



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 02:38 PM UTC

PDB ID : 4WQF / pdb_00004wqf
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G and fusidic acid in the post-translocational state
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-21
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

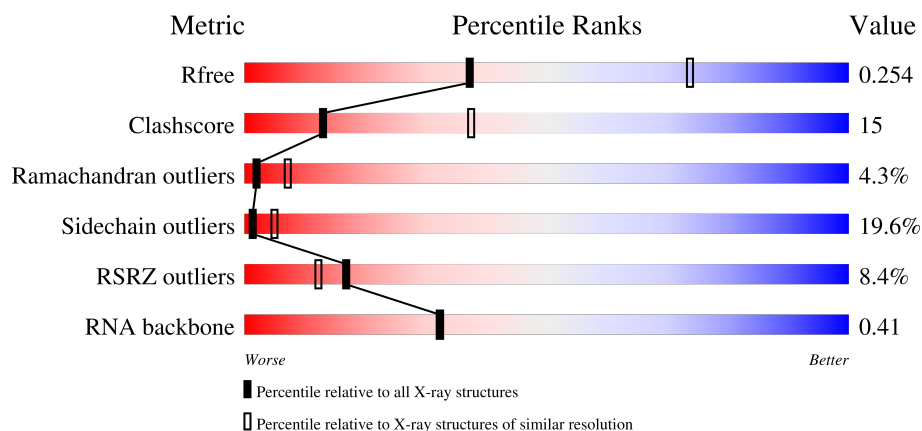
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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 $\leq 5\%$. 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	2% 54% 35% 9% ..
1	CA	2915	3% 47% 41% 9% .
2	AB	121	% 55% 34% 11% .
2	CB	121	% 47% 45% 7% .

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

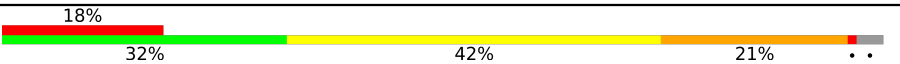
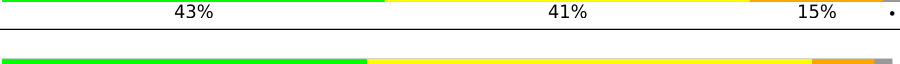
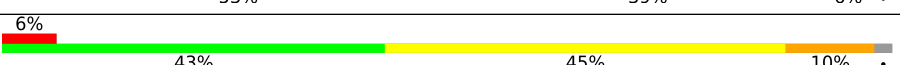
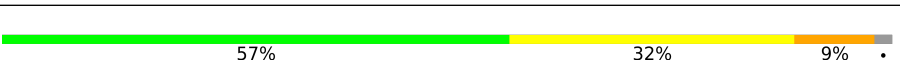
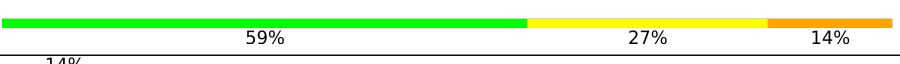
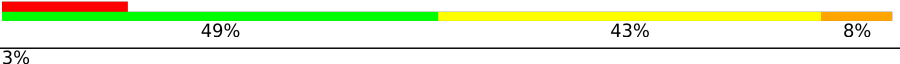
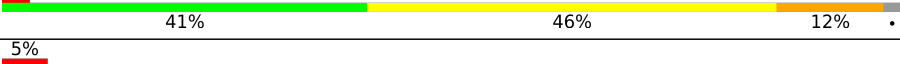
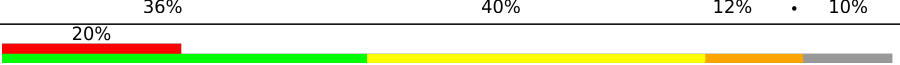
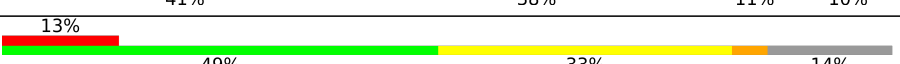
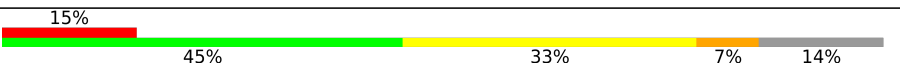
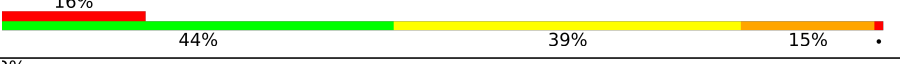
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Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
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
40	DG	156	
41	BH	138	
41	DH	138	
42	BI	128	
42	DI	128	
43	BJ	105	
43	DJ	105	
44	BK	129	
44	DK	129	
45	BL	132	
45	DL	132	
46	BM	126	
46	DM	126	
47	BN	61	
47	DN	61	
48	BO	89	
48	DO	89	
49	BP	88	
49	DP	88	
50	BQ	105	
50	DQ	105	
51	BR	88	
51	DR	88	
52	BS	93	
52	DS	93	

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

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	3094	-	-	-	X
58	MG	CA	3180	-	-	-	X
60	SF4	DD	501	-	-	X	-
62	GDP	DZ	704	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 310279 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	0	0	0
			61426	27339	11489	19747	2851			
1	CA	2848	Total	C	N	O	P	0	0	0
			61337	27299	11470	19721	2847			

- 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	0	0	0
			2573	1146	476	832	119			
2	CB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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	0	0	0
			1063	669	201	192	1			
3	CC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			

- 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	0	0	0
			2136	1349	423	361	3			
4	CD	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- 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	0	0	0
			1559	985	298	270	6			
5	CE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- 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	0	0	1
			1584	1009	298	275	2			
6	CF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- 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	0	0	0
			1425	914	256	251	4			
7	CG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- 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	0	0	0
			1330	845	248	236	1			
8	CH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

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

- 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	0	0	0
			1025	653	181	186	5			

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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	C	N	O	0	0	0
			877	553	175	149			
16	CS	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

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

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

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

- 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	0	0	0
			588	365	118	103	2			

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

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

- 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	0	0	0
			558	352	102	99	5			
28	C4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- 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	0	0	0
			455	285	89	76	5			
29	C5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- 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	0	0	0
			453	281	91	77	4			
30	C6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- 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	0	0	0
			418	257	104	55	2			
31	C7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- 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	C	N	O	S	0	0	0
			1659	1040	326	286	7			
37	DD	208	Total	C	N	O	S	0	0	0
			1678	1052	333	286	7			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			
57	DZ	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	815	Total Mg 815 815	0	0
58	AB	23	Total Mg 23 23	0	0
58	AD	12	Total Mg 12 12	0	0
58	AE	5	Total Mg 5 5	0	0
58	AF	8	Total Mg 8 8	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	3	Total Mg 3 3	0	0
58	AQ	3	Total Mg 3 3	0	0
58	AR	2	Total Mg 2 2	0	0
58	AU	4	Total Mg 4 4	0	0
58	AV	6	Total Mg 6 6	0	0
58	AW	4	Total Mg 4 4	0	0
58	AX	1	Total Mg 1 1	0	0
58	AY	1	Total Mg 1 1	0	0
58	AZ	2	Total Mg 2 2	0	0
58	A0	3	Total Mg 3 3	0	0
58	A2	2	Total Mg 2 2	0	0
58	A4	1	Total Mg 1 1	0	0
58	A5	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	A6	1	Total 1	Mg 1	0	0
58	A7	6	Total 6	Mg 6	0	0
58	A8	2	Total 2	Mg 2	0	0
58	A9	1	Total 1	Mg 1	0	0
58	BA	213	Total 213	Mg 213	0	0
58	BB	1	Total 1	Mg 1	0	0
58	BD	1	Total 1	Mg 1	0	0
58	BE	1	Total 1	Mg 1	0	0
58	BF	1	Total 1	Mg 1	0	0
58	BK	1	Total 1	Mg 1	0	0
58	BL	2	Total 2	Mg 2	0	0
58	BM	2	Total 2	Mg 2	0	0
58	BN	1	Total 1	Mg 1	0	0
58	BT	1	Total 1	Mg 1	0	0
58	BV	1	Total 1	Mg 1	0	0
58	BW	3	Total 3	Mg 3	0	0
58	BZ	2	Total 2	Mg 2	0	0
58	CA	664	Total 664	Mg 664	0	0
58	CB	13	Total 13	Mg 13	0	0
58	CD	3	Total 3	Mg 3	0	0
58	CE	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CF	5	Total 5	Mg 5	0	0
58	CG	1	Total 1	Mg 1	0	0
58	CN	1	Total 1	Mg 1	0	0
58	CO	2	Total 2	Mg 2	0	0
58	CP	3	Total 3	Mg 3	0	0
58	CQ	5	Total 5	Mg 5	0	0
58	CR	1	Total 1	Mg 1	0	0
58	CU	1	Total 1	Mg 1	0	0
58	CV	2	Total 2	Mg 2	0	0
58	CW	1	Total 1	Mg 1	0	0
58	CY	1	Total 1	Mg 1	0	0
58	C3	1	Total 1	Mg 1	0	0
58	C5	1	Total 1	Mg 1	0	0
58	C7	1	Total 1	Mg 1	0	0
58	C8	1	Total 1	Mg 1	0	0
58	DA	168	Total 168	Mg 168	0	0
58	DD	1	Total 1	Mg 1	0	0
58	DE	2	Total 2	Mg 2	0	0
58	DF	1	Total 1	Mg 1	0	0
58	DJ	1	Total 1	Mg 1	0	0
58	DK	1	Total 1	Mg 1	0	0

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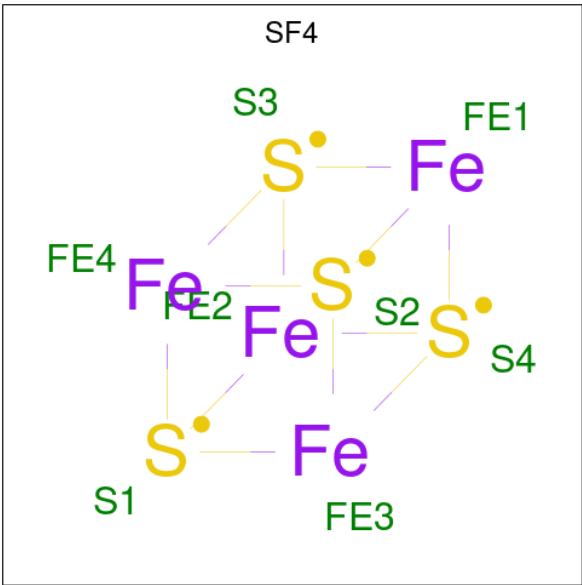
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DT	1	Total 1	Mg 1	0	0
58	DW	3	Total 3	Mg 3	0	0
58	DZ	2	Total 2	Mg 2	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

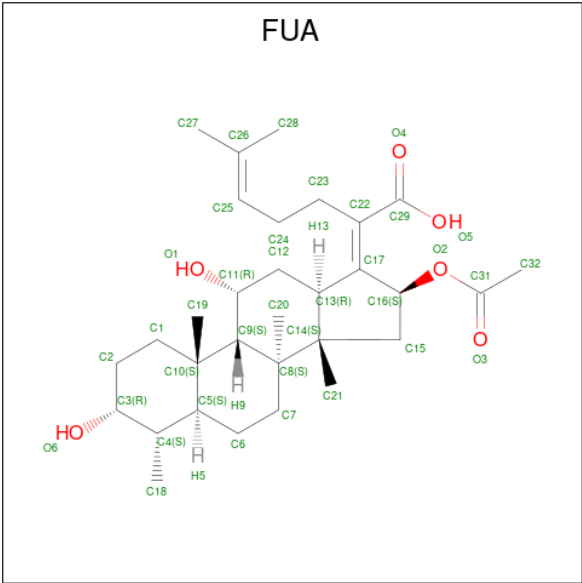
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AY	1	Total 1	Zn 1	0	0
59	A4	1	Total 1	Zn 1	0	0
59	A5	1	Total 1	Zn 1	0	0
59	A6	1	Total 1	Zn 1	0	0
59	A9	1	Total 1	Zn 1	0	0
59	BN	1	Total 1	Zn 1	0	0
59	CY	1	Total 1	Zn 1	0	0
59	C4	1	Total 1	Zn 1	0	0
59	C5	1	Total 1	Zn 1	0	0
59	C6	1	Total 1	Zn 1	0	0
59	C9	1	Total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

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



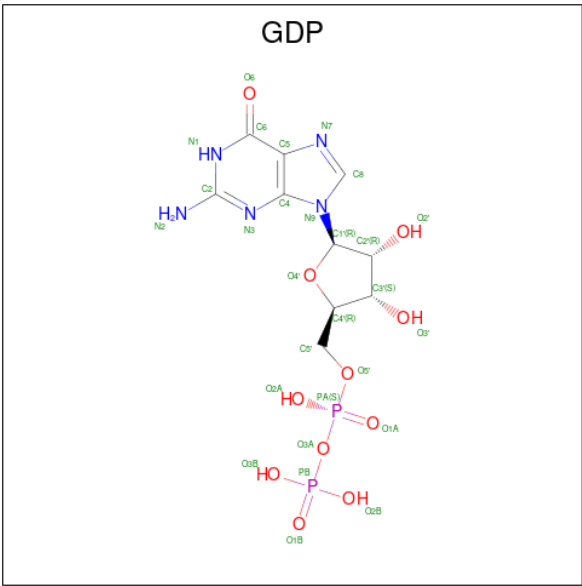
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	BD	1	Total	Fe	S	0	0
			8	4	4		
60	DD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is FUSIDIC ACID (CCD ID: FUA) (formula: C₃₁H₄₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	BZ	1	Total	C	O	0	0
			37	31	6		
61	DZ	1	Total	C	O	0	0
			37	31	6		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AA	1408	Total	O	0	0
			1408	1408		
63	AB	36	Total	O	0	0
			36	36		
63	AD	15	Total	O	0	0
			15	15		
63	AE	19	Total	O	0	0
			19	19		
63	AF	8	Total	O	0	0
			8	8		
63	AG	3	Total	O	0	0
			3	3		
63	AH	1	Total	O	0	0
			1	1		
63	AN	2	Total	O	0	0
			2	2		
63	AO	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AP	15	Total 15	O 15	0	0
63	AQ	3	Total 3	O 3	0	0
63	AR	3	Total 3	O 3	0	0
63	AS	1	Total 1	O 1	0	0
63	AT	2	Total 2	O 2	0	0
63	AU	6	Total 6	O 6	0	0
63	AW	1	Total 1	O 1	0	0
63	AX	2	Total 2	O 2	0	0
63	AZ	1	Total 1	O 1	0	0
63	A0	7	Total 7	O 7	0	0
63	A1	3	Total 3	O 3	0	0
63	A3	1	Total 1	O 1	0	0
63	A5	2	Total 2	O 2	0	0
63	A6	1	Total 1	O 1	0	0
63	A7	3	Total 3	O 3	0	0
63	A8	11	Total 11	O 11	0	0
63	BA	205	Total 205	O 205	0	0
63	BD	3	Total 3	O 3	0	0
63	BE	3	Total 3	O 3	0	0
63	BJ	1	Total 1	O 1	0	0
63	BL	2	Total 2	O 2	0	0

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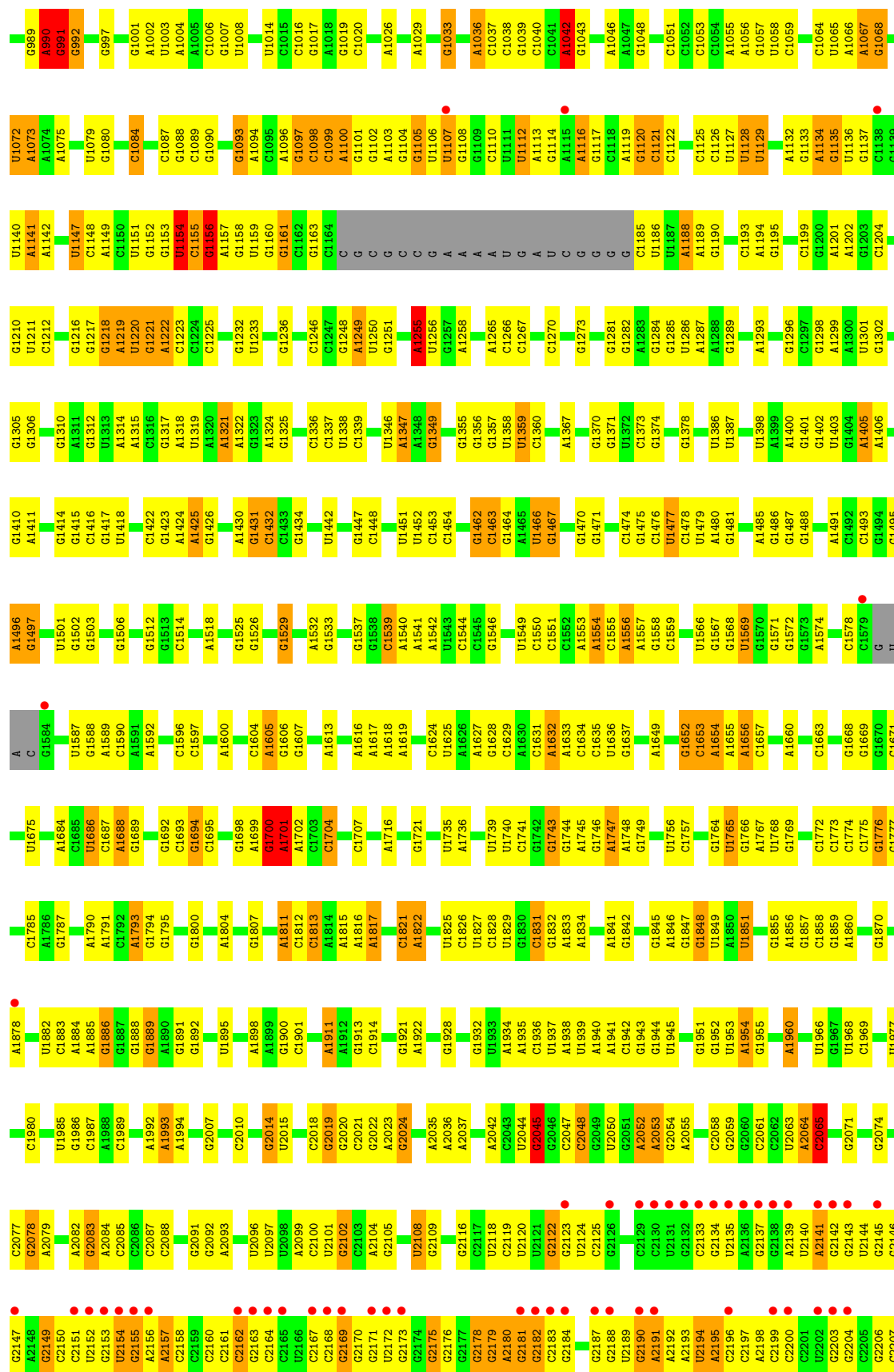
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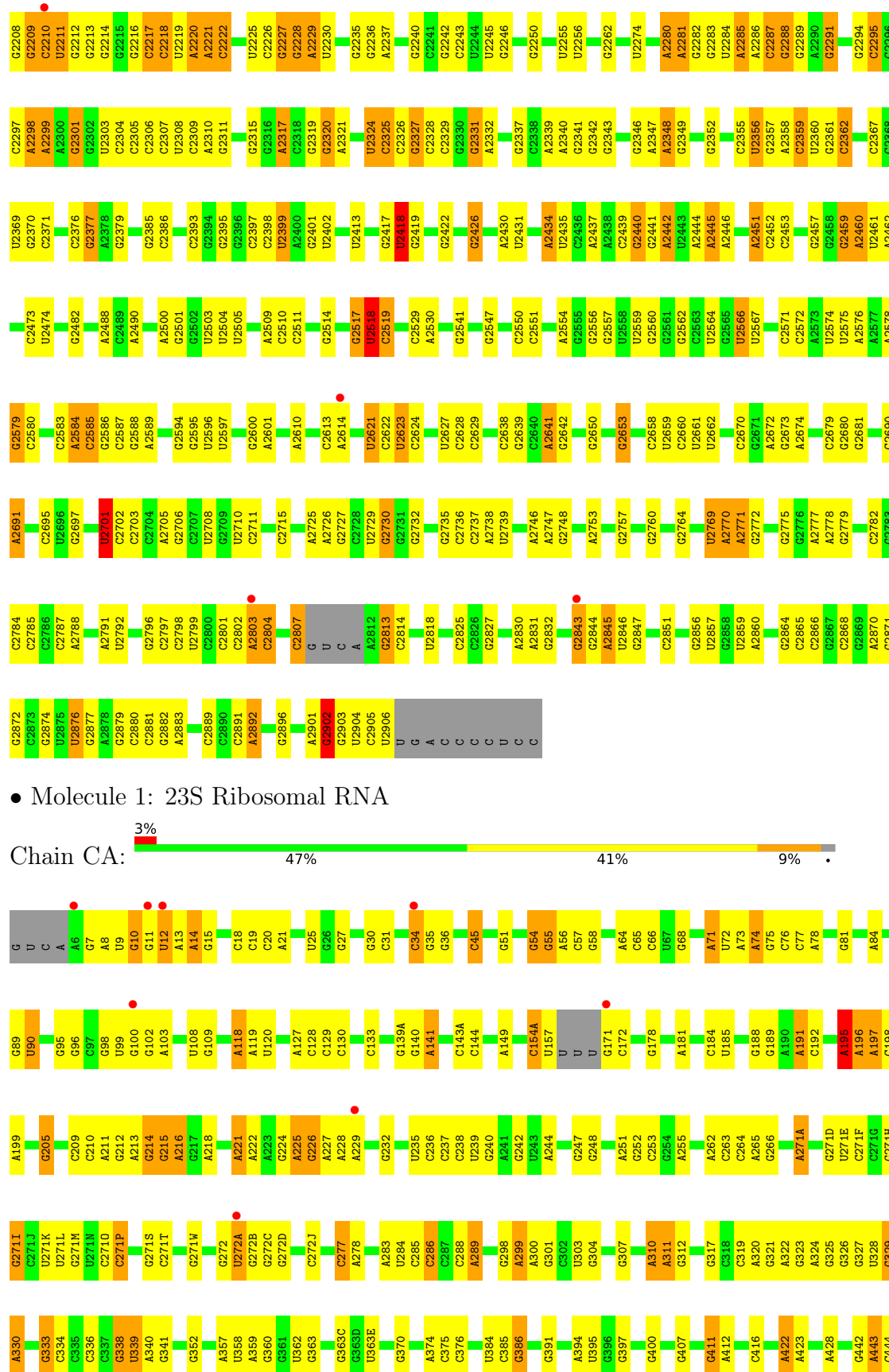
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BM	1	Total 1	O 1	0	0
63	BO	1	Total 1	O 1	0	0
63	BV	2	Total 2	O 2	0	0
63	BW	1	Total 1	O 1	0	0
63	BZ	3	Total 3	O 3	0	0
63	CA	981	Total 981	O 981	0	0
63	CB	9	Total 9	O 9	0	0
63	CD	15	Total 15	O 15	0	0
63	CE	9	Total 9	O 9	0	0
63	CF	6	Total 6	O 6	0	0
63	CP	13	Total 13	O 13	0	0
63	CQ	1	Total 1	O 1	0	0
63	CT	3	Total 3	O 3	0	0
63	CU	4	Total 4	O 4	0	0
63	CV	1	Total 1	O 1	0	0
63	CW	1	Total 1	O 1	0	0
63	CX	1	Total 1	O 1	0	0
63	CY	1	Total 1	O 1	0	0
63	C0	5	Total 5	O 5	0	0
63	C1	3	Total 3	O 3	0	0
63	C3	1	Total 1	O 1	0	0

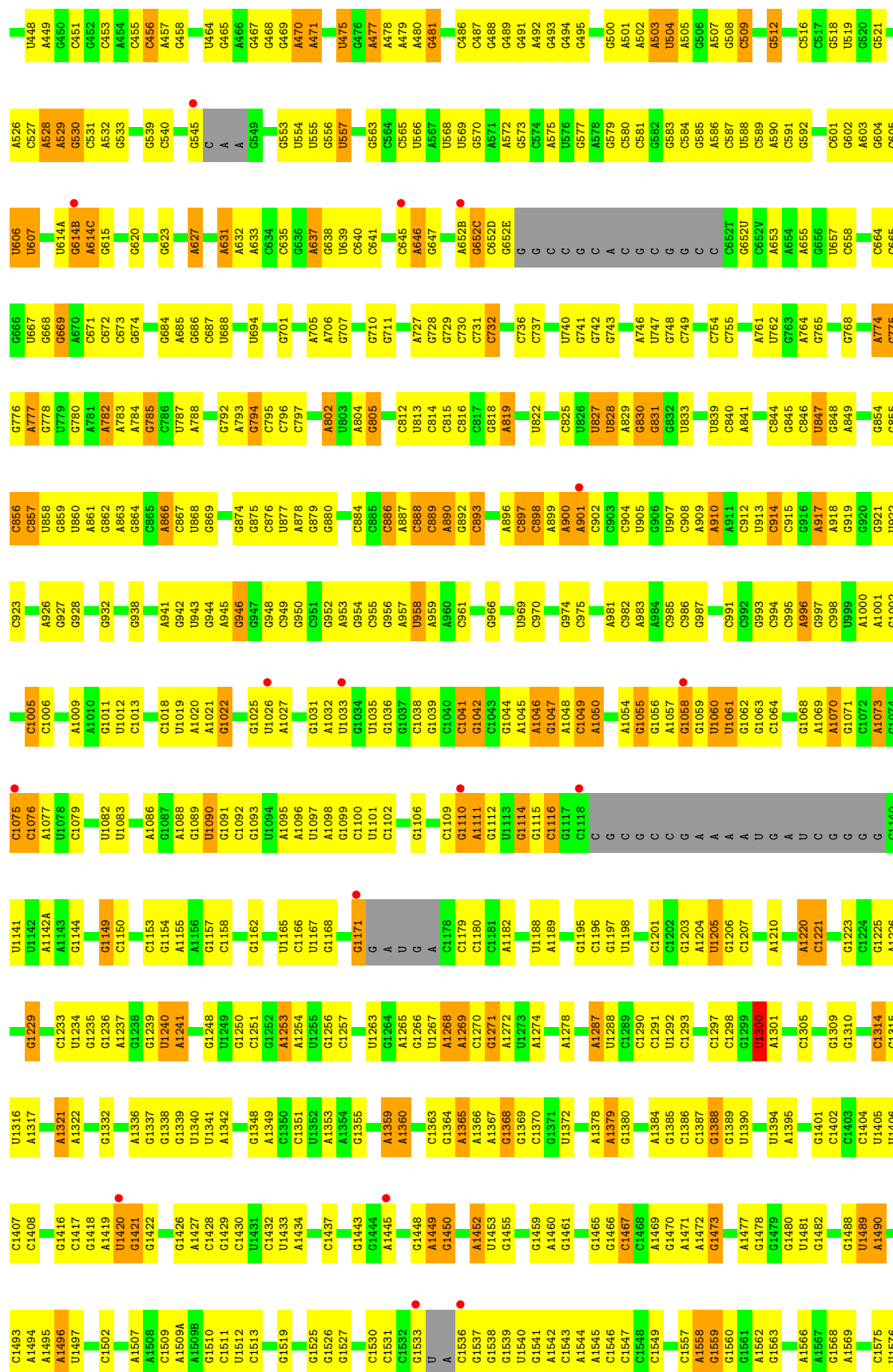
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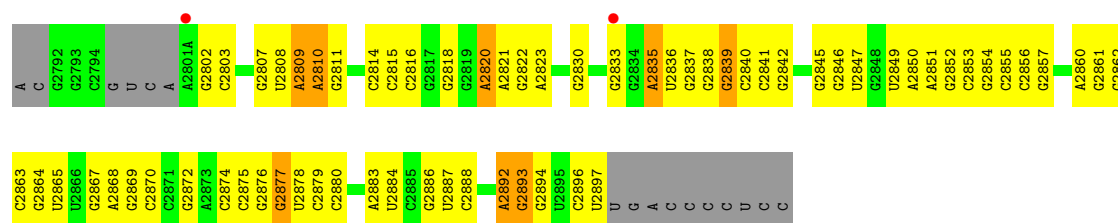
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	C5	1	Total	O	0	0
			1	1		
63	C7	3	Total	O	0	0
			3	3		
63	C8	3	Total	O	0	0
			3	3		
63	DA	153	Total	O	0	0
			153	153		
63	DE	2	Total	O	0	0
			2	2		
63	DH	1	Total	O	0	0
			1	1		
63	DJ	1	Total	O	0	0
			1	1		
63	DK	2	Total	O	0	0
			2	2		
63	DL	1	Total	O	0	0
			1	1		
63	DP	1	Total	O	0	0
			1	1		
63	DT	1	Total	O	0	0
			1	1		
63	DY	1	Total	O	0	0
			1	1		
63	DZ	2	Total	O	0	0
			2	2		



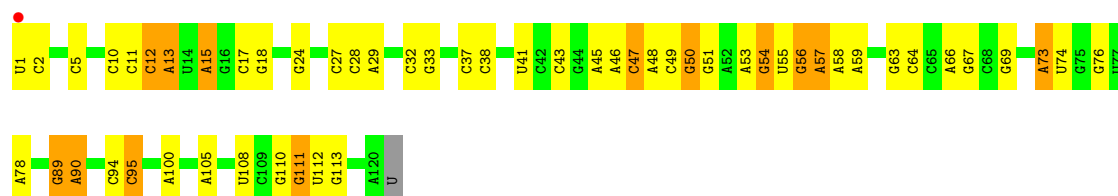




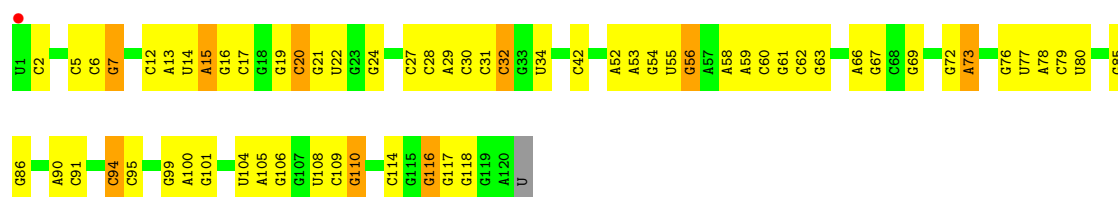
A2713	C2538	G2633	C2539	A2451	G2365	C2293	A2198	A2135	A2060	C1967	G1858	A1783	U1680	C1577
G2714	C2539	G2634	C2540	G2454	G2373	C2294	U2203	C2136	G2061	G1968	A1859	A1784	G1680	U1578
G2717	A2542	U2635	A2543	G2455	G2379	C2295	C2205	C2137	A2062	G1860	A1785	G1681	C1682	A1580
G2718	G2544	U2636	G2545	U2457	G2380	G2299	G2206	C2142	C2064	C1866	A1876	C1790	C1685	A1583
G2719	G2544	G2642	G2544	U2458	G2381	G2299	A2208	U2144	G2070	A1877	A1877	G1791	C1686	C1584
U2720	U2554	G2643	U2555	U2460	G2382	G2304	U2218	C2145	A2071	C1877	A1877	G1792	C1687	A1586
A2721	U2555	G2643	U2556	C2461	G2383	G2304	A2225	G2147	U2075	C1882	A1882	G1793	U1688	A1587
G2722	G2557	G2646	G2558	G2465	G2384	G2305	G2228	C2148	U2076	C1883	A1883	G1794	C1689	C1588
C2723	G2557	U2647	G2558	G2466	G2385	G2306	G2229	G2149	U2077	C1886	A1886	U1693	A1689	C1589
A2725	C2558	U2649	U2559	G2468	G2386	G2307	G2230	U2150	U2078	C1887	A1887	U1694	U1590	
U2726	U2562	U2649	U2562	A2469	A2388	A2309	G2231	G2151	G2080	C1888	A1888	U1695	G1696	G1595
G2727	U2563	U2652	U2564	G2470	G2389	A2310	U2233	G2152	G2081	C1889	A1889	G1799	G1697	C1607
U2728	A2564	U2653	U2565	G2471	G2390	A2311	G2234	G2153	A2082	C1890	A1890	U1700	C1608	C1607
G2729	A2565	U2654	U2566	G2472	G2391	U2312	U2244	G2154	U2098	C1891	A1891	G1701	A1609	A1609
C2730	A2566	G2655	U2567	G2473	G2392	G2315	G2238	G2155	U2099	C2006	A1900	G1702	C1612	C1612
G2731	A2567	G2656	U2568	G2474	G2393	G2316	G2239	G2156	G2094	C2007	A1901	G1703	G1613	G1613
G2732	G2568	G2657	U2569	G2475	G2394	G2317	G2240	G2157	G2095	C2008	A1902	G1704	A1614	A1614
A2733	U2659	G2658	U2570	G2476	G2395	G2318	G2241	G2158	U2096	G2009	A1903	G1705	C1617	C1617
A2734	G2661	G2659	U2571	G2477	G2396	G2319	U2242	G2159	G2097	C2010	A1904	C1708	A1618	A1618
G2735	A2662	G2660	U2572	G2478	G2397	G2320	U2243	G2160	A2013	C2011	A1905	U1709	G1626	G1626
U2744	G2663	G2661	U2573	G2479	G2398	G2321	U2244	G2161	U2098	C2012	A1906	G1710	G1627	G1627
G2745	G2663	G2662	U2574	G2480	G2399	G2322	U2245	G2162	U2099	C2013	A1907	C1711	C1712	C1712
U2746	G2663	G2663	U2575	G2481	G2400	G2323	U2246	G2163	U2099	C2014	A1908	C1712	C1713	C1713
U2747	G2663	G2663	U2576	G2482	G2401	G2324	U2247	G2164	U2099	C2015	A1909	C1713	C1714	C1714
U2748	G2663	G2663	U2577	G2483	G2402	G2325	U2248	G2165	U2099	C2016	A1910	C1714	C1715	C1715
A2749	G2663	G2663	U2578	G2484	G2403	G2326	U2249	G2166	U2099	C2017	A1911	C1715	C1716	C1716
U2750	G2663	G2663	U2579	G2485	G2404	G2327	U2250	G2167	U2099	C2018	A1912	C1716	C1717	C1717
G2751	G2663	G2663	U2580	G2486	G2405	G2328	U2251	G2168	U2099	C2019	A1913	C1717	C1718	C1718
U2752	G2663	G2663	U2581	G2487	G2406	G2329	U2252	G2169	U2099	C2020	A1914	C1718	C1719	C1719
U2753	G2663	G2663	U2582	G2488	G2407	G2330	U2253	G2170	U2099	C2021	A1915	C1719	C1720	C1720
U2754	G2663	G2663	U2583	G2489	G2408	G2331	U2254	G2171	U2099	C2022	A1916	C1720	C1721	C1721
U2755	G2663	G2663	U2584	G2490	G2409	G2332	U2255	G2172	U2099	C2023	A1917	C1721	C1722	C1722
U2756	G2663	G2663	U2585	G2491	G2410	G2333	U2256	G2173	U2099	C2024	A1918	C1722	C1723	C1723
U2757	G2663	G2663	U2586	G2492	G2411	G2334	U2257	G2174	U2099	C2025	A1919	C1723	C1724	C1724
U2758	G2663	G2663	U2587	G2493	G2412	G2335	U2258	G2175	U2099	C2026	A1920	C1724	C1725	C1725
U2759	G2663	G2663	U2588	G2494	G2413	G2336	U2259	G2176	U2099	C2027	A1921	C1725	C1726	C1726
U2760	G2663	G2663	U2589	G2495	G2414	G2337	U2260	G2177	U2099	C2028	A1922	C1726	C1727	C1727
U2761	G2663	G2663	U2590	G2496	G2415	G2338	U2261	G2178	U2099	C2029	A1923	C1727	C1728	C1728
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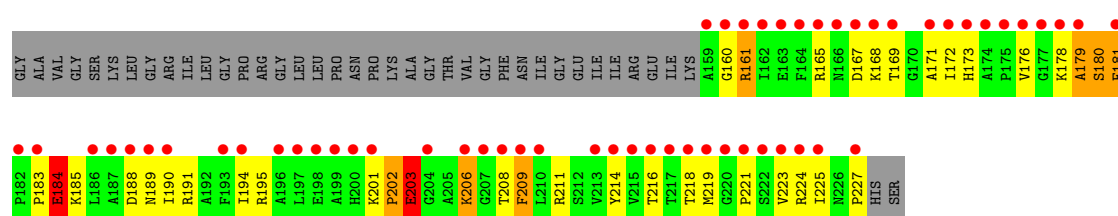
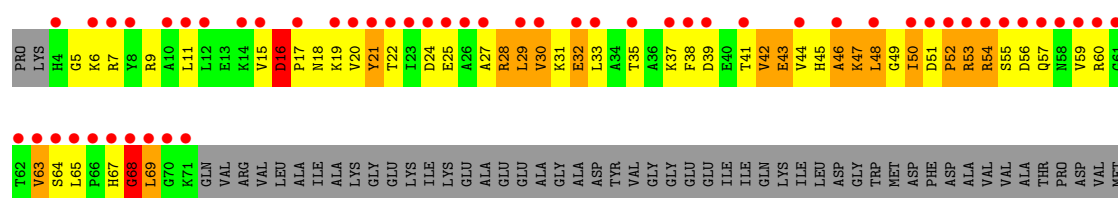
• Molecule 2: 5S Ribosomal RNA



