/1	0.96	0.17	42,42,42,42	0
58	MG	CA	3368	1/1	0.96	0.30	64,64,64,64	0
58	MG	AA	3305	1/1	0.96	0.26	53,53,53,53	0
58	MG	CA	3372	1/1	0.96	0.21	53,53,53,53	0
58	MG	AU	201	1/1	0.96	0.34	44,44,44,44	0
58	MG	AA	3033	1/1	0.96	0.31	34,34,34,34	0
58	MG	BA	3080	1/1	0.96	0.08	52,52,52,52	0
58	MG	AV	201	1/1	0.96	0.27	37,37,37,37	0
58	MG	AA	3599	1/1	0.96	0.13	52,52,52,52	0
58	MG	AA	3346	1/1	0.96	0.17	45,45,45,45	0
58	MG	AA	3782	1/1	0.96	0.31	72,72,72,72	0
58	MG	BA	3085	1/1	0.96	0.14	49,49,49,49	0
58	MG	CA	3567	1/1	0.96	0.32	49,49,49,49	0
58	MG	CA	3384	1/1	0.96	0.26	44,44,44,44	0
58	MG	AA	3602	1/1	0.96	0.34	47,47,47,47	0
58	MG	AA	3604	1/1	0.96	0.15	65,65,65,65	0
58	MG	DA	1649	1/1	0.96	0.21	60,60,60,60	0
58	MG	AA	3525	1/1	0.96	0.17	26,26,26,26	0
58	MG	CA	3219	1/1	0.96	0.36	52,52,52,52	0
58	MG	CA	3220	1/1	0.96	0.14	30,30,30,30	0
58	MG	AA	3008	1/1	0.96	0.26	18,18,18,18	0
58	MG	AA	3157	1/1	0.96	0.18	40,40,40,40	1
58	MG	CA	3092	1/1	0.96	0.41	107,107,107,107	0
58	MG	CA	3578	1/1	0.96	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	AA	3788	1/1	0.96	0.26	60,60,60,60	0
58	MG	AA	3457	1/1	0.96	0.23	65,65,65,65	0
58	MG	AA	3790	1/1	0.96	0.11	48,48,48,48	0
58	MG	AA	3534	1/1	0.96	0.12	22,22,22,22	0
58	MG	AA	3051	1/1	0.96	0.29	34,34,34,34	0
58	MG	AA	3227	1/1	0.96	0.21	31,31,31,31	0
58	MG	CA	3586	1/1	0.96	0.19	46,46,46,46	0
58	MG	AA	3405	1/1	0.96	0.09	54,54,54,54	0
58	MG	AA	3697	1/1	0.96	0.23	69,69,69,69	0
58	MG	CA	3589	1/1	0.96	0.09	35,35,35,35	0
58	MG	CA	3403	1/1	0.96	0.12	70,70,70,70	0
58	MG	AA	3542	1/1	0.96	0.12	45,45,45,45	0
58	MG	A7	101	1/1	0.96	0.07	44,44,44,44	0
58	MG	AA	3288	1/1	0.96	0.23	25,25,25,25	0
58	MG	CA	3594	1/1	0.96	0.57	74,74,74,74	0
58	MG	CA	3236	1/1	0.96	0.22	52,52,52,52	0
58	MG	AA	3463	1/1	0.96	0.28	46,46,46,46	0
58	MG	A9	502	1/1	0.96	0.34	58,58,58,58	0
58	MG	AA	3316	1/1	0.96	0.22	59,59,59,59	0
58	MG	AA	3468	1/1	0.96	0.24	51,51,51,51	0
58	MG	DA	1679	1/1	0.96	0.35	60,60,60,60	0
58	MG	DA	1680	1/1	0.96	0.23	56,56,56,56	0
58	MG	DA	1681	1/1	0.96	0.19	46,46,46,46	0
58	MG	CA	3111	1/1	0.96	0.41	62,62,62,62	0
58	MG	CA	3415	1/1	0.96	0.13	52,52,52,52	0
58	MG	CA	3418	1/1	0.96	0.21	39,39,39,39	0
58	MG	AA	3358	1/1	0.96	0.12	61,61,61,61	0
58	MG	CA	3113	1/1	0.96	0.23	60,60,60,60	0
58	MG	CA	3605	1/1	0.96	0.17	63,63,63,63	0
58	MG	AA	3549	1/1	0.96	0.15	58,58,58,58	0
58	MG	CA	3115	1/1	0.96	0.53	37,37,37,37	0
58	MG	AA	3228	1/1	0.96	0.15	55,55,55,55	0
58	MG	AA	3623	1/1	0.96	0.12	43,43,43,43	0
58	MG	AA	3413	1/1	0.96	0.16	36,36,36,36	0
58	MG	AA	3290	1/1	0.96	0.27	63,63,63,63	0
58	MG	CA	3120	1/1	0.96	0.15	127,127,127,127	0
58	MG	DA	1696	1/1	0.96	0.28	64,64,64,64	0