• Molecule 2: 5S Ribosomal RNA

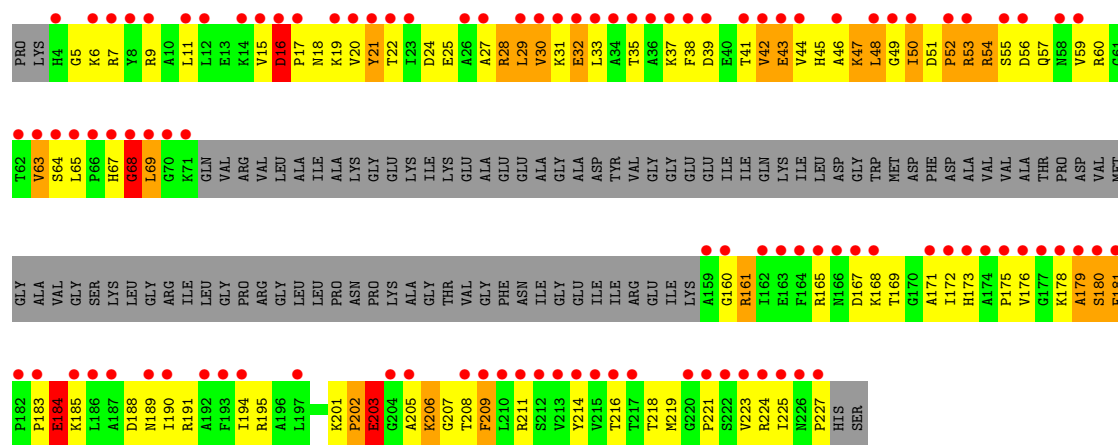


• Molecule 3: 50S ribosomal protein L1

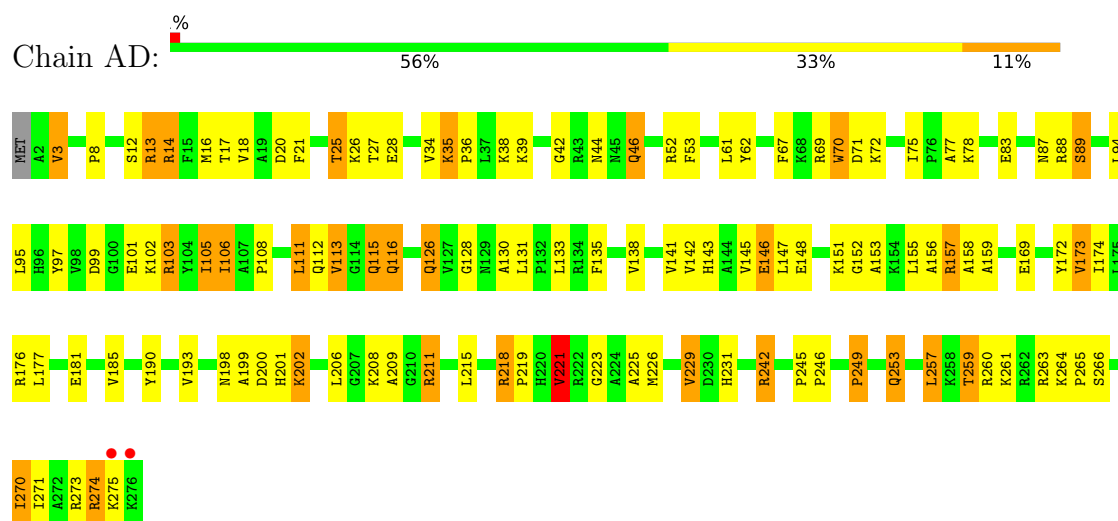


• Molecule 3: 50S ribosomal protein L1

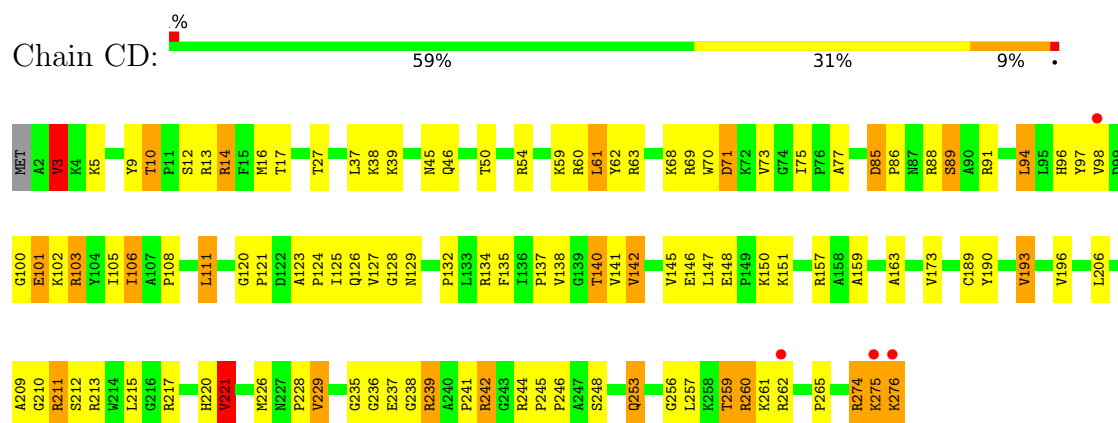




• Molecule 4: 50S ribosomal protein L2

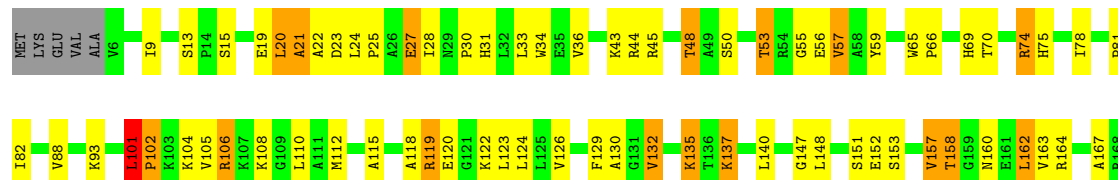


• Molecule 4: 50S ribosomal protein L2

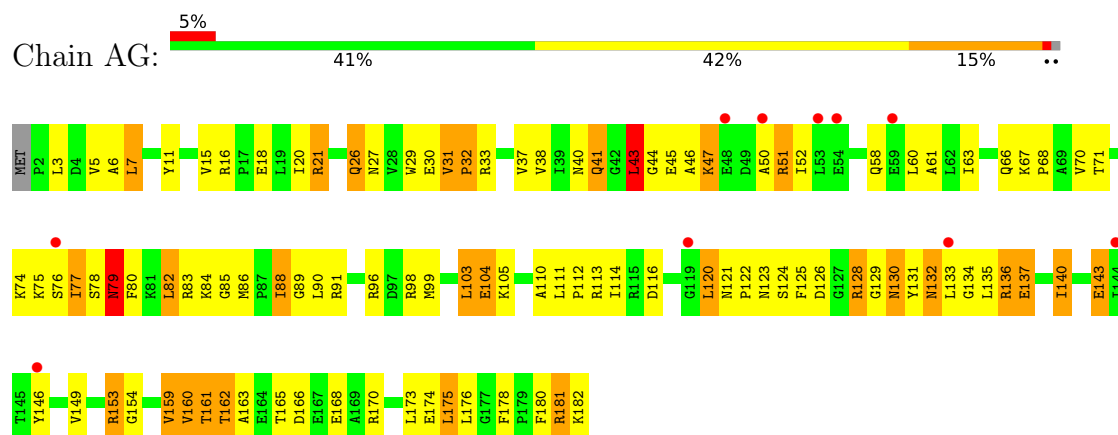


• Molecule 5: 50S ribosomal protein L3

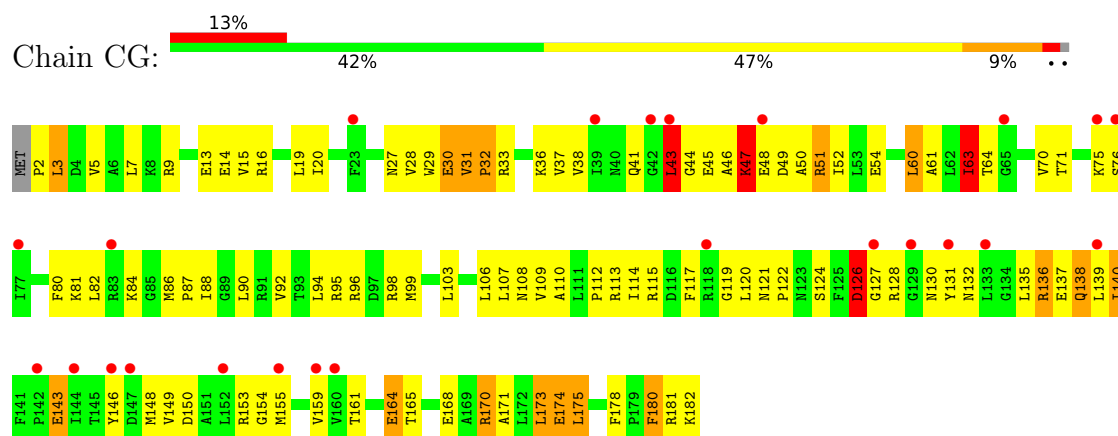




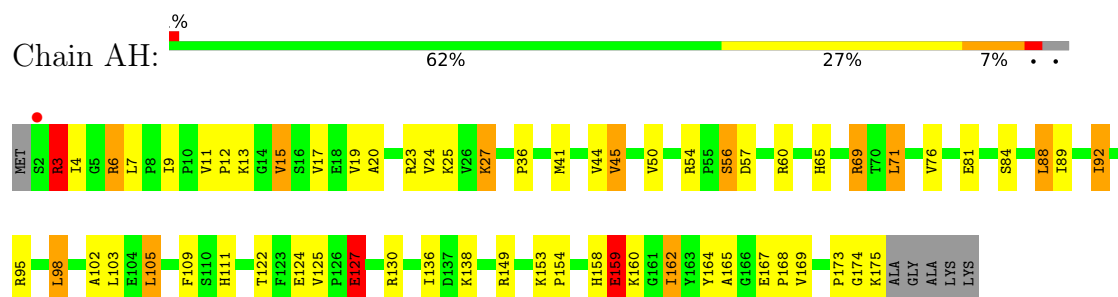
- Molecule 7: 50S ribosomal protein L5



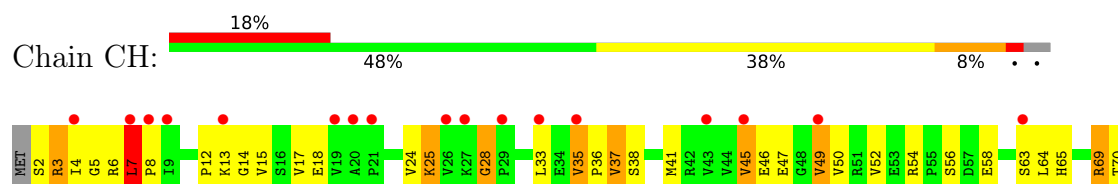
- Molecule 7: 50S ribosomal protein L5

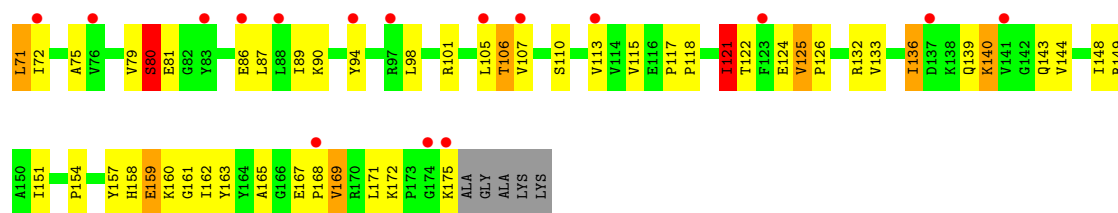


- Molecule 8: 50S ribosomal protein L6

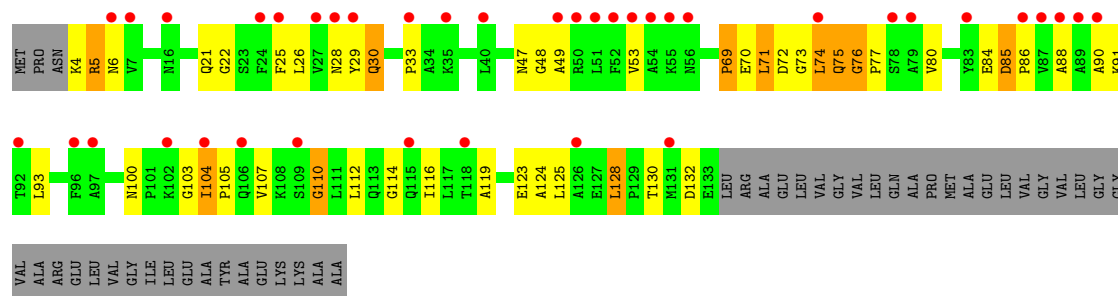


- Molecule 8: 50S ribosomal protein L6

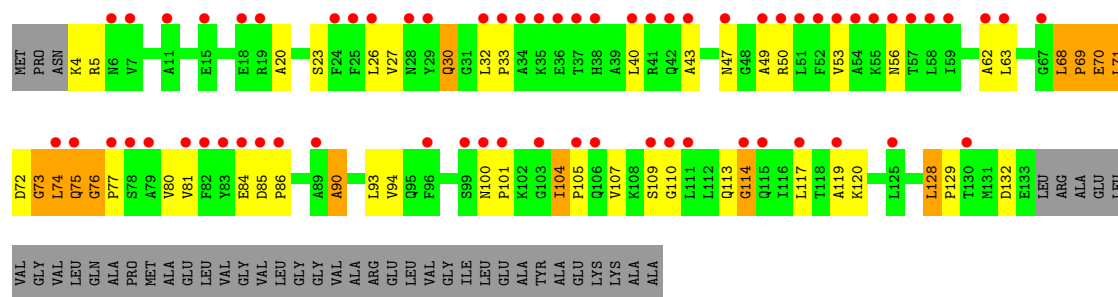
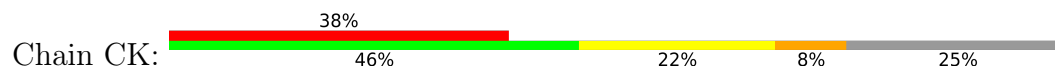




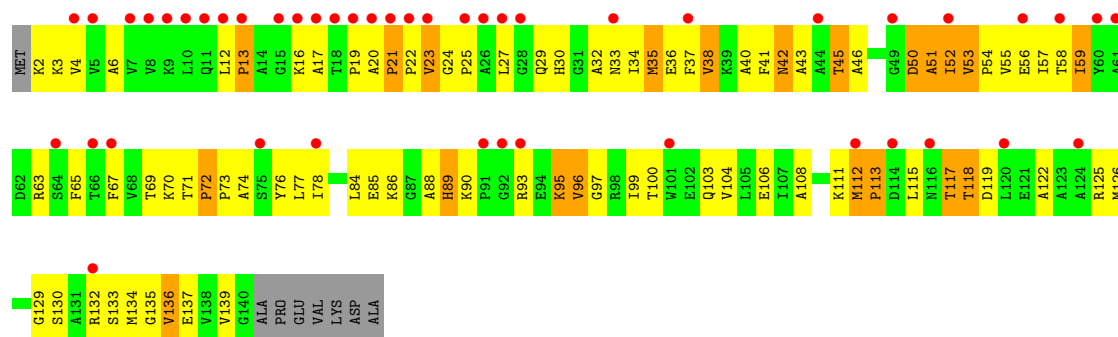
• Molecule 9: 50S ribosomal protein L10



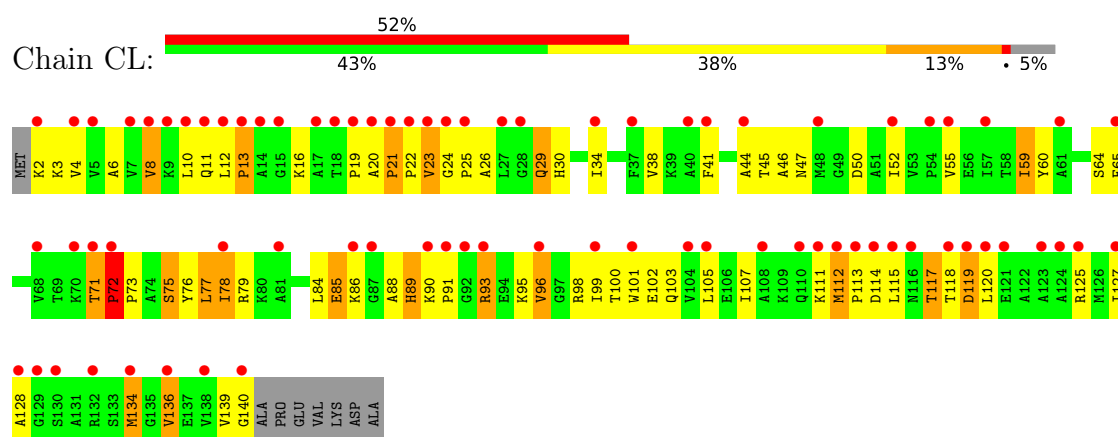
• Molecule 9: 50S ribosomal protein L10



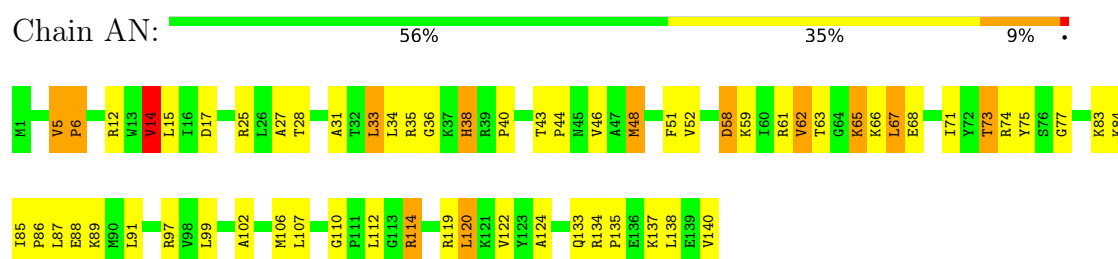
• Molecule 10: 50S ribosomal protein L11



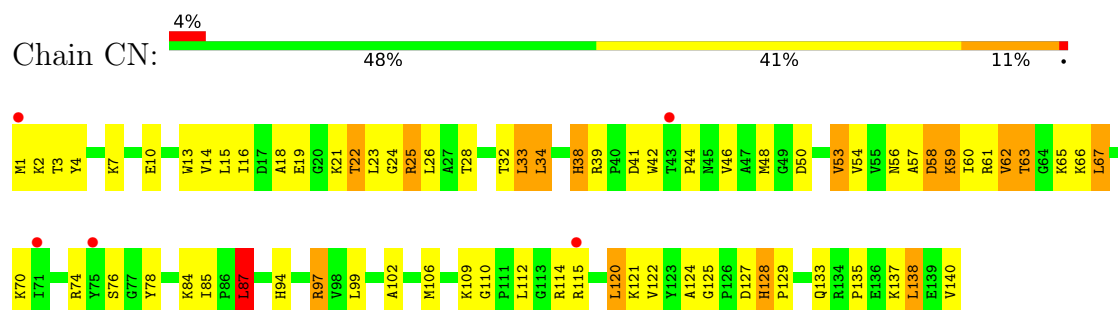
• Molecule 10: 50S ribosomal protein L11



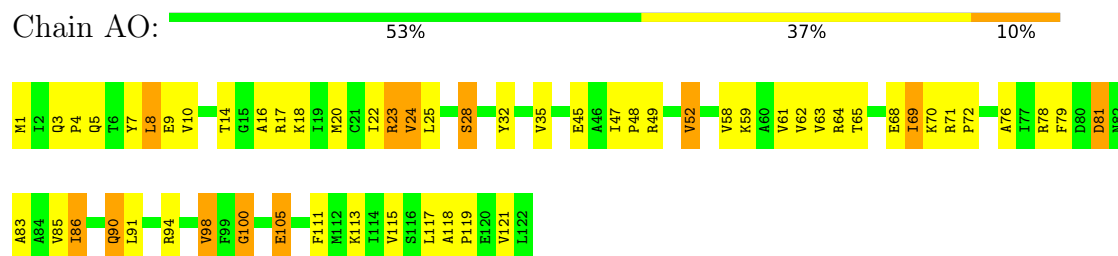
- Molecule 11: 50S ribosomal protein L13



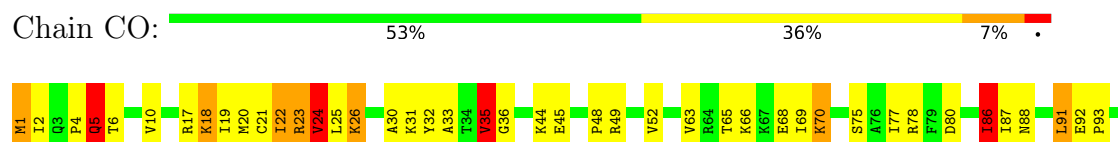
- Molecule 11: 50S ribosomal protein L13

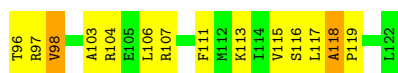


- Molecule 12: 50S ribosomal protein L14



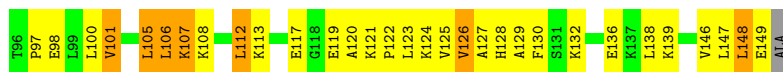
- Molecule 12: 50S ribosomal protein L14





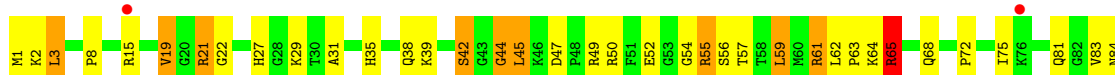
• Molecule 13: 50S ribosomal protein L15

Chain AP: 53% 35% 11% ..



• Molecule 13: 50S ribosomal protein L15

Chain CP: 3% 51% 37% 11% ..



• Molecule 14: 50S ribosomal protein L16

Chain AQ: 67% 27% 6%



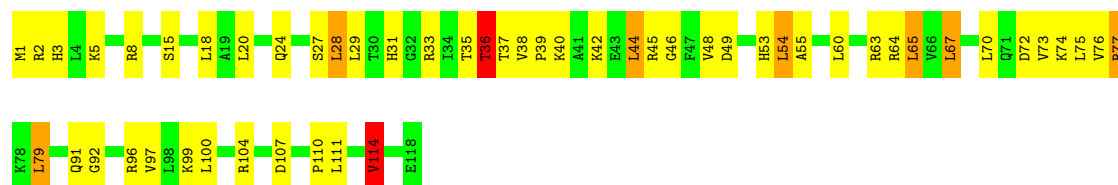
• Molecule 14: 50S ribosomal protein L16

Chain CQ: 5% 48% 39% 11%

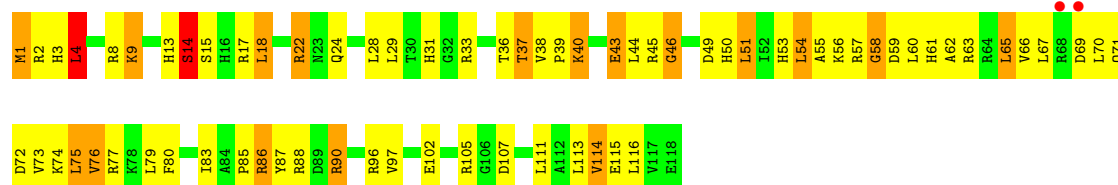
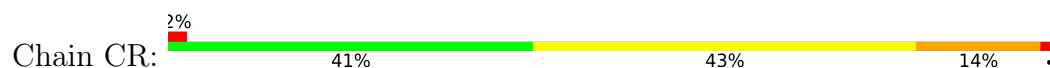


• Molecule 15: 50S ribosomal protein L17

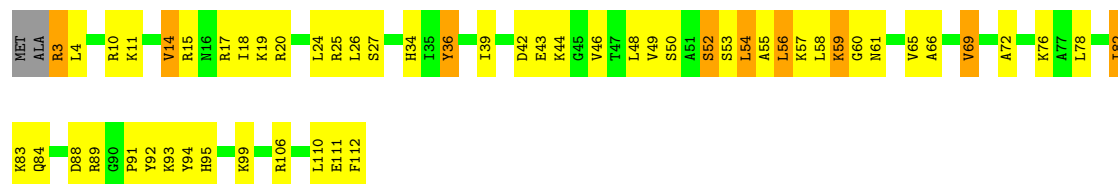
Chain AR: 55% 37% 6%



- Molecule 15: 50S ribosomal protein L17



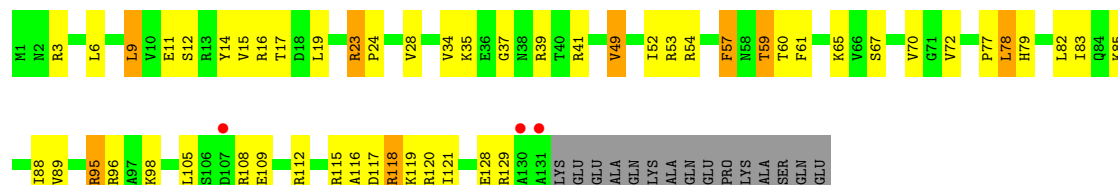
- Molecule 16: 50S ribosomal protein L18



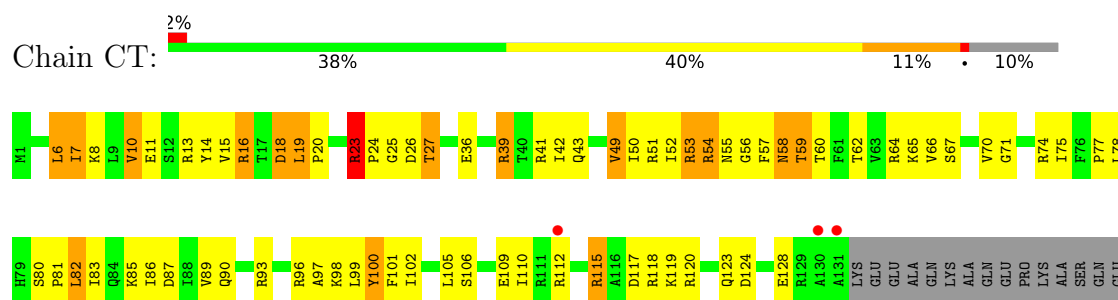
- Molecule 16: 50S ribosomal protein L18



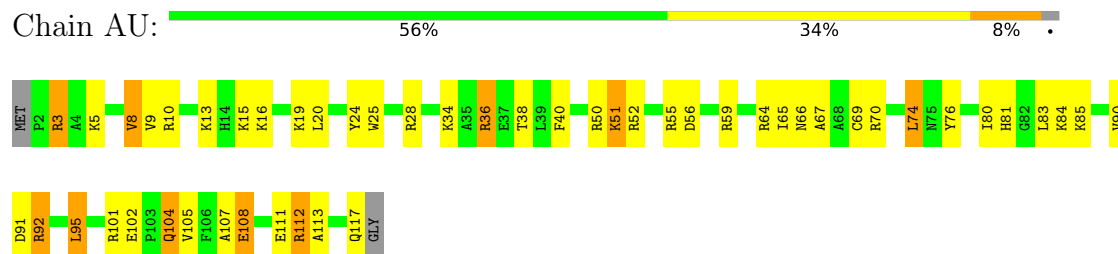
- Molecule 17: 50S ribosomal protein L19



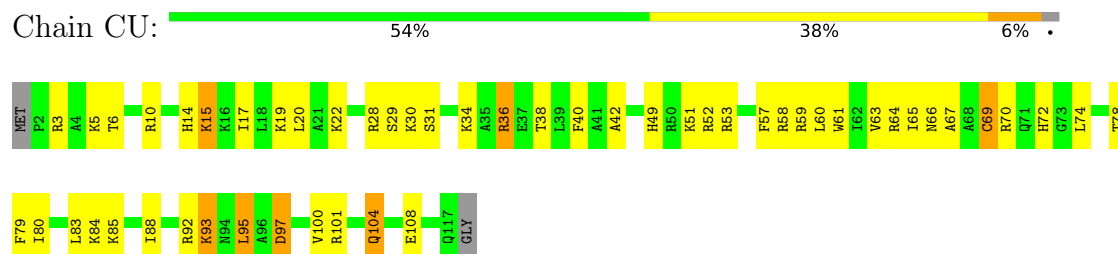
- Molecule 17: 50S ribosomal protein L19



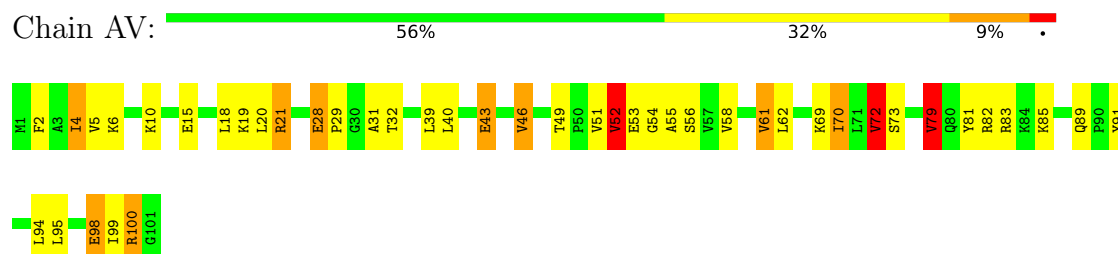
- Molecule 18: 50S ribosomal protein L20



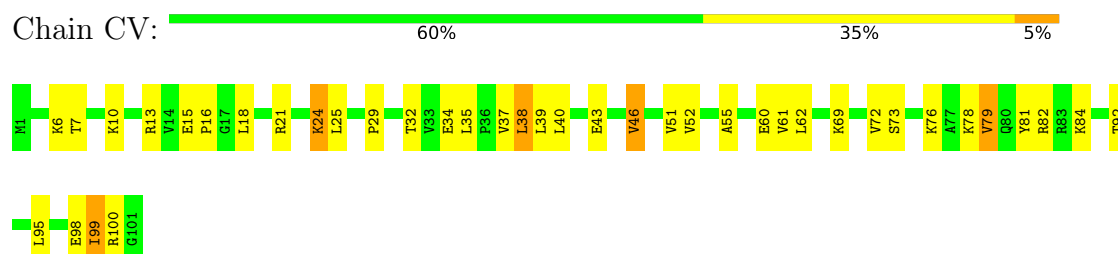
- Molecule 18: 50S ribosomal protein L20



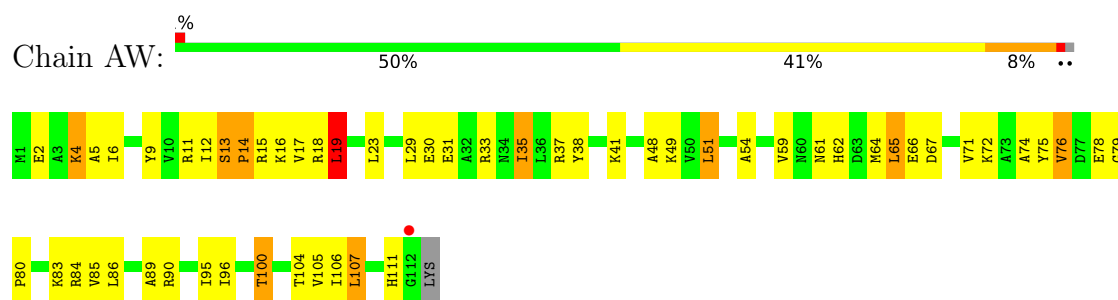
- Molecule 19: 50S ribosomal protein L21



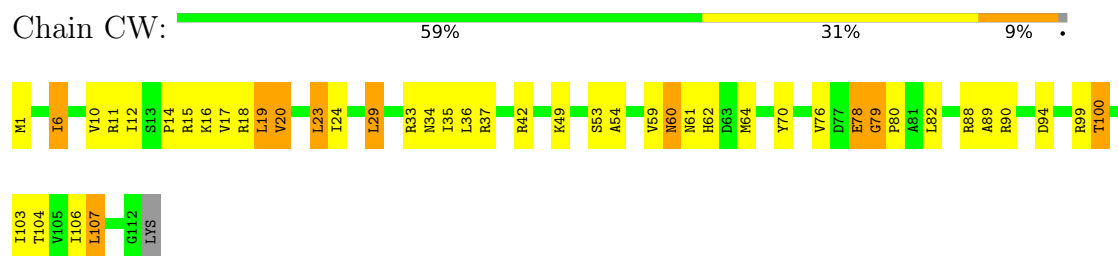
- Molecule 19: 50S ribosomal protein L21



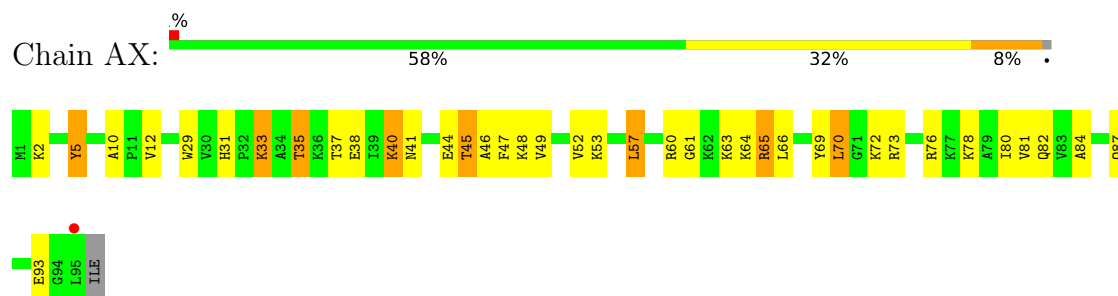
- Molecule 20: 50S ribosomal protein L22



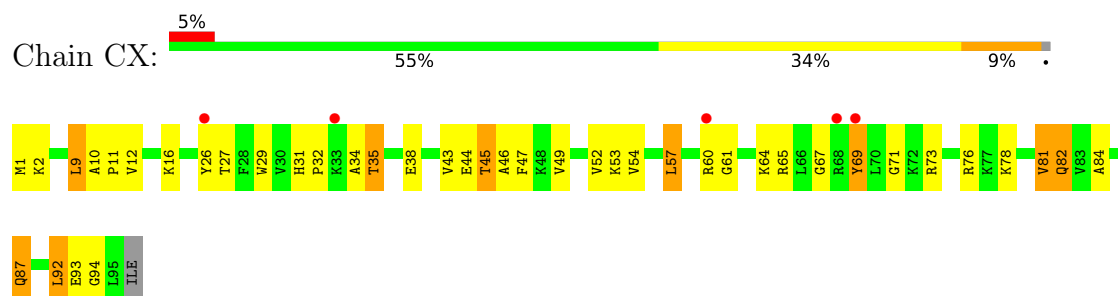
- Molecule 20: 50S ribosomal protein L22



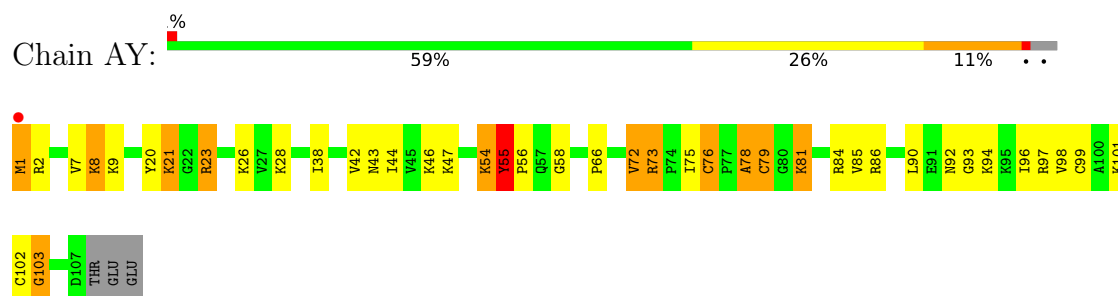
- Molecule 21: 50S ribosomal protein L23



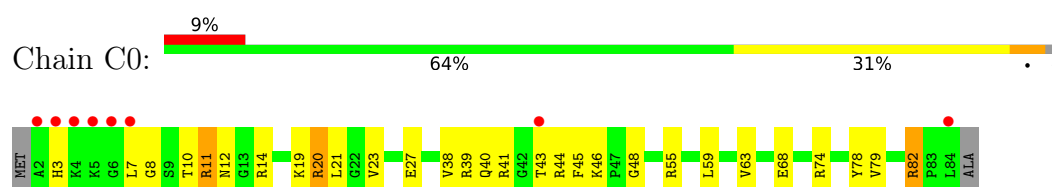
- Molecule 21: 50S ribosomal protein L23



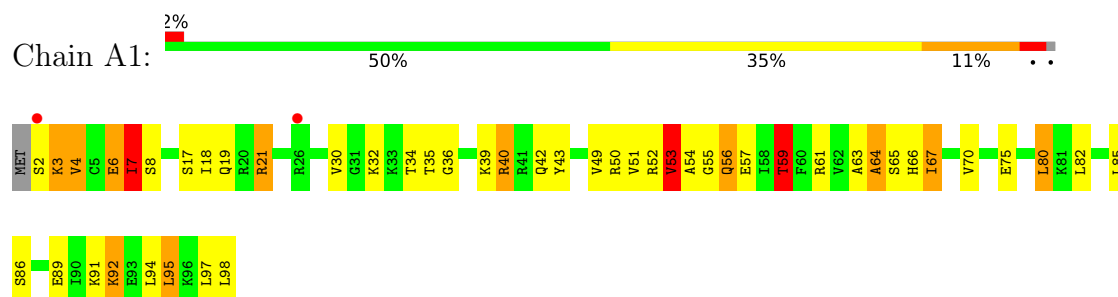
- Molecule 22: 50S ribosomal protein L24



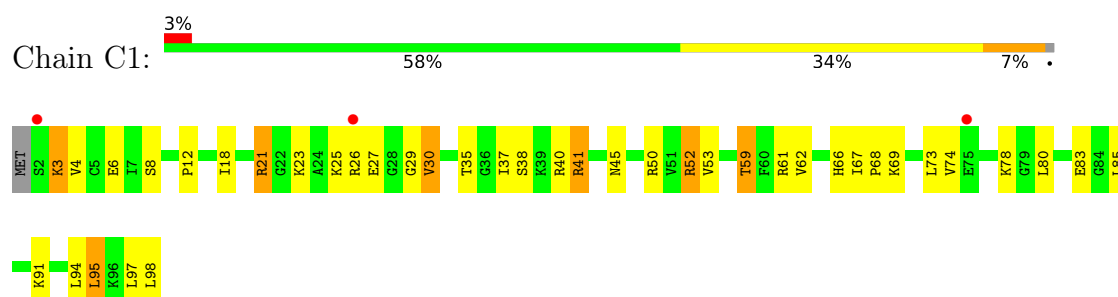
- Molecule 24: 50S ribosomal protein L27



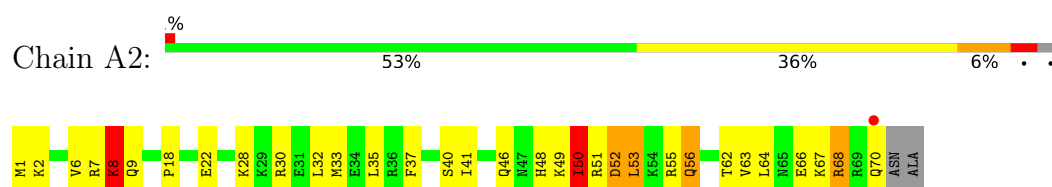
- Molecule 25: 50S ribosomal protein L28



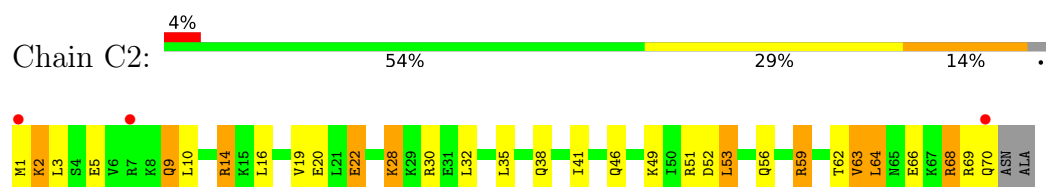
- Molecule 25: 50S ribosomal protein L28



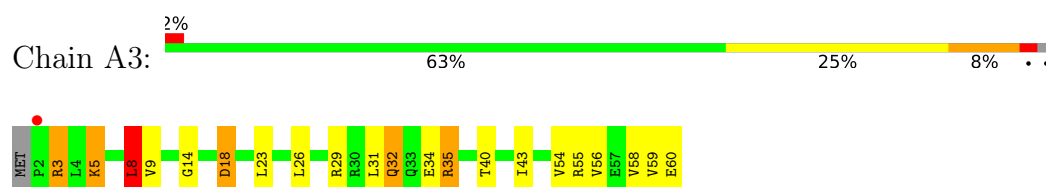
- Molecule 26: 50S ribosomal protein L29



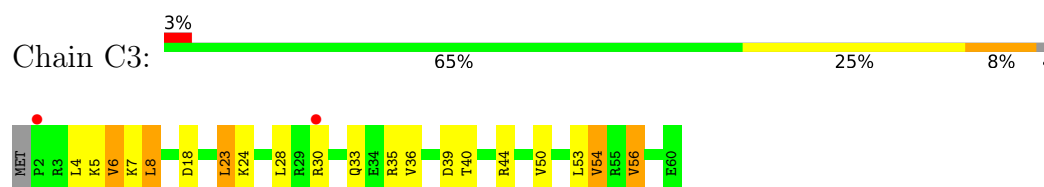
- Molecule 26: 50S ribosomal protein L29



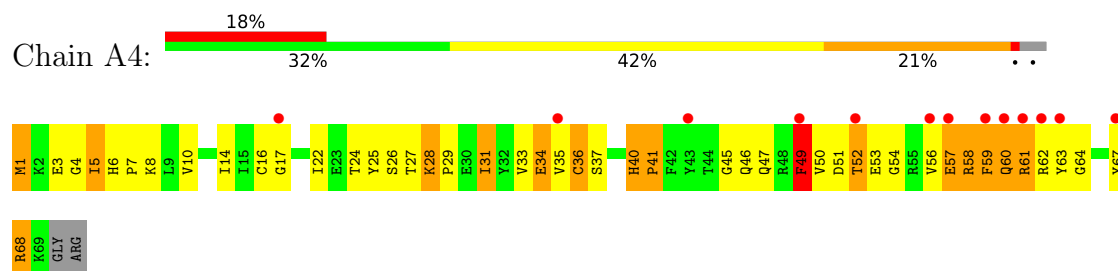
- Molecule 27: 50S ribosomal protein L30



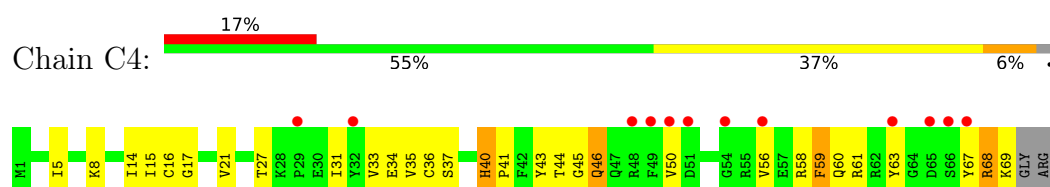
- Molecule 27: 50S ribosomal protein L30



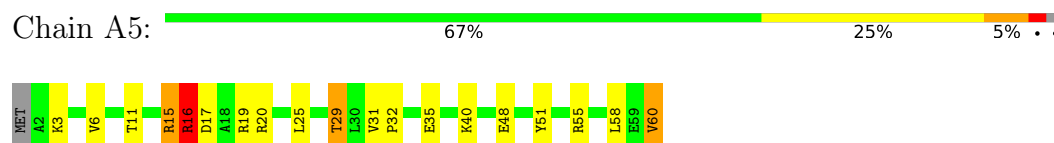
- Molecule 28: 50S ribosomal protein L31



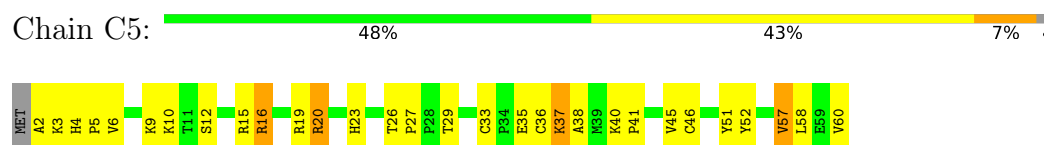
- Molecule 28: 50S ribosomal protein L31



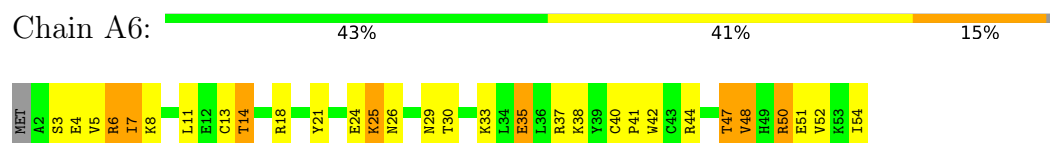
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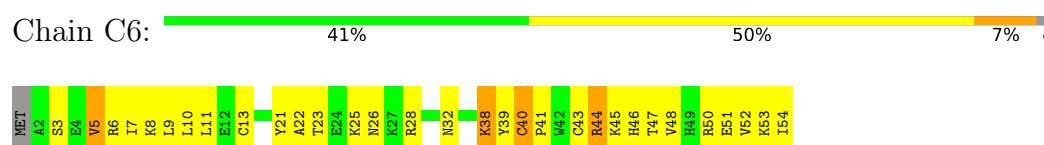
- Molecule 29: 50S ribosomal protein L32



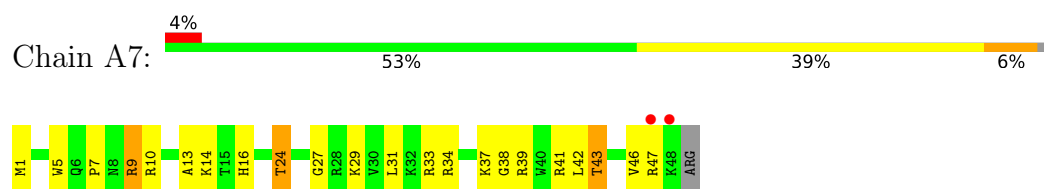
- Molecule 30: 50S ribosomal protein L33



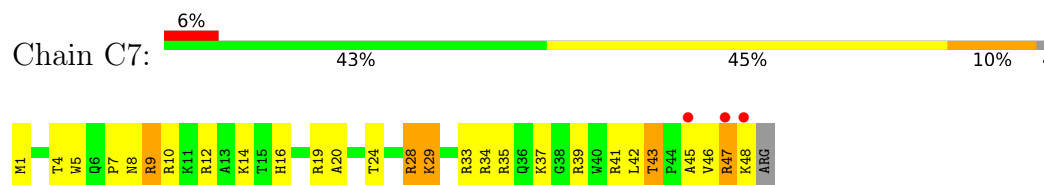
- Molecule 30: 50S ribosomal protein L33



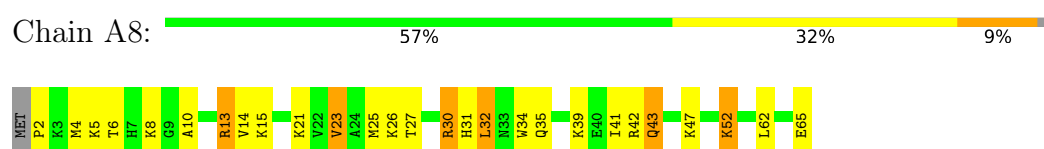
- Molecule 31: 50S ribosomal protein L34



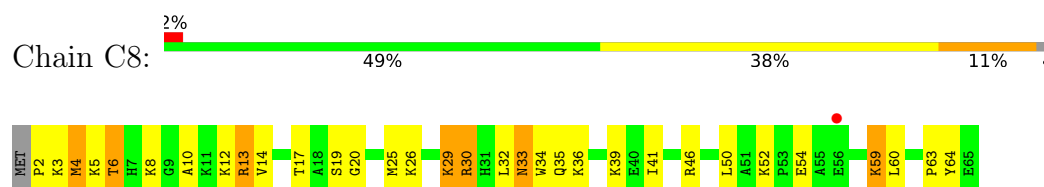
- Molecule 31: 50S ribosomal protein L34



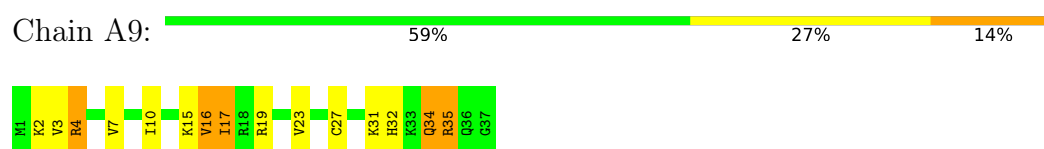
- Molecule 32: 50S ribosomal protein L35



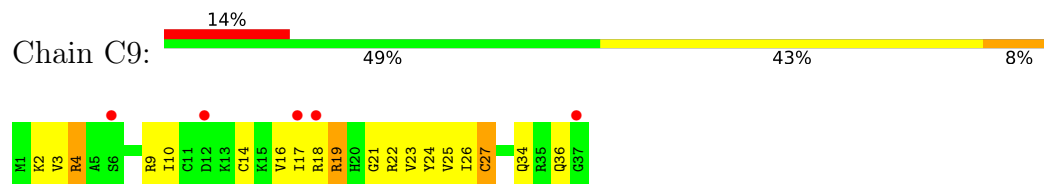
- Molecule 32: 50S ribosomal protein L35



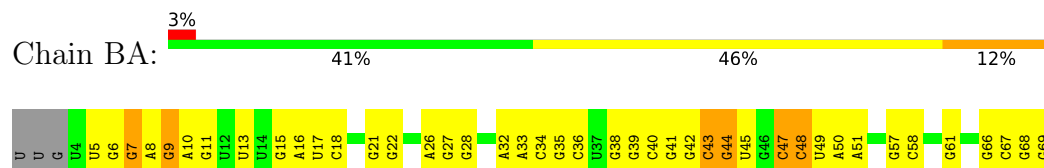
- Molecule 33: 50S ribosomal protein L36

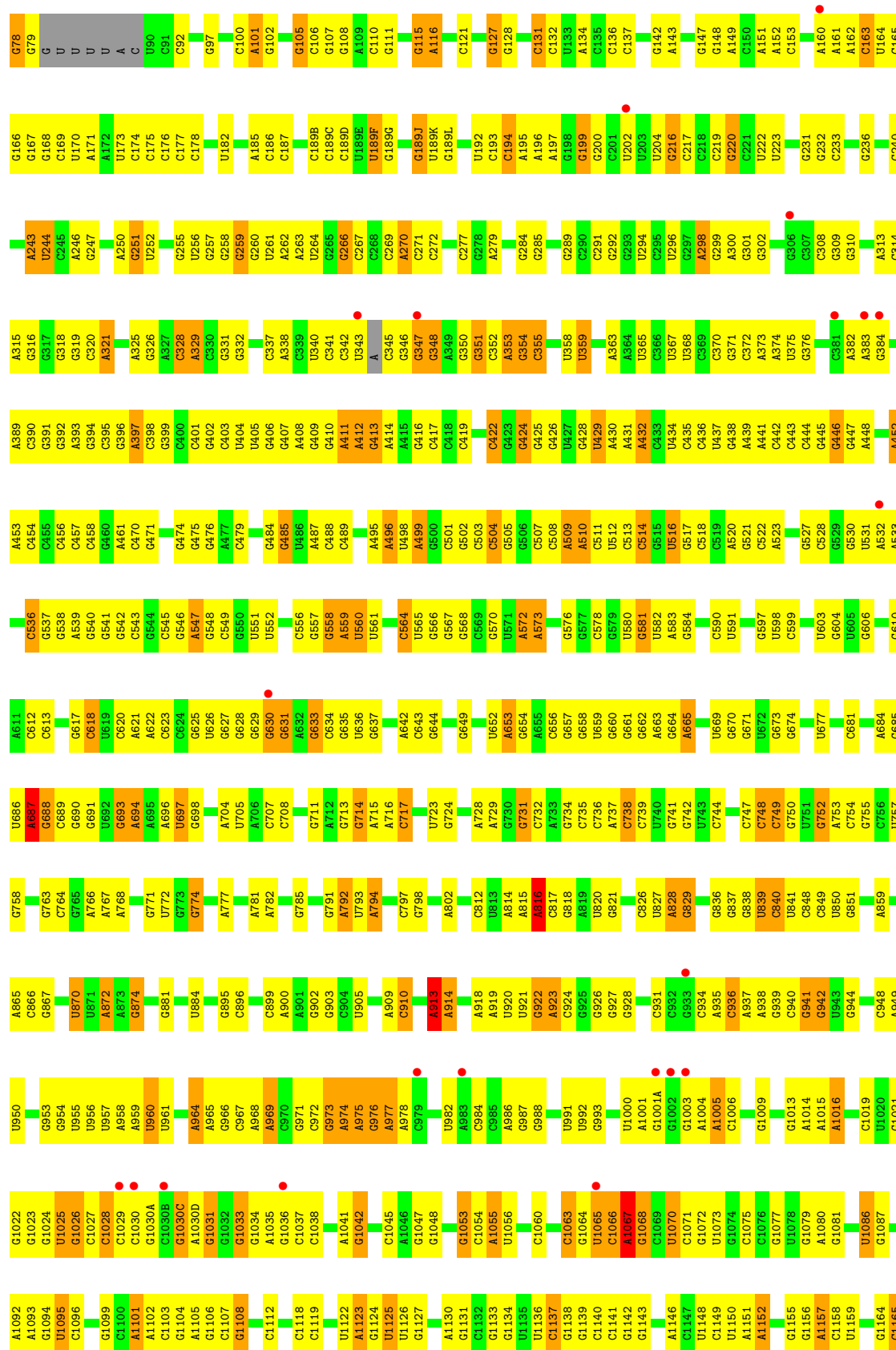


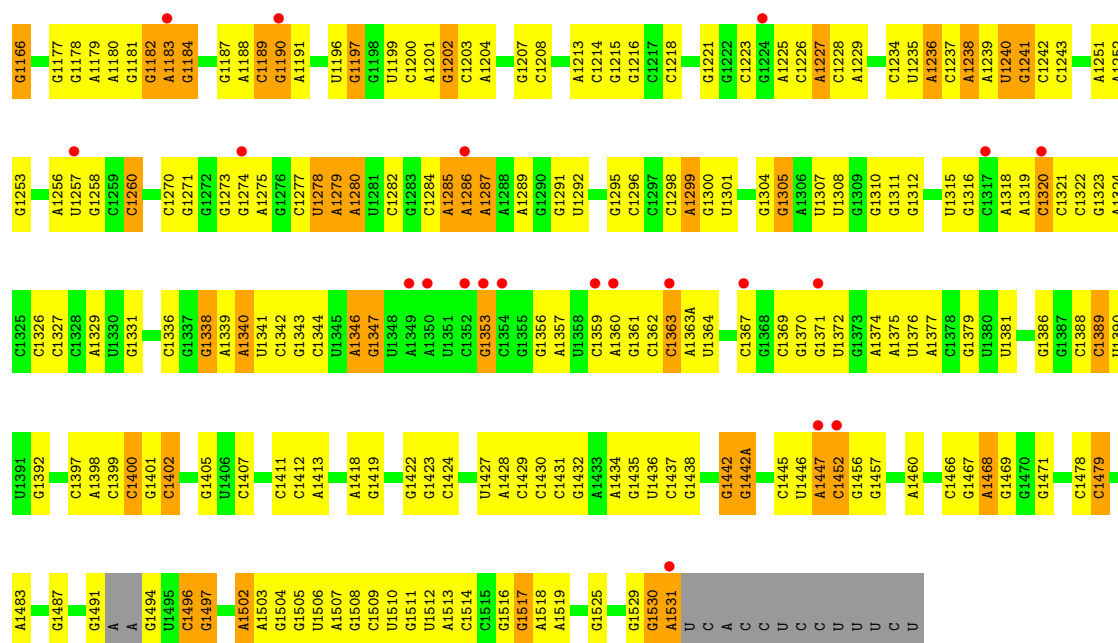
- Molecule 33: 50S ribosomal protein L36



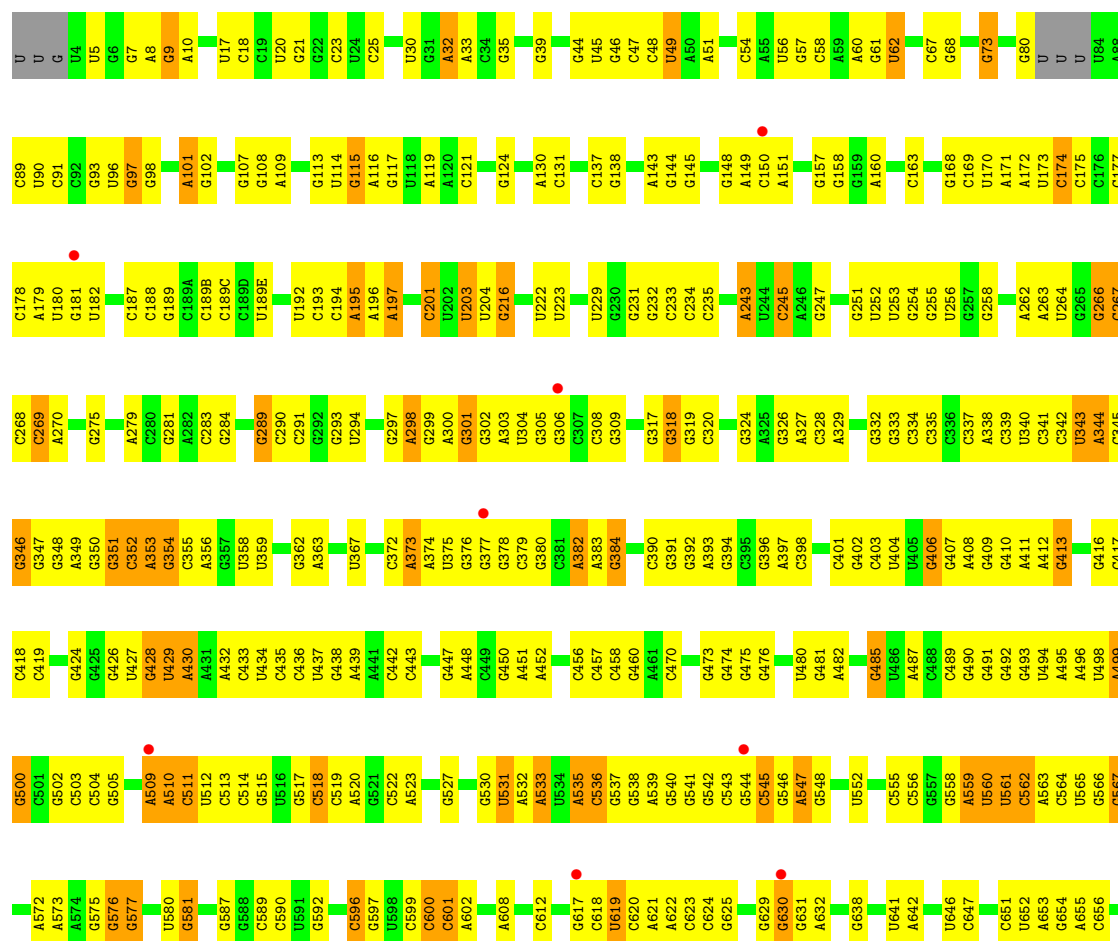
- Molecule 34: 16S Ribosomal RNA

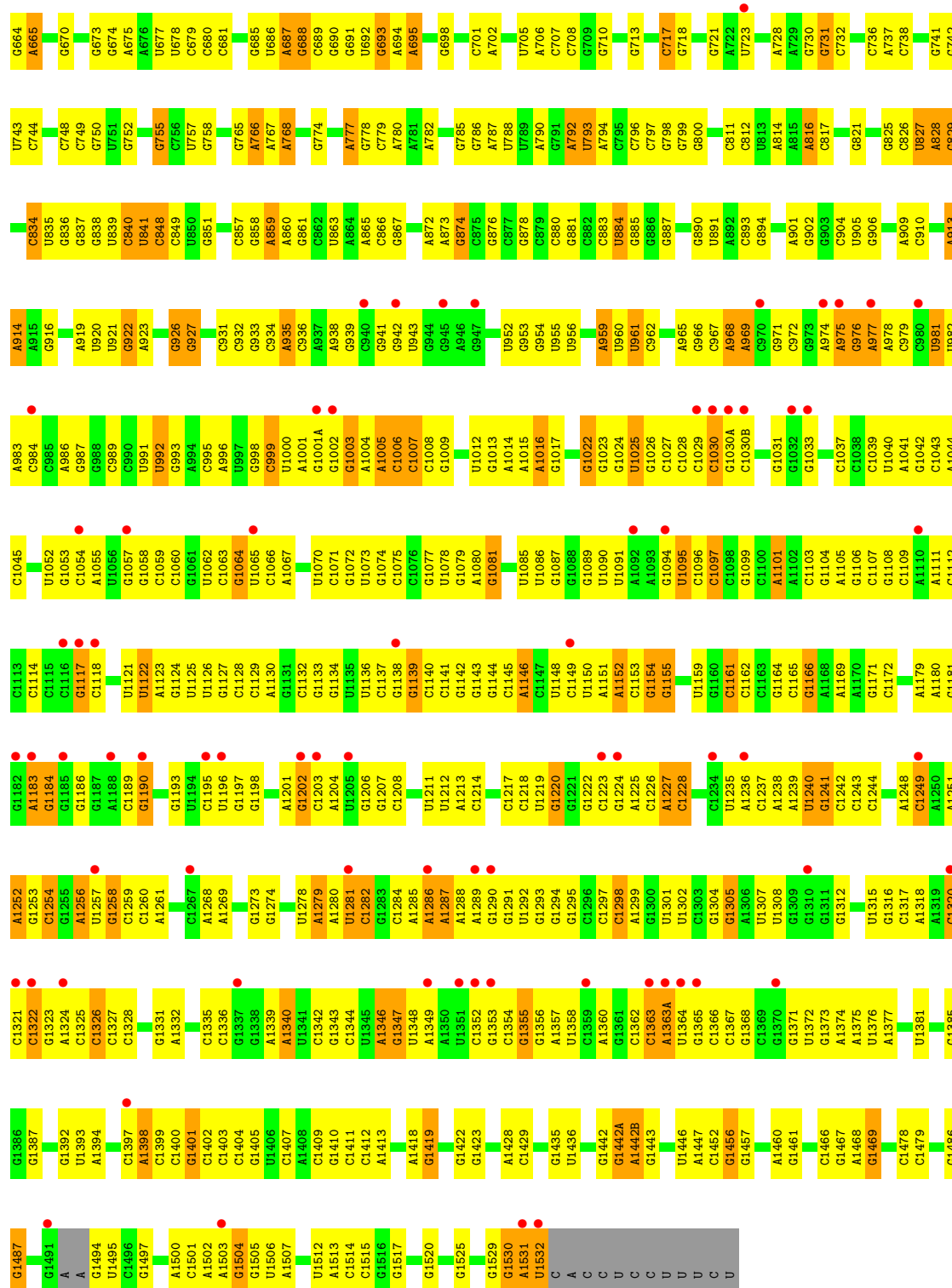


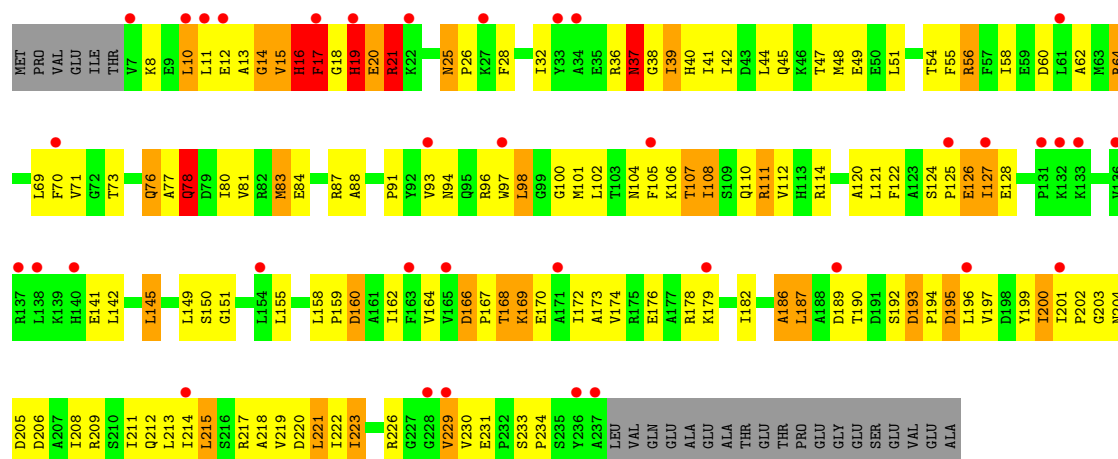




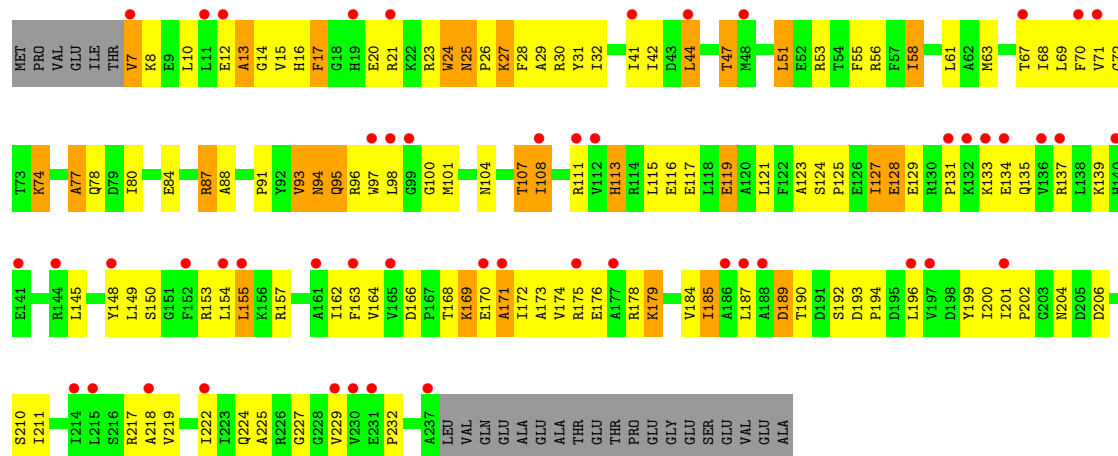
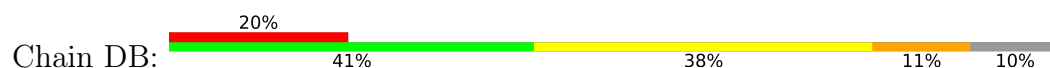
• Molecule 34: 16S Ribosomal RNA



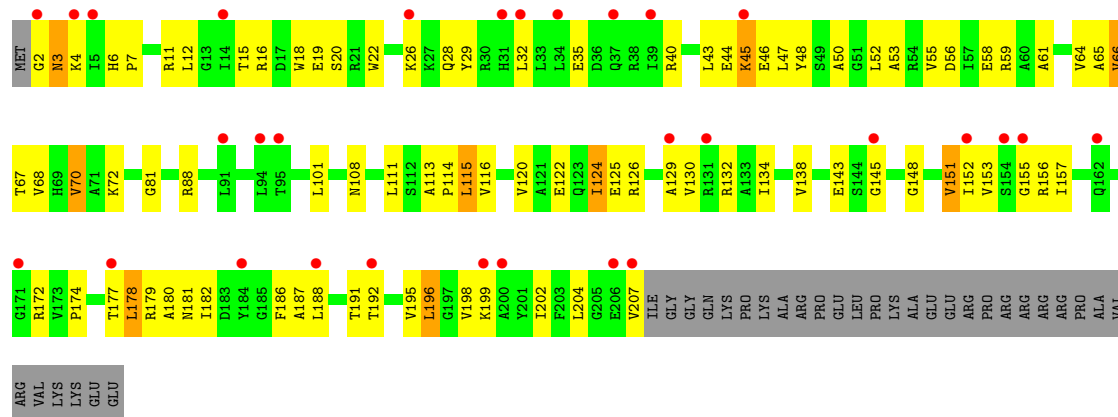




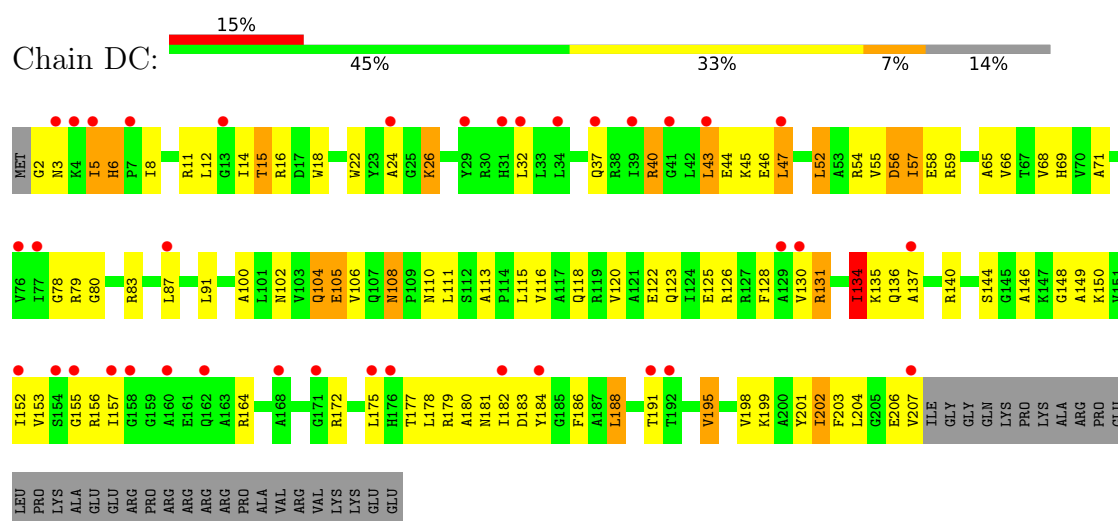
• Molecule 35: 30S ribosomal protein S2



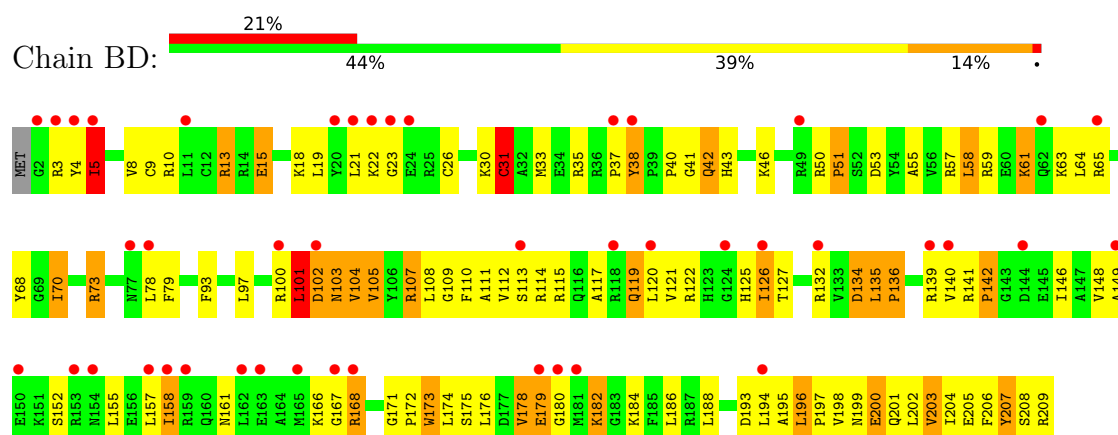
• Molecule 36: 30S ribosomal protein S3



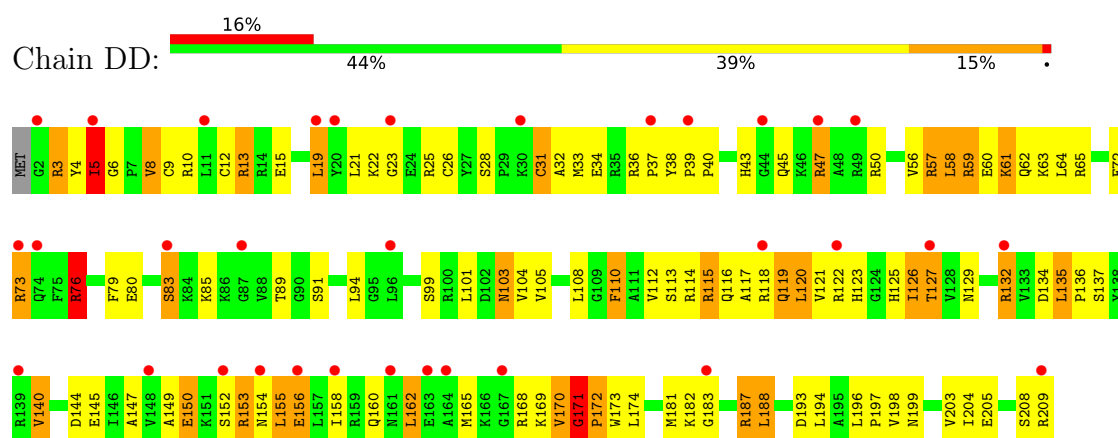
• Molecule 36: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S4



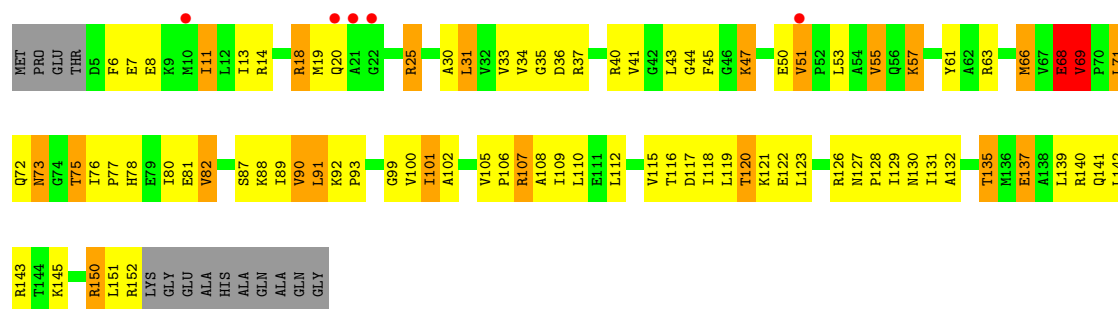
• Molecule 37: 30S ribosomal protein S4



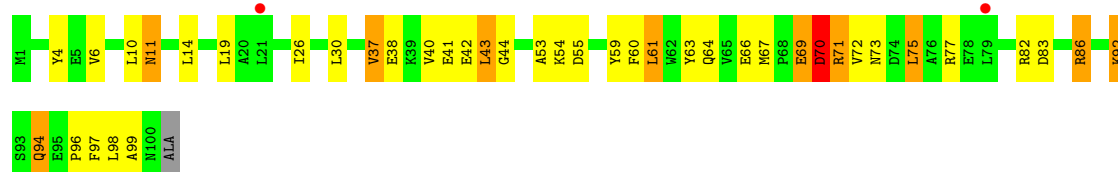
• Molecule 38: 30S ribosomal protein S5



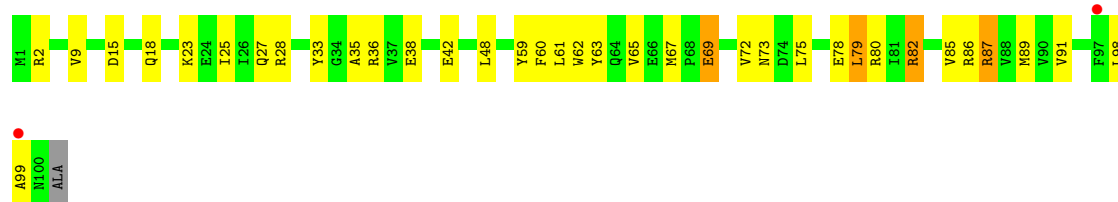
- Molecule 38: 30S ribosomal protein S5



- Molecule 39: 30S ribosomal protein S6

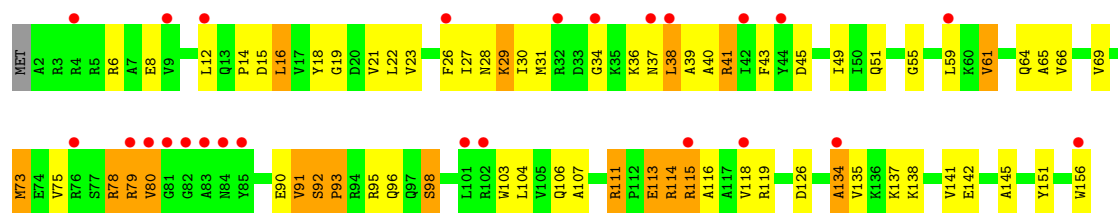


- Molecule 39: 30S ribosomal protein S6

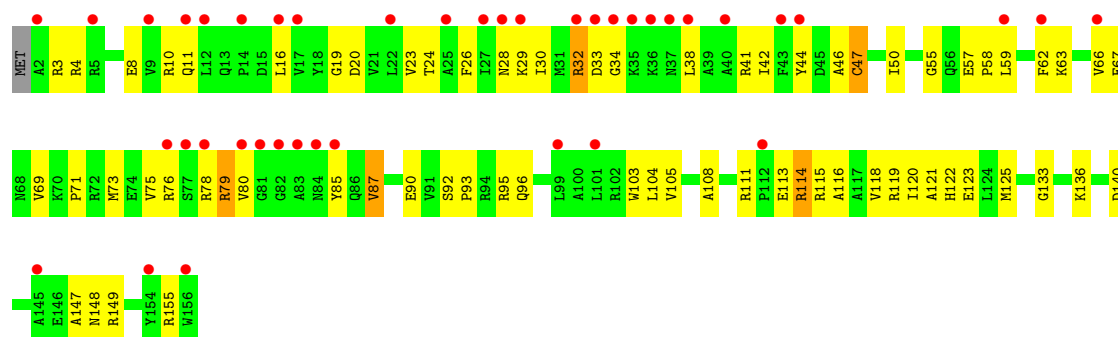


- Molecule 40: 30S ribosomal protein S7

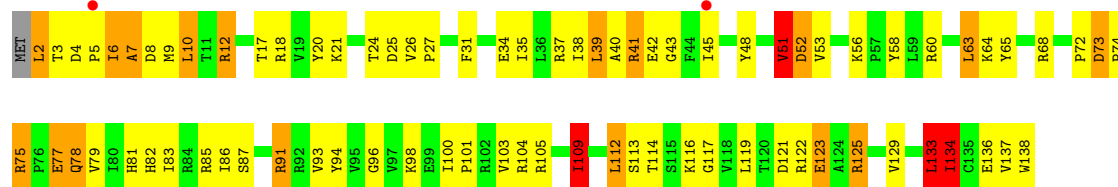




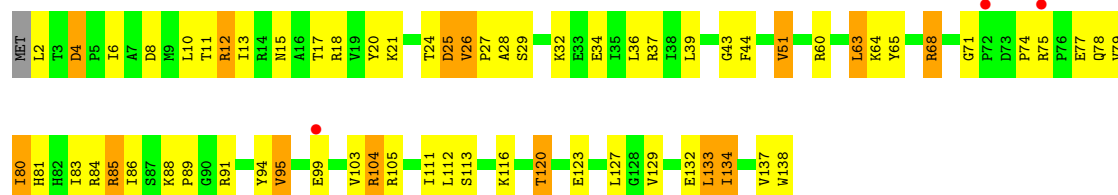
• Molecule 40: 30S ribosomal protein S7



• Molecule 41: 30S ribosomal protein S8

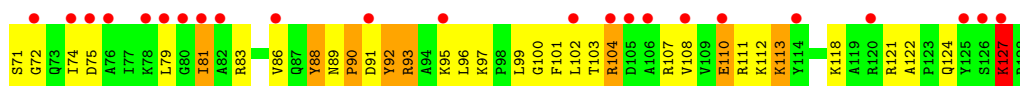


• Molecule 41: 30S ribosomal protein S8

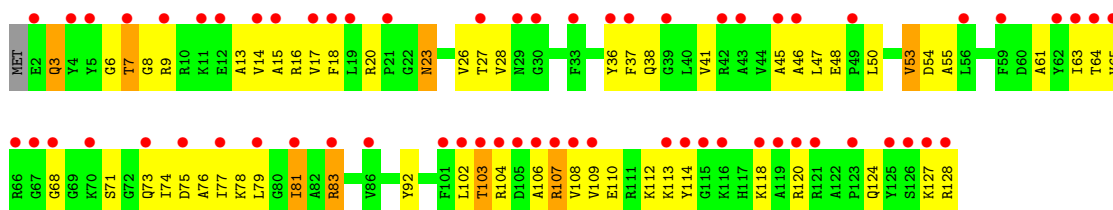


• Molecule 42: 30S ribosomal protein S9

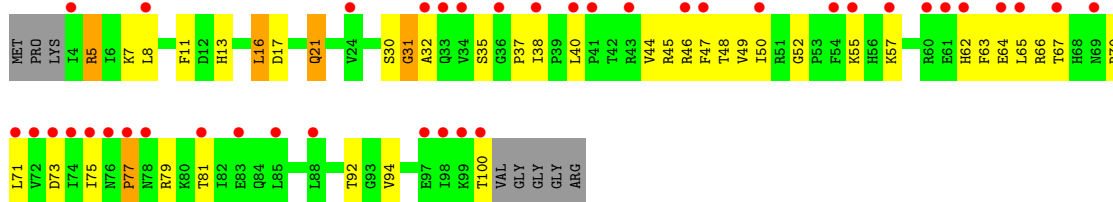
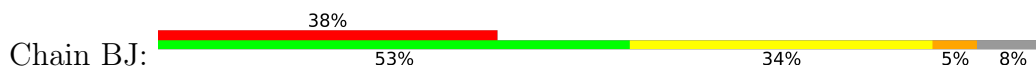




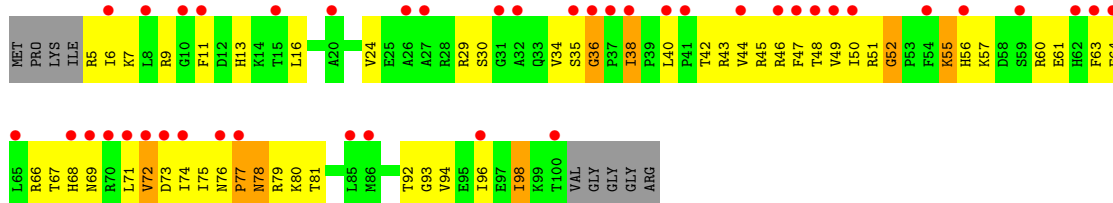
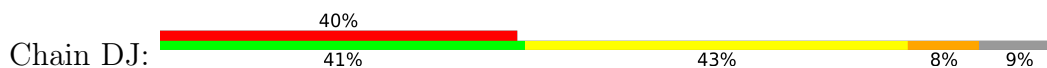
• Molecule 42: 30S ribosomal protein S9



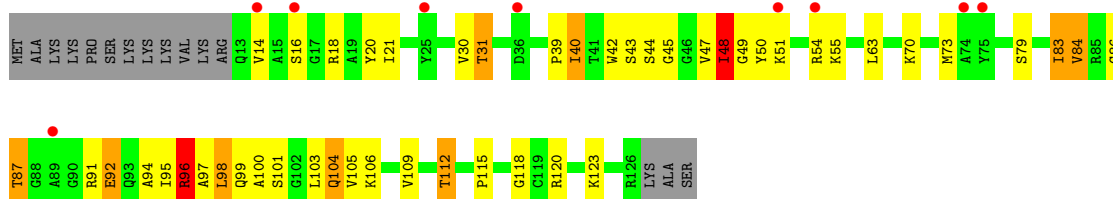
• Molecule 43: 30S ribosomal protein S10



• Molecule 43: 30S ribosomal protein S10

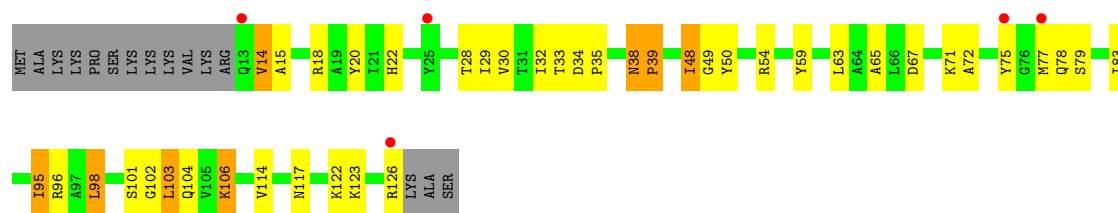


• Molecule 44: 30S ribosomal protein S11

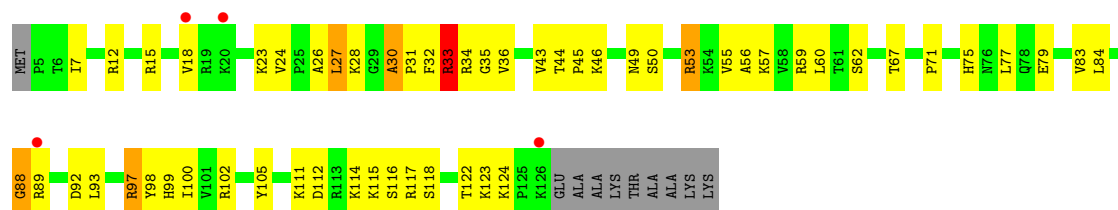


• Molecule 44: 30S ribosomal protein S11

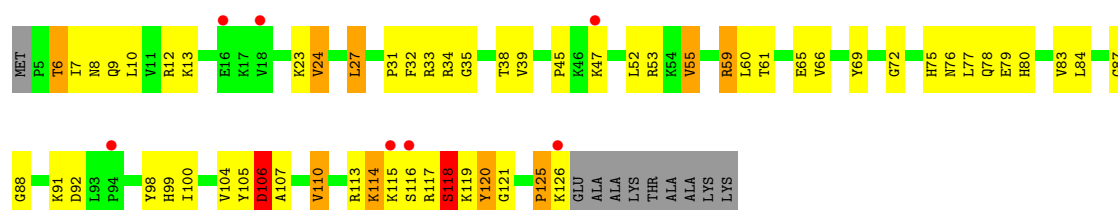




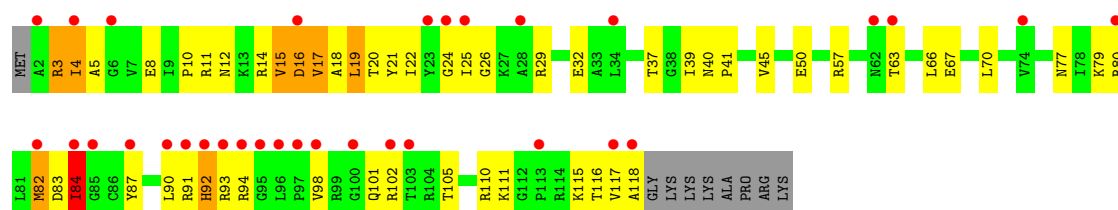
- Molecule 45: 30S ribosomal protein S12



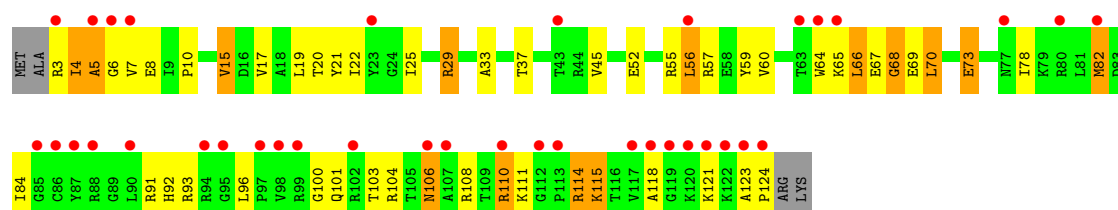
- Molecule 45: 30S ribosomal protein S12



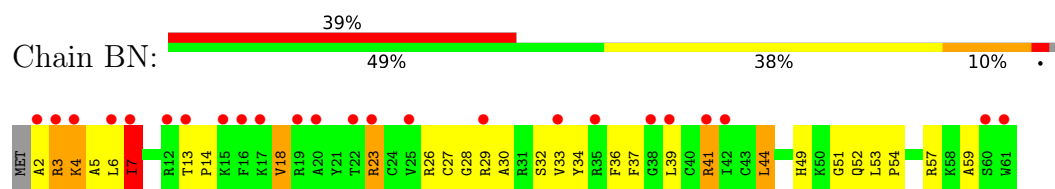
- Molecule 46: 30S ribosomal protein S13



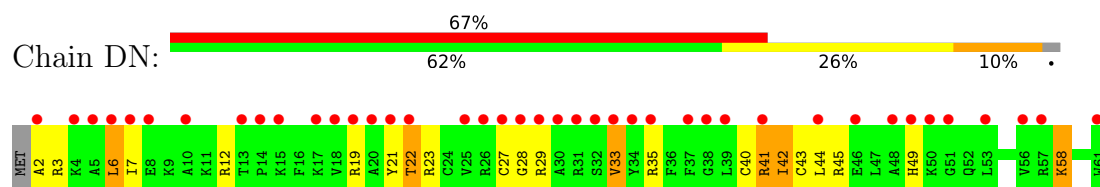
- Molecule 46: 30S ribosomal protein S13