58	MG	DA	1697	1/1	0.96	0.38	65,65,65,65	0
58	MG	CA	3614	1/1	0.96	0.60	89,89,89,89	0
58	MG	CA	3615	1/1	0.96	0.28	65,65,65,65	0
58	MG	AA	3023	1/1	0.96	0.24	37,37,37,37	0
58	MG	BZ	800	1/1	0.96	0.17	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3253	1/1	0.96	0.13	56,56,56,56	0
58	MG	AA	3812	1/1	0.96	0.31	57,57,57,57	0
58	MG	AA	3416	1/1	0.96	0.14	25,25,25,25	0
58	MG	AA	3557	1/1	0.96	0.13	39,39,39,39	0
58	MG	CA	3441	1/1	0.96	0.35	56,56,56,56	0
58	MG	AA	3419	1/1	0.96	0.20	26,26,26,26	0
58	MG	DA	1708	1/1	0.96	0.32	68,68,68,68	0
58	MG	AA	3719	1/1	0.96	0.13	41,41,41,41	0
58	MG	AA	3363	1/1	0.96	0.31	28,28,28,28	0
58	MG	AA	3322	1/1	0.96	0.09	33,33,33,33	0
58	MG	CA	3629	1/1	0.96	0.38	73,73,73,73	0
58	MG	AA	3722	1/1	0.96	0.14	11,11,11,11	0
58	MG	AA	3725	1/1	0.96	0.29	39,39,39,39	0
58	MG	AA	3128	1/1	0.96	0.34	71,71,71,71	0
58	MG	CA	3454	1/1	0.96	0.20	38,38,38,38	0
58	MG	CA	3267	1/1	0.96	0.13	39,39,39,39	0
58	MG	CA	3456	1/1	0.96	0.17	46,46,46,46	0
58	MG	AA	3293	1/1	0.96	0.19	32,32,32,32	0
58	MG	DA	1721	1/1	0.96	0.18	65,65,65,65	0
58	MG	CA	3639	1/1	0.96	0.34	79,79,79,79	0
58	MG	CA	3640	1/1	0.96	0.25	57,57,57,57	0
58	MG	AA	3245	1/1	0.96	0.29	28,28,28,28	1
58	MG	CA	3270	1/1	0.96	0.24	66,66,66,66	0
58	MG	AA	3829	1/1	0.96	0.19	19,19,19,19	0
58	MG	AA	3426	1/1	0.96	0.14	33,33,33,33	0
58	MG	CA	3016	1/1	0.96	0.45	79,79,79,79	0
58	MG	AA	3731	1/1	0.96	0.28	31,31,31,31	0
58	MG	CA	3276	1/1	0.96	0.11	51,51,51,51	0
58	MG	BA	3026	1/1	0.96	0.26	57,57,57,57	0
58	MG	AA	3568	1/1	0.96	0.21	51,51,51,51	0
58	MG	AA	3484	1/1	0.96	0.22	35,35,35,35	0
58	MG	CA	3470	1/1	0.96	0.19	69,69,69,69	0
58	MG	CA	3021	1/1	0.96	0.15	27,27,27,27	0
58	MG	CA	3655	1/1	0.96	0.17	52,52,52,52	0
58	MG	CA	3022	1/1	0.96	0.10	35,35,35,35	0
58	MG	AA	3643	1/1	0.96	0.22	47,47,47,47	0
58	MG	CA	3658	1/1	0.96	0.41	50,50,50,50	0
58	MG	DA	1741	1/1	0.96	0.44	68,68,68,68	0
58	MG	CA	3474	1/1	0.96	0.14	52,52,52,52	0
58	MG	DA	1743	1/1	0.96	0.13	60,60,60,60	0
58	MG	CA	3661	1/1	0.96	0.20	60,60,60,60	0
58	MG	CA	3475	1/1	0.96	0.30	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3644	1/1	0.96	0.11	49,49,49,49	0
58	MG	CA	3146	1/1	0.96	0.16	80,80,80,80	0
58	MG	DA	1748	1/1	0.96	0.21	66,66,66,66	0
58	MG	AB	3002	1/1	0.96	0.15	58,58,58,58	0
58	MG	AA	3570	1/1	0.96	0.12	18,18,18,18	0
58	MG	CA	3028	1/1	0.96	0.23	42,42,42,42	0
58	MG	CB	3003	1/1	0.96	0.07	76,76,76,76	0
58	MG	AA	3486	1/1	0.96	0.14	28,28,28,28	0
58	MG	AB	3005	1/1	0.96	0.11	67,67,67,67	0
58	MG	DA	1756	1/1	0.96	0.20	68,68,68,68	0
58	MG	BA	3145	1/1	0.96	0.08	37,37,37,37	0
58	MG	AA	3487	1/1	0.96	0.14	39,39,39,39	0
58	MG	AA	3427	1/1	0.96	0.10	34,34,34,34	0