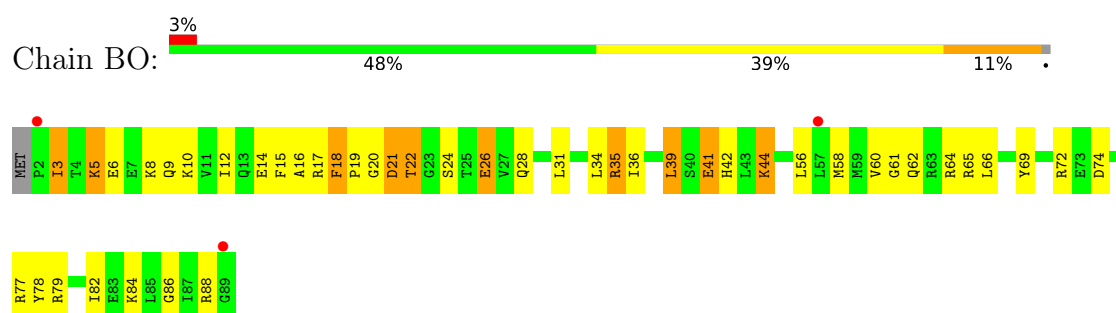
• Molecule 47: 30S ribosomal protein S14 type Z



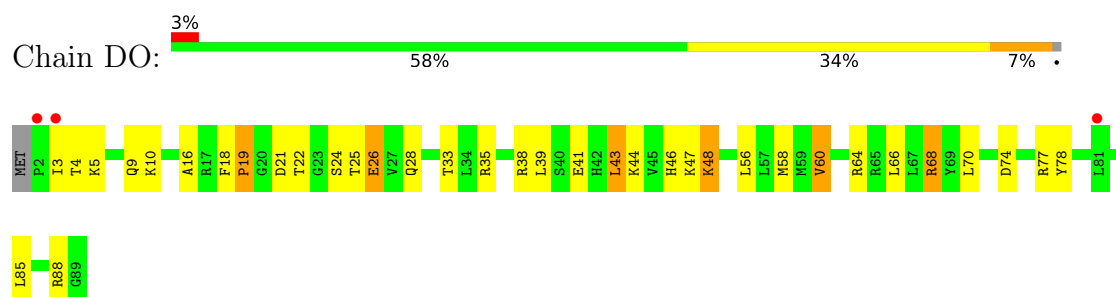
• Molecule 47: 30S ribosomal protein S14 type Z



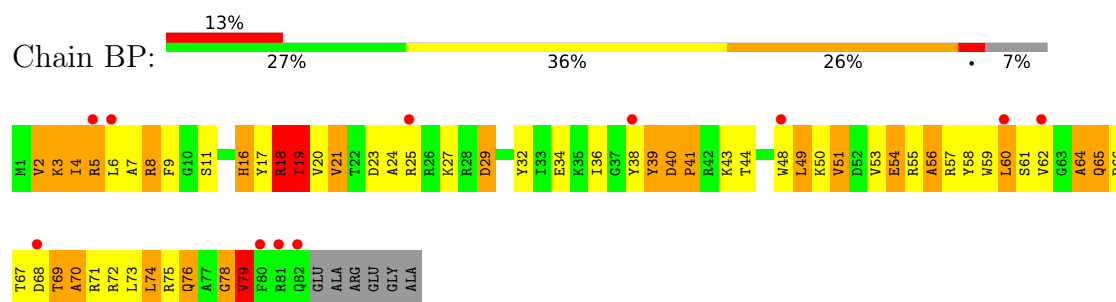
• Molecule 48: 30S ribosomal protein S15



• Molecule 48: 30S ribosomal protein S15

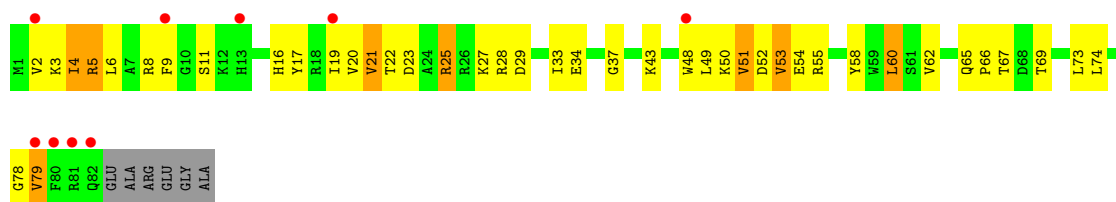


• Molecule 49: 30S ribosomal protein S16

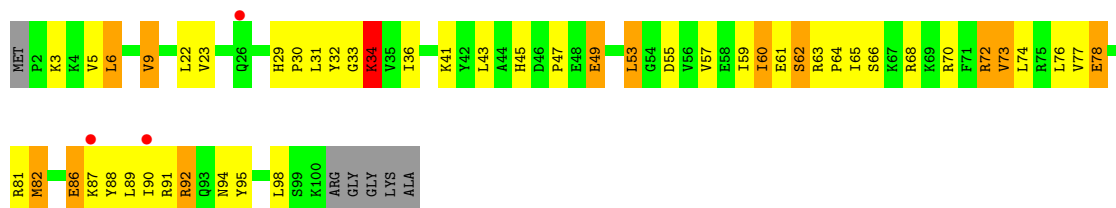


• Molecule 49: 30S ribosomal protein S16

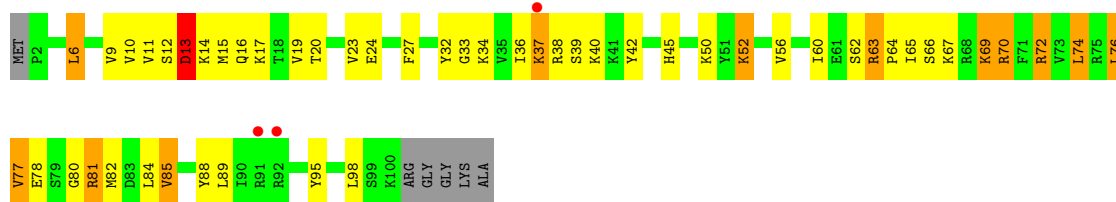




- Molecule 50: 30S ribosomal protein S17



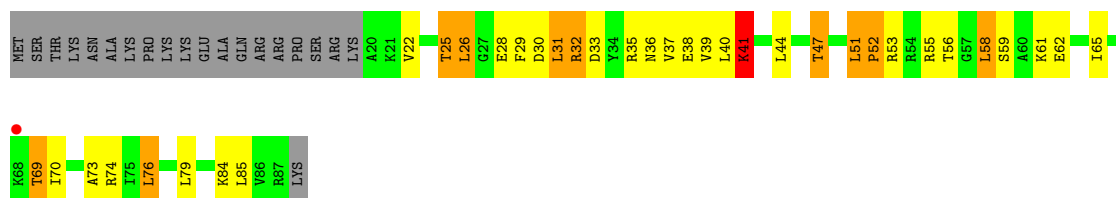
- Molecule 50: 30S ribosomal protein S17



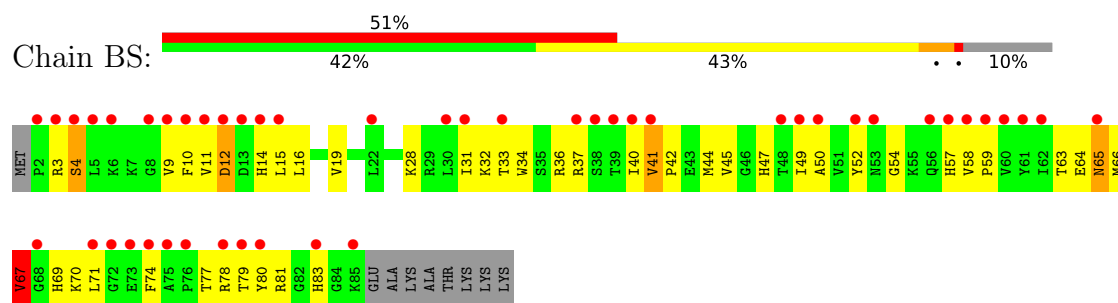
- Molecule 51: 30S ribosomal protein S18



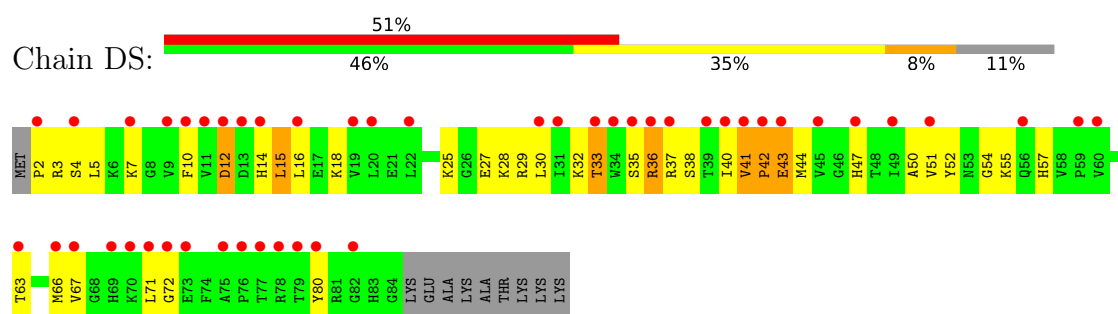
- Molecule 51: 30S ribosomal protein S18



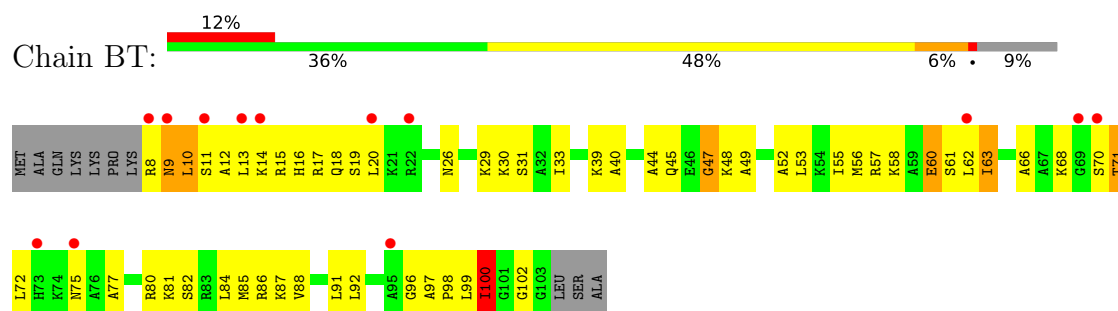
- Molecule 52: 30S ribosomal protein S19



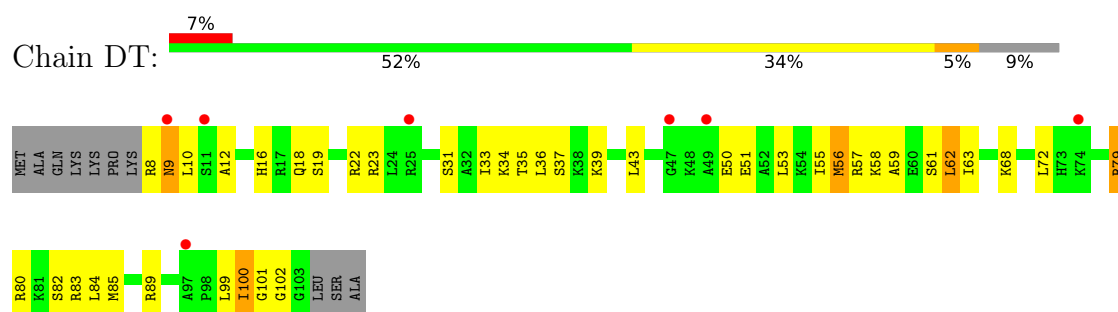
- Molecule 52: 30S ribosomal protein S19



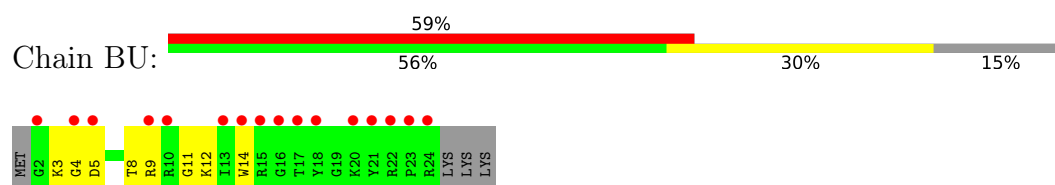
- Molecule 53: 30S ribosomal protein S20



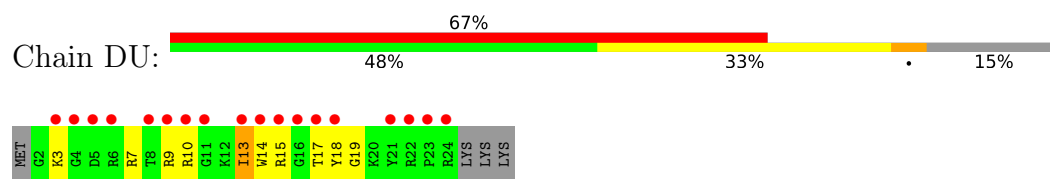
- Molecule 53: 30S ribosomal protein S20



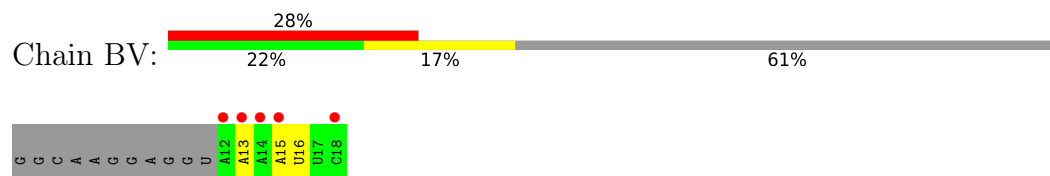
- Molecule 54: 30S ribosomal protein Thx



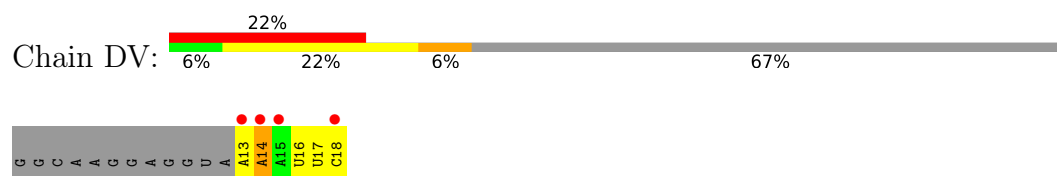
- Molecule 54: 30S ribosomal protein Thx



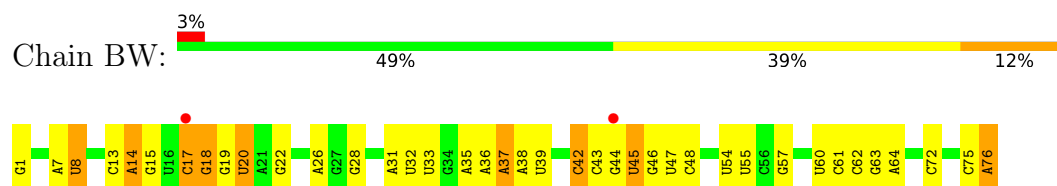
- Molecule 55: mRNA



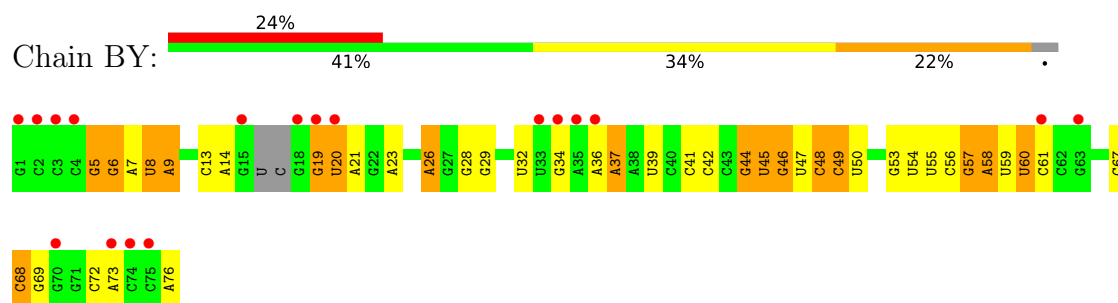
- Molecule 55: mRNA



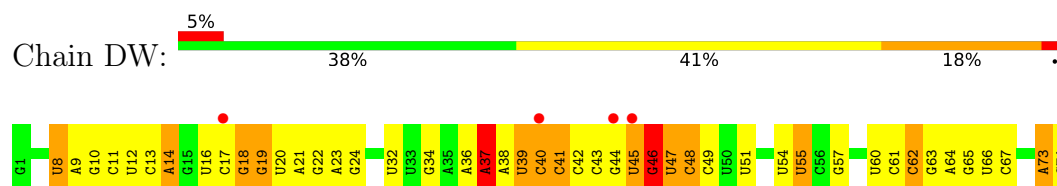
- Molecule 56: P-site tRNA



- Molecule 56: P-site tRNA

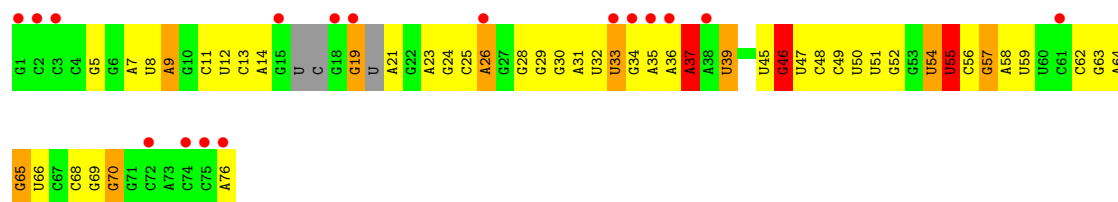


- Molecule 56: P-site tRNA

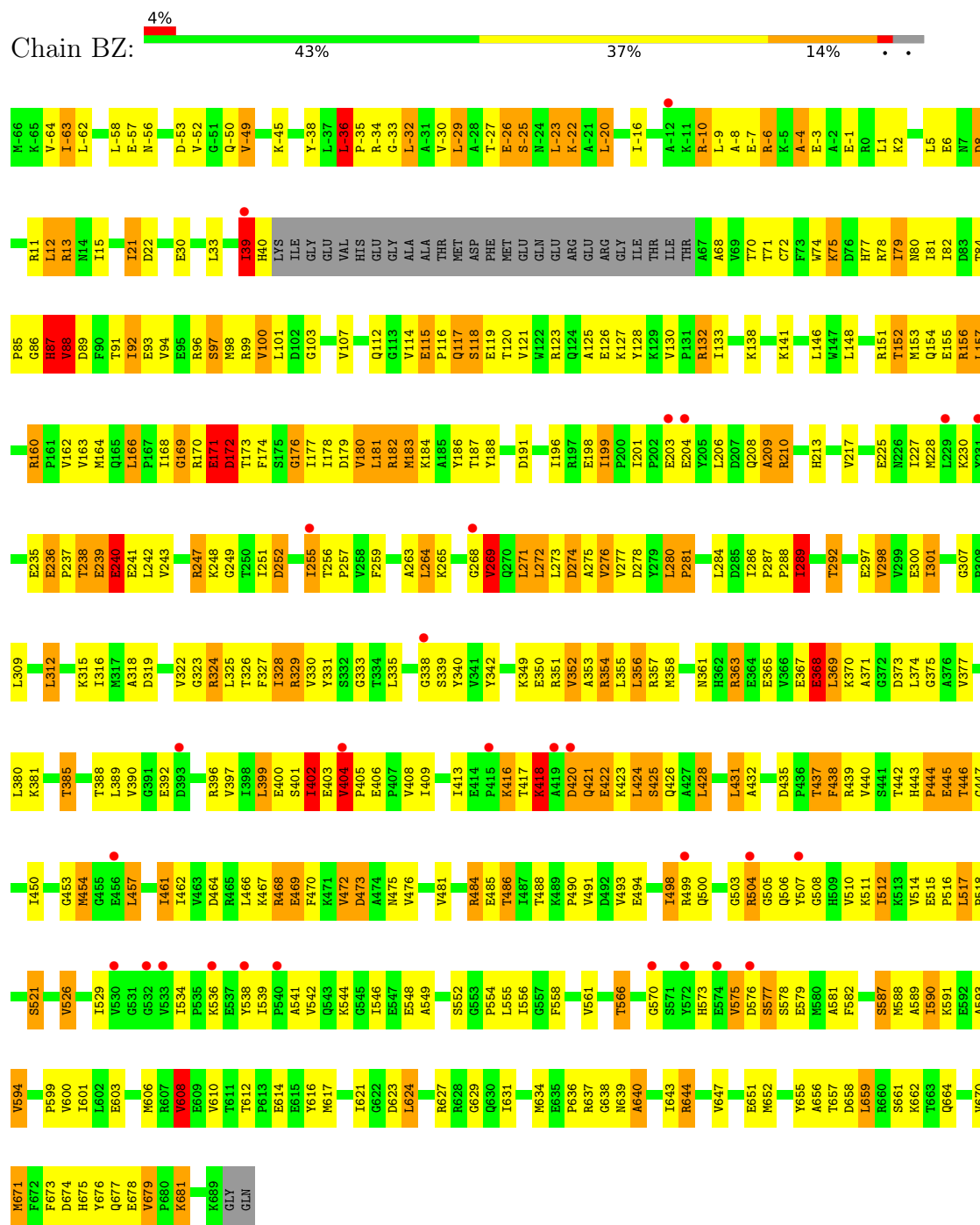


- Molecule 56: P-site tRNA

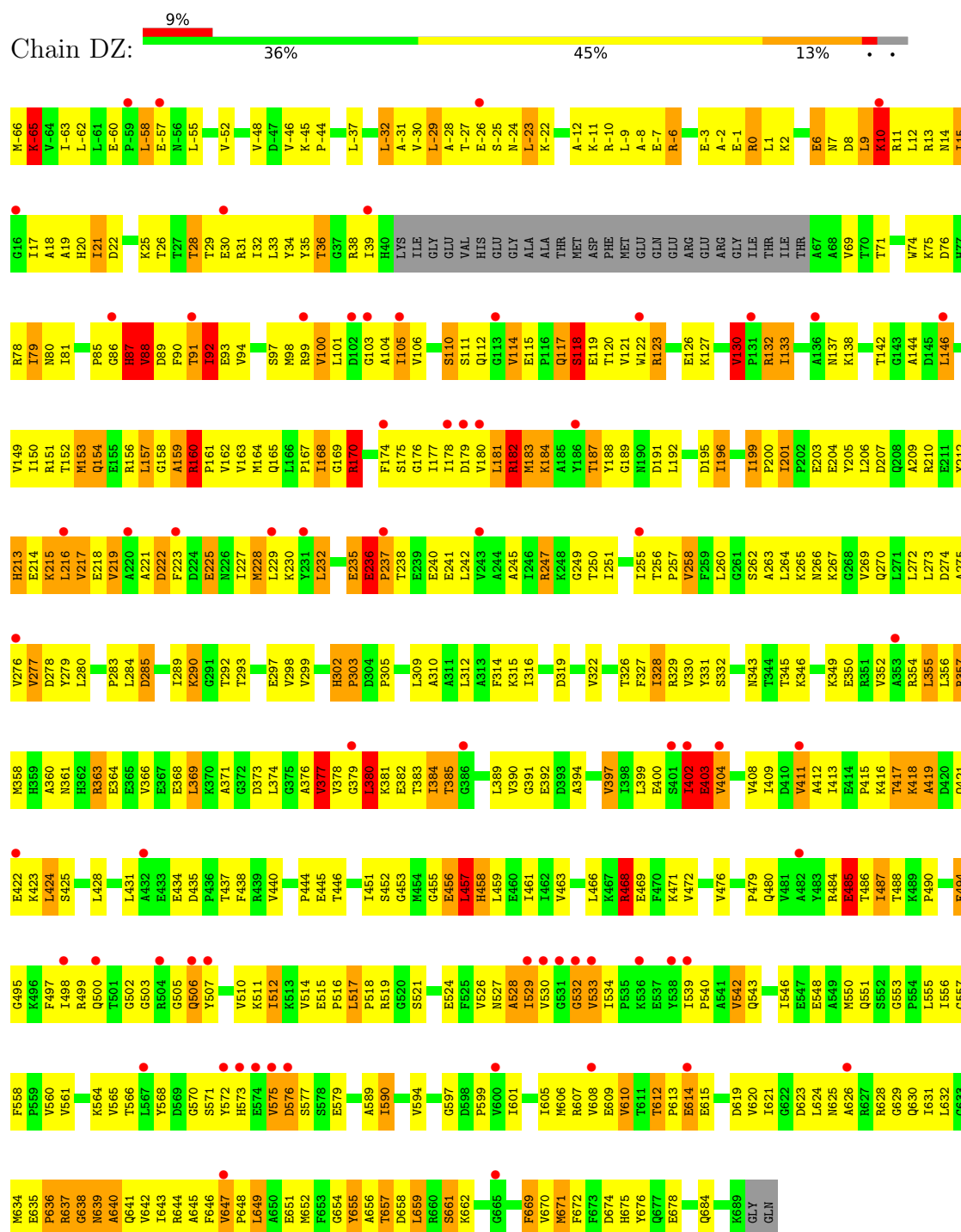




- Molecule 57: 50S ribosomal protein L9, Elongation factor G



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.45Å 449.00Å 625.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.80 49.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.74-2.80) 99.8 (49.74-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.200 , 0.255 0.202 , 0.254	Depositor DCC
R_{free} test set	72267 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	310279	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 4SU, MG, GDP, MIA, SF4, 5MU, 7MG, PSU, FUA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.81	2/68792 (0.0%)	0.97	73/107377 (0.1%)
1	CA	0.55	0/68691	0.77	14/107219 (0.0%)
2	AB	0.66	0/2878	0.93	0/4490
2	CB	0.39	0/2878	0.62	0/4490
3	AC	0.42	0/1083	0.97	6/1460 (0.4%)
3	CC	0.42	0/1083	0.97	5/1460 (0.3%)
4	AD	1.18	5/2186 (0.2%)	1.49	24/2944 (0.8%)
4	CD	0.94	0/2192	1.33	21/2951 (0.7%)
5	AE	1.28	4/1592 (0.3%)	1.52	23/2149 (1.1%)
5	CE	0.91	0/1592	1.26	20/2149 (0.9%)
6	AF	1.18	5/1619 (0.3%)	1.42	14/2193 (0.6%)
6	CF	0.79	1/1615 (0.1%)	1.25	11/2188 (0.5%)
7	AG	0.71	1/1450 (0.1%)	1.16	11/1959 (0.6%)
7	CG	0.51	0/1449	1.05	11/1958 (0.6%)
8	AH	1.06	1/1356 (0.1%)	1.36	10/1834 (0.5%)
8	CH	0.58	1/1356 (0.1%)	1.11	11/1834 (0.6%)
9	AK	0.72	0/640	1.64	14/889 (1.6%)
9	CK	0.49	0/640	1.65	10/889 (1.1%)
10	AL	0.50	0/1044	1.09	10/1416 (0.7%)
10	CL	0.49	0/1044	1.11	13/1416 (0.9%)
11	AN	1.31	3/1144 (0.3%)	1.47	14/1543 (0.9%)
11	CN	0.70	0/1144	1.18	7/1543 (0.5%)
12	AO	1.25	4/943 (0.4%)	1.50	11/1269 (0.9%)
12	CO	0.86	0/943	1.21	6/1269 (0.5%)
13	AP	1.09	0/1156	1.35	4/1537 (0.3%)
13	CP	0.71	0/1152	1.23	16/1533 (1.0%)
14	AQ	1.18	3/1143 (0.3%)	1.40	6/1527 (0.4%)
14	CQ	0.74	0/1143	1.16	6/1527 (0.4%)
15	AR	1.21	0/982	1.36	7/1312 (0.5%)
15	CR	0.82	0/982	1.20	2/1312 (0.2%)
16	AS	0.91	0/887	1.24	3/1180 (0.3%)
16	CS	0.68	0/880	1.07	3/1172 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	1.08	0/1105	1.35	7/1477 (0.5%)
17	CT	0.84	0/1097	1.29	11/1468 (0.7%)
18	AU	1.35	3/977 (0.3%)	1.44	10/1301 (0.8%)
18	CU	0.86	0/977	1.11	3/1301 (0.2%)
19	AV	1.25	1/782 (0.1%)	1.53	11/1049 (1.0%)
19	CV	0.68	0/782	1.02	0/1049
20	AW	1.49	7/897 (0.8%)	1.50	13/1205 (1.1%)
20	CW	1.01	1/897 (0.1%)	1.27	3/1205 (0.2%)
21	AX	1.13	0/764	1.33	4/1025 (0.4%)
21	CX	0.86	0/764	1.18	4/1025 (0.4%)
22	AY	1.08	1/819 (0.1%)	1.44	9/1095 (0.8%)
22	CY	0.75	0/819	1.13	4/1095 (0.4%)
23	AZ	0.96	0/1483	1.44	19/2017 (0.9%)
23	CZ	0.59	0/1483	1.14	14/2017 (0.7%)
24	A0	1.19	0/662	1.32	4/881 (0.5%)
24	C0	0.75	0/662	1.08	2/881 (0.2%)
25	A1	1.18	4/762 (0.5%)	1.43	10/1014 (1.0%)
25	C1	0.88	0/762	1.20	3/1014 (0.3%)
26	A2	1.08	1/590 (0.2%)	1.26	4/781 (0.5%)
26	C2	0.71	0/590	1.05	2/781 (0.3%)
27	A3	1.23	0/474	1.47	5/635 (0.8%)
27	C3	0.65	0/469	1.15	3/630 (0.5%)
28	A4	0.55	0/571	1.30	10/768 (1.3%)
28	C4	0.52	0/545	0.99	2/737 (0.3%)
29	A5	1.39	0/469	1.55	4/635 (0.6%)
29	C5	0.95	0/469	1.41	8/635 (1.3%)
30	A6	1.03	0/460	1.29	2/613 (0.3%)
30	C6	0.82	0/456	1.09	1/608 (0.2%)
31	A7	1.33	1/426 (0.2%)	1.40	2/561 (0.4%)
31	C7	1.06	1/426 (0.2%)	1.26	3/561 (0.5%)
32	A8	1.24	0/525	1.35	4/691 (0.6%)
32	C8	0.87	0/525	1.30	6/691 (0.9%)
33	A9	1.30	2/310 (0.6%)	1.29	2/407 (0.5%)
33	C9	0.69	0/310	0.97	1/407 (0.2%)
34	BA	0.44	0/35976	0.67	5/56145 (0.0%)
34	DA	0.39	0/36119	0.61	2/56370 (0.0%)
35	BB	0.60	0/1881	1.15	15/2542 (0.6%)
35	DB	0.52	0/1860	1.03	8/2518 (0.3%)
36	BC	0.51	0/1576	0.91	1/2130 (0.0%)
36	DC	0.49	0/1568	0.91	5/2122 (0.2%)
37	BD	0.64	0/1689	1.12	10/2267 (0.4%)
37	DD	0.64	0/1708	1.13	12/2289 (0.5%)
38	BE	0.78	0/1145	1.21	8/1543 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.73	0/1149	1.18	8/1548 (0.5%)
39	BF	0.68	0/825	1.02	2/1118 (0.2%)
39	DF	0.70	0/833	1.09	1/1128 (0.1%)
40	BG	0.52	0/1250	1.00	5/1679 (0.3%)
40	DG	0.45	0/1254	0.91	1/1683 (0.1%)
41	BH	0.74	0/1108	1.21	8/1494 (0.5%)
41	DH	0.62	0/1108	1.16	10/1494 (0.7%)
42	BI	0.50	0/1005	1.03	7/1350 (0.5%)
42	DI	0.46	0/997	0.94	0/1343
43	BJ	0.56	0/722	1.05	3/982 (0.3%)
43	DJ	0.50	0/727	0.99	3/988 (0.3%)
44	BK	0.71	0/848	1.15	3/1149 (0.3%)
44	DK	0.64	0/848	1.12	4/1149 (0.3%)
45	BL	0.86	0/946	1.18	5/1274 (0.4%)
45	DL	0.70	0/946	1.11	5/1274 (0.4%)
46	BM	0.53	0/933	1.01	2/1253 (0.2%)
46	DM	0.47	0/961	0.87	0/1291
47	BN	0.54	0/501	1.00	1/664 (0.2%)
47	DN	0.46	0/501	0.82	0/664
48	BO	0.71	0/739	1.09	3/985 (0.3%)
48	DO	0.68	0/739	1.03	3/985 (0.3%)
49	BP	0.74	1/697 (0.1%)	1.19	8/939 (0.9%)
49	DP	0.69	0/693	1.05	1/935 (0.1%)
50	BQ	0.74	0/836	1.15	5/1117 (0.4%)
50	DQ	0.64	0/836	1.09	4/1117 (0.4%)
51	BR	0.69	0/560	1.12	1/746 (0.1%)
51	DR	0.67	0/560	1.12	2/746 (0.3%)
52	BS	0.50	0/676	0.97	2/911 (0.2%)
52	DS	0.45	0/661	0.98	2/893 (0.2%)
53	BT	0.62	0/730	1.14	1/965 (0.1%)
53	DT	0.62	0/733	1.05	1/969 (0.1%)
54	BU	0.49	0/203	1.03	0/266
54	DU	0.43	0/203	0.87	1/266 (0.4%)
55	BV	0.54	0/165	0.64	0/254
55	DV	0.50	0/137	0.56	0/211
56	BW	0.51	0/1650	0.75	0/2569
56	BY	0.27	1/1602 (0.1%)	0.43	0/2493
56	DW	0.41	0/1650	0.63	0/2569
56	DY	0.23	0/1579	0.33	0/2455
57	BZ	0.76	2/5792 (0.0%)	1.18	26/7844 (0.3%)
57	DZ	0.64	0/5792	1.10	42/7844 (0.5%)
All	All	0.68	56/330005 (0.0%)	0.93	812/491779 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	0	1
17	CT	0	1
19	AV	0	1
21	AX	0	1
21	CX	0	1
23	AZ	0	1
24	A0	0	1
25	A1	0	1
28	A4	0	1
53	BT	0	1
53	DT	0	1
57	BZ	0	1
57	DZ	0	3
All	All	0	15

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	AW	95	ILE	CA-CB	-7.85	1.44	1.53
31	A7	13	ALA	CA-CB	-6.58	1.42	1.53
12	AO	121	VAL	CA-CB	-6.57	1.46	1.54
7	AG	159	VAL	CA-CB	6.28	1.61	1.53
14	AQ	73	PRO	CA-C	6.20	1.59	1.52

The worst 5 of 812 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AK	128	LEU	CA-C-N	19.29	144.38	121.04
9	AK	128	LEU	C-N-CA	19.29	144.38	121.04
9	CK	76	GLY	CA-C-N	16.86	140.91	119.84
9	CK	76	GLY	C-N-CA	16.86	140.91	119.84
9	CK	128	LEU	CA-C-N	13.01	136.11	119.84

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	A0	11	ARG	Peptide

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Mol	Chain	Res	Type	Group
25	A1	2	SER	Peptide
19	AV	54	GLY	Peptide
21	AX	93	GLU	Peptide
23	AZ	176	PRO	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	30937	937	0
1	CA	61337	0	30928	1114	0
2	AB	2573	0	1306	39	0
2	CB	2573	0	1306	50	0
3	AC	1063	0	1089	168	0
3	CC	1063	0	1091	209	0
4	AD	2136	0	2218	77	0
4	CD	2142	0	2229	75	0
5	AE	1559	0	1618	48	0
5	CE	1559	0	1618	95	0
6	AF	1584	0	1625	64	0
6	CF	1580	0	1619	69	0
7	AG	1425	0	1443	72	0
7	CG	1424	0	1434	63	0
8	AH	1330	0	1407	41	0
8	CH	1330	0	1407	52	0
9	AK	641	0	309	13	0
9	CK	641	0	309	13	0
10	AL	1025	0	1066	58	0
10	CL	1025	0	1066	51	0
11	AN	1117	0	1184	33	0
11	CN	1117	0	1184	45	0
12	AO	933	0	996	35	0
12	CO	933	0	996	39	0
13	AP	1139	0	1223	50	0
13	CP	1135	0	1212	48	0
14	AQ	1122	0	1179	37	0
14	CQ	1122	0	1179	60	0
15	AR	968	0	1033	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CR	968	0	1033	49	0
16	AS	877	0	938	31	0
16	CS	870	0	923	45	0
17	AT	1091	0	1151	36	0
17	CT	1083	0	1136	56	0
18	AU	959	0	1019	30	0
18	CU	959	0	1018	38	0
19	AV	771	0	829	25	0
19	CV	771	0	830	17	0
20	AW	886	0	940	27	0
20	CW	886	0	940	32	0
21	AX	750	0	814	29	0
21	CX	750	0	814	29	0
22	AY	806	0	881	24	0
22	CY	806	0	881	39	0
23	AZ	1451	0	1457	56	0
23	CZ	1451	0	1457	68	0
24	A0	653	0	674	29	0
24	C0	653	0	674	22	0
25	A1	755	0	826	25	0
25	C1	755	0	826	23	0
26	A2	588	0	643	15	0
26	C2	588	0	643	20	0
27	A3	469	0	518	14	0
27	C3	464	0	514	11	0
28	A4	558	0	547	24	0
28	C4	532	0	505	14	0
29	A5	455	0	465	18	0
29	C5	455	0	465	20	0
30	A6	453	0	473	19	0
30	C6	449	0	469	12	0
31	A7	418	0	467	17	0
31	C7	418	0	467	18	0
32	A8	517	0	582	22	0
32	C8	517	0	582	30	0
33	A9	307	0	335	10	0
33	C9	307	0	335	15	0
34	BA	32141	0	16224	677	0
34	DA	32268	0	16287	694	0
35	BB	1846	0	1867	106	0
35	DB	1825	0	1828	85	0
36	BC	1552	0	1546	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DC	1544	0	1524	64	0
37	BD	1659	0	1678	96	0
37	DD	1678	0	1720	93	0
38	BE	1129	0	1185	74	0
38	DE	1133	0	1191	66	0
39	BF	812	0	804	27	0
39	DF	820	0	814	23	0
40	BG	1231	0	1238	44	0
40	DG	1235	0	1249	32	0
41	BH	1088	0	1126	65	0
41	DH	1088	0	1126	37	0
42	BI	986	0	995	42	0
42	DI	978	0	966	40	0
43	BJ	709	0	650	37	0
43	DJ	714	0	672	47	0
44	BK	833	0	836	32	0
44	DK	833	0	836	25	0
45	BL	930	0	980	37	0
45	DL	930	0	980	44	0
46	BM	923	0	970	30	0
46	DM	950	0	988	49	0
47	BN	492	0	529	31	0
47	DN	492	0	531	20	0
48	BO	728	0	760	30	0
48	DO	728	0	760	20	0
49	BP	681	0	697	52	0
49	DP	677	0	686	33	0
50	BQ	823	0	891	30	0
50	DQ	823	0	891	39	0
51	BR	555	0	618	23	0
51	DR	555	0	618	25	0
52	BS	661	0	675	35	0
52	DS	646	0	644	33	0
53	BT	728	0	798	37	0
53	DT	731	0	807	25	0
54	BU	199	0	208	5	0
54	DU	199	0	208	8	0
55	BV	148	0	76	6	0
55	DV	123	0	66	6	0
56	BW	1631	0	839	24	0
56	BY	1581	0	805	25	0
56	DW	1631	0	839	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DY	1561	0	796	38	0
57	BZ	5690	0	5783	286	0
57	DZ	5690	0	5783	332	0
58	A0	3	0	0	0	0
58	A2	2	0	0	0	0
58	A4	1	0	0	0	0
58	A5	4	0	0	0	0
58	A6	1	0	0	0	0
58	A7	6	0	0	0	0
58	A8	2	0	0	0	0
58	A9	1	0	0	0	0
58	AA	815	0	0	0	0
58	AB	23	0	0	0	0
58	AD	12	0	0	0	0
58	AE	5	0	0	0	0
58	AF	8	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	3	0	0	0	0
58	AQ	3	0	0	0	0
58	AR	2	0	0	0	0
58	AU	4	0	0	0	0
58	AV	6	0	0	0	0
58	AW	4	0	0	0	0
58	AX	1	0	0	0	0
58	AY	1	0	0	0	0
58	AZ	2	0	0	0	0
58	BA	213	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	2	0	0	0	0
58	BM	2	0	0	0	0
58	BN	1	0	0	0	0
58	BT	1	0	0	0	0
58	BV	1	0	0	0	0
58	BW	3	0	0	0	0
58	BZ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	C3	1	0	0	0	0
58	C5	1	0	0	0	0
58	C7	1	0	0	0	0
58	C8	1	0	0	0	0
58	CA	664	0	0	0	0
58	CB	13	0	0	0	0
58	CD	3	0	0	0	0
58	CE	6	0	0	0	0
58	CF	5	0	0	0	0
58	CG	1	0	0	0	0
58	CN	1	0	0	0	0
58	CO	2	0	0	0	0
58	CP	3	0	0	0	0
58	CQ	5	0	0	0	0
58	CR	1	0	0	0	0
58	CU	1	0	0	0	0
58	CV	2	0	0	0	0
58	CW	1	0	0	0	0
58	CY	1	0	0	0	0
58	DA	168	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	DT	1	0	0	0	0
58	DW	3	0	0	0	0
58	DZ	2	0	0	0	0
59	A4	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	1	0	0	0	0
59	A9	1	0	0	0	0
59	AY	1	0	0	0	0
59	BN	1	0	0	0	0
59	C4	1	0	0	0	0
59	C5	1	0	0	0	0
59	C6	1	0	0	0	0
59	C9	1	0	0	0	0
59	CY	1	0	0	0	0
59	DN	1	0	0	0	0
60	BD	8	0	0	1	0
60	DD	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BZ	37	0	47	11	0
61	DZ	37	0	47	17	0
62	BZ	28	0	12	5	0
62	DZ	28	0	12	9	0
63	A0	7	0	0	1	0
63	A1	3	0	0	0	0
63	A3	1	0	0	0	0
63	A5	2	0	0	0	0
63	A6	1	0	0	0	0
63	A7	3	0	0	2	0
63	A8	11	0	0	2	0
63	AA	1408	0	0	60	0
63	AB	36	0	0	1	0
63	AD	15	0	0	1	0
63	AE	19	0	0	5	0
63	AF	8	0	0	1	0
63	AG	3	0	0	1	0
63	AH	1	0	0	0	0
63	AN	2	0	0	1	0
63	AO	3	0	0	0	0
63	AP	15	0	0	0	0
63	AQ	3	0	0	0	0
63	AR	3	0	0	0	0
63	AS	1	0	0	0	0
63	AT	2	0	0	0	0
63	AU	6	0	0	0	0
63	AW	1	0	0	0	0
63	AX	2	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	205	0	0	13	0
63	BD	3	0	0	0	0
63	BE	3	0	0	0	0
63	BJ	1	0	0	0	0
63	BL	2	0	0	0	0
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BV	2	0	0	0	0
63	BW	1	0	0	0	0
63	BZ	3	0	0	0	0
63	C0	5	0	0	0	0
63	C1	3	0	0	0	0
63	C3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C5	1	0	0	0	0
63	C7	3	0	0	0	0
63	C8	3	0	0	1	0
63	CA	981	0	0	65	0
63	CB	9	0	0	0	0
63	CD	15	0	0	0	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CP	13	0	0	3	0
63	CQ	1	0	0	0	0
63	CT	3	0	0	0	0
63	CU	4	0	0	1	0
63	CV	1	0	0	0	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	1	0	0	0	0
63	DA	153	0	0	11	0
63	DE	2	0	0	0	0
63	DH	1	0	0	1	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DP	1	0	0	0	0
63	DT	1	0	0	0	0
63	DY	1	0	0	0	0
63	DZ	2	0	0	0	0
All	All	310279	0	209988	7477	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 7477 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1891:G:C5'	3:AC:206:LYS:CG	1.80	1.55
1:AA:1891:G:H5''	3:AC:206:LYS:CG	1.26	1.54
1:AA:1891:G:C5'	3:AC:206:LYS:HG3	1.40	1.40
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.55	1.37
1:AA:2143:G:N2	3:AC:169:THR:OG1	1.57	1.36