58	MG	AA	3489	1/1	0.96	0.09	63,63,63,63	0
58	MG	AA	3329	1/1	0.96	0.17	17,17,17,17	0
58	MG	BA	3039	1/1	0.96	0.58	78,78,78,78	0
58	MG	AB	3012	1/1	0.96	0.20	30,30,30,30	1
58	MG	CA	3301	1/1	0.96	0.15	58,58,58,58	0
58	MG	CA	3492	1/1	0.96	0.22	52,52,52,52	0
58	MG	AB	3013	1/1	0.96	0.19	53,53,53,53	0
58	MG	AA	3747	1/1	0.96	0.20	62,62,62,62	0
58	MG	AB	3015	1/1	0.96	0.17	38,38,38,38	0
58	MG	AB	3016	1/1	0.96	0.21	33,33,33,33	0
58	MG	DF	3001	1/1	0.96	0.17	49,49,49,49	0
58	MG	AA	3009	1/1	0.96	0.13	23,23,23,23	0
58	MG	AA	3655	1/1	0.96	0.15	59,59,59,59	0
58	MG	AB	3019	1/1	0.96	0.13	64,64,64,64	0
58	MG	AA	3331	1/1	0.96	0.28	34,34,34,34	0
58	MG	CA	3172	1/1	0.96	0.30	53,53,53,53	0
58	MG	CF	304	1/1	0.96	0.16	54,54,54,54	0
58	MG	AA	3378	1/1	0.96	0.18	18,18,18,18	0
58	MG	AB	3022	1/1	0.96	0.06	56,56,56,56	0
58	MG	CA	3319	1/1	0.96	0.23	33,33,33,33	0
58	MG	CA	3507	1/1	0.96	0.08	71,71,71,71	0
58	MG	AA	3332	1/1	0.96	0.16	44,44,44,44	0
60	ZN	C9	501	1/1	0.96	0.11	93,93,93,93	0
58	MG	CA	3321	1/1	0.96	0.15	30,30,30,30	0
62	GDP	BZ	801	28/28	0.96	0.15	52,52,52,52	0
58	MG	AA	3439	1/1	0.96	0.23	33,33,33,33	0
58	MG	CA	3388	1/1	0.97	0.53	68,68,68,68	0
58	MG	AA	3168	1/1	0.97	0.13	64,64,64,64	0
58	MG	AA	3522	1/1	0.97	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	AA	3146	1/1	0.97	0.14	34,34,34,34	0
58	MG	AA	3022	1/1	0.97	0.11	9,9,9,9	0
58	MG	AA	3814	1/1	0.97	0.21	43,43,43,43	0
58	MG	CA	3554	1/1	0.97	0.08	67,67,67,67	0
58	MG	AA	3446	1/1	0.97	0.10	59,59,59,59	0
58	MG	AA	3528	1/1	0.97	0.13	25,25,25,25	0
58	MG	AA	3327	1/1	0.97	0.16	13,13,13,13	0
58	MG	CA	3558	1/1	0.97	0.10	47,47,47,47	0
58	MG	BX	110	1/1	0.97	0.16	57,57,57,57	0
58	MG	CA	3561	1/1	0.97	0.15	55,55,55,55	1
58	MG	CA	3398	1/1	0.97	0.10	58,58,58,58	0
58	MG	CA	3564	1/1	0.97	0.14	75,75,75,75	0
58	MG	AA	3617	1/1	0.97	0.09	30,30,30,30	0
58	MG	BA	3118	1/1	0.97	0.15	43,43,43,43	0
58	MG	AA	3820	1/1	0.97	0.26	44,44,44,44	0
58	MG	CA	3568	1/1	0.97	0.08	40,40,40,40	0
58	MG	AA	3530	1/1	0.97	0.15	15,15,15,15	0
58	MG	AA	3328	1/1	0.97	0.16	17,17,17,17	0
58	MG	AA	3532	1/1	0.97	0.15	60,60,60,60	0
58	MG	BA	3123	1/1	0.97	0.26	54,54,54,54	0
58	MG	DA	1636	1/1	0.97	0.46	64,64,64,64	0
58	MG	AA	3384	1/1	0.97	0.12	28,28,28,28	0
58	MG	AA	3286	1/1	0.97	0.12	53,53,53,53	0
58	MG	AA	3085	1/1	0.97	0.15	30,30,30,30	0
58	MG	CA	3409	1/1	0.97	0.19	61,61,61,61	0
58	MG	BA	3127	1/1	0.97	0.20	50,50,50,50	0
58	MG	CA	3411	1/1	0.97	0.20	31,31,31,31	0
58	MG	AA	3131	1/1	0.97	0.25	36,36,36,36	0
58	MG	AA	3723	1/1	0.97	0.14	19,19,19,19	0
58	MG	AA	3152	1/1	0.97	0.23	49,49,49,49	0
58	MG	AA	3075	1/1	0.97	0.31	13,13,13,13	0
58	MG	DA	1647	1/1	0.97	0.09	49,49,49,49	0
58	MG	CA	3416	1/1	0.97	0.22	34,34,34,34	0
58	MG	CA	3417	1/1	0.97	0.15	48,48,48,48	0
58	MG	CA	3263	1/1	0.97	0.21	29,29,29,29	0
58	MG	BA	3024	1/1	0.97	0.43	63,63,63,63	0
58	MG	CA	3421	1/1	0.97	0.26	69,69,69,69	0
58	MG	AA	3199	1/1	0.97	0.10	55,55,55,55	0
58	MG	CA	3423	1/1	0.97	0.19	54,54,54,54	0
58	MG	BA	3134	1/1	0.97	0.26	62,62,62,62	0
58	MG	CA	3426	1/1	0.97	0.14	51,51,51,51	0
58	MG	AA	3628	1/1	0.97	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3393	1/1	0.97	0.15	26,26,26,26	0
58	MG	AA	3230	1/1	0.97	0.24	49,49,49,49	0
58	MG	AA	3632	1/1	0.97	0.21	45,45,45,45	0
58	MG	CA	3272	1/1	0.97	0.12	34,34,34,34	0
58	MG	AA	3734	1/1	0.97	0.33	65,65,65,65	0
58	MG	AA	3395	1/1	0.97	0.18	22,22,22,22	0
58	MG	CA	3434	1/1	0.97	0.11	68,68,68,68	0
58	MG	AA	3120	1/1	0.97	0.18	43,43,43,43	0
58	MG	AB	3007	1/1	0.97	0.19	45,45,45,45	0
58	MG	CA	3277	1/1	0.97	0.20	42,42,42,42	0
58	MG	AA	3739	1/1	0.97	0.24	74,74,74,74	0
58	MG	AA	3338	1/1	0.97	0.12	29,29,29,29	0
58	MG	CA	3440	1/1	0.97	0.20	39,39,39,39	0
58	MG	AA	3636	1/1	0.97	0.13	24,24,24,24	0
58	MG	AA	3551	1/1	0.97	0.16	46,46,46,46	0
58	MG	AA	3398	1/1	0.97	0.07	17,17,17,17	0
58	MG	AA	3465	1/1	0.97	0.15	40,40,40,40	0
58	MG	CA	3446	1/1	0.97	0.31	39,39,39,39	0
58	MG	BA	3150	1/1	0.97	0.16	47,47,47,47	0
58	MG	CA	3449	1/1	0.97	0.21	42,42,42,42	0
58	MG	AA	3155	1/1	0.97	0.20	48,48,48,48	0
58	MG	AA	3467	1/1	0.97	0.07	44,44,44,44	0
58	MG	BA	3153	1/1	0.97	0.14	48,48,48,48	0
58	MG	CA	3288	1/1	0.97	0.22	63,63,63,63	0
58	MG	AA	3296	1/1	0.97	0.14	18,18,18,18	0
58	MG	CA	3621	1/1	0.97	0.51	65,65,65,65	0
58	MG	AA	3558	1/1	0.97	0.22	18,18,18,18	0
58	MG	CA	3040	1/1	0.97	0.19	64,64,64,64	0
58	MG	CA	3161	1/1	0.97	0.13	40,40,40,40	0
58	MG	CA	3162	1/1	0.97	0.35	63,63,63,63	0
58	MG	CA	3460	1/1	0.97	0.18	49,49,49,49	0
58	MG	AA	3050	1/1	0.97	0.23	53,53,53,53	0
58	MG	CA	3462	1/1	0.97	0.25	43,43,43,43	0
58	MG	AA	3646	1/1	0.97	0.10	57,57,57,57	0
58	MG	DA	1694	1/1	0.97	0.23	65,65,65,65	0
58	MG	CA	3630	1/1	0.97	0.23	61,61,61,61	0
58	MG	CA	3631	1/1	0.97	0.23	66,66,66,66	0
58	MG	AA	3343	1/1	0.97	0.14	65,65,65,65	0
58	MG	CA	3167	1/1	0.97	0.35	43,43,43,43	0
58	MG	AA	3135	1/1	0.97	0.45	62,62,62,62	0
58	MG	AA	3180	1/1	0.97	0.33	72,72,72,72	0
58	MG	AA	3301	1/1	0.97	0.25	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3303	1/1	0.97	0.28	45,45,45,45	0
58	MG	AD	302	1/1	0.97	0.33	18,18,18,18	0
58	MG	CA	3306	1/1	0.97	0.19	61,61,61,61	0
58	MG	CA	3307	1/1	0.97	0.16	39,39,39,39	0
58	MG	AA	3236	1/1	0.97	0.31	37,37,37,37	1
58	MG	AA	3409	1/1	0.97	0.18	30,30,30,30	0
58	MG	AA	3654	1/1	0.97	0.30	65,65,65,65	0
58	MG	AA	3136	1/1	0.97	0.34	66,66,66,66	0
58	MG	AA	3182	1/1	0.97	0.09	23,23,23,23	1