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	249 (91%)	20 (7%)	4 (2%)	8	28
4	CD	273/276 (99%)	242 (89%)	26 (10%)	5 (2%)	6	23
5	AE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	12	38
5	CE	202/206 (98%)	174 (86%)	19 (9%)	9 (4%)	2	7
6	AF	201/210 (96%)	187 (93%)	11 (6%)	3 (2%)	8	28
6	CF	201/210 (96%)	186 (92%)	12 (6%)	3 (2%)	8	28
7	AG	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	1	3
7	CG	179/182 (98%)	148 (83%)	20 (11%)	11 (6%)	1	3
8	AH	172/180 (96%)	150 (87%)	20 (12%)	2 (1%)	10	34
8	CH	172/180 (96%)	148 (86%)	19 (11%)	5 (3%)	3	13
9	AK	128/173 (74%)	68 (53%)	33 (26%)	27 (21%)	0	0
9	CK	128/173 (74%)	69 (54%)	24 (19%)	35 (27%)	0	0
10	AL	137/147 (93%)	105 (77%)	23 (17%)	9 (7%)	1	3
10	CL	137/147 (93%)	95 (69%)	33 (24%)	9 (7%)	1	3
11	AN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18	47
11	CN	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	9	30
12	AO	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	7	25
12	CO	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	16
13	AP	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	9	30
13	CP	147/150 (98%)	128 (87%)	16 (11%)	3 (2%)	6	21
14	AQ	139/141 (99%)	124 (89%)	13 (9%)	2 (1%)	9	30
14	CQ	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	5	19
15	AR	116/118 (98%)	100 (86%)	13 (11%)	3 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CR	116/118 (98%)	92 (79%)	16 (14%)	8 (7%)	1	2
16	AS	108/112 (96%)	92 (85%)	12 (11%)	4 (4%)	2	9
16	CS	108/112 (96%)	86 (80%)	17 (16%)	5 (5%)	2	6
17	AT	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	44
17	CT	129/146 (88%)	109 (84%)	15 (12%)	5 (4%)	2	8
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	103 (90%)	10 (9%)	1 (1%)	14	41
19	AV	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	21
19	CV	99/101 (98%)	87 (88%)	9 (9%)	3 (3%)	3	12
20	AW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
20	CW	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
21	AX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
21	CX	93/96 (97%)	80 (86%)	11 (12%)	2 (2%)	5	19
22	AY	105/110 (96%)	91 (87%)	11 (10%)	3 (3%)	3	13
22	CY	105/110 (96%)	90 (86%)	13 (12%)	2 (2%)	6	22
23	AZ	183/206 (89%)	146 (80%)	24 (13%)	13 (7%)	1	2
23	CZ	183/206 (89%)	140 (76%)	31 (17%)	12 (7%)	1	3
24	A0	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	10	34
24	C0	81/85 (95%)	70 (86%)	11 (14%)	0	100	100
25	A1	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	5	20
25	C1	95/98 (97%)	87 (92%)	4 (4%)	4 (4%)	2	7
26	A2	68/72 (94%)	62 (91%)	5 (7%)	1 (2%)	8	28
26	C2	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	8	28
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	A4	67/71 (94%)	41 (61%)	19 (28%)	7 (10%)	0	1
28	C4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	7
29	A5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
29	C5	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	6	23
30	A6	51/54 (94%)	48 (94%)	2 (4%)	1 (2%)	6	21
30	C6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	6	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	A7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
31	C7	46/49 (94%)	43 (94%)	1 (2%)	2 (4%)	2	7
32	A8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
32	C8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	27
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	176 (77%)	42 (18%)	11 (5%)	2	6
35	DB	229/256 (90%)	177 (77%)	37 (16%)	15 (7%)	1	3
36	BC	204/239 (85%)	169 (83%)	28 (14%)	7 (3%)	3	11
36	DC	204/239 (85%)	175 (86%)	26 (13%)	3 (2%)	8	28
37	BD	206/209 (99%)	154 (75%)	34 (16%)	18 (9%)	0	1
37	DD	206/209 (99%)	161 (78%)	31 (15%)	14 (7%)	1	2
38	BE	146/162 (90%)	111 (76%)	26 (18%)	9 (6%)	1	3
38	DE	146/162 (90%)	122 (84%)	21 (14%)	3 (2%)	5	20
39	BF	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	3	12
39	DF	98/101 (97%)	82 (84%)	15 (15%)	1 (1%)	12	38
40	BG	153/156 (98%)	131 (86%)	17 (11%)	5 (3%)	3	11
40	DG	153/156 (98%)	133 (87%)	14 (9%)	6 (4%)	2	8
41	BH	135/138 (98%)	111 (82%)	18 (13%)	6 (4%)	2	7
41	DH	135/138 (98%)	122 (90%)	13 (10%)	0	100	100
42	BI	125/128 (98%)	104 (83%)	16 (13%)	5 (4%)	2	8
42	DI	125/128 (98%)	104 (83%)	18 (14%)	3 (2%)	4	17
43	BJ	95/105 (90%)	80 (84%)	12 (13%)	3 (3%)	3	11
43	DJ	94/105 (90%)	76 (81%)	9 (10%)	9 (10%)	0	1
44	BK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	2	10
44	DK	112/129 (87%)	98 (88%)	11 (10%)	3 (3%)	4	15
45	BL	120/132 (91%)	111 (92%)	7 (6%)	2 (2%)	7	25
45	DL	120/132 (91%)	103 (86%)	13 (11%)	4 (3%)	3	11
46	BM	115/126 (91%)	89 (77%)	23 (20%)	3 (3%)	4	15
46	DM	120/126 (95%)	100 (83%)	12 (10%)	8 (7%)	1	3
47	BN	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DN	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
48	BO	86/89 (97%)	72 (84%)	8 (9%)	6 (7%)	1	2
48	DO	86/89 (97%)	75 (87%)	8 (9%)	3 (4%)	3	10
49	BP	80/88 (91%)	52 (65%)	19 (24%)	9 (11%)	0	1
49	DP	80/88 (91%)	65 (81%)	12 (15%)	3 (4%)	2	9
50	BQ	97/105 (92%)	82 (84%)	9 (9%)	6 (6%)	1	3
50	DQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	3	12
51	BR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
51	DR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	3	12
52	BS	82/93 (88%)	66 (80%)	14 (17%)	2 (2%)	4	17
52	DS	81/93 (87%)	68 (84%)	8 (10%)	5 (6%)	1	3
53	BT	94/106 (89%)	77 (82%)	10 (11%)	7 (7%)	1	2
53	DT	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	3	11
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	6
57	BZ	726/758 (96%)	569 (78%)	106 (15%)	51 (7%)	1	2
57	DZ	726/758 (96%)	554 (76%)	121 (17%)	51 (7%)	1	2
All	All	13389/14444 (93%)	11230 (84%)	1582 (12%)	577 (4%)	2	7

5 of 577 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%)	100 (90%)	11 (10%)	7	24
3	CC	111/180 (62%)	100 (90%)	11 (10%)	7	24
4	AD	215/218 (99%)	175 (81%)	40 (19%)	1	5
4	CD	216/218 (99%)	177 (82%)	39 (18%)	2	6
5	AE	164/166 (99%)	127 (77%)	37 (23%)	1	3
5	CE	164/166 (99%)	125 (76%)	39 (24%)	1	3
6	AF	160/166 (96%)	124 (78%)	36 (22%)	1	3
6	CF	159/166 (96%)	120 (76%)	39 (24%)	1	2
7	AG	143/156 (92%)	113 (79%)	30 (21%)	1	4
7	CG	142/156 (91%)	108 (76%)	34 (24%)	1	3
8	AH	144/148 (97%)	117 (81%)	27 (19%)	1	5
8	CH	144/148 (97%)	119 (83%)	25 (17%)	2	7
10	AL	104/111 (94%)	82 (79%)	22 (21%)	1	4
10	CL	104/111 (94%)	84 (81%)	20 (19%)	1	5
11	AN	118/119 (99%)	95 (80%)	23 (20%)	1	5
11	CN	118/119 (99%)	88 (75%)	30 (25%)	0	2
12	AO	100/100 (100%)	85 (85%)	15 (15%)	3	10
12	CO	100/100 (100%)	80 (80%)	20 (20%)	1	4
13	AP	116/116 (100%)	87 (75%)	29 (25%)	0	2
13	CP	115/116 (99%)	90 (78%)	25 (22%)	1	3
14	AQ	111/111 (100%)	97 (87%)	14 (13%)	4	15
14	CQ	111/111 (100%)	88 (79%)	23 (21%)	1	4
15	AR	101/101 (100%)	79 (78%)	22 (22%)	1	3
15	CR	101/101 (100%)	74 (73%)	27 (27%)	0	1
16	AS	87/88 (99%)	67 (77%)	20 (23%)	1	3
16	CS	85/88 (97%)	67 (79%)	18 (21%)	1	4
17	AT	115/127 (91%)	95 (83%)	20 (17%)	2	7
17	CT	113/127 (89%)	87 (77%)	26 (23%)	1	3
18	AU	93/94 (99%)	74 (80%)	19 (20%)	1	4
18	CU	93/94 (99%)	77 (83%)	16 (17%)	2	7
19	AV	80/82 (98%)	58 (72%)	22 (28%)	0	1
19	CV	80/82 (98%)	63 (79%)	17 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AW	90/92 (98%)	74 (82%)	16 (18%)	2	6
20	CW	90/92 (98%)	79 (88%)	11 (12%)	5	16
21	AX	77/78 (99%)	65 (84%)	12 (16%)	2	9
21	CX	77/78 (99%)	65 (84%)	12 (16%)	2	9
22	AY	85/91 (93%)	70 (82%)	15 (18%)	2	7
22	CY	85/91 (93%)	69 (81%)	16 (19%)	1	5
23	AZ	156/179 (87%)	116 (74%)	40 (26%)	0	2
23	CZ	156/179 (87%)	124 (80%)	32 (20%)	1	4
24	A0	65/67 (97%)	59 (91%)	6 (9%)	8	27
24	C0	65/67 (97%)	59 (91%)	6 (9%)	8	27
25	A1	80/83 (96%)	66 (82%)	14 (18%)	2	7
25	C1	80/83 (96%)	64 (80%)	16 (20%)	1	4
26	A2	65/67 (97%)	52 (80%)	13 (20%)	1	4
26	C2	65/67 (97%)	50 (77%)	15 (23%)	1	3
27	A3	51/52 (98%)	39 (76%)	12 (24%)	1	3
27	C3	50/52 (96%)	41 (82%)	9 (18%)	2	6
28	A4	60/63 (95%)	44 (73%)	16 (27%)	0	1
28	C4	53/63 (84%)	40 (76%)	13 (24%)	1	2
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	12
29	C5	50/52 (96%)	42 (84%)	8 (16%)	2	9
30	A6	51/52 (98%)	36 (71%)	15 (29%)	0	1
30	C6	50/52 (96%)	37 (74%)	13 (26%)	0	2
31	A7	41/42 (98%)	34 (83%)	7 (17%)	2	7
31	C7	41/42 (98%)	32 (78%)	9 (22%)	1	3
32	A8	54/55 (98%)	46 (85%)	8 (15%)	3	10
32	C8	54/55 (98%)	44 (82%)	10 (18%)	1	6
33	A9	34/34 (100%)	31 (91%)	3 (9%)	9	29
33	C9	34/34 (100%)	30 (88%)	4 (12%)	5	17
35	BB	192/220 (87%)	153 (80%)	39 (20%)	1	4
35	DB	187/220 (85%)	150 (80%)	37 (20%)	1	5
36	BC	143/188 (76%)	129 (90%)	14 (10%)	7	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DC	141/188 (75%)	115 (82%)	26 (18%)	1	6
37	BD	170/181 (94%)	138 (81%)	32 (19%)	1	5
37	DD	174/181 (96%)	136 (78%)	38 (22%)	1	3
38	BE	113/123 (92%)	87 (77%)	26 (23%)	1	3
38	DE	114/123 (93%)	87 (76%)	27 (24%)	1	3
39	BF	84/90 (93%)	65 (77%)	19 (23%)	1	3
39	DF	86/90 (96%)	73 (85%)	13 (15%)	3	10
40	BG	119/127 (94%)	99 (83%)	20 (17%)	2	8
40	DG	120/127 (94%)	100 (83%)	20 (17%)	2	8
41	BH	114/119 (96%)	89 (78%)	25 (22%)	1	3
41	DH	114/119 (96%)	89 (78%)	25 (22%)	1	3
42	BI	91/99 (92%)	70 (77%)	21 (23%)	1	3
42	DI	89/99 (90%)	76 (85%)	13 (15%)	3	11
43	BJ	66/92 (72%)	59 (89%)	7 (11%)	6	22
43	DJ	69/92 (75%)	66 (96%)	3 (4%)	26	60
44	BK	83/99 (84%)	67 (81%)	16 (19%)	1	5
44	DK	83/99 (84%)	73 (88%)	10 (12%)	5	17
45	BL	97/109 (89%)	81 (84%)	16 (16%)	2	8
45	DL	97/109 (89%)	77 (79%)	20 (21%)	1	4
46	BM	91/101 (90%)	71 (78%)	20 (22%)	1	3
46	DM	92/101 (91%)	80 (87%)	12 (13%)	4	14
47	BN	49/50 (98%)	41 (84%)	8 (16%)	2	8
47	DN	49/50 (98%)	40 (82%)	9 (18%)	1	6
48	BO	78/80 (98%)	68 (87%)	10 (13%)	4	15
48	DO	78/80 (98%)	67 (86%)	11 (14%)	3	12
49	BP	69/74 (93%)	53 (77%)	16 (23%)	1	3
49	DP	68/74 (92%)	56 (82%)	12 (18%)	2	7
50	BQ	94/97 (97%)	75 (80%)	19 (20%)	1	4
50	DQ	94/97 (97%)	81 (86%)	13 (14%)	3	12
51	BR	59/77 (77%)	49 (83%)	10 (17%)	2	7
51	DR	59/77 (77%)	46 (78%)	13 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	BS	70/80 (88%)	61 (87%)	9 (13%)	4	14
52	DS	67/80 (84%)	61 (91%)	6 (9%)	9	28
53	BT	70/82 (85%)	55 (79%)	15 (21%)	1	4
53	DT	71/82 (87%)	62 (87%)	9 (13%)	4	15
54	BU	18/22 (82%)	17 (94%)	1 (6%)	19	50
54	DU	18/22 (82%)	18 (100%)	0	100	100
57	BZ	609/636 (96%)	464 (76%)	145 (24%)	1	3
57	DZ	609/636 (96%)	457 (75%)	152 (25%)	0	2
All	All	10785/11672 (92%)	8674 (80%)	2111 (20%)	1	5

5 of 2111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	DK	103	LEU
49	DP	4	ILE
44	DK	96	ARG
57	DZ	485	GLU
44	BK	31	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 207 such sidechains are listed below:

Mol	Chain	Res	Type
5	CE	143	ASN
21	CX	31	HIS
57	DZ	302	HIS
6	CF	75	HIS
11	CN	133	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2845/2915 (97%)	540 (18%)	56 (1%)
1	CA	2839/2915 (97%)	582 (20%)	39 (1%)
2	AB	119/121 (98%)	23 (19%)	0
2	CB	119/121 (98%)	21 (17%)	0
34	BA	1491/1521 (98%)	311 (20%)	22 (1%)
34	DA	1498/1521 (98%)	304 (20%)	24 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	BV	6/18 (33%)	1 (16%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	75/76 (98%)	15 (20%)	0
56	BY	72/76 (94%)	24 (33%)	2 (2%)
56	DW	75/76 (98%)	20 (26%)	2 (2%)
56	DY	71/76 (93%)	23 (32%)	1 (1%)
All	All	9215/9454 (97%)	1865 (20%)	146 (1%)

5 of 1865 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	U
1	AA	12	U
1	AA	13	A
1	AA	34	C
1	AA	45	C

5 of 146 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	2566	A
56	DW	13	C
34	DA	115	G
34	DA	748	C
1	AA	2434	A

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

28 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	PSU	DW	55	56	18,21,22	1.37	3 (16%)	21,30,33	1.87	3 (14%)
56	7MG	BY	46	56	23,26,27	1.28	3 (13%)	27,39,42	2.70	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	DW	32	56	18,21,22	1.41	3 (16%)	21,30,33	1.88	4 (19%)
56	5MU	BW	54	56	19,22,23	1.52	6 (31%)	27,32,35	2.29	6 (22%)
56	4SU	DY	8	56	18,21,22	1.84	4 (22%)	25,30,33	2.34	5 (20%)
56	PSU	BY	39	56	18,21,22	1.38	2 (11%)	21,30,33	1.93	3 (14%)
56	PSU	BW	39	56	18,21,22	1.37	2 (11%)	21,30,33	1.95	5 (23%)
56	MIA	BY	37	56	21,24,32	1.67	3 (14%)	30,35,47	2.04	8 (26%)
56	4SU	BY	8	56	18,21,22	1.75	5 (27%)	25,30,33	2.12	6 (24%)
56	MIA	DY	37	56	21,24,32	1.59	4 (19%)	30,35,47	2.07	7 (23%)
56	7MG	DY	46	56	23,26,27	1.25	3 (13%)	27,39,42	2.76	7 (25%)
56	4SU	DW	8	56	18,21,22	1.73	3 (16%)	25,30,33	2.04	5 (20%)
56	7MG	DW	46	56	23,26,27	1.32	4 (17%)	27,39,42	2.64	7 (25%)
56	MIA	BW	37	56	28,31,32	2.46	6 (21%)	38,44,47	3.23	15 (39%)
56	PSU	DY	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.96	3 (14%)
56	PSU	BW	55	56	18,21,22	1.28	2 (11%)	21,30,33	1.94	4 (19%)
56	5MU	DW	54	56	19,22,23	1.48	6 (31%)	27,32,35	2.21	8 (29%)
56	PSU	BW	32	56	18,21,22	1.40	3 (16%)	21,30,33	2.19	6 (28%)
56	PSU	BY	32	56	18,21,22	1.42	2 (11%)	21,30,33	1.93	4 (19%)
56	7MG	BW	46	56	23,26,27	1.31	3 (13%)	27,39,42	2.97	7 (25%)
56	PSU	DW	39	56	18,21,22	1.38	2 (11%)	21,30,33	2.17	5 (23%)
56	5MU	BY	54	56	19,22,23	1.53	5 (26%)	27,32,35	2.19	9 (33%)
56	MIA	DW	37	56	28,31,32	2.57	7 (25%)	38,44,47	2.51	11 (28%)
56	4SU	BW	8	56	18,21,22	1.56	3 (16%)	25,30,33	2.30	5 (20%)
56	5MU	DY	54	56	19,22,23	1.44	6 (31%)	27,32,35	2.09	5 (18%)
56	PSU	BY	55	56	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
56	PSU	DY	55	56	18,21,22	1.42	3 (16%)	21,30,33	2.02	3 (14%)
56	PSU	DY	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.96	4 (19%)

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	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
56	7MG	BY	46	56	-	4/7/37/38	0/3/3/3
56	PSU	DW	32	56	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	BW	54	56	-	0/7/25/26	0/2/2/2
56	4SU	DY	8	56	-	1/7/25/26	0/2/2/2
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
56	MIA	BY	37	56	-	2/7/25/34	0/3/3/3
56	4SU	BY	8	56	-	1/7/25/26	0/2/2/2
56	MIA	DY	37	56	-	3/7/25/34	0/3/3/3
56	7MG	DY	46	56	-	3/7/37/38	0/3/3/3
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
56	7MG	DW	46	56	-	2/7/37/38	0/3/3/3
56	MIA	BW	37	56	-	5/15/33/34	0/3/3/3
56	PSU	DY	39	56	-	2/7/25/26	0/2/2/2
56	PSU	BW	55	56	-	0/7/25/26	0/2/2/2
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	56	-	4/7/25/26	0/2/2/2
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
56	7MG	BW	46	56	-	0/7/37/38	0/3/3/3
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
56	5MU	BY	54	56	-	2/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	6/15/33/34	0/3/3/3
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2
56	5MU	DY	54	56	-	2/7/25/26	0/2/2/2
56	PSU	BY	55	56	-	2/7/25/26	0/2/2/2
56	PSU	DY	55	56	-	3/7/25/26	0/2/2/2
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DW	37	MIA	C2-S10	-8.05	1.69	1.75
56	BW	37	MIA	C13-C14	7.46	1.54	1.32
56	BW	37	MIA	C2-S10	-7.31	1.69	1.75
56	DW	37	MIA	C13-C14	7.29	1.54	1.32
56	BY	37	MIA	C5-C4	5.34	1.48	1.39

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BW	37	MIA	C11-S10-C2	-11.58	93.56	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DY	46	7MG	N9-C4-N3	9.62	139.55	125.46
56	BW	46	7MG	N9-C4-N3	9.54	139.44	125.46
56	BY	46	7MG	N9-C4-N3	9.19	138.93	125.46
56	DW	46	7MG	N9-C4-N3	8.89	138.48	125.46

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

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

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DW	55	PSU	1	0
56	BY	8	4SU	1	0
56	DY	37	MIA	1	0
56	DY	46	7MG	2	0
56	DW	46	7MG	2	0
56	BW	37	MIA	2	0
56	DW	39	PSU	4	0
56	DW	37	MIA	3	0
56	DY	55	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2058 ligands modelled in this entry, 2052 are monoatomic - leaving 6 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
60	SF4	BD	501	37	0,12,12	-	-	-		
62	GDP	BZ	704	58	29,30,30	1.26	5 (17%)	45,47,47	1.89	11 (24%)
62	GDP	DZ	704	58	29,30,30	1.12	2 (6%)	45,47,47	1.82	6 (13%)
61	FUA	DZ	703	-	39,40,40	1.70	7 (17%)	50,64,64	1.70	8 (16%)
60	SF4	DD	501	37	0,12,12	-	-	-		
61	FUA	BZ	703	-	39,40,40	1.70	7 (17%)	50,64,64	1.70	8 (16%)

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
60	SF4	BD	501	37	-	-	0/6/5/5
62	GDP	DZ	704	58	-	2/16/32/32	0/3/3/3
62	GDP	BZ	704	58	-	4/16/32/32	0/3/3/3
61	FUA	DZ	703	-	-	7/16/92/92	0/4/4/4
60	SF4	DD	501	37	-	-	0/6/5/5
61	FUA	BZ	703	-	-	7/16/92/92	0/4/4/4

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BZ	703	FUA	C23-C22	-4.44	1.39	1.51
61	DZ	703	FUA	C23-C22	-4.41	1.40	1.51
61	BZ	703	FUA	C23-C24	-4.35	1.39	1.53
61	DZ	703	FUA	C23-C24	-4.34	1.39	1.53
61	BZ	703	FUA	C29-C22	4.24	1.53	1.47

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	704	GDP	C5-C4-N3	-5.90	119.00	128.39
62	DZ	704	GDP	C5-C4-N3	-5.86	119.06	128.39
61	BZ	703	FUA	C24-C23-C22	5.35	124.11	112.72
61	DZ	703	FUA	C24-C23-C22	5.34	124.09	112.72
62	BZ	704	GDP	C2-N3-C4	4.99	120.90	112.30

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

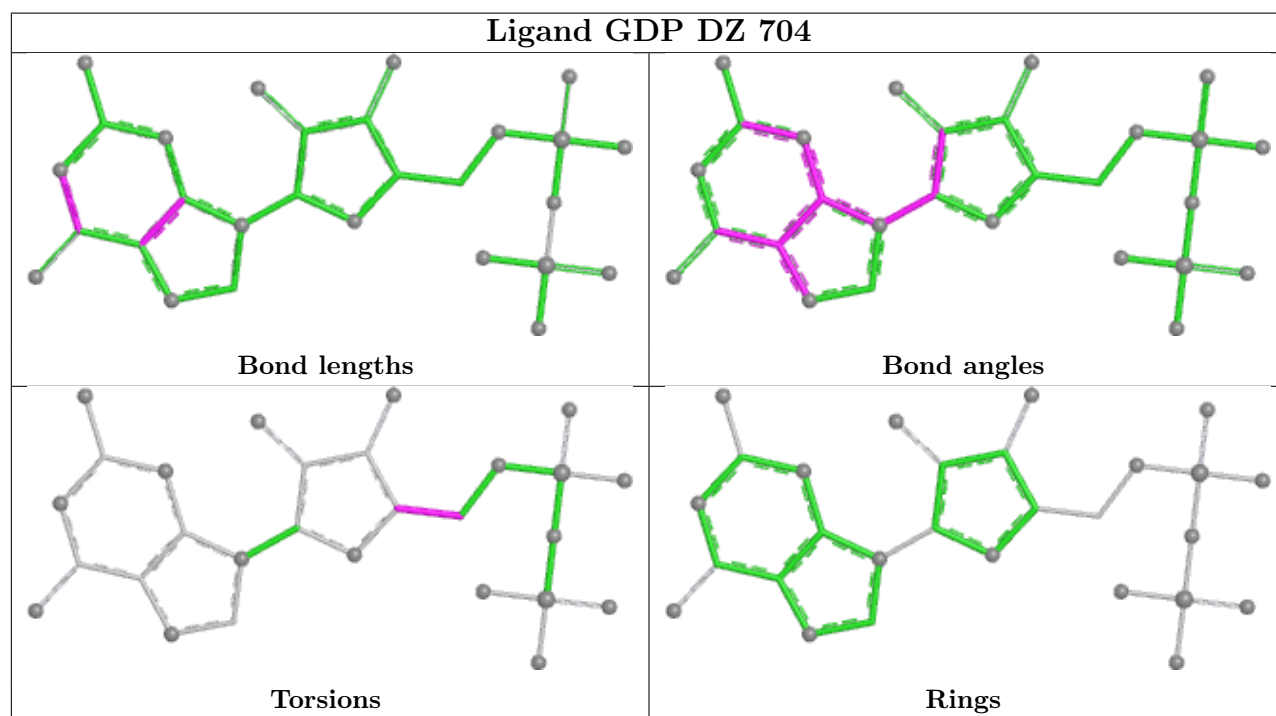
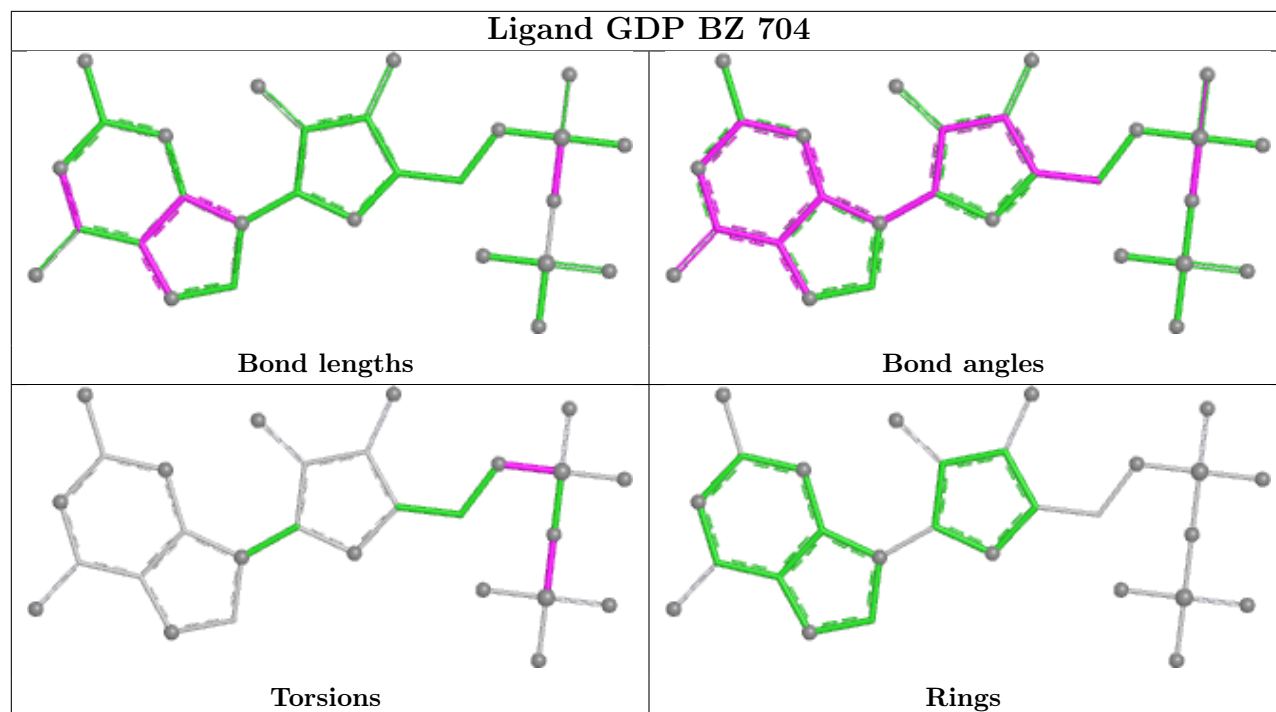
Mol	Chain	Res	Type	Atoms
61	BZ	703	FUA	C13-C17-C22-C23
61	BZ	703	FUA	C13-C17-C22-C29
61	DZ	703	FUA	C13-C17-C22-C23
61	DZ	703	FUA	C13-C17-C22-C29
62	BZ	704	GDP	PA-O3A-PB-O3B

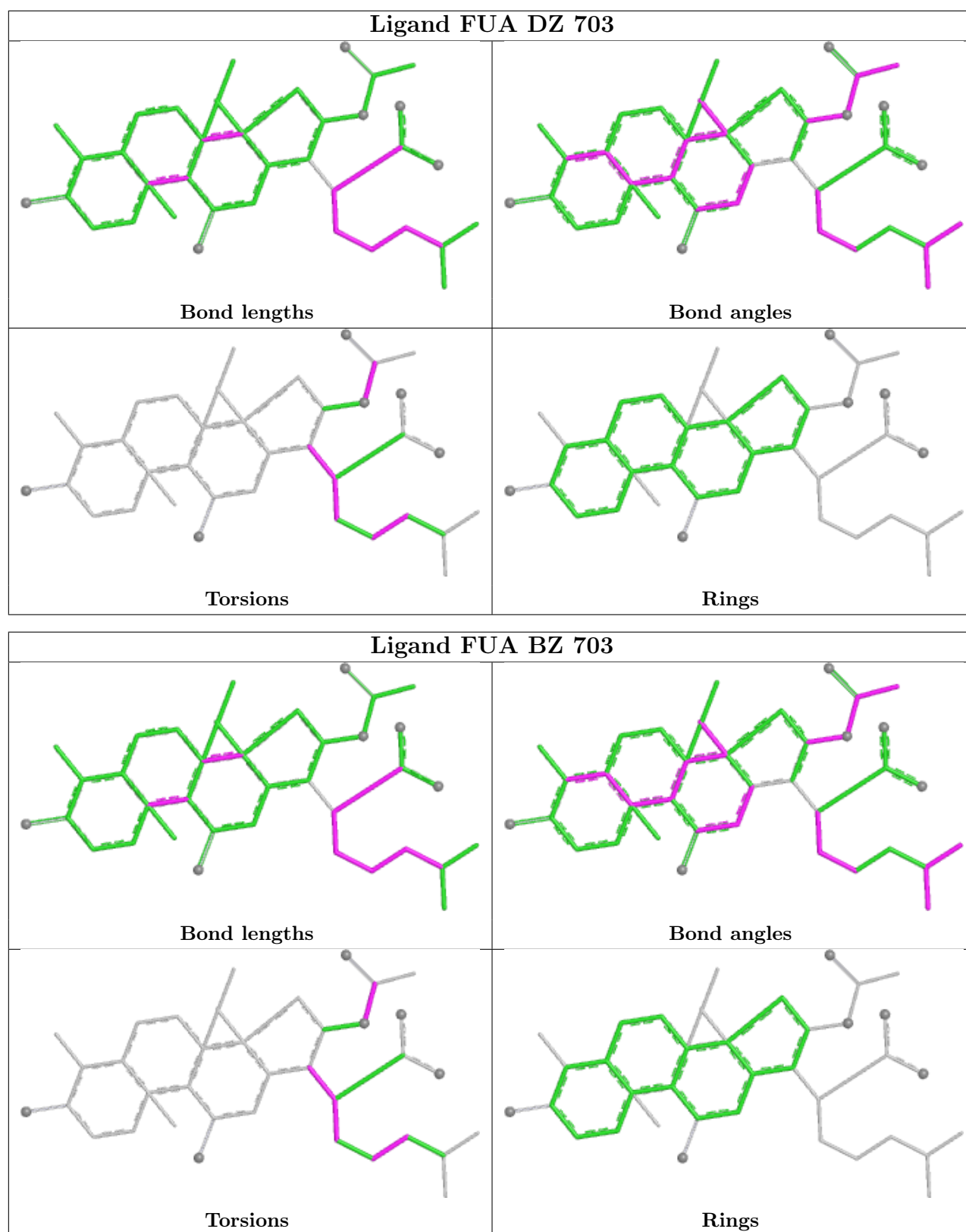
There are no ring outliers.

6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BD	501	SF4	1	0
62	BZ	704	GDP	5	0
62	DZ	704	GDP	9	0
61	DZ	703	FUA	17	0
60	DD	501	SF4	2	0
61	BZ	703	FUA	11	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	AA	2852/2915 (97%)	-0.78	69 (2%)	59	49	14, 33, 136, 352	4 (0%)
1	CA	2848/2915 (97%)	-0.25	85 (2%)	52	42	26, 56, 178, 343	0
2	AB	120/121 (99%)	-0.55	1 (0%)	82	75	22, 48, 72, 108	0
2	CB	120/121 (99%)	0.36	1 (0%)	82	75	61, 90, 117, 168	0
3	AC	137/228 (60%)	2.97	109 (79%)	0	0	258, 289, 307, 313	0
3	CC	137/228 (60%)	2.93	104 (75%)	0	0	281, 312, 331, 336	0
4	AD	275/276 (99%)	-0.48	2 (0%)	84	77	12, 34, 57, 136	0
4	CD	275/276 (99%)	-0.27	4 (1%)	72	63	16, 47, 73, 129	2 (0%)
5	AE	204/206 (99%)	-0.71	0	100	100	5, 33, 55, 75	1 (0%)
5	CE	204/206 (99%)	0.33	7 (3%)	48	39	21, 61, 106, 132	0
6	AF	203/210 (96%)	-0.57	1 (0%)	87	82	10, 35, 76, 172	0
6	CF	203/210 (96%)	0.04	1 (0%)	87	82	21, 62, 106, 154	0
7	AG	181/182 (99%)	0.67	10 (5%)	30	23	31, 76, 134, 206	0
7	CG	181/182 (99%)	1.08	24 (13%)	7	5	72, 110, 174, 203	0
8	AH	174/180 (96%)	-0.32	1 (0%)	85	80	26, 45, 69, 111	0
8	CH	174/180 (96%)	1.22	33 (18%)	3	2	64, 111, 158, 195	0
9	AK	130/173 (75%)	1.59	39 (30%)	1	1	47, 105, 170, 221	0
9	CK	130/173 (75%)	2.14	65 (50%)	0	0	73, 159, 203, 217	0
10	AL	139/147 (94%)	1.79	46 (33%)	1	1	95, 170, 225, 245	0
10	CL	139/147 (94%)	2.30	76 (54%)	0	0	123, 192, 241, 279	1 (0%)
11	AN	140/140 (100%)	-0.72	0	100	100	13, 28, 60, 95	1 (0%)
11	CN	140/140 (100%)	0.37	5 (3%)	46	37	29, 71, 107, 150	0
12	AO	122/122 (100%)	-0.60	0	100	100	16, 37, 62, 76	0
12	CO	122/122 (100%)	0.01	0	100	100	36, 58, 82, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.32	0 100 100	10, 42, 79, 102	1 (0%)
13	CP	149/150 (99%)	0.19	4 (2%) 56 46	29, 66, 115, 134	0
14	AQ	141/141 (100%)	-0.59	1 (0%) 84 77	11, 33, 52, 78	0
14	CQ	141/141 (100%)	0.40	7 (4%) 34 26	35, 69, 99, 118	0
15	AR	118/118 (100%)	-0.75	0 100 100	16, 28, 43, 54	0
15	CR	118/118 (100%)	0.15	2 (1%) 69 60	32, 55, 87, 105	0
16	AS	110/112 (98%)	-0.26	0 100 100	28, 49, 79, 91	0
16	CS	110/112 (98%)	0.92	11 (10%) 12 9	43, 83, 119, 152	0
17	AT	131/146 (89%)	-0.35	3 (2%) 61 51	23, 40, 91, 164	0
17	CT	131/146 (89%)	0.28	3 (2%) 61 51	41, 64, 102, 142	0
18	AU	116/118 (98%)	-0.83	0 100 100	8, 22, 36, 89	1 (0%)
18	CU	116/118 (98%)	0.28	0 100 100	26, 64, 91, 105	0
19	AV	101/101 (100%)	-0.90	0 100 100	9, 27, 48, 73	0
19	CV	101/101 (100%)	0.25	0 100 100	34, 79, 112, 171	0
20	AW	112/113 (99%)	-0.81	1 (0%) 81 74	13, 25, 43, 109	1 (0%)
20	CW	112/113 (99%)	-0.14	0 100 100	25, 48, 80, 118	0
21	AX	95/96 (98%)	-0.49	1 (1%) 78 70	16, 34, 66, 97	1 (1%)
21	CX	95/96 (98%)	0.20	5 (5%) 32 24	36, 60, 85, 106	0
22	AY	107/110 (97%)	-0.26	1 (0%) 81 74	24, 43, 86, 156	0
22	CY	107/110 (97%)	0.44	4 (3%) 45 36	45, 74, 115, 162	0
23	AZ	185/206 (89%)	-0.04	2 (1%) 78 70	28, 55, 91, 147	0
23	CZ	185/206 (89%)	0.92	12 (6%) 25 18	59, 105, 148, 213	0
24	A0	83/85 (97%)	-0.20	5 (6%) 27 21	11, 34, 77, 219	0
24	C0	83/85 (97%)	0.63	8 (9%) 13 10	39, 65, 120, 225	0
25	A1	97/98 (98%)	-0.18	2 (2%) 63 54	18, 43, 79, 99	1 (1%)
25	C1	97/98 (98%)	-0.05	3 (3%) 51 41	29, 51, 89, 125	0
26	A2	70/72 (97%)	-0.18	1 (1%) 73 64	25, 42, 67, 123	1 (1%)
26	C2	70/72 (97%)	0.42	3 (4%) 40 31	47, 70, 99, 117	0
27	A3	59/60 (98%)	-0.61	1 (1%) 69 60	13, 30, 55, 98	1 (1%)
27	C3	59/60 (98%)	0.47	2 (3%) 48 39	44, 73, 110, 150	0
28	A4	69/71 (97%)	1.10	13 (18%) 3 2	56, 116, 206, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.31	12 (17%)	4	3	78, 159, 204, 220	0
29	A5	59/60 (98%)	-0.87	0	100	100	8, 25, 38, 50	0
29	C5	59/60 (98%)	-0.11	0	100	100	27, 50, 89, 102	0
30	A6	53/54 (98%)	-0.59	0	100	100	23, 40, 52, 71	0
30	C6	53/54 (98%)	-0.04	0	100	100	39, 60, 78, 103	0
31	A7	48/49 (97%)	-0.45	2 (4%)	40	32	13, 24, 69, 131	1 (2%)
31	C7	48/49 (97%)	-0.17	3 (6%)	26	19	24, 38, 95, 117	0
32	A8	64/65 (98%)	-0.64	0	100	100	16, 28, 43, 60	0
32	C8	64/65 (98%)	0.01	1 (1%)	70	61	36, 52, 72, 80	0
33	A9	37/37 (100%)	-0.50	0	100	100	22, 34, 56, 65	1 (2%)
33	C9	37/37 (100%)	0.92	5 (13%)	7	5	44, 77, 96, 126	0
34	BA	1495/1521 (98%)	0.35	42 (2%)	55	45	30, 82, 185, 333	0
34	DA	1501/1521 (98%)	0.41	80 (5%)	32	24	37, 88, 194, 340	0
35	BB	231/256 (90%)	1.09	37 (16%)	5	4	41, 104, 170, 215	0
35	DB	231/256 (90%)	1.26	51 (22%)	2	2	68, 123, 175, 213	0
36	BC	206/239 (86%)	1.07	30 (14%)	6	4	52, 117, 172, 191	0
36	DC	206/239 (86%)	1.22	37 (17%)	3	3	67, 135, 179, 211	0
37	BD	208/209 (99%)	1.19	44 (21%)	2	2	42, 85, 137, 190	0
37	DD	208/209 (99%)	1.15	33 (15%)	5	4	58, 85, 134, 195	0
38	BE	148/162 (91%)	0.42	3 (2%)	65	56	34, 70, 104, 128	0
38	DE	148/162 (91%)	0.50	5 (3%)	48	39	45, 79, 115, 180	0
39	BF	100/101 (99%)	0.58	2 (2%)	65	56	54, 85, 116, 137	0
39	DF	100/101 (99%)	0.56	2 (2%)	65	56	45, 86, 113, 133	0
40	BG	155/156 (99%)	1.07	25 (16%)	4	4	65, 110, 182, 221	0
40	DG	155/156 (99%)	1.41	41 (26%)	1	1	68, 129, 190, 217	0
41	BH	137/138 (99%)	0.33	2 (1%)	72	63	45, 71, 97, 116	0
41	DH	137/138 (99%)	0.60	3 (2%)	62	52	53, 80, 109, 140	0
42	BI	127/128 (99%)	1.70	46 (36%)	1	0	64, 123, 164, 190	0
42	DI	127/128 (99%)	2.26	64 (50%)	0	0	89, 143, 191, 213	0
43	BJ	97/105 (92%)	1.84	40 (41%)	0	0	80, 128, 182, 213	0
43	DJ	96/105 (91%)	1.90	42 (43%)	0	0	91, 149, 196, 225	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	0.51	9 (7%) 18 13	34, 78, 125, 151	0
44	DK	114/129 (88%)	0.54	5 (4%) 39 31	51, 90, 115, 173	0
45	BL	122/132 (92%)	0.18	4 (3%) 49 39	35, 58, 77, 112	0
45	DL	122/132 (92%)	0.52	7 (5%) 29 22	44, 71, 95, 116	0
46	BM	117/126 (92%)	1.61	32 (27%) 1 1	76, 132, 181, 208	0
46	DM	122/126 (96%)	1.85	37 (30%) 1 1	93, 149, 195, 250	0
47	BN	60/61 (98%)	1.82	24 (40%) 1 0	66, 111, 145, 164	0
47	DN	60/61 (98%)	2.81	41 (68%) 0 0	95, 135, 176, 196	0
48	BO	88/89 (98%)	0.36	3 (3%) 48 39	34, 71, 104, 119	0
48	DO	88/89 (98%)	0.37	3 (3%) 48 39	47, 70, 104, 152	0
49	BP	82/88 (93%)	1.07	11 (13%) 7 5	46, 79, 116, 170	0
49	DP	82/88 (93%)	0.93	9 (10%) 10 8	53, 77, 111, 151	0
50	BQ	99/105 (94%)	0.44	3 (3%) 52 42	41, 70, 98, 122	0
50	DQ	99/105 (94%)	0.51	3 (3%) 52 42	42, 77, 104, 118	0
51	BR	68/88 (77%)	0.34	2 (2%) 53 43	42, 79, 122, 135	0
51	DR	68/88 (77%)	0.52	1 (1%) 72 63	52, 82, 127, 143	0
52	BS	84/93 (90%)	2.22	47 (55%) 0 0	94, 143, 191, 207	0
52	DS	83/93 (89%)	2.22	47 (56%) 0 0	86, 163, 214, 226	0
53	BT	96/106 (90%)	1.01	13 (13%) 7 5	60, 84, 121, 158	0
53	DT	96/106 (90%)	0.84	7 (7%) 21 15	56, 85, 134, 157	0
54	BU	23/27 (85%)	3.08	16 (69%) 0 0	58, 118, 156, 174	0
54	DU	23/27 (85%)	2.87	18 (78%) 0 0	92, 132, 170, 187	0
55	BV	7/18 (38%)	2.44	5 (71%) 0 0	51, 85, 207, 222	0
55	DV	6/18 (33%)	2.65	4 (66%) 0 0	82, 102, 210, 222	0
56	BW	69/76 (90%)	-0.10	2 (2%) 53 43	36, 69, 104, 210	0
56	BY	67/76 (88%)	1.61	18 (26%) 1 1	75, 278, 314, 346	0
56	DW	69/76 (90%)	0.29	4 (5%) 29 22	51, 95, 137, 251	0
56	DY	66/76 (86%)	1.72	17 (25%) 1 1	208, 287, 320, 345	0
57	BZ	730/758 (96%)	0.41	28 (3%) 44 35	35, 77, 134, 188	0
57	DZ	730/758 (96%)	0.82	67 (9%) 14 10	35, 99, 164, 218	0
All	All	22825/23898 (95%)	0.27	1917 (8%) 17 12	5, 69, 186, 352	18 (0%)