58	MG	AA	3352	1/1	0.97	0.12	51,51,51,51	0
58	MG	AA	3047	1/1	0.97	0.27	31,31,31,31	0
58	MG	AA	3011	1/1	0.97	0.22	39,39,39,39	0
58	MG	BA	3172	1/1	0.97	0.23	55,55,55,55	0
58	MG	AA	3661	1/1	0.97	0.33	43,43,43,43	0
58	MG	AA	3053	1/1	0.97	0.16	13,13,13,13	0
58	MG	CA	3653	1/1	0.97	0.20	25,25,25,25	0
58	MG	AA	3575	1/1	0.97	0.15	30,30,30,30	0
58	MG	AF	302	1/1	0.97	0.16	40,40,40,40	0
58	MG	AA	3418	1/1	0.97	0.17	30,30,30,30	0
58	MG	BA	3064	1/1	0.97	0.07	78,78,78,78	0
58	MG	CA	3327	1/1	0.97	0.13	33,33,33,33	0
58	MG	BA	3180	1/1	0.97	0.07	41,41,41,41	0
58	MG	CA	3660	1/1	0.97	0.17	38,38,38,38	0
58	MG	AA	3357	1/1	0.97	0.19	27,27,27,27	0
58	MG	CA	3662	1/1	0.97	0.18	48,48,48,48	0
58	MG	AA	3140	1/1	0.97	0.09	56,56,56,56	0
58	MG	BA	3183	1/1	0.97	0.17	60,60,60,60	0
58	MG	AA	3065	1/1	0.97	0.24	28,28,28,28	0
58	MG	AA	3072	1/1	0.97	0.64	40,40,40,40	0
58	MG	AA	3312	1/1	0.97	0.19	52,52,52,52	0
58	MG	CA	3497	1/1	0.97	0.14	63,63,63,63	0
58	MG	CA	3335	1/1	0.97	0.20	43,43,43,43	0
58	MG	AA	3214	1/1	0.97	0.39	39,39,39,39	1
58	MG	AA	3315	1/1	0.97	0.16	34,34,34,34	0
58	MG	AN	3003	1/1	0.97	0.10	45,45,45,45	0
58	MG	AA	3673	1/1	0.97	0.13	66,66,66,66	0
58	MG	AA	3777	1/1	0.97	0.14	20,20,20,20	0
58	MG	CA	3504	1/1	0.97	0.19	69,69,69,69	0
58	MG	AA	3143	1/1	0.97	0.17	28,28,28,28	0
58	MG	CB	3011	1/1	0.97	0.32	51,51,51,51	0
58	MG	AQ	202	1/1	0.97	0.33	40,40,40,40	0
58	MG	AA	3779	1/1	0.97	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3494	1/1	0.97	0.19	33,33,33,33	1
58	MG	AA	3366	1/1	0.97	0.14	52,52,52,52	0
58	MG	AA	3496	1/1	0.97	0.12	58,58,58,58	0
58	MG	AA	3678	1/1	0.97	0.19	32,32,32,32	0
58	MG	DA	1750	1/1	0.97	0.20	71,71,71,71	0
58	MG	CA	3208	1/1	0.97	0.28	69,69,69,69	0
58	MG	AA	3497	1/1	0.97	0.12	51,51,51,51	0
58	MG	AA	3429	1/1	0.97	0.18	42,42,42,42	0
58	MG	AA	3499	1/1	0.97	0.12	35,35,35,35	0
58	MG	AA	3430	1/1	0.97	0.08	25,25,25,25	0
58	MG	CA	3213	1/1	0.97	0.11	68,68,68,68	0
58	MG	CA	3519	1/1	0.97	0.21	62,62,62,62	0
58	MG	BA	3086	1/1	0.97	0.25	51,51,51,51	0
58	MG	CA	3358	1/1	0.97	0.11	78,78,78,78	0
58	MG	AX	101	1/1	0.97	0.16	30,30,30,30	1
58	MG	AA	3216	1/1	0.97	0.12	36,36,36,36	0
58	MG	AA	3684	1/1	0.97	0.10	28,28,28,28	0
58	MG	BA	3207	1/1	0.97	0.22	66,66,66,66	0
58	MG	AA	3432	1/1	0.97	0.28	28,28,28,28	0
58	MG	AA	3433	1/1	0.97	0.18	18,18,18,18	0
58	MG	AA	3368	1/1	0.97	0.22	39,39,39,39	0
58	MG	CA	3367	1/1	0.97	0.37	59,59,59,59	0
58	MG	AA	3506	1/1	0.97	0.17	32,32,32,32	0
58	MG	BA	3212	1/1	0.97	0.11	73,73,73,73	0
58	MG	AA	3507	1/1	0.97	0.28	31,31,31,31	0
58	MG	CA	3373	1/1	0.97	0.18	42,42,42,42	0
58	MG	AA	3318	1/1	0.97	0.32	53,53,53,53	0
58	MG	AA	3103	1/1	0.97	0.24	48,48,48,48	0
58	MG	AA	3511	1/1	0.97	0.34	56,56,56,56	0
58	MG	AA	3800	1/1	0.97	0.13	30,30,30,30	0
58	MG	AA	3603	1/1	0.97	0.17	35,35,35,35	0
58	MG	AA	3438	1/1	0.97	0.13	19,19,19,19	0
58	MG	AA	3220	1/1	0.97	0.11	34,34,34,34	0
58	MG	AA	3374	1/1	0.97	0.09	17,17,17,17	0
58	MG	CA	3382	1/1	0.97	0.15	37,37,37,37	0
58	MG	CA	3383	1/1	0.97	0.16	40,40,40,40	0
58	MG	AA	3699	1/1	0.97	0.22	38,38,38,38	1
58	MG	AA	3607	1/1	0.97	0.34	59,59,59,59	0
61	SF4	DD	501	8/8	0.97	0.10	90,90,90,90	0
58	MG	AA	3104	1/1	0.97	0.13	13,13,13,13	0
58	MG	AA	3376	1/1	0.97	0.18	18,18,18,18	0
58	MG	DA	1667	1/1	0.98	0.35	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	AA	3370	1/1	0.98	0.20	57,57,57,57	0
58	MG	AA	3512	1/1	0.98	0.22	11,11,11,11	0
58	MG	CA	3442	1/1	0.98	0.26	75,75,75,75	0
58	MG	AA	3750	1/1	0.98	0.11	14,14,14,14	0
58	MG	AA	3565	1/1	0.98	0.24	17,17,17,17	0
58	MG	AA	3434	1/1	0.98	0.18	22,22,22,22	0
58	MG	CA	3341	1/1	0.98	0.13	48,48,48,48	0
58	MG	AA	3823	1/1	0.98	0.25	43,43,43,43	0
58	MG	CA	3065	1/1	0.98	0.12	41,41,41,41	0
58	MG	AA	3032	1/1	0.98	0.15	37,37,37,37	0
58	MG	AA	3114	1/1	0.98	0.23	62,62,62,62	0
58	MG	AA	3826	1/1	0.98	0.29	66,66,66,66	0
58	MG	CA	3560	1/1	0.98	0.21	56,56,56,56	0
58	MG	CA	3453	1/1	0.98	0.32	59,59,59,59	0
58	MG	AA	3516	1/1	0.98	0.17	20,20,20,20	0
58	MG	AA	3517	1/1	0.98	0.16	18,18,18,18	0
58	MG	AA	3571	1/1	0.98	0.17	14,14,14,14	0
58	MG	CA	3350	1/1	0.98	0.20	39,39,39,39	0
58	MG	BA	3142	1/1	0.98	0.08	47,47,47,47	0
58	MG	AA	3831	1/1	0.98	0.20	51,51,51,51	0
58	MG	CA	3353	1/1	0.98	0.11	66,66,66,66	0
58	MG	A0	104	1/1	0.98	0.13	36,36,36,36	0
58	MG	CE	301	1/1	0.98	0.34	64,64,64,64	0
58	MG	AA	3037	1/1	0.98	0.26	44,44,44,44	0
58	MG	AA	3403	1/1	0.98	0.17	18,18,18,18	0
58	MG	AA	3326	1/1	0.98	0.12	59,59,59,59	0
58	MG	CA	3165	1/1	0.98	0.31	41,41,41,41	0
58	MG	A5	101	1/1	0.98	0.34	40,40,40,40	0
58	MG	AA	3521	1/1	0.98	0.13	37,37,37,37	0
58	MG	AA	3074	1/1	0.98	0.23	59,59,59,59	0
58	MG	AA	3692	1/1	0.98	0.17	51,51,51,51	0
58	MG	CA	3170	1/1	0.98	0.24	32,32,32,32	0
58	MG	AA	3406	1/1	0.98	0.17	50,50,50,50	0
58	MG	CA	3581	1/1	0.98	0.12	51,51,51,51	0
58	MG	CA	3365	1/1	0.98	0.29	29,29,29,29	0
58	MG	CO	202	1/1	0.98	0.22	52,52,52,52	0
58	MG	AA	3524	1/1	0.98	0.23	29,29,29,29	0
58	MG	CA	3265	1/1	0.98	0.13	55,55,55,55	0
58	MG	AA	3054	1/1	0.98	0.10	38,38,38,38	0
58	MG	CA	3369	1/1	0.98	0.16	58,58,58,58	0
58	MG	AA	3526	1/1	0.98	0.25	38,38,38,38	0
58	MG	AA	3377	1/1	0.98	0.15	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3351	1/1	0.98	0.16	29,29,29,29	0
58	MG	DA	1712	1/1	0.98	0.14	51,51,51,51	0
58	MG	CV	201	1/1	0.98	0.21	69,69,69,69	0
58	MG	CA	3480	1/1	0.98	0.20	44,44,44,44	0