The worst 5 of 1917 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	DM	123	ALA	10.9
46	DM	124	PRO	8.7
47	DN	25	VAL	8.6
24	C0	2	ALA	8.5
9	AK	51	LEU	7.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	DY	32	20/21	0.14	0.21	268,268,268,268	0
56	MIA	BY	37	22/30	0.15	0.19	284,284,284,284	0
56	5MU	DY	54	21/22	0.18	0.14	305,305,305,305	1
56	PSU	BY	32	20/21	0.22	0.18	254,254,254,254	1
56	PSU	BY	55	20/21	0.22	0.15	302,302,302,302	1
56	PSU	DY	39	20/21	0.24	0.15	284,284,284,284	0
56	MIA	DY	37	22/30	0.24	0.25	319,319,319,319	1
56	PSU	DY	55	20/21	0.27	0.12	246,246,246,246	0
56	PSU	BY	39	20/21	0.29	0.14	316,316,316,316	0
56	7MG	BY	46	24/25	0.38	0.14	302,302,302,302	0
56	5MU	BY	54	21/22	0.41	0.15	315,315,315,315	0
56	4SU	BY	8	20/21	0.62	0.11	300,300,300,300	0
56	7MG	DY	46	24/25	0.69	0.13	302,302,302,302	0
56	4SU	DY	8	20/21	0.73	0.11	275,275,275,275	0
56	7MG	DW	46	24/25	0.77	0.12	114,114,114,114	2
56	PSU	DW	55	20/21	0.78	0.13	106,106,106,106	2
56	PSU	DW	32	20/21	0.85	0.12	106,106,106,106	1
56	5MU	DW	54	21/22	0.87	0.12	114,114,114,114	1
56	PSU	BW	32	20/21	0.88	0.12	81,81,81,81	1
56	7MG	BW	46	24/25	0.88	0.09	63,63,63,63	5
56	PSU	DW	39	20/21	0.89	0.17	93,93,93,93	3
56	MIA	BW	37	29/30	0.90	0.14	79,79,79,79	2
56	MIA	DW	37	29/30	0.92	0.14	94,94,94,94	0
56	4SU	DW	8	20/21	0.92	0.09	88,88,88,88	3
56	PSU	BW	55	20/21	0.93	0.08	74,74,74,74	5
56	4SU	BW	8	20/21	0.93	0.07	51,51,51,51	6
56	5MU	BW	54	21/22	0.94	0.08	74,74,74,74	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	PSU	BW	39	20/21	0.95	0.10	65,65,65,65	3

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
58	MG	CA	3107	1/1	0.11	0.25	108,108,108,108	0
58	MG	DA	1700	1/1	0.35	0.18	124,124,124,124	0
58	MG	CA	3046	1/1	0.43	0.29	114,114,114,114	0
58	MG	DA	1660	1/1	0.46	0.32	90,90,90,90	0
58	MG	BA	1773	1/1	0.46	0.24	115,115,115,115	0
58	MG	CA	3253	1/1	0.47	0.22	95,95,95,95	0
58	MG	CA	3209	1/1	0.50	0.18	93,93,93,93	0
58	MG	BA	1707	1/1	0.50	0.18	92,92,92,92	0
58	MG	CA	3624	1/1	0.53	0.20	104,104,104,104	0
58	MG	A4	502	1/1	0.54	0.13	123,123,123,123	0
58	MG	AA	3273	1/1	0.55	0.20	90,90,90,90	0
58	MG	BA	1711	1/1	0.55	0.19	104,104,104,104	0
58	MG	CA	3555	1/1	0.56	0.24	83,83,83,83	0
58	MG	DJ	5001	1/1	0.56	0.21	105,105,105,105	0
58	MG	DA	1606	1/1	0.57	0.28	84,84,84,84	0
58	MG	AA	3766	1/1	0.57	0.16	72,72,72,72	0
58	MG	AA	3610	1/1	0.58	0.10	51,51,51,51	1
58	MG	CA	3126	1/1	0.58	0.35	93,93,93,93	0
58	MG	BZ	701	1/1	0.59	0.18	137,137,137,137	0
58	MG	CA	3205	1/1	0.59	0.17	105,105,105,105	0
58	MG	CA	3481	1/1	0.59	0.21	91,91,91,91	0
58	MG	CA	3180	1/1	0.60	0.43	108,108,108,108	0
58	MG	CB	3013	1/1	0.60	0.20	98,98,98,98	0
58	MG	DA	1755	1/1	0.61	0.20	86,86,86,86	0
58	MG	AA	3200	1/1	0.61	0.25	91,91,91,91	0
58	MG	CA	3590	1/1	0.62	0.15	95,95,95,95	0
58	MG	BA	1787	1/1	0.62	0.21	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DZ	701	1/1	0.62	0.18	111,111,111,111	0
58	MG	CA	3618	1/1	0.63	0.19	65,65,65,65	0
58	MG	AA	3758	1/1	0.63	0.24	81,81,81,81	0
58	MG	CA	3513	1/1	0.63	0.14	75,75,75,75	0
58	MG	CA	3507	1/1	0.64	0.16	100,100,100,100	0
58	MG	DA	1657	1/1	0.64	0.13	93,93,93,93	0
58	MG	DA	1754	1/1	0.64	0.21	81,81,81,81	0
58	MG	BA	1697	1/1	0.65	0.21	98,98,98,98	0
58	MG	CA	3071	1/1	0.65	0.35	97,97,97,97	0
58	MG	AA	3265	1/1	0.66	0.36	77,77,77,77	0
58	MG	BA	1618	1/1	0.66	0.21	134,134,134,134	0
58	MG	CA	3314	1/1	0.67	0.22	77,77,77,77	0
58	MG	CA	3002	1/1	0.67	0.20	114,114,114,114	0
58	MG	BA	1807	1/1	0.67	0.13	83,83,83,83	0
58	MG	AA	3268	1/1	0.67	0.22	88,88,88,88	0
58	MG	DA	1677	1/1	0.67	0.14	74,74,74,74	0
58	MG	BA	1626	1/1	0.68	0.23	87,87,87,87	0
58	MG	CA	3544	1/1	0.68	0.12	81,81,81,81	0
58	MG	CA	3080	1/1	0.69	0.37	87,87,87,87	0
58	MG	AA	3613	1/1	0.69	0.15	104,104,104,104	0
58	MG	CA	3593	1/1	0.69	0.14	73,73,73,73	0
58	MG	BA	1691	1/1	0.69	0.17	91,91,91,91	0
58	MG	CA	3620	1/1	0.69	0.15	69,69,69,69	0
58	MG	DA	1673	1/1	0.69	0.31	100,100,100,100	0
58	MG	CA	3056	1/1	0.70	0.24	85,85,85,85	0
58	MG	CA	3537	1/1	0.70	0.18	78,78,78,78	0
58	MG	CA	3295	1/1	0.70	0.11	84,84,84,84	0
58	MG	DA	1706	1/1	0.70	0.28	128,128,128,128	0
58	MG	BA	1617	1/1	0.70	0.12	74,74,74,74	0
58	MG	BA	1636	1/1	0.70	0.33	100,100,100,100	0
58	MG	AB	3018	1/1	0.70	0.14	84,84,84,84	0
58	MG	CA	3594	1/1	0.70	0.22	80,80,80,80	0
58	MG	BA	1661	1/1	0.71	0.28	84,84,84,84	0
58	MG	CA	3460	1/1	0.71	0.30	109,109,109,109	0
58	MG	BA	1713	1/1	0.71	0.33	71,71,71,71	0
58	MG	CG	3001	1/1	0.71	0.21	83,83,83,83	0
58	MG	CA	3610	1/1	0.71	0.21	98,98,98,98	0
58	MG	DA	1623	1/1	0.71	0.14	117,117,117,117	0
58	MG	CA	3616	1/1	0.71	0.20	79,79,79,79	0
58	MG	AA	3751	1/1	0.71	0.21	56,56,56,56	1
58	MG	CA	3300	1/1	0.72	0.19	86,86,86,86	0
58	MG	DA	1720	1/1	0.72	0.18	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3066	1/1	0.72	0.29	84,84,84,84	0
58	MG	BA	1795	1/1	0.73	0.22	86,86,86,86	0
58	MG	DA	1614	1/1	0.73	0.33	87,87,87,87	0
58	MG	AA	3690	1/1	0.73	0.15	71,71,71,71	0
58	MG	DA	1649	1/1	0.73	0.26	93,93,93,93	0
58	MG	CA	3604	1/1	0.73	0.13	69,69,69,69	0
58	MG	CA	3561	1/1	0.73	0.21	95,95,95,95	0
58	MG	DA	1669	1/1	0.73	0.23	84,84,84,84	0
58	MG	CA	3076	1/1	0.73	0.15	84,84,84,84	0
58	MG	CA	3058	1/1	0.74	0.25	77,77,77,77	0
58	MG	CA	3467	1/1	0.74	0.29	80,80,80,80	0
58	MG	AA	3224	1/1	0.74	0.28	75,75,75,75	0
58	MG	AA	3744	1/1	0.74	0.15	86,86,86,86	0
58	MG	AB	3021	1/1	0.74	0.15	61,61,61,61	0
58	MG	AA	3192	1/1	0.74	0.27	76,76,76,76	0
58	MG	AA	3108	1/1	0.74	0.38	125,125,125,125	0
58	MG	BA	1692	1/1	0.74	0.21	89,89,89,89	0
58	MG	CA	3389	1/1	0.74	0.21	75,75,75,75	0
58	MG	CA	3553	1/1	0.75	0.11	81,81,81,81	0
58	MG	AA	3672	1/1	0.75	0.19	25,25,25,25	1
58	MG	CA	3621	1/1	0.75	0.19	73,73,73,73	0
58	MG	BA	1768	1/1	0.75	0.15	86,86,86,86	0
58	MG	CA	3571	1/1	0.75	0.13	65,65,65,65	0
58	MG	CA	3220	1/1	0.75	0.22	78,78,78,78	0
58	MG	BA	1616	1/1	0.75	0.26	88,88,88,88	0
58	MG	CA	3286	1/1	0.75	0.15	64,64,64,64	0
58	MG	AA	3626	1/1	0.75	0.22	74,74,74,74	0
58	MG	CA	3008	1/1	0.75	0.36	100,100,100,100	0
58	MG	CA	3202	1/1	0.75	0.33	77,77,77,77	0
58	MG	BA	1683	1/1	0.76	0.32	84,84,84,84	0
58	MG	AA	3112	1/1	0.76	0.35	98,98,98,98	0
58	MG	BV	101	1/1	0.76	0.21	110,110,110,110	0
58	MG	BA	1721	1/1	0.76	0.18	80,80,80,80	0
58	MG	AQ	201	1/1	0.76	0.23	62,62,62,62	0
58	MG	AA	3621	1/1	0.76	0.15	46,46,46,46	0
58	MG	CA	3016	1/1	0.76	0.24	80,80,80,80	0
58	MG	CA	3290	1/1	0.76	0.31	75,75,75,75	0
58	MG	CA	3294	1/1	0.76	0.11	83,83,83,83	0
58	MG	CA	3644	1/1	0.76	0.32	84,84,84,84	0
58	MG	BA	1669	1/1	0.76	0.11	89,89,89,89	0
58	MG	CA	3139	1/1	0.76	0.22	123,123,123,123	0
58	MG	CA	3140	1/1	0.76	0.32	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3388	1/1	0.76	0.15	83,83,83,83	0
58	MG	AA	3248	1/1	0.77	0.18	64,64,64,64	0
58	MG	CA	3596	1/1	0.77	0.17	72,72,72,72	0
58	MG	CA	3070	1/1	0.77	0.37	87,87,87,87	0
58	MG	CA	3212	1/1	0.77	0.17	69,69,69,69	0
58	MG	AA	3784	1/1	0.77	0.17	74,74,74,74	0
58	MG	AB	3017	1/1	0.77	0.11	77,77,77,77	0
58	MG	BA	1748	1/1	0.77	0.11	83,83,83,83	0
58	MG	DA	1678	1/1	0.77	0.22	82,82,82,82	0
58	MG	DA	1687	1/1	0.77	0.14	100,100,100,100	0
58	MG	A8	5001	1/1	0.77	0.17	59,59,59,59	0
58	MG	DA	1701	1/1	0.77	0.22	63,63,63,63	0
58	MG	CA	3125	1/1	0.77	0.29	73,73,73,73	0
58	MG	DA	1715	1/1	0.77	0.13	76,76,76,76	0
58	MG	BA	1653	1/1	0.77	0.18	102,102,102,102	0
58	MG	DA	1746	1/1	0.77	0.14	91,91,91,91	0
58	MG	CA	3042	1/1	0.77	0.26	95,95,95,95	0
58	MG	BA	1777	1/1	0.77	0.14	75,75,75,75	0
58	MG	BA	1704	1/1	0.77	0.29	89,89,89,89	0
58	MG	AA	3623	1/1	0.77	0.15	74,74,74,74	0
58	MG	AA	3771	1/1	0.78	0.21	31,31,31,31	1
58	MG	BA	1736	1/1	0.78	0.14	81,81,81,81	0
58	MG	CA	3304	1/1	0.78	0.15	93,93,93,93	0
58	MG	BA	1802	1/1	0.78	0.12	84,84,84,84	0
58	MG	AA	3375	1/1	0.78	0.19	57,57,57,57	0
58	MG	CB	3006	1/1	0.78	0.12	83,83,83,83	0
58	MG	BA	1758	1/1	0.78	0.14	68,68,68,68	0
58	MG	CD	302	1/1	0.78	0.25	95,95,95,95	0
58	MG	CA	3131	1/1	0.78	0.19	62,62,62,62	0
58	MG	CA	3267	1/1	0.78	0.14	56,56,56,56	0
58	MG	AA	3028	1/1	0.78	0.27	51,51,51,51	1
58	MG	CA	3485	1/1	0.78	0.20	83,83,83,83	0
58	MG	CA	3500	1/1	0.78	0.18	64,64,64,64	0
58	MG	DA	1765	1/1	0.78	0.17	95,95,95,95	0
58	MG	AA	3640	1/1	0.78	0.34	77,77,77,77	0
58	MG	BA	1720	1/1	0.78	0.19	83,83,83,83	0
58	MG	CA	3155	1/1	0.79	0.10	86,86,86,86	0
58	MG	BA	1813	1/1	0.79	0.24	75,75,75,75	0
58	MG	AA	3321	1/1	0.79	0.20	70,70,70,70	0
58	MG	CA	3634	1/1	0.79	0.17	81,81,81,81	0
58	MG	AA	3094	1/1	0.79	0.70	111,111,111,111	0
58	MG	CA	3001	1/1	0.79	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3583	1/1	0.79	0.13	78,78,78,78	1
58	MG	AA	3476	1/1	0.79	0.15	69,69,69,69	0
58	MG	CA	3093	1/1	0.79	0.22	84,84,84,84	0
58	MG	AA	3728	1/1	0.79	0.18	61,61,61,61	0
58	MG	BA	1658	1/1	0.79	0.23	90,90,90,90	0
58	MG	AA	3242	1/1	0.79	0.28	72,72,72,72	0
58	MG	DA	1639	1/1	0.79	0.28	75,75,75,75	0
58	MG	AA	3803	1/1	0.79	0.14	62,62,62,62	0
58	MG	AB	3004	1/1	0.79	0.28	89,89,89,89	0
58	MG	AB	3014	1/1	0.79	0.15	67,67,67,67	0
58	MG	CQ	205	1/1	0.80	0.21	81,81,81,81	0
58	MG	CA	3323	1/1	0.80	0.14	67,67,67,67	0
58	MG	CA	3357	1/1	0.80	0.11	80,80,80,80	0
58	MG	AA	3630	1/1	0.80	0.26	71,71,71,71	0
58	MG	BA	1665	1/1	0.80	0.13	79,79,79,79	0
58	MG	CA	3431	1/1	0.80	0.19	100,100,100,100	0
58	MG	CA	3031	1/1	0.80	0.13	76,76,76,76	0
58	MG	CA	3123	1/1	0.80	0.20	88,88,88,88	0
58	MG	CA	3246	1/1	0.80	0.22	59,59,59,59	0
58	MG	AD	311	1/1	0.80	0.19	57,57,57,57	0
58	MG	DA	1676	1/1	0.80	0.11	78,78,78,78	0
58	MG	BA	1670	1/1	0.80	0.18	83,83,83,83	0
58	MG	CA	3272	1/1	0.80	0.23	75,75,75,75	0
58	MG	BA	1673	1/1	0.80	0.22	75,75,75,75	0
58	MG	AA	3697	1/1	0.80	0.15	63,63,63,63	0
58	MG	AA	3105	1/1	0.80	0.16	81,81,81,81	0
58	MG	CA	3646	1/1	0.80	0.12	95,95,95,95	0
58	MG	DA	1708	1/1	0.80	0.14	87,87,87,87	0
58	MG	CA	3656	1/1	0.80	0.18	61,61,61,61	0
58	MG	CB	3001	1/1	0.80	0.20	99,99,99,99	0
58	MG	DA	1730	1/1	0.80	0.15	88,88,88,88	0
58	MG	CB	3002	1/1	0.80	0.12	66,66,66,66	0
58	MG	DA	1753	1/1	0.80	0.15	70,70,70,70	0
58	MG	BA	1649	1/1	0.80	0.07	75,75,75,75	0
58	MG	AA	3732	1/1	0.80	0.12	68,68,68,68	0
58	MG	CA	3190	1/1	0.80	0.23	83,83,83,83	0
58	MG	AA	3464	1/1	0.80	0.13	63,63,63,63	0
58	MG	CQ	201	1/1	0.80	0.16	62,62,62,62	0
61	FUA	BZ	703	37/37	0.80	0.18	69,69,69,69	0
58	MG	CA	3631	1/1	0.81	0.14	77,77,77,77	0
58	MG	DA	1665	1/1	0.81	0.28	61,61,61,61	0
58	MG	AA	3597	1/1	0.81	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3270	1/1	0.81	0.15	54,54,54,54	0
58	MG	CA	3034	1/1	0.81	0.26	101,101,101,101	0
58	MG	CA	3653	1/1	0.81	0.25	95,95,95,95	0
58	MG	CA	3097	1/1	0.81	0.14	80,80,80,80	0
58	MG	DA	1685	1/1	0.81	0.24	65,65,65,65	0
58	MG	CA	3661	1/1	0.81	0.20	74,74,74,74	0
58	MG	DA	1692	1/1	0.81	0.15	76,76,76,76	0
58	MG	CA	3105	1/1	0.81	0.12	80,80,80,80	0
58	MG	A7	106	1/1	0.81	0.28	38,38,38,38	1
58	MG	CA	3122	1/1	0.81	0.16	67,67,67,67	0
58	MG	CA	3045	1/1	0.81	0.21	67,67,67,67	0
58	MG	AA	3774	1/1	0.81	0.17	80,80,80,80	0
58	MG	DA	1716	1/1	0.81	0.18	78,78,78,78	0
58	MG	BA	1605	1/1	0.81	0.21	67,67,67,67	0
58	MG	CO	202	1/1	0.81	0.10	53,53,53,53	0
58	MG	DA	1731	1/1	0.81	0.21	82,82,82,82	0
58	MG	DA	1737	1/1	0.81	0.13	72,72,72,72	0
58	MG	AA	3164	1/1	0.81	0.12	58,58,58,58	0
58	MG	CA	3134	1/1	0.81	0.34	86,86,86,86	0
58	MG	CA	3493	1/1	0.81	0.18	88,88,88,88	0
58	MG	AA	3016	1/1	0.81	0.20	59,59,59,59	0
58	MG	AA	3807	1/1	0.81	0.18	62,62,62,62	1
58	MG	BA	1625	1/1	0.81	0.12	65,65,65,65	0
58	MG	CA	3528	1/1	0.81	0.25	79,79,79,79	0
58	MG	CA	3533	1/1	0.81	0.11	81,81,81,81	0
58	MG	CA	3441	1/1	0.82	0.26	77,77,77,77	0
58	MG	DA	1641	1/1	0.82	0.09	77,77,77,77	0
58	MG	CA	3607	1/1	0.82	0.18	97,97,97,97	0
58	MG	CA	3444	1/1	0.82	0.17	91,91,91,91	0
58	MG	AB	3006	1/1	0.82	0.19	72,72,72,72	0
58	MG	CA	3090	1/1	0.82	0.29	65,65,65,65	0
58	MG	BA	1652	1/1	0.82	0.23	72,72,72,72	0
58	MG	CA	3094	1/1	0.82	0.23	87,87,87,87	0
58	MG	AA	3460	1/1	0.82	0.21	72,72,72,72	0
58	MG	BA	1694	1/1	0.82	0.22	86,86,86,86	0
58	MG	AA	3733	1/1	0.82	0.13	68,68,68,68	0
58	MG	CA	3641	1/1	0.82	0.21	67,67,67,67	0
58	MG	BA	1701	1/1	0.82	0.19	75,75,75,75	0
58	MG	DA	1691	1/1	0.82	0.09	85,85,85,85	0
58	MG	BA	1624	1/1	0.82	0.30	75,75,75,75	0
58	MG	AA	3221	1/1	0.82	0.16	56,56,56,56	0
58	MG	BA	1789	1/1	0.82	0.16	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3543	1/1	0.82	0.13	63,63,63,63	0
58	MG	BA	1710	1/1	0.82	0.13	79,79,79,79	0
58	MG	AA	3026	1/1	0.82	0.19	86,86,86,86	0
58	MG	BA	1804	1/1	0.82	0.12	68,68,68,68	1
58	MG	AD	307	1/1	0.82	0.17	53,53,53,53	1
58	MG	DA	1722	1/1	0.82	0.13	65,65,65,65	0
58	MG	CA	3569	1/1	0.82	0.19	79,79,79,79	0
58	MG	CA	3145	1/1	0.82	0.14	79,79,79,79	0
58	MG	BA	1717	1/1	0.82	0.16	83,83,83,83	0
58	MG	CA	3585	1/1	0.82	0.16	78,78,78,78	0
58	MG	BD	502	1/1	0.82	0.26	82,82,82,82	0
58	MG	DA	1603	1/1	0.82	0.16	74,74,74,74	0
58	MG	BA	1640	1/1	0.82	0.36	78,78,78,78	0
58	MG	DA	1607	1/1	0.82	0.18	61,61,61,61	0
58	MG	CA	3421	1/1	0.82	0.21	76,76,76,76	0
58	MG	DW	503	1/1	0.82	0.19	84,84,84,84	0
58	MG	DA	1622	1/1	0.82	0.27	77,77,77,77	0
58	MG	CA	3077	1/1	0.82	0.20	66,66,66,66	0
58	MG	AA	3575	1/1	0.83	0.10	69,69,69,69	0
58	MG	AA	3283	1/1	0.83	0.30	62,62,62,62	0
58	MG	DA	1640	1/1	0.83	0.13	79,79,79,79	0
58	MG	CA	3363	1/1	0.83	0.11	66,66,66,66	0
58	MG	CA	3059	1/1	0.83	0.19	60,60,60,60	0
58	MG	DA	1652	1/1	0.83	0.18	71,71,71,71	0
58	MG	AA	3696	1/1	0.83	0.14	69,69,69,69	0
58	MG	CA	3152	1/1	0.83	0.15	56,56,56,56	0
58	MG	DA	1663	1/1	0.83	0.13	72,72,72,72	0
58	MG	AA	3193	1/1	0.83	0.25	62,62,62,62	0
58	MG	BA	1629	1/1	0.83	0.22	87,87,87,87	0
58	MG	CA	3073	1/1	0.83	0.21	91,91,91,91	0
58	MG	BA	1632	1/1	0.83	0.11	63,63,63,63	0
58	MG	BL	201	1/1	0.83	0.09	80,80,80,80	0
58	MG	AA	3801	1/1	0.83	0.15	88,88,88,88	0
58	MG	AA	3645	1/1	0.83	0.23	79,79,79,79	0
58	MG	CA	3636	1/1	0.83	0.11	80,80,80,80	0
58	MG	DA	1690	1/1	0.83	0.23	82,82,82,82	0
58	MG	CA	3489	1/1	0.83	0.22	80,80,80,80	0
58	MG	BA	1646	1/1	0.83	0.19	75,75,75,75	0
58	MG	CA	3235	1/1	0.83	0.27	75,75,75,75	0
58	MG	CA	3649	1/1	0.83	0.24	85,85,85,85	0
58	MG	CA	3241	1/1	0.83	0.28	107,107,107,107	0
58	MG	CA	3243	1/1	0.83	0.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	1709	1/1	0.83	0.20	72,72,72,72	0
58	MG	CA	3525	1/1	0.83	0.18	83,83,83,83	0
58	MG	CA	3245	1/1	0.83	0.22	57,57,57,57	0
58	MG	BA	1759	1/1	0.83	0.23	65,65,65,65	0
58	MG	BA	1647	1/1	0.83	0.08	61,61,61,61	0
58	MG	CB	3010	1/1	0.83	0.13	55,55,55,55	0
58	MG	CA	3098	1/1	0.83	0.13	83,83,83,83	0
58	MG	BA	1612	1/1	0.83	0.08	79,79,79,79	0
58	MG	CA	3273	1/1	0.83	0.16	69,69,69,69	0
58	MG	CA	3024	1/1	0.83	0.36	88,88,88,88	0
58	MG	CA	3113	1/1	0.83	0.21	92,92,92,92	0
58	MG	BA	1774	1/1	0.83	0.11	70,70,70,70	0
58	MG	DA	1763	1/1	0.83	0.13	77,77,77,77	0
58	MG	AB	3023	1/1	0.83	0.33	76,76,76,76	0
58	MG	CA	3581	1/1	0.83	0.11	81,81,81,81	0
58	MG	BA	1785	1/1	0.83	0.24	69,69,69,69	0
58	MG	AA	3760	1/1	0.83	0.10	27,27,27,27	0
58	MG	BA	1655	1/1	0.83	0.26	78,78,78,78	0
61	FUA	DZ	703	37/37	0.83	0.18	85,85,85,85	0
58	MG	BA	1737	1/1	0.84	0.29	72,72,72,72	0
58	MG	BA	1747	1/1	0.84	0.17	66,66,66,66	0
58	MG	CA	3619	1/1	0.84	0.20	47,47,47,47	1
58	MG	CA	3230	1/1	0.84	0.25	51,51,51,51	0
58	MG	CA	3095	1/1	0.84	0.18	64,64,64,64	0
58	MG	AA	3041	1/1	0.84	0.23	75,75,75,75	0
58	MG	DA	1672	1/1	0.84	0.31	73,73,73,73	0
58	MG	BA	1750	1/1	0.84	0.13	84,84,84,84	0
58	MG	AA	3362	1/1	0.84	0.19	69,69,69,69	0
58	MG	BA	1675	1/1	0.84	0.32	77,77,77,77	0
58	MG	AA	3599	1/1	0.84	0.16	58,58,58,58	0
58	MG	CA	3255	1/1	0.84	0.21	67,67,67,67	0
58	MG	CA	3645	1/1	0.84	0.14	82,82,82,82	0
58	MG	CA	3032	1/1	0.84	0.32	67,67,67,67	0
58	MG	AA	3227	1/1	0.84	0.14	55,55,55,55	0
58	MG	CA	3536	1/1	0.84	0.13	71,71,71,71	0
58	MG	AA	3611	1/1	0.84	0.16	51,51,51,51	0
58	MG	CA	3660	1/1	0.84	0.34	101,101,101,101	0
58	MG	CA	3538	1/1	0.84	0.09	71,71,71,71	0
58	MG	CA	3540	1/1	0.84	0.22	85,85,85,85	0
58	MG	AA	3775	1/1	0.84	0.09	45,45,45,45	0
58	MG	DA	1711	1/1	0.84	0.11	45,45,45,45	0
58	MG	AZ	301	1/1	0.84	0.15	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3779	1/1	0.84	0.12	62,62,62,62	0
58	MG	BA	1648	1/1	0.84	0.33	75,75,75,75	0
58	MG	AA	3443	1/1	0.84	0.19	65,65,65,65	0
58	MG	AA	3710	1/1	0.84	0.20	75,75,75,75	0
58	MG	AA	3458	1/1	0.84	0.15	72,72,72,72	0
58	MG	CA	3574	1/1	0.84	0.08	72,72,72,72	0
58	MG	DA	1739	1/1	0.84	0.19	79,79,79,79	0
58	MG	AA	3204	1/1	0.84	0.20	57,57,57,57	0
58	MG	DA	1749	1/1	0.84	0.23	80,80,80,80	0
58	MG	DA	1751	1/1	0.84	0.19	81,81,81,81	0
58	MG	CA	3159	1/1	0.84	0.14	69,69,69,69	0
58	MG	CA	3178	1/1	0.84	0.17	57,57,57,57	0
58	MG	AA	3244	1/1	0.84	0.22	100,100,100,100	0
58	MG	AA	3739	1/1	0.84	0.27	94,94,94,94	0
58	MG	CA	3396	1/1	0.84	0.14	58,58,58,58	0
58	MG	CA	3199	1/1	0.84	0.25	74,74,74,74	0
58	MG	CA	3599	1/1	0.84	0.13	80,80,80,80	0
58	MG	AA	3096	1/1	0.84	0.19	63,63,63,63	0
58	MG	BM	202	1/1	0.84	0.10	65,65,65,65	0
58	MG	AA	3639	1/1	0.84	0.14	77,77,77,77	0
58	MG	CA	3049	1/1	0.85	0.20	81,81,81,81	0
58	MG	CA	3052	1/1	0.85	0.23	69,69,69,69	0
58	MG	AA	3434	1/1	0.85	0.08	17,17,17,17	0
58	MG	AA	3814	1/1	0.85	0.11	93,93,93,93	0
58	MG	AA	3649	1/1	0.85	0.14	92,92,92,92	0
58	MG	CA	3133	1/1	0.85	0.16	69,69,69,69	0
58	MG	CA	3062	1/1	0.85	0.11	68,68,68,68	0
58	MG	BA	1662	1/1	0.85	0.15	70,70,70,70	0
58	MG	A5	105	1/1	0.85	0.14	60,60,60,60	0
58	MG	AA	3713	1/1	0.85	0.26	52,52,52,52	1
58	MG	AA	3720	1/1	0.85	0.23	77,77,77,77	0
58	MG	CA	3153	1/1	0.85	0.23	78,78,78,78	0
58	MG	AA	3652	1/1	0.85	0.12	77,77,77,77	0
58	MG	DA	1696	1/1	0.85	0.11	91,91,91,91	0
58	MG	CA	3158	1/1	0.85	0.21	70,70,70,70	0
58	MG	BA	1786	1/1	0.85	0.14	60,60,60,60	0
58	MG	AA	3656	1/1	0.85	0.13	56,56,56,56	0
58	MG	CA	3081	1/1	0.85	0.10	68,68,68,68	0
58	MG	CA	3563	1/1	0.85	0.12	91,91,91,91	0
58	MG	CA	3189	1/1	0.85	0.10	68,68,68,68	0
58	MG	CA	3373	1/1	0.85	0.26	58,58,58,58	0
58	MG	CE	306	1/1	0.85	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3374	1/1	0.85	0.14	76,76,76,76	0
58	MG	CA	3579	1/1	0.85	0.11	51,51,51,51	0
58	MG	DA	1725	1/1	0.85	0.12	70,70,70,70	0
58	MG	CA	3378	1/1	0.85	0.14	84,84,84,84	0
58	MG	CA	3088	1/1	0.85	0.41	75,75,75,75	0
58	MG	DA	1733	1/1	0.85	0.15	83,83,83,83	0
58	MG	CA	3018	1/1	0.85	0.29	64,64,64,64	0
58	MG	DA	1604	1/1	0.85	0.29	76,76,76,76	0
58	MG	BA	1679	1/1	0.85	0.18	87,87,87,87	0
58	MG	DA	1748	1/1	0.85	0.13	78,78,78,78	0
58	MG	CA	3402	1/1	0.85	0.10	70,70,70,70	0
58	MG	CA	3407	1/1	0.85	0.12	55,55,55,55	0
58	MG	BA	1793	1/1	0.85	0.10	63,63,63,63	0
58	MG	AA	3017	1/1	0.85	0.19	78,78,78,78	0
58	MG	DA	1634	1/1	0.85	0.18	90,90,90,90	0
58	MG	CA	3033	1/1	0.85	0.30	89,89,89,89	0
58	MG	BA	1800	1/1	0.85	0.13	69,69,69,69	0
58	MG	CA	3223	1/1	0.85	0.32	65,65,65,65	0
58	MG	DK	5001	1/1	0.85	0.06	100,100,100,100	0
58	MG	AA	3689	1/1	0.85	0.11	55,55,55,55	1
58	MG	CA	3477	1/1	0.85	0.13	74,74,74,74	0
58	MG	AA	3067	1/1	0.85	0.17	55,55,55,55	0
58	MG	AA	3547	1/1	0.85	0.11	31,31,31,31	0
58	MG	AA	3657	1/1	0.86	0.14	43,43,43,43	1
58	MG	AA	3665	1/1	0.86	0.21	85,85,85,85	0
58	MG	CA	3395	1/1	0.86	0.21	65,65,65,65	0
58	MG	BA	1663	1/1	0.86	0.18	82,82,82,82	0
58	MG	AA	3445	1/1	0.86	0.19	75,75,75,75	0
58	MG	CA	3406	1/1	0.86	0.10	70,70,70,70	0
58	MG	BA	1739	1/1	0.86	0.18	63,63,63,63	0
58	MG	AA	3590	1/1	0.86	0.13	69,69,69,69	0
58	MG	BA	1620	1/1	0.86	0.19	57,57,57,57	0
58	MG	CA	3440	1/1	0.86	0.16	57,57,57,57	0
58	MG	CA	3208	1/1	0.86	0.20	84,84,84,84	0
58	MG	CA	3085	1/1	0.86	0.17	66,66,66,66	0
58	MG	AA	3596	1/1	0.86	0.19	40,40,40,40	0
58	MG	AA	3636	1/1	0.86	0.15	65,65,65,65	0
58	MG	CA	3004	1/1	0.86	0.29	64,64,64,64	0
58	MG	DA	1684	1/1	0.86	0.33	72,72,72,72	0
58	MG	CA	3005	1/1	0.86	0.20	59,59,59,59	0
58	MG	DA	1686	1/1	0.86	0.11	53,53,53,53	0
58	MG	CA	3633	1/1	0.86	0.16	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AB	3019	1/1	0.86	0.10	65,65,65,65	0
58	MG	CA	3635	1/1	0.86	0.09	79,79,79,79	0
58	MG	CA	3010	1/1	0.86	0.08	41,41,41,41	0
58	MG	CA	3492	1/1	0.86	0.21	105,105,105,105	0
58	MG	CA	3642	1/1	0.86	0.45	80,80,80,80	0
58	MG	AA	3767	1/1	0.86	0.13	63,63,63,63	1
58	MG	CA	3499	1/1	0.86	0.20	83,83,83,83	0
58	MG	CA	3099	1/1	0.86	0.16	92,92,92,92	0
58	MG	AA	3638	1/1	0.86	0.21	72,72,72,72	0
58	MG	CA	3512	1/1	0.86	0.26	65,65,65,65	0
58	MG	AA	3448	1/1	0.86	0.18	78,78,78,78	0
58	MG	BA	1775	1/1	0.86	0.15	78,78,78,78	0
58	MG	CA	3115	1/1	0.86	0.22	76,76,76,76	0
58	MG	CA	3532	1/1	0.86	0.09	79,79,79,79	0
58	MG	AA	3360	1/1	0.86	0.16	114,114,114,114	0
58	MG	CB	3003	1/1	0.86	0.13	77,77,77,77	0
58	MG	CB	3005	1/1	0.86	0.14	62,62,62,62	0
58	MG	BA	1784	1/1	0.86	0.09	50,50,50,50	0
58	MG	CA	3285	1/1	0.86	0.19	57,57,57,57	0
58	MG	AA	3057	1/1	0.86	0.20	57,57,57,57	0
58	MG	DA	1740	1/1	0.86	0.12	81,81,81,81	0
58	MG	CA	3037	1/1	0.86	0.12	58,58,58,58	0
58	MG	AA	3274	1/1	0.86	0.16	55,55,55,55	0
58	MG	CA	3043	1/1	0.86	0.37	102,102,102,102	0
58	MG	DA	1750	1/1	0.86	0.21	68,68,68,68	0
58	MG	AA	3788	1/1	0.86	0.16	58,58,58,58	1
58	MG	AA	3731	1/1	0.86	0.12	42,42,42,42	0
58	MG	CA	3557	1/1	0.86	0.09	76,76,76,76	0
58	MG	DA	1602	1/1	0.86	0.11	80,80,80,80	0
58	MG	BA	1791	1/1	0.86	0.15	68,68,68,68	0
58	MG	BA	1792	1/1	0.86	0.10	72,72,72,72	0
58	MG	DA	1768	1/1	0.86	0.19	73,73,73,73	0
58	MG	AA	3269	1/1	0.86	0.18	84,84,84,84	0
58	MG	AA	3806	1/1	0.86	0.14	61,61,61,61	0
58	MG	AA	3065	1/1	0.86	0.22	48,48,48,48	0
58	MG	BA	1607	1/1	0.86	0.07	67,67,67,67	0
58	MG	CA	3375	1/1	0.86	0.20	71,71,71,71	0
58	MG	BA	1718	1/1	0.86	0.11	67,67,67,67	0
58	MG	AN	3001	1/1	0.87	0.17	85,85,85,85	0
58	MG	AA	3018	1/1	0.87	0.70	78,78,78,78	0
58	MG	AB	3001	1/1	0.87	0.23	87,87,87,87	0
58	MG	AB	3002	1/1	0.87	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3385	1/1	0.87	0.18	64,64,64,64	0
58	MG	CA	3067	1/1	0.87	0.21	72,72,72,72	0
58	MG	CA	3546	1/1	0.87	0.12	119,119,119,119	0
58	MG	CA	3221	1/1	0.87	0.15	54,54,54,54	0
58	MG	AA	3107	1/1	0.87	0.20	76,76,76,76	0
58	MG	AA	3438	1/1	0.87	0.15	57,57,57,57	0
58	MG	CA	3662	1/1	0.87	0.19	55,55,55,55	0
58	MG	CA	3132	1/1	0.87	0.07	30,30,30,30	0
58	MG	CA	3237	1/1	0.87	0.23	75,75,75,75	0
58	MG	CA	3568	1/1	0.87	0.13	41,41,41,41	0
58	MG	AA	3201	1/1	0.87	0.24	65,65,65,65	0
58	MG	CA	3412	1/1	0.87	0.17	81,81,81,81	0
58	MG	CB	3007	1/1	0.87	0.17	65,65,65,65	0
58	MG	AA	3781	1/1	0.87	0.19	44,44,44,44	1
58	MG	AA	3633	1/1	0.87	0.16	48,48,48,48	1
58	MG	BA	1732	1/1	0.87	0.10	78,78,78,78	0
58	MG	CA	3141	1/1	0.87	0.14	54,54,54,54	0
58	MG	BA	1680	1/1	0.87	0.22	69,69,69,69	0
58	MG	BA	1611	1/1	0.87	0.11	69,69,69,69	0
58	MG	BA	1684	1/1	0.87	0.12	69,69,69,69	0
58	MG	BA	1689	1/1	0.87	0.21	72,72,72,72	0
58	MG	CA	3595	1/1	0.87	0.10	53,53,53,53	0
58	MG	CA	3283	1/1	0.87	0.14	60,60,60,60	0
58	MG	CA	3484	1/1	0.87	0.15	76,76,76,76	0
58	MG	BA	1803	1/1	0.87	0.19	69,69,69,69	0
58	MG	BA	1690	1/1	0.87	0.33	70,70,70,70	0
58	MG	CA	3172	1/1	0.87	0.24	83,83,83,83	0
58	MG	DA	1619	1/1	0.87	0.14	71,71,71,71	0
58	MG	AA	3755	1/1	0.87	0.09	63,63,63,63	0
58	MG	BA	1755	1/1	0.87	0.09	94,94,94,94	0
58	MG	DA	1630	1/1	0.87	0.16	61,61,61,61	0
58	MG	AA	3059	1/1	0.87	0.12	51,51,51,51	0
58	MG	DA	1636	1/1	0.87	0.29	70,70,70,70	0
58	MG	AA	3367	1/1	0.87	0.10	52,52,52,52	0
58	MG	CA	3508	1/1	0.87	0.13	96,96,96,96	0
58	MG	CA	3194	1/1	0.87	0.30	72,72,72,72	0
58	MG	DA	1647	1/1	0.87	0.21	58,58,58,58	0
58	MG	CA	3625	1/1	0.87	0.15	79,79,79,79	0
58	MG	AA	3578	1/1	0.87	0.10	55,55,55,55	0
58	MG	CA	3350	1/1	0.87	0.10	85,85,85,85	0
58	MG	DA	1658	1/1	0.87	0.20	72,72,72,72	0
58	MG	AA	3682	1/1	0.87	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3360	1/1	0.87	0.09	49,49,49,49	0
58	MG	CA	3204	1/1	0.87	0.17	74,74,74,74	0
58	MG	AA	3049	1/1	0.88	0.13	52,52,52,52	0
58	MG	CA	3100	1/1	0.88	0.24	79,79,79,79	0
58	MG	AA	3573	1/1	0.88	0.09	50,50,50,50	0
58	MG	AD	308	1/1	0.88	0.17	73,73,73,73	0
58	MG	AA	3136	1/1	0.88	0.10	52,52,52,52	0
58	MG	AA	3029	1/1	0.88	0.13	53,53,53,53	0
58	MG	AA	3589	1/1	0.88	0.16	21,21,21,21	1
58	MG	CA	3292	1/1	0.88	0.10	73,73,73,73	0
58	MG	AA	3080	1/1	0.88	0.22	57,57,57,57	0
58	MG	DA	1628	1/1	0.88	0.29	74,74,74,74	0
58	MG	AZ	302	1/1	0.88	0.13	68,68,68,68	0
58	MG	AA	3230	1/1	0.88	0.38	80,80,80,80	0
58	MG	AA	3674	1/1	0.88	0.15	75,75,75,75	0
58	MG	DA	1637	1/1	0.88	0.11	76,76,76,76	0
58	MG	DA	1638	1/1	0.88	0.22	83,83,83,83	0
58	MG	BA	1756	1/1	0.88	0.08	98,98,98,98	0
58	MG	AA	3027	1/1	0.88	0.39	77,77,77,77	0
58	MG	AA	3109	1/1	0.88	0.10	50,50,50,50	0
58	MG	CA	3577	1/1	0.88	0.11	83,83,83,83	0
58	MG	BA	1601	1/1	0.88	0.10	58,58,58,58	0
58	MG	CA	3035	1/1	0.88	0.28	60,60,60,60	0
58	MG	AA	3600	1/1	0.88	0.10	60,60,60,60	0
58	MG	AA	3794	1/1	0.88	0.13	58,58,58,58	1
58	MG	BA	1608	1/1	0.88	0.11	74,74,74,74	0
58	MG	AA	3795	1/1	0.88	0.20	68,68,68,68	1
58	MG	CA	3154	1/1	0.88	0.26	72,72,72,72	0
58	MG	BA	1781	1/1	0.88	0.10	46,46,46,46	1
58	MG	CA	3386	1/1	0.88	0.14	65,65,65,65	0
58	MG	AA	3605	1/1	0.88	0.13	68,68,68,68	0
58	MG	BA	1686	1/1	0.88	0.13	81,81,81,81	0
58	MG	CA	3165	1/1	0.88	0.12	62,62,62,62	0
58	MG	CA	3609	1/1	0.88	0.20	76,76,76,76	0
58	MG	AA	3455	1/1	0.88	0.17	58,58,58,58	0
58	MG	CA	3173	1/1	0.88	0.18	65,65,65,65	0
58	MG	AA	3704	1/1	0.88	0.14	59,59,59,59	0
58	MG	CA	3179	1/1	0.88	0.27	75,75,75,75	0
58	MG	AA	3245	1/1	0.88	0.21	69,69,69,69	0
58	MG	CA	3420	1/1	0.88	0.17	71,71,71,71	0
58	MG	CA	3060	1/1	0.88	0.23	77,77,77,77	0
58	MG	BA	1790	1/1	0.88	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	1698	1/1	0.88	0.25	68,68,68,68	0
58	MG	CA	3432	1/1	0.88	0.18	61,61,61,61	0
58	MG	CA	3436	1/1	0.88	0.09	75,75,75,75	0
58	MG	CA	3063	1/1	0.88	0.15	53,53,53,53	0
58	MG	DA	1707	1/1	0.88	0.11	87,87,87,87	0
58	MG	AA	3339	1/1	0.88	0.14	43,43,43,43	0
58	MG	AA	3461	1/1	0.88	0.16	66,66,66,66	0
58	MG	CA	3447	1/1	0.88	0.18	80,80,80,80	0
58	MG	CA	3454	1/1	0.88	0.12	81,81,81,81	0
58	MG	BA	1695	1/1	0.88	0.15	67,67,67,67	0
58	MG	AA	3246	1/1	0.88	0.19	72,72,72,72	0
58	MG	BA	1799	1/1	0.88	0.10	63,63,63,63	0
58	MG	CA	3075	1/1	0.88	0.19	71,71,71,71	0
58	MG	BA	1699	1/1	0.88	0.17	78,78,78,78	0
58	MG	BA	1700	1/1	0.88	0.30	74,74,74,74	0
58	MG	DA	1732	1/1	0.88	0.17	76,76,76,76	0
58	MG	AA	3111	1/1	0.88	0.17	48,48,48,48	0
58	MG	BA	1628	1/1	0.88	0.18	75,75,75,75	0
58	MG	CA	3226	1/1	0.88	0.21	69,69,69,69	0
58	MG	AA	3477	1/1	0.88	0.10	58,58,58,58	0
58	MG	CA	3233	1/1	0.88	0.26	71,71,71,71	0
58	MG	CA	3506	1/1	0.88	0.10	58,58,58,58	0
58	MG	BA	1809	1/1	0.88	0.18	83,83,83,83	0
58	MG	CA	3236	1/1	0.88	0.12	87,87,87,87	0
58	MG	AA	3480	1/1	0.88	0.09	54,54,54,54	0
58	MG	CA	3091	1/1	0.88	0.26	111,111,111,111	0
58	MG	CA	3515	1/1	0.88	0.11	79,79,79,79	0
58	MG	AA	3489	1/1	0.88	0.11	64,64,64,64	0
58	MG	CE	303	1/1	0.88	0.15	54,54,54,54	0
58	MG	CE	304	1/1	0.88	0.24	68,68,68,68	0
58	MG	CA	3527	1/1	0.88	0.08	78,78,78,78	0
58	MG	AA	3510	1/1	0.88	0.19	58,58,58,58	0
58	MG	AA	3526	1/1	0.88	0.08	20,20,20,20	0
58	MG	CP	203	1/1	0.88	0.14	67,67,67,67	0
58	MG	BT	3001	1/1	0.88	0.17	62,62,62,62	0
58	MG	CQ	203	1/1	0.88	0.16	67,67,67,67	0
58	MG	AA	3538	1/1	0.88	0.19	61,61,61,61	1
58	MG	CA	3257	1/1	0.89	0.30	57,57,57,57	0
58	MG	C5	101	1/1	0.89	0.28	65,65,65,65	0
58	MG	CA	3263	1/1	0.89	0.12	57,57,57,57	0
58	MG	BA	1667	1/1	0.89	0.12	55,55,55,55	0
58	MG	CA	3116	1/1	0.89	0.18	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1668	1/1	0.89	0.31	75,75,75,75	0
58	MG	AA	3263	1/1	0.89	0.17	80,80,80,80	0
58	MG	AA	3430	1/1	0.89	0.12	44,44,44,44	0
58	MG	BA	1672	1/1	0.89	0.22	92,92,92,92	0
58	MG	CA	3545	1/1	0.89	0.13	68,68,68,68	0
58	MG	AA	3282	1/1	0.89	0.25	40,40,40,40	0
58	MG	DA	1625	1/1	0.89	0.29	73,73,73,73	0
58	MG	AA	3264	1/1	0.89	0.11	62,62,62,62	0
58	MG	AA	3804	1/1	0.89	0.15	68,68,68,68	0
58	MG	AA	3442	1/1	0.89	0.12	49,49,49,49	0
58	MG	DA	1635	1/1	0.89	0.12	65,65,65,65	0
58	MG	AA	3319	1/1	0.89	0.09	69,69,69,69	0
58	MG	AA	3212	1/1	0.89	0.17	34,34,34,34	1
58	MG	BA	1685	1/1	0.89	0.20	69,69,69,69	0
58	MG	BA	1779	1/1	0.89	0.14	79,79,79,79	0
58	MG	AA	3580	1/1	0.89	0.08	23,23,23,23	0
58	MG	BA	1782	1/1	0.89	0.13	81,81,81,81	0
58	MG	AA	3736	1/1	0.89	0.12	78,78,78,78	0
58	MG	CA	3053	1/1	0.89	0.18	58,58,58,58	0
58	MG	AA	3586	1/1	0.89	0.11	62,62,62,62	0
58	MG	AB	3005	1/1	0.89	0.23	69,69,69,69	0
58	MG	AA	3647	1/1	0.89	0.18	72,72,72,72	0
58	MG	CA	3586	1/1	0.89	0.08	69,69,69,69	0
58	MG	CA	3376	1/1	0.89	0.13	66,66,66,66	0
58	MG	DA	1664	1/1	0.89	0.15	64,64,64,64	0
58	MG	CA	3168	1/1	0.89	0.27	56,56,56,56	0
58	MG	BA	1693	1/1	0.89	0.34	74,74,74,74	0
58	MG	DA	1671	1/1	0.89	0.25	83,83,83,83	0
58	MG	AA	3336	1/1	0.89	0.11	54,54,54,54	0
58	MG	CA	3387	1/1	0.89	0.12	70,70,70,70	0
58	MG	CA	3174	1/1	0.89	0.30	61,61,61,61	0
58	MG	AB	3015	1/1	0.89	0.10	40,40,40,40	0
58	MG	AA	3199	1/1	0.89	0.19	54,54,54,54	0
58	MG	BA	1698	1/1	0.89	0.16	68,68,68,68	0
58	MG	CA	3401	1/1	0.89	0.11	69,69,69,69	0
58	MG	CA	3611	1/1	0.89	0.22	91,91,91,91	0
58	MG	CA	3614	1/1	0.89	0.09	52,52,52,52	0
58	MG	CA	3183	1/1	0.89	0.50	86,86,86,86	0
58	MG	AA	3354	1/1	0.89	0.16	60,60,60,60	0
58	MG	BA	1797	1/1	0.89	0.16	69,69,69,69	0
58	MG	BA	1635	1/1	0.89	0.22	62,62,62,62	0
58	MG	CA	3196	1/1	0.89	0.34	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3074	1/1	0.89	0.16	53,53,53,53	0
58	MG	AA	3355	1/1	0.89	0.11	58,58,58,58	0
58	MG	DA	1703	1/1	0.89	0.16	74,74,74,74	0
58	MG	CA	3628	1/1	0.89	0.16	66,66,66,66	0
58	MG	AA	3765	1/1	0.89	0.13	63,63,63,63	0
58	MG	BA	1706	1/1	0.89	0.11	61,61,61,61	0
58	MG	AA	3356	1/1	0.89	0.10	35,35,35,35	0
58	MG	AA	3463	1/1	0.89	0.10	46,46,46,46	0
58	MG	CA	3210	1/1	0.89	0.24	75,75,75,75	0
58	MG	CA	3082	1/1	0.89	0.12	70,70,70,70	0
58	MG	DA	1718	1/1	0.89	0.09	77,77,77,77	0
58	MG	AA	3770	1/1	0.89	0.26	37,37,37,37	0
58	MG	BA	1811	1/1	0.89	0.09	68,68,68,68	0
58	MG	CA	3089	1/1	0.89	0.20	80,80,80,80	0
58	MG	DA	1726	1/1	0.89	0.13	77,77,77,77	0
58	MG	CA	3469	1/1	0.89	0.11	69,69,69,69	0
58	MG	CA	3470	1/1	0.89	0.15	72,72,72,72	0
58	MG	AA	3174	1/1	0.89	0.20	63,63,63,63	0
58	MG	CA	3228	1/1	0.89	0.15	63,63,63,63	0
58	MG	CA	3483	1/1	0.89	0.21	69,69,69,69	0
58	MG	BA	1716	1/1	0.89	0.14	88,88,88,88	0
58	MG	CA	3231	1/1	0.89	0.29	57,57,57,57	0
58	MG	AA	3679	1/1	0.89	0.11	65,65,65,65	0
58	MG	AA	3606	1/1	0.89	0.21	61,61,61,61	0
58	MG	BA	1719	1/1	0.89	0.09	44,44,44,44	0
58	MG	AA	3778	1/1	0.89	0.10	54,54,54,54	0
58	MG	AA	3015	1/1	0.89	0.31	64,64,64,64	0
58	MG	CA	3505	1/1	0.89	0.14	73,73,73,73	0
58	MG	AA	3365	1/1	0.89	0.19	57,57,57,57	0
58	MG	CA	3244	1/1	0.89	0.27	78,78,78,78	0
58	MG	A5	102	1/1	0.89	0.30	88,88,88,88	0
58	MG	AA	3133	1/1	0.89	0.17	69,69,69,69	0
58	MG	CA	3248	1/1	0.89	0.24	77,77,77,77	0
58	MG	CA	3252	1/1	0.89	0.16	64,64,64,64	0
58	MG	CA	3516	1/1	0.89	0.11	62,62,62,62	0
58	MG	DW	502	1/1	0.89	0.13	84,84,84,84	0
58	MG	CA	3523	1/1	0.89	0.11	40,40,40,40	0
58	MG	AA	3370	1/1	0.89	0.22	58,58,58,58	0
58	MG	BA	1744	1/1	0.89	0.13	79,79,79,79	0
58	MG	CA	3256	1/1	0.89	0.13	40,40,40,40	0
58	MG	CA	3393	1/1	0.90	0.08	82,82,82,82	0
58	MG	DA	1626	1/1	0.90	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1722	1/1	0.90	0.16	62,62,62,62	0
58	MG	BA	1727	1/1	0.90	0.11	59,59,59,59	0
58	MG	CA	3399	1/1	0.90	0.13	75,75,75,75	0
58	MG	AA	3309	1/1	0.90	0.18	44,44,44,44	0
58	MG	BA	1733	1/1	0.90	0.18	63,63,63,63	0
58	MG	CA	3405	1/1	0.90	0.17	91,91,91,91	0
58	MG	AA	3310	1/1	0.90	0.11	58,58,58,58	0
58	MG	AA	3462	1/1	0.90	0.27	71,71,71,71	0
58	MG	CA	3409	1/1	0.90	0.12	40,40,40,40	0
58	MG	AA	3232	1/1	0.90	0.18	79,79,79,79	0
58	MG	DA	1642	1/1	0.90	0.11	66,66,66,66	0
58	MG	CA	3413	1/1	0.90	0.10	39,39,39,39	0
58	MG	BA	1606	1/1	0.90	0.15	65,65,65,65	0
58	MG	BA	1671	1/1	0.90	0.22	73,73,73,73	0
58	MG	DA	1653	1/1	0.90	0.10	60,60,60,60	0
58	MG	CA	3424	1/1	0.90	0.10	55,55,55,55	0
58	MG	CA	3426	1/1	0.90	0.14	55,55,55,55	0
58	MG	DA	1659	1/1	0.90	0.12	64,64,64,64	0
58	MG	CA	3428	1/1	0.90	0.18	54,54,54,54	1
58	MG	CA	3429	1/1	0.90	0.17	74,74,74,74	0
58	MG	AA	3184	1/1	0.90	0.17	68,68,68,68	0
58	MG	AA	3738	1/1	0.90	0.10	75,75,75,75	0
58	MG	CA	3433	1/1	0.90	0.15	71,71,71,71	0
58	MG	AA	3811	1/1	0.90	0.13	58,58,58,58	0
58	MG	AA	3415	1/1	0.90	0.06	56,56,56,56	0
58	MG	BA	1614	1/1	0.90	0.08	75,75,75,75	0
58	MG	DA	1674	1/1	0.90	0.11	62,62,62,62	0
58	MG	CA	3025	1/1	0.90	0.14	77,77,77,77	0
58	MG	AA	3743	1/1	0.90	0.14	80,80,80,80	0
58	MG	CA	3622	1/1	0.90	0.11	55,55,55,55	0
58	MG	CA	3239	1/1	0.90	0.24	75,75,75,75	0
58	MG	CA	3117	1/1	0.90	0.20	68,68,68,68	0
58	MG	AA	3139	1/1	0.90	0.07	58,58,58,58	0
58	MG	AA	3747	1/1	0.90	0.15	58,58,58,58	0
58	MG	AA	3750	1/1	0.90	0.08	24,24,24,24	0
58	MG	BA	1687	1/1	0.90	0.19	50,50,50,50	0
58	MG	CA	3478	1/1	0.90	0.10	58,58,58,58	0
58	MG	CA	3480	1/1	0.90	0.17	55,55,55,55	0
58	MG	CA	3127	1/1	0.90	0.12	63,63,63,63	0
58	MG	CA	3482	1/1	0.90	0.16	70,70,70,70	0
58	MG	CA	3128	1/1	0.90	0.23	71,71,71,71	0
58	MG	DA	1702	1/1	0.90	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1688	1/1	0.90	0.20	52,52,52,52	0
58	MG	AA	3163	1/1	0.90	0.18	40,40,40,40	0
58	MG	AA	3660	1/1	0.90	0.14	70,70,70,70	0
58	MG	AA	3437	1/1	0.90	0.12	54,54,54,54	0
58	MG	CA	3137	1/1	0.90	0.32	73,73,73,73	0
58	MG	CA	3498	1/1	0.90	0.17	68,68,68,68	0
58	MG	AA	3491	1/1	0.90	0.14	35,35,35,35	0
58	MG	AA	3762	1/1	0.90	0.13	53,53,53,53	1
58	MG	CA	3663	1/1	0.90	0.21	91,91,91,91	0
58	MG	AA	3345	1/1	0.90	0.08	68,68,68,68	0
58	MG	BA	1633	1/1	0.90	0.09	48,48,48,48	0
58	MG	CA	3284	1/1	0.90	0.15	92,92,92,92	0
58	MG	CB	3004	1/1	0.90	0.13	68,68,68,68	0
58	MG	AA	3024	1/1	0.90	0.11	57,57,57,57	0
58	MG	CA	3057	1/1	0.90	0.12	49,49,49,49	0
58	MG	AA	3010	1/1	0.90	0.26	68,68,68,68	0
58	MG	BA	1638	1/1	0.90	0.14	64,64,64,64	0
58	MG	DA	1736	1/1	0.90	0.07	79,79,79,79	0
58	MG	CA	3157	1/1	0.90	0.11	55,55,55,55	0
58	MG	AD	305	1/1	0.90	0.20	63,63,63,63	0
58	MG	AA	3252	1/1	0.90	0.13	66,66,66,66	0
58	MG	DA	1744	1/1	0.90	0.13	79,79,79,79	0
58	MG	AA	3625	1/1	0.90	0.10	60,60,60,60	0
58	MG	CA	3167	1/1	0.90	0.12	60,60,60,60	0
58	MG	AA	3695	1/1	0.90	0.17	78,78,78,78	0
58	MG	CA	3341	1/1	0.90	0.17	71,71,71,71	0
58	MG	AA	3563	1/1	0.90	0.10	49,49,49,49	1
58	MG	AA	3446	1/1	0.90	0.19	61,61,61,61	0
58	MG	AA	3632	1/1	0.90	0.11	76,76,76,76	0
58	MG	CA	3072	1/1	0.90	0.14	56,56,56,56	0
58	MG	DA	1757	1/1	0.90	0.15	75,75,75,75	0
58	MG	DA	1761	1/1	0.90	0.17	66,66,66,66	0
58	MG	BA	1654	1/1	0.90	0.07	69,69,69,69	0
58	MG	AA	3708	1/1	0.90	0.22	53,53,53,53	1
58	MG	DA	1766	1/1	0.90	0.09	58,58,58,58	0
58	MG	A0	103	1/1	0.90	0.07	37,37,37,37	0
58	MG	DF	3001	1/1	0.90	0.12	49,49,49,49	0
58	MG	BA	1660	1/1	0.90	0.29	76,76,76,76	0
58	MG	AA	3260	1/1	0.90	0.22	71,71,71,71	0
58	MG	CA	3079	1/1	0.90	0.16	57,57,57,57	0
58	MG	AA	3178	1/1	0.90	0.13	78,78,78,78	0
58	MG	BB	3001	1/1	0.90	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3364	1/1	0.90	0.24	81,81,81,81	0
58	MG	BK	201	1/1	0.90	0.11	57,57,57,57	0
58	MG	BA	1619	1/1	0.91	0.08	73,73,73,73	0
58	MG	CA	3269	1/1	0.91	0.10	86,86,86,86	0
58	MG	CA	3514	1/1	0.91	0.22	105,105,105,105	0
58	MG	CA	3114	1/1	0.91	0.17	39,39,39,39	0
58	MG	AA	3802	1/1	0.91	0.15	55,55,55,55	0
58	MG	CA	3518	1/1	0.91	0.19	86,86,86,86	0
58	MG	AA	3698	1/1	0.91	0.18	32,32,32,32	1
58	MG	AA	3702	1/1	0.91	0.19	35,35,35,35	1
58	MG	BA	1702	1/1	0.91	0.17	61,61,61,61	0
58	MG	AA	3186	1/1	0.91	0.11	37,37,37,37	0
58	MG	DA	1613	1/1	0.91	0.19	72,72,72,72	0
58	MG	BA	1627	1/1	0.91	0.25	57,57,57,57	0
58	MG	AA	3358	1/1	0.91	0.16	63,63,63,63	0
58	MG	CA	3534	1/1	0.91	0.11	79,79,79,79	0
58	MG	AA	3062	1/1	0.91	0.23	67,67,67,67	0
58	MG	BA	1630	1/1	0.91	0.23	55,55,55,55	0
58	MG	AA	3095	1/1	0.91	0.21	82,82,82,82	0
58	MG	CA	3302	1/1	0.91	0.19	68,68,68,68	0
58	MG	CA	3541	1/1	0.91	0.10	71,71,71,71	0
58	MG	DA	1632	1/1	0.91	0.20	61,61,61,61	0
58	MG	AA	3718	1/1	0.91	0.08	43,43,43,43	0
58	MG	AA	3194	1/1	0.91	0.16	44,44,44,44	0
58	MG	AA	3237	1/1	0.91	0.17	71,71,71,71	0
58	MG	BA	1637	1/1	0.91	0.22	72,72,72,72	0
58	MG	CA	3551	1/1	0.91	0.11	88,88,88,88	0
58	MG	AA	3729	1/1	0.91	0.07	38,38,38,38	0
58	MG	AA	3070	1/1	0.91	0.21	60,60,60,60	0
58	MG	BA	1644	1/1	0.91	0.23	69,69,69,69	0
58	MG	CA	3030	1/1	0.91	0.19	57,57,57,57	1
58	MG	DA	1643	1/1	0.91	0.09	55,55,55,55	0