58	MG	AA	3255	1/1	0.98	0.21	40,40,40,40	0
58	MG	AA	3485	1/1	0.98	0.19	15,15,15,15	0
58	MG	AA	3702	1/1	0.98	0.31	46,46,46,46	1
58	MG	C3	101	1/1	0.98	0.22	69,69,69,69	0
58	MG	CA	3007	1/1	0.98	0.11	27,27,27,27	0
58	MG	AB	3011	1/1	0.98	0.13	31,31,31,31	0
58	MG	CA	3093	1/1	0.98	0.16	68,68,68,68	0
58	MG	AA	3380	1/1	0.98	0.14	15,15,15,15	0
58	MG	AA	3642	1/1	0.98	0.18	41,41,41,41	0
58	MG	AA	3256	1/1	0.98	0.19	54,54,54,54	0
58	MG	CA	3097	1/1	0.98	0.24	65,65,65,65	0
58	MG	AA	3706	1/1	0.98	0.28	29,29,29,29	1
58	MG	DA	1727	1/1	0.98	0.09	57,57,57,57	0
58	MG	AA	3707	1/1	0.98	0.24	31,31,31,31	1
58	MG	AA	3533	1/1	0.98	0.15	24,24,24,24	0
58	MG	AA	3038	1/1	0.98	0.16	10,10,10,10	0
58	MG	AA	3084	1/1	0.98	0.23	41,41,41,41	0
58	MG	AA	3537	1/1	0.98	0.11	35,35,35,35	0
58	MG	CA	3104	1/1	0.98	0.39	60,60,60,60	0
58	MG	BA	3171	1/1	0.98	0.16	61,61,61,61	0
58	MG	AA	3356	1/1	0.98	0.23	33,33,33,33	0
58	MG	CA	3610	1/1	0.98	0.32	98,98,98,98	0
58	MG	AA	3417	1/1	0.98	0.24	42,42,42,42	0
58	MG	AA	3540	1/1	0.98	0.09	29,29,29,29	0
58	MG	CA	3291	1/1	0.98	0.32	40,40,40,40	0
58	MG	BA	3095	1/1	0.98	0.16	99,99,99,99	0
58	MG	CA	3023	1/1	0.98	0.17	45,45,45,45	0
58	MG	AA	3594	1/1	0.98	0.11	27,27,27,27	0
58	MG	AA	3541	1/1	0.98	0.19	29,29,29,29	0
58	MG	CA	3618	1/1	0.98	0.19	37,37,37,37	0
58	MG	BA	3178	1/1	0.98	0.26	63,63,63,63	0
58	MG	AA	3150	1/1	0.98	0.27	62,62,62,62	0
58	MG	AD	304	1/1	0.98	0.24	41,41,41,41	0
58	MG	AA	3260	1/1	0.98	0.19	23,23,23,23	0
58	MG	AA	3420	1/1	0.98	0.18	12,12,12,12	0
58	MG	AA	3545	1/1	0.98	0.15	15,15,15,15	0
58	MG	AA	3600	1/1	0.98	0.38	57,57,57,57	0
58	MG	CA	3304	1/1	0.98	0.26	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	3659	1/1	0.98	0.20	14,14,14,14	0
58	MG	AA	3726	1/1	0.98	0.20	37,37,37,37	0
58	MG	AA	3175	1/1	0.98	0.34	60,60,60,60	0
58	MG	CA	3518	1/1	0.98	0.08	61,61,61,61	0
58	MG	AA	3797	1/1	0.98	0.22	39,39,39,39	0
58	MG	AA	3388	1/1	0.98	0.20	17,17,17,17	0
58	MG	CA	3310	1/1	0.98	0.20	29,29,29,29	0
58	MG	AA	3151	1/1	0.98	0.23	14,14,14,14	0
58	MG	CA	3312	1/1	0.98	0.15	49,49,49,49	0
58	MG	AA	3459	1/1	0.98	0.20	18,18,18,18	0
58	MG	AA	3337	1/1	0.98	0.22	10,10,10,10	0
58	MG	AA	3101	1/1	0.98	0.43	51,51,51,51	0
58	MG	CA	3419	1/1	0.98	0.24	40,40,40,40	0
58	MG	AA	3666	1/1	0.98	0.16	62,62,62,62	0
58	MG	BA	3114	1/1	0.98	0.32	55,55,55,55	0
58	MG	CA	3642	1/1	0.98	0.32	53,53,53,53	0
58	MG	AA	3735	1/1	0.98	0.18	21,21,21,21	0
58	MG	AA	3552	1/1	0.98	0.28	51,51,51,51	0
58	MG	AA	3392	1/1	0.98	0.15	21,21,21,21	0
58	MG	CA	3425	1/1	0.98	0.15	54,54,54,54	0
58	MG	AA	3339	1/1	0.98	0.19	41,41,41,41	0
58	MG	AA	3464	1/1	0.98	0.10	59,59,59,59	0
58	MG	AA	3504	1/1	0.98	0.14	62,62,62,62	0
58	MG	CA	3325	1/1	0.98	0.32	39,39,39,39	0
58	MG	AA	3810	1/1	0.98	0.27	62,62,62,62	0
58	MG	DZ	703	1/1	0.98	0.22	56,56,56,56	0
58	MG	AP	201	1/1	0.98	0.20	31,31,31,31	0
58	MG	AA	3219	1/1	0.98	0.10	4,4,4,4	0
58	MG	CA	3230	1/1	0.98	0.22	50,50,50,50	0
58	MG	AA	3320	1/1	0.98	0.24	23,23,23,23	0
60	ZN	C5	101	1/1	0.98	0.10	66,66,66,66	0
60	ZN	C6	501	1/1	0.98	0.07	60,60,60,60	0
58	MG	AA	3077	1/1	0.98	0.34	92,92,92,92	0
58	MG	AA	3031	1/1	0.98	0.23	22,22,22,22	1
61	SF4	BD	501	8/8	0.98	0.06	79,79,79,79	0
58	MG	AA	3561	1/1	0.98	0.23	56,56,56,56	0
58	MG	AA	3369	1/1	0.98	0.22	27,27,27,27	0
58	MG	AU	203	1/1	0.98	0.21	34,34,34,34	1
58	MG	CA	3323	1/1	0.99	0.24	45,45,45,45	0
58	MG	AA	3471	1/1	0.99	0.19	34,34,34,34	0
58	MG	AA	3631	1/1	0.99	0.23	68,68,68,68	0
58	MG	AA	3791	1/1	0.99	0.27	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DA	1678	1/1	0.99	0.26	57,57,57,57	0
58	MG	AE	302	1/1	0.99	0.14	17,17,17,17	0
58	MG	AA	3648	1/1	0.99	0.17	38,38,38,38	0
58	MG	AA	3287	1/1	0.99	0.36	46,46,46,46	0
58	MG	AA	3003	1/1	0.99	0.08	19,19,19,19	0
58	MG	CA	3298	1/1	0.99	0.42	42,42,42,42	0
58	MG	CA	3176	1/1	0.99	0.15	41,41,41,41	0
58	MG	AA	3348	1/1	0.99	0.23	31,31,31,31	0
58	MG	CE	302	1/1	0.99	0.15	46,46,46,46	0
58	MG	DA	1610	1/1	0.99	0.22	45,45,45,45	0
58	MG	AA	3724	1/1	0.99	0.17	22,22,22,22	0
58	MG	AA	3313	1/1	0.99	0.19	33,33,33,33	0
58	MG	AA	3412	1/1	0.99	0.16	20,20,20,20	0
58	MG	AA	3307	1/1	0.99	0.23	6,6,6,6	0
58	MG	CA	3371	1/1	0.99	0.20	46,46,46,46	0
58	MG	AA	3454	1/1	0.99	0.13	49,49,49,49	0
58	MG	BE	3001	1/1	0.99	0.04	59,59,59,59	0
58	MG	AA	3708	1/1	0.99	0.21	32,32,32,32	1
58	MG	AA	3208	1/1	0.99	0.30	26,26,26,26	1
58	MG	AA	3710	1/1	0.99	0.23	32,32,32,32	1
58	MG	AA	3830	1/1	0.99	0.14	40,40,40,40	0
58	MG	AA	3732	1/1	0.99	0.25	41,41,41,41	0
58	MG	CA	3447	1/1	0.99	0.17	62,62,62,62	0
58	MG	AA	3217	1/1	0.99	0.15	46,46,46,46	0
60	ZN	AY	501	1/1	0.99	0.06	63,63,63,63	0
58	MG	AA	3535	1/1	0.99	0.17	27,27,27,27	0
60	ZN	A5	102	1/1	0.99	0.10	36,36,36,36	0
60	ZN	A9	501	1/1	0.99	0.10	41,41,41,41	0
58	MG	AA	3361	1/1	0.99	0.23	28,28,28,28	0
60	ZN	CY	501	1/1	0.99	0.05	92,92,92,92	0
58	MG	AA	3835	1/1	0.99	0.20	39,39,39,39	0
58	MG	AA	3694	1/1	0.99	0.15	47,47,47,47	0
58	MG	AA	3508	1/1	0.99	0.21	13,13,13,13	0
58	MG	AA	3738	1/1	0.99	0.16	28,28,28,28	0
58	MG	CA	3256	1/1	0.99	0.24	40,40,40,40	0
58	MG	AA	3469	1/1	0.99	0.07	42,42,42,42	0
58	MG	CA	3562	1/1	0.99	0.15	36,36,36,36	0
58	MG	AA	3763	1/1	0.99	0.32	62,62,62,62	0
58	MG	AA	3299	1/1	0.99	0.12	21,21,21,21	0
58	MG	AN	3002	1/1	1.00	0.10	26,26,26,26	0
60	ZN	A6	103	1/1	1.00	0.10	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.