58	MG	BA	1725	1/1	0.91	0.16	71,71,71,71	0
58	MG	BA	1726	1/1	0.91	0.08	64,64,64,64	0
58	MG	AA	3165	1/1	0.91	0.20	57,57,57,57	0
58	MG	AA	3493	1/1	0.91	0.08	30,30,30,30	1
58	MG	AA	3100	1/1	0.91	0.18	53,53,53,53	0
58	MG	CA	3379	1/1	0.91	0.09	65,65,65,65	0
58	MG	AA	3203	1/1	0.91	0.21	46,46,46,46	1
58	MG	CA	3039	1/1	0.91	0.40	71,71,71,71	0
58	MG	BA	1651	1/1	0.91	0.19	68,68,68,68	0
58	MG	CA	3166	1/1	0.91	0.19	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3531	1/1	0.91	0.15	62,62,62,62	0
58	MG	DA	1668	1/1	0.91	0.28	62,62,62,62	0
58	MG	AA	3247	1/1	0.91	0.13	63,63,63,63	0
58	MG	CA	3591	1/1	0.91	0.10	83,83,83,83	0
58	MG	AA	3317	1/1	0.91	0.09	58,58,58,58	0
58	MG	AA	3642	1/1	0.91	0.07	49,49,49,49	0
58	MG	CA	3398	1/1	0.91	0.09	65,65,65,65	0
58	MG	DA	1675	1/1	0.91	0.17	74,74,74,74	0
58	MG	CA	3051	1/1	0.91	0.23	63,63,63,63	0
58	MG	CA	3598	1/1	0.91	0.08	73,73,73,73	0
58	MG	AA	3558	1/1	0.91	0.10	51,51,51,51	0
58	MG	DA	1679	1/1	0.91	0.22	58,58,58,58	0
58	MG	CA	3601	1/1	0.91	0.10	75,75,75,75	0
58	MG	CA	3603	1/1	0.91	0.09	51,51,51,51	0
58	MG	BA	1659	1/1	0.91	0.16	73,73,73,73	0
58	MG	AA	3561	1/1	0.91	0.13	58,58,58,58	0
58	MG	AA	3436	1/1	0.91	0.10	38,38,38,38	0
58	MG	CA	3185	1/1	0.91	0.24	59,59,59,59	0
58	MG	AE	302	1/1	0.91	0.17	69,69,69,69	0
58	MG	BA	1761	1/1	0.91	0.10	63,63,63,63	0
58	MG	DA	1697	1/1	0.91	0.19	62,62,62,62	0
58	MG	CA	3192	1/1	0.91	0.12	58,58,58,58	0
58	MG	CA	3414	1/1	0.91	0.10	50,50,50,50	0
58	MG	CA	3418	1/1	0.91	0.11	41,41,41,41	0
58	MG	BA	1762	1/1	0.91	0.09	89,89,89,89	0
58	MG	BA	1767	1/1	0.91	0.08	61,61,61,61	0
58	MG	DA	1705	1/1	0.91	0.12	62,62,62,62	0
58	MG	CA	3197	1/1	0.91	0.23	64,64,64,64	0
58	MG	AH	3002	1/1	0.91	0.19	74,74,74,74	0
58	MG	AA	3756	1/1	0.91	0.15	40,40,40,40	1
58	MG	BA	1666	1/1	0.91	0.12	59,59,59,59	0
58	MG	CA	3069	1/1	0.91	0.20	81,81,81,81	0
58	MG	DA	1713	1/1	0.91	0.20	72,72,72,72	0
58	MG	AA	3177	1/1	0.91	0.24	61,61,61,61	0
58	MG	AW	3001	1/1	0.91	0.21	52,52,52,52	0
58	MG	AW	3004	1/1	0.91	0.18	65,65,65,65	0
58	MG	AY	502	1/1	0.91	0.14	58,58,58,58	0
58	MG	CA	3216	1/1	0.91	0.10	66,66,66,66	0
58	MG	AA	3249	1/1	0.91	0.09	24,24,24,24	1
58	MG	AA	3208	1/1	0.91	0.15	61,61,61,61	0
58	MG	AA	3338	1/1	0.91	0.06	30,30,30,30	0
58	MG	CA	3224	1/1	0.91	0.39	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3661	1/1	0.91	0.17	43,43,43,43	0
58	MG	BA	1676	1/1	0.91	0.11	68,68,68,68	0
58	MG	DA	1735	1/1	0.91	0.19	83,83,83,83	0
58	MG	AA	3258	1/1	0.91	0.05	22,22,22,22	0
58	MG	CA	3657	1/1	0.91	0.14	67,67,67,67	0
58	MG	DA	1738	1/1	0.91	0.15	80,80,80,80	0
58	MG	AA	3343	1/1	0.91	0.13	65,65,65,65	0
58	MG	AA	3673	1/1	0.91	0.17	67,67,67,67	0
58	MG	AA	3344	1/1	0.91	0.09	84,84,84,84	0
58	MG	CA	3086	1/1	0.91	0.12	36,36,36,36	0
58	MG	CA	3087	1/1	0.91	0.12	67,67,67,67	0
58	MG	AA	3678	1/1	0.91	0.12	31,31,31,31	0
58	MG	AA	3450	1/1	0.91	0.14	53,53,53,53	0
58	MG	AA	3002	1/1	0.91	0.17	55,55,55,55	0
58	MG	CA	3488	1/1	0.91	0.09	51,51,51,51	0
58	MG	AA	3457	1/1	0.91	0.12	67,67,67,67	0
58	MG	AA	3349	1/1	0.91	0.09	40,40,40,40	0
58	MG	CB	3009	1/1	0.91	0.12	67,67,67,67	0
58	MG	DA	1759	1/1	0.91	0.12	76,76,76,76	0
58	MG	DA	1760	1/1	0.91	0.23	66,66,66,66	0
58	MG	BA	1610	1/1	0.91	0.14	60,60,60,60	0
58	MG	CB	3012	1/1	0.91	0.18	76,76,76,76	0
58	MG	AA	3785	1/1	0.91	0.11	72,72,72,72	0
58	MG	CD	301	1/1	0.91	0.27	81,81,81,81	0
58	MG	DA	1767	1/1	0.91	0.09	74,74,74,74	0
58	MG	AA	3694	1/1	0.91	0.09	45,45,45,45	0
58	MG	DD	502	1/1	0.91	0.29	62,62,62,62	0
58	MG	DE	202	1/1	0.91	0.08	94,94,94,94	0
58	MG	BA	1805	1/1	0.91	0.10	64,64,64,64	0
58	MG	AA	3604	1/1	0.91	0.11	38,38,38,38	1
58	MG	AA	3091	1/1	0.91	0.12	38,38,38,38	1
58	MG	CF	301	1/1	0.91	0.14	63,63,63,63	0
58	MG	CF	303	1/1	0.91	0.17	62,62,62,62	0
58	MG	AA	3797	1/1	0.91	0.13	15,15,15,15	1
58	MG	CO	201	1/1	0.91	0.11	64,64,64,64	0
58	MG	AA	3223	1/1	0.91	0.12	35,35,35,35	0
58	MG	AA	3019	1/1	0.92	0.10	58,58,58,58	0
58	MG	CA	3006	1/1	0.92	0.21	67,67,67,67	0
58	MG	AA	3271	1/1	0.92	0.24	69,69,69,69	0
58	MG	BA	1703	1/1	0.92	0.29	58,58,58,58	0
58	MG	CA	3013	1/1	0.92	0.08	63,63,63,63	0
58	MG	CA	3430	1/1	0.92	0.19	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3772	1/1	0.92	0.23	17,17,17,17	1
58	MG	CA	3171	1/1	0.92	0.14	55,55,55,55	0
58	MG	CB	3008	1/1	0.92	0.10	59,59,59,59	0
58	MG	AA	3773	1/1	0.92	0.18	30,30,30,30	1
58	MG	CA	3020	1/1	0.92	0.08	63,63,63,63	0
58	MG	AA	3492	1/1	0.92	0.14	45,45,45,45	0
58	MG	BA	1708	1/1	0.92	0.18	62,62,62,62	0
58	MG	CA	3442	1/1	0.92	0.22	67,67,67,67	0
58	MG	CA	3027	1/1	0.92	0.13	44,44,44,44	0
58	MG	AA	3272	1/1	0.92	0.21	52,52,52,52	0
58	MG	CA	3181	1/1	0.92	0.20	47,47,47,47	0
58	MG	AA	3068	1/1	0.92	0.17	65,65,65,65	0
58	MG	CA	3465	1/1	0.92	0.21	66,66,66,66	0
58	MG	AA	3518	1/1	0.92	0.08	33,33,33,33	0
58	MG	CF	304	1/1	0.92	0.14	65,65,65,65	0
58	MG	CA	3468	1/1	0.92	0.11	61,61,61,61	0
58	MG	CN	5001	1/1	0.92	0.07	77,77,77,77	0
58	MG	AA	3122	1/1	0.92	0.12	54,54,54,54	0
58	MG	AA	3783	1/1	0.92	0.08	54,54,54,54	0
58	MG	CA	3472	1/1	0.92	0.33	72,72,72,72	0
58	MG	CA	3473	1/1	0.92	0.08	54,54,54,54	0
58	MG	CA	3191	1/1	0.92	0.29	65,65,65,65	0
58	MG	AA	3658	1/1	0.92	0.17	62,62,62,62	0
58	MG	CV	201	1/1	0.92	0.29	100,100,100,100	0
58	MG	AA	3368	1/1	0.92	0.06	37,37,37,37	0
58	MG	C8	5001	1/1	0.92	0.12	51,51,51,51	0
58	MG	AA	3537	1/1	0.92	0.08	95,95,95,95	0
58	MG	CA	3040	1/1	0.92	0.15	66,66,66,66	0
58	MG	AA	3236	1/1	0.92	0.11	57,57,57,57	0
58	MG	CA	3200	1/1	0.92	0.16	54,54,54,54	0
58	MG	AA	3182	1/1	0.92	0.16	76,76,76,76	0
58	MG	DA	1609	1/1	0.92	0.18	46,46,46,46	0
58	MG	AA	3548	1/1	0.92	0.09	57,57,57,57	1
58	MG	AA	3799	1/1	0.92	0.12	47,47,47,47	0
58	MG	CA	3207	1/1	0.92	0.14	71,71,71,71	0
58	MG	AA	3382	1/1	0.92	0.07	36,36,36,36	1
58	MG	CA	3494	1/1	0.92	0.12	63,63,63,63	0
58	MG	CA	3495	1/1	0.92	0.12	65,65,65,65	0
58	MG	AA	3286	1/1	0.92	0.08	52,52,52,52	0
58	MG	AA	3426	1/1	0.92	0.09	50,50,50,50	0
58	MG	AA	3292	1/1	0.92	0.13	74,74,74,74	0
58	MG	DA	1631	1/1	0.92	0.18	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3501	1/1	0.92	0.12	45,45,45,45	1
58	MG	DA	1633	1/1	0.92	0.27	73,73,73,73	0
58	MG	CA	3054	1/1	0.92	0.16	71,71,71,71	0
58	MG	CA	3217	1/1	0.92	0.16	52,52,52,52	0
58	MG	AA	3686	1/1	0.92	0.11	73,73,73,73	0
58	MG	BA	1643	1/1	0.92	0.24	71,71,71,71	0
58	MG	BA	1741	1/1	0.92	0.07	93,93,93,93	0
58	MG	AA	3294	1/1	0.92	0.13	66,66,66,66	0
58	MG	AA	3809	1/1	0.92	0.18	62,62,62,62	0
58	MG	CA	3227	1/1	0.92	0.14	53,53,53,53	0
58	MG	AA	3123	1/1	0.92	0.13	37,37,37,37	1
58	MG	AA	3579	1/1	0.92	0.07	38,38,38,38	0
58	MG	CA	3522	1/1	0.92	0.14	56,56,56,56	0
58	MG	DA	1648	1/1	0.92	0.14	50,50,50,50	0
58	MG	AA	3060	1/1	0.92	0.33	65,65,65,65	0
58	MG	DA	1650	1/1	0.92	0.22	61,61,61,61	0
58	MG	BA	1650	1/1	0.92	0.12	37,37,37,37	0
58	MG	AA	3312	1/1	0.92	0.09	55,55,55,55	0
58	MG	AA	3316	1/1	0.92	0.19	60,60,60,60	0
58	MG	CA	3531	1/1	0.92	0.10	51,51,51,51	0
58	MG	AA	3073	1/1	0.92	0.13	58,58,58,58	0
58	MG	AA	3701	1/1	0.92	0.23	43,43,43,43	1
58	MG	DA	1662	1/1	0.92	0.15	64,64,64,64	0
58	MG	CA	3240	1/1	0.92	0.12	64,64,64,64	0
58	MG	BA	1766	1/1	0.92	0.22	63,63,63,63	0
58	MG	AB	3009	1/1	0.92	0.07	56,56,56,56	0
58	MG	AA	3591	1/1	0.92	0.14	65,65,65,65	0
58	MG	CA	3539	1/1	0.92	0.22	73,73,73,73	0
58	MG	AA	3592	1/1	0.92	0.15	52,52,52,52	0
58	MG	AA	3706	1/1	0.92	0.14	27,27,27,27	1
58	MG	CA	3542	1/1	0.92	0.22	68,68,68,68	0
58	MG	AA	3138	1/1	0.92	0.19	50,50,50,50	0
58	MG	AA	3052	1/1	0.92	0.34	65,65,65,65	0
58	MG	AA	3447	1/1	0.92	0.09	61,61,61,61	0
58	MG	CA	3254	1/1	0.92	0.09	42,42,42,42	0
58	MG	CA	3549	1/1	0.92	0.07	57,57,57,57	0
58	MG	BA	1664	1/1	0.92	0.13	53,53,53,53	0
58	MG	CA	3552	1/1	0.92	0.09	69,69,69,69	0
58	MG	CA	3084	1/1	0.92	0.19	59,59,59,59	1
58	MG	AA	3715	1/1	0.92	0.12	66,66,66,66	0
58	MG	CA	3556	1/1	0.92	0.09	48,48,48,48	0
58	MG	DA	1689	1/1	0.92	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3143	1/1	0.92	0.13	47,47,47,47	0
58	MG	AA	3148	1/1	0.92	0.13	68,68,68,68	0
58	MG	CA	3562	1/1	0.92	0.14	76,76,76,76	0
58	MG	AA	3451	1/1	0.92	0.13	48,48,48,48	0
58	MG	CA	3567	1/1	0.92	0.12	56,56,56,56	0
58	MG	AA	3452	1/1	0.92	0.12	69,69,69,69	0
58	MG	AA	3151	1/1	0.92	0.14	50,50,50,50	0
58	MG	AF	307	1/1	0.92	0.11	62,62,62,62	0
58	MG	AA	3456	1/1	0.92	0.08	30,30,30,30	0
58	MG	AA	3256	1/1	0.92	0.09	21,21,21,21	1
58	MG	CA	3578	1/1	0.92	0.13	80,80,80,80	0
58	MG	BA	1674	1/1	0.92	0.14	61,61,61,61	0
58	MG	CA	3096	1/1	0.92	0.20	68,68,68,68	0
58	MG	BA	1794	1/1	0.92	0.19	75,75,75,75	0
58	MG	AA	3616	1/1	0.92	0.10	28,28,28,28	0
58	MG	DA	1710	1/1	0.92	0.12	70,70,70,70	0
58	MG	AA	3618	1/1	0.92	0.09	38,38,38,38	0
58	MG	BA	1677	1/1	0.92	0.12	57,57,57,57	0
58	MG	CA	3103	1/1	0.92	0.22	62,62,62,62	0
58	MG	CA	3592	1/1	0.92	0.21	76,76,76,76	0
58	MG	AA	3620	1/1	0.92	0.13	40,40,40,40	0
58	MG	CA	3310	1/1	0.92	0.09	48,48,48,48	0
58	MG	BA	1801	1/1	0.92	0.10	65,65,65,65	0
58	MG	CA	3109	1/1	0.92	0.09	54,54,54,54	0
58	MG	CA	3327	1/1	0.92	0.14	53,53,53,53	0
58	MG	CA	3340	1/1	0.92	0.09	48,48,48,48	0
58	MG	CA	3111	1/1	0.92	0.05	71,71,71,71	0
58	MG	CA	3602	1/1	0.92	0.09	66,66,66,66	0
58	MG	CA	3343	1/1	0.92	0.07	36,36,36,36	0
58	MG	AA	3741	1/1	0.92	0.13	34,34,34,34	1
58	MG	AA	3155	1/1	0.92	0.10	64,64,64,64	0
58	MG	AA	3158	1/1	0.92	0.19	97,97,97,97	0
58	MG	AA	3624	1/1	0.92	0.08	65,65,65,65	0
58	MG	CA	3365	1/1	0.92	0.10	48,48,48,48	0
58	MG	A2	101	1/1	0.92	0.08	35,35,35,35	0
58	MG	DA	1742	1/1	0.92	0.15	79,79,79,79	0
58	MG	DA	1743	1/1	0.92	0.17	72,72,72,72	0
58	MG	CA	3118	1/1	0.92	0.12	57,57,57,57	0
58	MG	CA	3121	1/1	0.92	0.09	45,45,45,45	0
58	MG	BA	1808	1/1	0.92	0.13	81,81,81,81	0
58	MG	A2	102	1/1	0.92	0.10	54,54,54,54	0
58	MG	AA	3347	1/1	0.92	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1812	1/1	0.92	0.11	66,66,66,66	0
58	MG	AA	3348	1/1	0.92	0.07	32,32,32,32	0
58	MG	AA	3752	1/1	0.92	0.14	72,72,72,72	0
58	MG	AA	3629	1/1	0.92	0.14	61,61,61,61	0
58	MG	AA	3159	1/1	0.92	0.24	46,46,46,46	1
58	MG	AA	3088	1/1	0.92	0.09	34,34,34,34	0
58	MG	BL	202	1/1	0.92	0.15	67,67,67,67	0
58	MG	CA	3135	1/1	0.92	0.17	66,66,66,66	0
58	MG	BA	1603	1/1	0.92	0.13	93,93,93,93	0
58	MG	BN	502	1/1	0.92	0.09	66,66,66,66	0
58	MG	AA	3468	1/1	0.92	0.18	52,52,52,52	0
58	MG	CA	3643	1/1	0.92	0.07	76,76,76,76	0
58	MG	BA	1696	1/1	0.92	0.08	80,80,80,80	0
58	MG	BW	501	1/1	0.92	0.22	48,48,48,48	0
58	MG	DE	201	1/1	0.92	0.16	84,84,84,84	0
58	MG	CA	3147	1/1	0.92	0.21	76,76,76,76	0
58	MG	CA	3148	1/1	0.92	0.18	65,65,65,65	0
58	MG	CA	3651	1/1	0.92	0.09	31,31,31,31	0
58	MG	CA	3150	1/1	0.92	0.07	54,54,54,54	0
58	MG	AA	3042	1/1	0.92	0.18	38,38,38,38	0
58	MG	BZ	702	1/1	0.92	0.18	46,46,46,46	0
58	MG	AA	3092	1/1	0.92	0.11	53,53,53,53	0
58	MG	AA	3479	1/1	0.92	0.10	54,54,54,54	0
58	MG	AA	3171	1/1	0.92	0.16	25,25,25,25	1
62	GDP	DZ	704	28/28	0.92	0.10	80,80,80,80	3
58	MG	CA	3535	1/1	0.93	0.17	69,69,69,69	0
58	MG	AA	3352	1/1	0.93	0.10	51,51,51,51	0
58	MG	AA	3699	1/1	0.93	0.14	46,46,46,46	1
58	MG	CA	3347	1/1	0.93	0.13	59,59,59,59	0
58	MG	CA	3161	1/1	0.93	0.13	66,66,66,66	0
58	MG	AA	3622	1/1	0.93	0.07	45,45,45,45	0
58	MG	CA	3358	1/1	0.93	0.14	45,45,45,45	0
58	MG	DA	1612	1/1	0.93	0.32	72,72,72,72	0
58	MG	AA	3291	1/1	0.93	0.07	44,44,44,44	0
58	MG	CA	3361	1/1	0.93	0.18	58,58,58,58	0
58	MG	DA	1615	1/1	0.93	0.20	53,53,53,53	0
58	MG	DA	1618	1/1	0.93	0.26	65,65,65,65	0
58	MG	AA	3261	1/1	0.93	0.15	51,51,51,51	0
58	MG	DA	1620	1/1	0.93	0.05	58,58,58,58	0
58	MG	AA	3543	1/1	0.93	0.10	52,52,52,52	1
58	MG	CA	3366	1/1	0.93	0.16	61,61,61,61	0
58	MG	BA	1604	1/1	0.93	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1678	1/1	0.93	0.17	44,44,44,44	0
58	MG	DA	1627	1/1	0.93	0.12	70,70,70,70	0
58	MG	AA	3118	1/1	0.93	0.16	64,64,64,64	0
58	MG	AA	3297	1/1	0.93	0.06	20,20,20,20	1
58	MG	CA	3177	1/1	0.93	0.07	36,36,36,36	0
58	MG	AA	3712	1/1	0.93	0.13	46,46,46,46	0
58	MG	AA	3551	1/1	0.93	0.10	52,52,52,52	0
58	MG	CA	3558	1/1	0.93	0.08	51,51,51,51	1
58	MG	AA	3714	1/1	0.93	0.17	56,56,56,56	0
58	MG	AA	3181	1/1	0.93	0.10	56,56,56,56	0
58	MG	AA	3137	1/1	0.93	0.11	56,56,56,56	0
58	MG	CA	3564	1/1	0.93	0.12	40,40,40,40	1
58	MG	CA	3565	1/1	0.93	0.13	51,51,51,51	0
58	MG	AA	3363	1/1	0.93	0.07	28,28,28,28	0
58	MG	CA	3186	1/1	0.93	0.10	69,69,69,69	0
58	MG	AA	3571	1/1	0.93	0.09	48,48,48,48	0
58	MG	CA	3570	1/1	0.93	0.18	77,77,77,77	0
58	MG	DA	1646	1/1	0.93	0.22	62,62,62,62	0
58	MG	AA	3106	1/1	0.93	0.18	52,52,52,52	0
58	MG	CA	3573	1/1	0.93	0.08	80,80,80,80	0
58	MG	AA	3313	1/1	0.93	0.06	35,35,35,35	0
58	MG	AA	3576	1/1	0.93	0.09	38,38,38,38	0
58	MG	CA	3400	1/1	0.93	0.09	62,62,62,62	0
58	MG	AA	3078	1/1	0.93	0.24	66,66,66,66	0
58	MG	DA	1655	1/1	0.93	0.28	58,58,58,58	0
58	MG	DA	1656	1/1	0.93	0.16	75,75,75,75	0
58	MG	CA	3580	1/1	0.93	0.08	100,100,100,100	0
58	MG	BA	1621	1/1	0.93	0.07	52,52,52,52	0
58	MG	CA	3404	1/1	0.93	0.09	54,54,54,54	0
58	MG	AB	3003	1/1	0.93	0.12	51,51,51,51	0
58	MG	AA	3128	1/1	0.93	0.15	59,59,59,59	0
58	MG	CA	3589	1/1	0.93	0.12	79,79,79,79	0
58	MG	AA	3648	1/1	0.93	0.10	40,40,40,40	0
58	MG	CA	3201	1/1	0.93	0.27	59,59,59,59	0
58	MG	DA	1666	1/1	0.93	0.10	66,66,66,66	0
58	MG	AA	3147	1/1	0.93	0.18	69,69,69,69	0
58	MG	AA	3585	1/1	0.93	0.09	65,65,65,65	0
58	MG	AB	3010	1/1	0.93	0.06	47,47,47,47	1
58	MG	CA	3206	1/1	0.93	0.30	56,56,56,56	0
58	MG	AA	3132	1/1	0.93	0.13	27,27,27,27	1
58	MG	CA	3597	1/1	0.93	0.13	39,39,39,39	0
58	MG	BA	1631	1/1	0.93	0.24	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3423	1/1	0.93	0.09	50,50,50,50	0
58	MG	AA	3250	1/1	0.93	0.13	46,46,46,46	0
58	MG	AB	3016	1/1	0.93	0.10	34,34,34,34	0
58	MG	BA	1634	1/1	0.93	0.22	54,54,54,54	0
58	MG	AA	3383	1/1	0.93	0.09	54,54,54,54	0
58	MG	CA	3605	1/1	0.93	0.15	73,73,73,73	0
58	MG	AA	3748	1/1	0.93	0.16	56,56,56,56	0
58	MG	BF	3001	1/1	0.93	0.15	74,74,74,74	0
58	MG	AA	3411	1/1	0.93	0.09	47,47,47,47	0
58	MG	CA	3222	1/1	0.93	0.14	75,75,75,75	0
58	MG	CA	3613	1/1	0.93	0.18	74,74,74,74	0
58	MG	AA	3172	1/1	0.93	0.32	71,71,71,71	0
58	MG	DA	1693	1/1	0.93	0.12	54,54,54,54	0
58	MG	BA	1639	1/1	0.93	0.08	66,66,66,66	0
58	MG	BM	201	1/1	0.93	0.07	57,57,57,57	0
58	MG	BA	1715	1/1	0.93	0.15	55,55,55,55	0
58	MG	AA	3664	1/1	0.93	0.12	57,57,57,57	0
58	MG	CA	3446	1/1	0.93	0.08	63,63,63,63	0
58	MG	CA	3101	1/1	0.93	0.11	78,78,78,78	0
58	MG	BA	1641	1/1	0.93	0.16	49,49,49,49	0
58	MG	DA	1704	1/1	0.93	0.10	69,69,69,69	0
58	MG	CA	3456	1/1	0.93	0.13	60,60,60,60	0
58	MG	BA	1642	1/1	0.93	0.12	55,55,55,55	0
58	MG	AD	301	1/1	0.93	0.15	43,43,43,43	0
58	MG	AD	303	1/1	0.93	0.19	70,70,70,70	0
58	MG	AA	3424	1/1	0.93	0.09	65,65,65,65	0
58	MG	AA	3667	1/1	0.93	0.09	28,28,28,28	0
58	MG	AA	3671	1/1	0.93	0.15	58,58,58,58	0
58	MG	CA	3637	1/1	0.93	0.25	59,59,59,59	0
58	MG	CA	3638	1/1	0.93	0.11	55,55,55,55	0
58	MG	CA	3640	1/1	0.93	0.11	59,59,59,59	0
58	MG	AD	309	1/1	0.93	0.09	37,37,37,37	0
58	MG	AA	3277	1/1	0.93	0.27	79,79,79,79	0
58	MG	CA	3474	1/1	0.93	0.16	76,76,76,76	0
58	MG	AA	3761	1/1	0.93	0.12	50,50,50,50	0
58	MG	AA	3598	1/1	0.93	0.17	54,54,54,54	0
58	MG	DA	1727	1/1	0.93	0.14	66,66,66,66	0
58	MG	DA	1728	1/1	0.93	0.12	63,63,63,63	0
58	MG	CA	3120	1/1	0.93	0.27	62,62,62,62	0
58	MG	AA	3428	1/1	0.93	0.09	35,35,35,35	0
58	MG	CA	3012	1/1	0.93	0.11	59,59,59,59	0
58	MG	AA	3278	1/1	0.93	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	1734	1/1	0.93	0.14	83,83,83,83	0
58	MG	CA	3655	1/1	0.93	0.11	70,70,70,70	0
58	MG	CA	3014	1/1	0.93	0.14	62,62,62,62	0
58	MG	BA	1738	1/1	0.93	0.06	73,73,73,73	0
58	MG	AP	203	1/1	0.93	0.06	40,40,40,40	0
58	MG	BA	1740	1/1	0.93	0.19	56,56,56,56	0
58	MG	CA	3490	1/1	0.93	0.09	67,67,67,67	0
58	MG	CA	3130	1/1	0.93	0.30	73,73,73,73	0
58	MG	AA	3431	1/1	0.93	0.11	25,25,25,25	0
58	MG	BA	1743	1/1	0.93	0.06	46,46,46,46	0
58	MG	AU	201	1/1	0.93	0.18	45,45,45,45	0
58	MG	DA	1747	1/1	0.93	0.10	70,70,70,70	0
58	MG	AV	201	1/1	0.93	0.06	17,17,17,17	1
58	MG	AA	3279	1/1	0.93	0.22	53,53,53,53	0
58	MG	AA	3063	1/1	0.93	0.23	67,67,67,67	0
58	MG	CA	3138	1/1	0.93	0.07	63,63,63,63	0
58	MG	BA	1751	1/1	0.93	0.08	48,48,48,48	0
58	MG	BA	1752	1/1	0.93	0.10	65,65,65,65	0
58	MG	AX	101	1/1	0.93	0.16	75,75,75,75	0
58	MG	CA	3143	1/1	0.93	0.28	57,57,57,57	0
58	MG	AA	3235	1/1	0.93	0.16	64,64,64,64	0
58	MG	AA	3496	1/1	0.93	0.13	52,52,52,52	0
58	MG	AA	3691	1/1	0.93	0.16	89,89,89,89	0
58	MG	AA	3152	1/1	0.93	0.18	71,71,71,71	0
58	MG	CA	3306	1/1	0.93	0.06	41,41,41,41	0
58	MG	AA	3512	1/1	0.93	0.15	60,60,60,60	0
58	MG	CA	3521	1/1	0.93	0.13	61,61,61,61	0
58	MG	CA	3313	1/1	0.93	0.13	50,50,50,50	0
58	MG	BA	1765	1/1	0.93	0.10	62,62,62,62	0
58	MG	CA	3524	1/1	0.93	0.06	77,77,77,77	0
58	MG	CA	3319	1/1	0.93	0.10	67,67,67,67	0
58	MG	CA	3526	1/1	0.93	0.06	40,40,40,40	0
58	MG	AA	3441	1/1	0.93	0.11	51,51,51,51	1
58	MG	CA	3324	1/1	0.93	0.13	40,40,40,40	0
58	MG	DT	3001	1/1	0.93	0.22	67,67,67,67	0
58	MG	DW	501	1/1	0.93	0.26	74,74,74,74	0
58	MG	CA	3530	1/1	0.93	0.13	59,59,59,59	0
58	MG	CA	3048	1/1	0.93	0.18	86,86,86,86	0
58	MG	CA	3332	1/1	0.93	0.08	42,42,42,42	0
58	MG	CA	3334	1/1	0.93	0.13	44,44,44,44	0
58	MG	CY	502	1/1	0.93	0.14	56,56,56,56	0
58	MG	AA	3290	1/1	0.93	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CV	202	1/1	0.94	0.21	85,85,85,85	0
58	MG	AD	302	1/1	0.94	0.14	61,61,61,61	0
58	MG	AA	3735	1/1	0.94	0.08	35,35,35,35	0
58	MG	CA	3316	1/1	0.94	0.11	50,50,50,50	0
58	MG	BA	1749	1/1	0.94	0.14	68,68,68,68	0
58	MG	AD	304	1/1	0.94	0.12	19,19,19,19	0
58	MG	AA	3058	1/1	0.94	0.13	35,35,35,35	0
58	MG	DA	1605	1/1	0.94	0.13	73,73,73,73	0
58	MG	AA	3503	1/1	0.94	0.08	64,64,64,64	0
58	MG	CA	3330	1/1	0.94	0.13	43,43,43,43	0
58	MG	CA	3331	1/1	0.94	0.11	52,52,52,52	0
58	MG	DA	1610	1/1	0.94	0.07	75,75,75,75	0
58	MG	AA	3390	1/1	0.94	0.11	35,35,35,35	0
58	MG	AA	3511	1/1	0.94	0.07	12,12,12,12	0
58	MG	CA	3335	1/1	0.94	0.12	62,62,62,62	0
58	MG	CA	3336	1/1	0.94	0.10	69,69,69,69	0
58	MG	DA	1616	1/1	0.94	0.17	64,64,64,64	0
58	MG	AA	3406	1/1	0.94	0.09	57,57,57,57	0
58	MG	CA	3162	1/1	0.94	0.20	46,46,46,46	0
58	MG	BA	1656	1/1	0.94	0.11	54,54,54,54	0
58	MG	CA	3344	1/1	0.94	0.14	87,87,87,87	0
58	MG	CA	3346	1/1	0.94	0.07	31,31,31,31	0
58	MG	DA	1624	1/1	0.94	0.06	44,44,44,44	0
58	MG	AA	3516	1/1	0.94	0.08	18,18,18,18	0
58	MG	CA	3348	1/1	0.94	0.13	54,54,54,54	0
58	MG	AF	301	1/1	0.94	0.12	25,25,25,25	1
58	MG	CA	3547	1/1	0.94	0.09	61,61,61,61	0
58	MG	CA	3352	1/1	0.94	0.11	68,68,68,68	0
58	MG	CA	3353	1/1	0.94	0.08	48,48,48,48	0
58	MG	AF	304	1/1	0.94	0.17	43,43,43,43	0
58	MG	CA	3169	1/1	0.94	0.11	34,34,34,34	0
58	MG	AA	3517	1/1	0.94	0.09	19,19,19,19	0
58	MG	AG	201	1/1	0.94	0.10	52,52,52,52	0
58	MG	CA	3362	1/1	0.94	0.08	44,44,44,44	0
58	MG	AA	3135	1/1	0.94	0.32	62,62,62,62	1
58	MG	AA	3519	1/1	0.94	0.09	21,21,21,21	0
58	MG	AA	3414	1/1	0.94	0.09	36,36,36,36	0
58	MG	CA	3368	1/1	0.94	0.11	59,59,59,59	0
58	MG	AA	3644	1/1	0.94	0.09	56,56,56,56	0
58	MG	AA	3110	1/1	0.94	0.17	79,79,79,79	0
58	MG	BA	1778	1/1	0.94	0.10	64,64,64,64	0
58	MG	AA	3422	1/1	0.94	0.06	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AV	205	1/1	0.94	0.15	55,55,55,55	1
58	MG	AA	3166	1/1	0.94	0.17	31,31,31,31	0
58	MG	CA	3380	1/1	0.94	0.15	71,71,71,71	0
58	MG	AA	3206	1/1	0.94	0.10	39,39,39,39	0
58	MG	DA	1651	1/1	0.94	0.27	59,59,59,59	0
58	MG	CA	3187	1/1	0.94	0.08	37,37,37,37	0
58	MG	AA	3651	1/1	0.94	0.08	52,52,52,52	0
58	MG	AA	3546	1/1	0.94	0.09	32,32,32,32	0
58	MG	AA	3763	1/1	0.94	0.16	65,65,65,65	0
58	MG	AA	3653	1/1	0.94	0.09	68,68,68,68	0
58	MG	A0	102	1/1	0.94	0.08	40,40,40,40	0
58	MG	CA	3195	1/1	0.94	0.17	60,60,60,60	0
58	MG	AA	3259	1/1	0.94	0.19	20,20,20,20	1
58	MG	DA	1661	1/1	0.94	0.18	70,70,70,70	0
58	MG	AA	3099	1/1	0.94	0.07	62,62,62,62	0
58	MG	CA	3588	1/1	0.94	0.16	63,63,63,63	0
58	MG	CA	3198	1/1	0.94	0.06	37,37,37,37	0
58	MG	AA	3079	1/1	0.94	0.05	34,34,34,34	0
58	MG	AA	3324	1/1	0.94	0.07	33,33,33,33	0
58	MG	DA	1667	1/1	0.94	0.13	49,49,49,49	0
58	MG	A5	101	1/1	0.94	0.13	37,37,37,37	1
58	MG	BA	1796	1/1	0.94	0.12	77,77,77,77	0
58	MG	CA	3203	1/1	0.94	0.06	60,60,60,60	0
58	MG	AA	3330	1/1	0.94	0.10	69,69,69,69	0
58	MG	AA	3663	1/1	0.94	0.16	62,62,62,62	0
58	MG	CA	3411	1/1	0.94	0.19	61,61,61,61	0
58	MG	A6	101	1/1	0.94	0.18	65,65,65,65	0
58	MG	AA	3262	1/1	0.94	0.32	70,70,70,70	0
58	MG	AA	3214	1/1	0.94	0.05	34,34,34,34	0
58	MG	CA	3416	1/1	0.94	0.10	48,48,48,48	0
58	MG	AA	3215	1/1	0.94	0.20	42,42,42,42	1
58	MG	CA	3419	1/1	0.94	0.07	60,60,60,60	0
58	MG	BA	1602	1/1	0.94	0.16	111,111,111,111	0
58	MG	CA	3606	1/1	0.94	0.17	65,65,65,65	0
58	MG	AA	3668	1/1	0.94	0.07	40,40,40,40	0
58	MG	CA	3608	1/1	0.94	0.09	56,56,56,56	0
58	MG	CA	3213	1/1	0.94	0.17	44,44,44,44	0
58	MG	CA	3215	1/1	0.94	0.16	73,73,73,73	0
58	MG	AA	3341	1/1	0.94	0.08	15,15,15,15	0
58	MG	AA	3220	1/1	0.94	0.21	62,62,62,62	0
58	MG	DA	1694	1/1	0.94	0.09	60,60,60,60	0
58	MG	AA	3266	1/1	0.94	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3615	1/1	0.94	0.10	38,38,38,38	0
58	MG	AA	3102	1/1	0.94	0.17	49,49,49,49	0
58	MG	AA	3176	1/1	0.94	0.08	50,50,50,50	0
58	MG	BA	1609	1/1	0.94	0.09	62,62,62,62	0
58	MG	AA	3789	1/1	0.94	0.14	54,54,54,54	0
58	MG	CA	3434	1/1	0.94	0.07	28,28,28,28	0
58	MG	CA	3225	1/1	0.94	0.14	65,65,65,65	0
58	MG	AA	3581	1/1	0.94	0.10	40,40,40,40	0
58	MG	AA	3120	1/1	0.94	0.15	46,46,46,46	0
58	MG	AA	3146	1/1	0.94	0.13	33,33,33,33	1
58	MG	BA	1615	1/1	0.94	0.05	101,101,101,101	0
58	MG	CA	3106	1/1	0.94	0.21	55,55,55,55	0
58	MG	AA	3007	1/1	0.94	0.04	21,21,21,21	0
58	MG	AA	3353	1/1	0.94	0.09	76,76,76,76	0
58	MG	DA	1712	1/1	0.94	0.11	81,81,81,81	0
58	MG	AA	3093	1/1	0.94	0.07	27,27,27,27	1
58	MG	CA	3112	1/1	0.94	0.09	61,61,61,61	0
58	MG	CA	3464	1/1	0.94	0.06	46,46,46,46	0
58	MG	AA	3233	1/1	0.94	0.09	55,55,55,55	0
58	MG	AA	3124	1/1	0.94	0.15	63,63,63,63	0
58	MG	AA	3127	1/1	0.94	0.16	71,71,71,71	0
58	MG	DA	1723	1/1	0.94	0.18	66,66,66,66	0
58	MG	DA	1724	1/1	0.94	0.14	61,61,61,61	0
58	MG	AA	3190	1/1	0.94	0.17	45,45,45,45	0
58	MG	BW	503	1/1	0.94	0.10	45,45,45,45	0
58	MG	AA	3280	1/1	0.94	0.14	47,47,47,47	0
58	MG	AA	3239	1/1	0.94	0.17	64,64,64,64	0
58	MG	DA	1729	1/1	0.94	0.07	57,57,57,57	0
58	MG	AA	3812	1/1	0.94	0.11	42,42,42,42	0
58	MG	AA	3603	1/1	0.94	0.11	63,63,63,63	0
58	MG	AA	3241	1/1	0.94	0.12	69,69,69,69	0
58	MG	AA	3703	1/1	0.94	0.06	76,76,76,76	0
58	MG	AA	3191	1/1	0.94	0.15	42,42,42,42	0
58	MG	AA	3466	1/1	0.94	0.06	63,63,63,63	0
58	MG	CA	3659	1/1	0.94	0.09	77,77,77,77	0
58	MG	AA	3607	1/1	0.94	0.08	30,30,30,30	0
58	MG	CA	3258	1/1	0.94	0.11	70,70,70,70	0
58	MG	CA	3261	1/1	0.94	0.11	29,29,29,29	0
58	MG	BA	1724	1/1	0.94	0.15	55,55,55,55	0
58	MG	CA	3664	1/1	0.94	0.10	54,54,54,54	0
58	MG	AA	3153	1/1	0.94	0.13	59,59,59,59	0
58	MG	CA	3268	1/1	0.94	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AB	3008	1/1	0.94	0.25	51,51,51,51	0
58	MG	AA	3081	1/1	0.94	0.06	40,40,40,40	0
58	MG	CA	3017	1/1	0.94	0.21	46,46,46,46	0
58	MG	CA	3280	1/1	0.94	0.06	30,30,30,30	0
58	MG	CA	3497	1/1	0.94	0.12	73,73,73,73	0
58	MG	AA	3129	1/1	0.94	0.18	66,66,66,66	1
58	MG	DA	1752	1/1	0.94	0.12	74,74,74,74	0
58	MG	CA	3136	1/1	0.94	0.19	53,53,53,53	0
58	MG	AA	3372	1/1	0.94	0.18	63,63,63,63	0
58	MG	CB	3011	1/1	0.94	0.15	53,53,53,53	0
58	MG	DA	1756	1/1	0.94	0.08	68,68,68,68	0
58	MG	AA	3617	1/1	0.94	0.12	49,49,49,49	0
58	MG	CA	3502	1/1	0.94	0.11	70,70,70,70	0
58	MG	AA	3373	1/1	0.94	0.18	59,59,59,59	0
58	MG	AA	3481	1/1	0.94	0.05	51,51,51,51	0
58	MG	AA	3487	1/1	0.94	0.09	39,39,39,39	0
58	MG	CA	3142	1/1	0.94	0.10	69,69,69,69	0
58	MG	CA	3509	1/1	0.94	0.10	76,76,76,76	0
58	MG	CA	3298	1/1	0.94	0.09	68,68,68,68	0
58	MG	CF	302	1/1	0.94	0.08	56,56,56,56	0
58	MG	CA	3299	1/1	0.94	0.08	61,61,61,61	0
58	MG	AA	3197	1/1	0.94	0.11	37,37,37,37	0
58	MG	CF	305	1/1	0.94	0.12	51,51,51,51	0
58	MG	CA	3301	1/1	0.94	0.08	47,47,47,47	0
58	MG	AA	3378	1/1	0.94	0.07	19,19,19,19	0
58	MG	CA	3517	1/1	0.94	0.22	64,64,64,64	0
58	MG	CA	3303	1/1	0.94	0.13	54,54,54,54	0
58	MG	CP	201	1/1	0.94	0.35	65,65,65,65	0
58	MG	CA	3520	1/1	0.94	0.12	59,59,59,59	0
58	MG	AA	3381	1/1	0.94	0.10	27,27,27,27	0
58	MG	AA	3087	1/1	0.94	0.19	72,72,72,72	0
58	MG	CA	3309	1/1	0.94	0.08	29,29,29,29	0
58	MG	CR	201	1/1	0.94	0.13	51,51,51,51	0
58	MG	CA	3149	1/1	0.94	0.05	66,66,66,66	0
58	MG	CA	3175	1/1	0.95	0.16	42,42,42,42	0
58	MG	AA	3013	1/1	0.95	0.07	35,35,35,35	0
58	MG	CA	3355	1/1	0.95	0.07	41,41,41,41	0
58	MG	AA	3634	1/1	0.95	0.07	62,62,62,62	0
58	MG	CA	3047	1/1	0.95	0.14	61,61,61,61	0
58	MG	AD	306	1/1	0.95	0.16	38,38,38,38	1
58	MG	AA	3737	1/1	0.95	0.07	29,29,29,29	0
58	MG	AA	3183	1/1	0.95	0.10	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3008	1/1	0.95	0.08	19,19,19,19	0
58	MG	AA	3061	1/1	0.95	0.11	27,27,27,27	0
58	MG	AE	301	1/1	0.95	0.07	19,19,19,19	0
58	MG	CA	3367	1/1	0.95	0.16	65,65,65,65	0
58	MG	AA	3050	1/1	0.95	0.08	53,53,53,53	0
58	MG	AE	304	1/1	0.95	0.05	41,41,41,41	0
58	MG	BA	1763	1/1	0.95	0.09	55,55,55,55	0
58	MG	AA	3051	1/1	0.95	0.14	36,36,36,36	0
58	MG	AA	3549	1/1	0.95	0.06	54,54,54,54	0
58	MG	DA	1629	1/1	0.95	0.17	58,58,58,58	0
58	MG	CA	3061	1/1	0.95	0.27	67,67,67,67	0
58	MG	AA	3157	1/1	0.95	0.07	34,34,34,34	0
58	MG	AF	308	1/1	0.95	0.09	55,55,55,55	0
58	MG	CA	3384	1/1	0.95	0.12	71,71,71,71	0
58	MG	CA	3065	1/1	0.95	0.09	52,52,52,52	0
58	MG	BA	1770	1/1	0.95	0.07	75,75,75,75	0
58	MG	AA	3646	1/1	0.95	0.08	58,58,58,58	0
58	MG	AG	202	1/1	0.95	0.06	73,73,73,73	0
58	MG	AH	3001	1/1	0.95	0.18	52,52,52,52	0
58	MG	CA	3392	1/1	0.95	0.06	35,35,35,35	0
58	MG	AA	3553	1/1	0.95	0.07	40,40,40,40	0
58	MG	CA	3394	1/1	0.95	0.11	55,55,55,55	0
58	MG	AA	3556	1/1	0.95	0.07	39,39,39,39	0
58	MG	AO	5001	1/1	0.95	0.08	55,55,55,55	0
58	MG	DA	1644	1/1	0.95	0.17	57,57,57,57	0
58	MG	DA	1645	1/1	0.95	0.12	64,64,64,64	0
58	MG	BA	1780	1/1	0.95	0.06	42,42,42,42	0
58	MG	AA	3030	1/1	0.95	0.15	26,26,26,26	1
58	MG	AA	3560	1/1	0.95	0.09	58,58,58,58	0
58	MG	CA	3584	1/1	0.95	0.08	46,46,46,46	0
58	MG	BA	1783	1/1	0.95	0.09	62,62,62,62	0
58	MG	AA	3054	1/1	0.95	0.10	38,38,38,38	0
58	MG	AA	3759	1/1	0.95	0.12	65,65,65,65	0
58	MG	AV	202	1/1	0.95	0.10	20,20,20,20	0
58	MG	AA	3281	1/1	0.95	0.27	61,61,61,61	0
58	MG	AA	3655	1/1	0.95	0.10	61,61,61,61	0
58	MG	AW	3003	1/1	0.95	0.13	52,52,52,52	0
58	MG	AA	3566	1/1	0.95	0.08	27,27,27,27	0
58	MG	AA	3449	1/1	0.95	0.06	15,15,15,15	0
58	MG	AA	3161	1/1	0.95	0.18	60,60,60,60	0
58	MG	AA	3198	1/1	0.95	0.11	58,58,58,58	0
58	MG	AA	3284	1/1	0.95	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3454	1/1	0.95	0.11	51,51,51,51	0
58	MG	AA	3361	1/1	0.95	0.07	29,29,29,29	0
58	MG	CA	3600	1/1	0.95	0.07	50,50,50,50	0
58	MG	AA	3055	1/1	0.95	0.11	35,35,35,35	0
58	MG	AA	3036	1/1	0.95	0.10	51,51,51,51	0
58	MG	CA	3229	1/1	0.95	0.14	51,51,51,51	0
58	MG	AA	3582	1/1	0.95	0.12	66,66,66,66	0
58	MG	CA	3425	1/1	0.95	0.07	53,53,53,53	0
58	MG	AA	3071	1/1	0.95	0.20	41,41,41,41	0
58	MG	CA	3232	1/1	0.95	0.05	60,60,60,60	0
58	MG	AA	3021	1/1	0.95	0.07	40,40,40,40	0
58	MG	AA	3366	1/1	0.95	0.08	53,53,53,53	0
58	MG	AA	3167	1/1	0.95	0.09	65,65,65,65	0
58	MG	BA	1806	1/1	0.95	0.13	67,67,67,67	0
58	MG	CA	3612	1/1	0.95	0.10	68,68,68,68	0
58	MG	A7	101	1/1	0.95	0.10	65,65,65,65	0
58	MG	DA	1681	1/1	0.95	0.11	55,55,55,55	0
58	MG	DA	1683	1/1	0.95	0.19	54,54,54,54	0
58	MG	A7	104	1/1	0.95	0.09	49,49,49,49	1
58	MG	CA	3435	1/1	0.95	0.07	52,52,52,52	0
58	MG	AA	3782	1/1	0.95	0.17	74,74,74,74	0
58	MG	BA	1810	1/1	0.95	0.10	50,50,50,50	0
58	MG	AA	3676	1/1	0.95	0.07	66,66,66,66	0
58	MG	CA	3110	1/1	0.95	0.09	63,63,63,63	0
58	MG	AA	3677	1/1	0.95	0.05	41,41,41,41	0
58	MG	CA	3247	1/1	0.95	0.14	66,66,66,66	0
58	MG	AA	3295	1/1	0.95	0.16	47,47,47,47	0
58	MG	CA	3449	1/1	0.95	0.07	66,66,66,66	0
58	MG	DA	1695	1/1	0.95	0.13	66,66,66,66	0
58	MG	CA	3626	1/1	0.95	0.15	75,75,75,75	0
58	MG	CA	3452	1/1	0.95	0.15	61,61,61,61	0
58	MG	CA	3251	1/1	0.95	0.10	56,56,56,56	0
58	MG	AA	3205	1/1	0.95	0.27	64,64,64,64	0
58	MG	AA	3681	1/1	0.95	0.12	65,65,65,65	0
58	MG	CA	3463	1/1	0.95	0.08	49,49,49,49	0
58	MG	BE	3001	1/1	0.95	0.08	60,60,60,60	0
58	MG	AA	3371	1/1	0.95	0.12	62,62,62,62	0
58	MG	CA	3466	1/1	0.95	0.18	57,57,57,57	0
58	MG	AA	3683	1/1	0.95	0.22	67,67,67,67	0
58	MG	AA	3796	1/1	0.95	0.11	50,50,50,50	0
58	MG	AA	3685	1/1	0.95	0.10	47,47,47,47	0
58	MG	AA	3798	1/1	0.95	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3299	1/1	0.95	0.07	20,20,20,20	0
58	MG	AA	3305	1/1	0.95	0.15	55,55,55,55	0
58	MG	BA	1705	1/1	0.95	0.16	78,78,78,78	0
58	MG	CA	3475	1/1	0.95	0.22	55,55,55,55	0
58	MG	CA	3476	1/1	0.95	0.07	55,55,55,55	0
58	MG	AA	3168	1/1	0.95	0.15	63,63,63,63	0
58	MG	CA	3654	1/1	0.95	0.17	51,51,51,51	0
58	MG	CA	3271	1/1	0.95	0.11	57,57,57,57	0
58	MG	DA	1721	1/1	0.95	0.12	67,67,67,67	0
58	MG	AA	3254	1/1	0.95	0.12	42,42,42,42	0
58	MG	BW	502	1/1	0.95	0.13	53,53,53,53	0
58	MG	CA	3275	1/1	0.95	0.08	42,42,42,42	0
58	MG	CA	3277	1/1	0.95	0.09	90,90,90,90	0
58	MG	CA	3278	1/1	0.95	0.08	37,37,37,37	0
58	MG	CA	3129	1/1	0.95	0.24	69,69,69,69	0
58	MG	AA	3601	1/1	0.95	0.18	47,47,47,47	0
58	MG	BA	1709	1/1	0.95	0.14	50,50,50,50	0
58	MG	AA	3311	1/1	0.95	0.11	33,33,33,33	0
58	MG	CA	3491	1/1	0.95	0.07	51,51,51,51	0
58	MG	AA	3113	1/1	0.95	0.14	64,64,64,64	0
58	MG	CA	3287	1/1	0.95	0.07	52,52,52,52	0
58	MG	BA	1712	1/1	0.95	0.37	73,73,73,73	0
58	MG	CA	3003	1/1	0.95	0.13	45,45,45,45	0
58	MG	CA	3293	1/1	0.95	0.10	71,71,71,71	0
58	MG	AA	3484	1/1	0.95	0.08	35,35,35,35	0
58	MG	AA	3486	1/1	0.95	0.09	27,27,27,27	0
58	MG	AA	3209	1/1	0.95	0.08	63,63,63,63	0
58	MG	AA	3115	1/1	0.95	0.24	67,67,67,67	1
58	MG	CA	3009	1/1	0.95	0.17	67,67,67,67	0
58	MG	CA	3503	1/1	0.95	0.09	62,62,62,62	0
58	MG	BA	1623	1/1	0.95	0.11	49,49,49,49	0
58	MG	AA	3391	1/1	0.95	0.07	45,45,45,45	0
58	MG	CE	301	1/1	0.95	0.11	66,66,66,66	0
58	MG	CE	302	1/1	0.95	0.09	47,47,47,47	0
58	MG	AA	3612	1/1	0.95	0.13	56,56,56,56	0
58	MG	AA	3404	1/1	0.95	0.07	19,19,19,19	0
58	MG	CE	305	1/1	0.95	0.14	43,43,43,43	0
58	MG	CA	3015	1/1	0.95	0.16	85,85,85,85	0
58	MG	AA	3614	1/1	0.95	0.07	56,56,56,56	0
58	MG	AA	3173	1/1	0.95	0.11	60,60,60,60	0
58	MG	AA	3142	1/1	0.95	0.13	26,26,26,26	1
58	MG	AA	3711	1/1	0.95	0.14	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3315	1/1	0.95	0.12	60,60,60,60	0
58	MG	AA	3216	1/1	0.95	0.13	51,51,51,51	0
58	MG	AA	3219	1/1	0.95	0.16	58,58,58,58	0
58	MG	CA	3026	1/1	0.95	0.15	81,81,81,81	0
58	MG	DA	1762	1/1	0.95	0.06	73,73,73,73	0
58	MG	CA	3156	1/1	0.95	0.14	68,68,68,68	0
58	MG	AA	3117	1/1	0.95	0.15	30,30,30,30	1
58	MG	CA	3328	1/1	0.95	0.07	55,55,55,55	0
58	MG	BA	1735	1/1	0.95	0.10	62,62,62,62	0
58	MG	CQ	202	1/1	0.95	0.23	64,64,64,64	0
58	MG	AA	3332	1/1	0.95	0.08	46,46,46,46	0
58	MG	AA	3335	1/1	0.95	0.09	41,41,41,41	0
58	MG	CA	3333	1/1	0.95	0.15	75,75,75,75	0
58	MG	AA	3144	1/1	0.95	0.09	40,40,40,40	0
58	MG	CA	3163	1/1	0.95	0.20	40,40,40,40	0
58	MG	AA	3725	1/1	0.95	0.08	39,39,39,39	0
58	MG	AA	3726	1/1	0.95	0.06	67,67,67,67	0
58	MG	AA	3222	1/1	0.95	0.12	28,28,28,28	0
58	MG	CA	3038	1/1	0.95	0.17	48,48,48,48	0
58	MG	AA	3076	1/1	0.95	0.16	92,92,92,92	0
58	MG	AA	3525	1/1	0.95	0.16	40,40,40,40	0
59	ZN	C4	501	1/1	0.95	0.06	189,189,189,189	0
58	MG	AA	3432	1/1	0.95	0.12	57,57,57,57	0
58	MG	AA	3098	1/1	0.95	0.23	58,58,58,58	0
58	MG	CA	3044	1/1	0.95	0.16	52,52,52,52	0
58	MG	AA	3255	1/1	0.96	0.11	53,53,53,53	0
58	MG	C7	101	1/1	0.96	0.21	42,42,42,42	1
58	MG	AA	3298	1/1	0.96	0.07	59,59,59,59	0
58	MG	CA	3325	1/1	0.96	0.06	38,38,38,38	0
58	MG	CA	3326	1/1	0.96	0.08	34,34,34,34	0
58	MG	AA	3654	1/1	0.96	0.14	66,66,66,66	0
58	MG	CA	3151	1/1	0.96	0.07	50,50,50,50	0
58	MG	AA	3564	1/1	0.96	0.08	19,19,19,19	0
58	MG	AA	3764	1/1	0.96	0.09	55,55,55,55	0
58	MG	DA	1608	1/1	0.96	0.07	47,47,47,47	0
58	MG	AA	3066	1/1	0.96	0.19	50,50,50,50	0
58	MG	AA	3569	1/1	0.96	0.08	19,19,19,19	0
58	MG	AA	3570	1/1	0.96	0.06	15,15,15,15	0
58	MG	AA	3769	1/1	0.96	0.14	57,57,57,57	0
58	MG	AA	3300	1/1	0.96	0.07	50,50,50,50	0
58	MG	AA	3301	1/1	0.96	0.07	23,23,23,23	0
58	MG	AA	3662	1/1	0.96	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3302	1/1	0.96	0.06	56,56,56,56	0
58	MG	AA	3114	1/1	0.96	0.06	17,17,17,17	0
58	MG	CA	3164	1/1	0.96	0.12	41,41,41,41	0
58	MG	AA	3577	1/1	0.96	0.05	32,32,32,32	0
58	MG	AA	3777	1/1	0.96	0.05	19,19,19,19	0
58	MG	CA	3349	1/1	0.96	0.16	41,41,41,41	0
58	MG	BA	1714	1/1	0.96	0.10	61,61,61,61	0
58	MG	CA	3351	1/1	0.96	0.06	46,46,46,46	0
58	MG	AA	3307	1/1	0.96	0.06	6,6,6,6	0
58	MG	A9	502	1/1	0.96	0.16	60,60,60,60	0
58	MG	CA	3548	1/1	0.96	0.04	48,48,48,48	1
58	MG	AA	3185	1/1	0.96	0.17	41,41,41,41	0
58	MG	AA	3780	1/1	0.96	0.12	42,42,42,42	0
58	MG	AA	3669	1/1	0.96	0.05	33,33,33,33	0
58	MG	AA	3670	1/1	0.96	0.08	33,33,33,33	0
58	MG	AA	3032	1/1	0.96	0.09	36,36,36,36	0
58	MG	CA	3176	1/1	0.96	0.20	50,50,50,50	0
58	MG	AA	3162	1/1	0.96	0.08	47,47,47,47	0
58	MG	BA	1723	1/1	0.96	0.07	60,60,60,60	0
58	MG	AA	3116	1/1	0.96	0.10	51,51,51,51	0
58	MG	AA	3786	1/1	0.96	0.17	59,59,59,59	0
58	MG	AA	3086	1/1	0.96	0.10	47,47,47,47	0
58	MG	CA	3371	1/1	0.96	0.11	55,55,55,55	0
58	MG	AA	3467	1/1	0.96	0.05	44,44,44,44	0
58	MG	CA	3184	1/1	0.96	0.12	66,66,66,66	0
58	MG	BA	1728	1/1	0.96	0.19	52,52,52,52	0
58	MG	BA	1731	1/1	0.96	0.08	49,49,49,49	0
58	MG	AA	3790	1/1	0.96	0.05	49,49,49,49	0
58	MG	CA	3188	1/1	0.96	0.14	58,58,58,58	0
58	MG	AA	3793	1/1	0.96	0.08	28,28,28,28	0
58	MG	AA	3014	1/1	0.96	0.19	45,45,45,45	0
58	MG	AA	3226	1/1	0.96	0.11	56,56,56,56	0
58	MG	AA	3103	1/1	0.96	0.07	15,15,15,15	0
58	MG	AA	3680	1/1	0.96	0.09	59,59,59,59	0
58	MG	AA	3386	1/1	0.96	0.09	29,29,29,29	0
58	MG	CA	3050	1/1	0.96	0.05	44,44,44,44	0
58	MG	CA	3582	1/1	0.96	0.07	44,44,44,44	0
58	MG	CA	3391	1/1	0.96	0.08	63,63,63,63	0
58	MG	AA	3594	1/1	0.96	0.09	43,43,43,43	0
58	MG	AA	3595	1/1	0.96	0.10	55,55,55,55	0
58	MG	BA	1742	1/1	0.96	0.09	50,50,50,50	0
58	MG	AA	3267	1/1	0.96	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1622	1/1	0.96	0.05	37,37,37,37	0
58	MG	CA	3397	1/1	0.96	0.08	59,59,59,59	0
58	MG	AA	3229	1/1	0.96	0.15	43,43,43,43	0
58	MG	AA	3688	1/1	0.96	0.06	25,25,25,25	1
58	MG	AA	3805	1/1	0.96	0.10	35,35,35,35	1
58	MG	AA	3326	1/1	0.96	0.09	58,58,58,58	0
58	MG	AA	3405	1/1	0.96	0.15	46,46,46,46	0
58	MG	AA	3808	1/1	0.96	0.08	28,28,28,28	1
58	MG	BA	1754	1/1	0.96	0.12	48,48,48,48	0
58	MG	AA	3195	1/1	0.96	0.13	50,50,50,50	0
58	MG	AA	3692	1/1	0.96	0.09	53,53,53,53	0
58	MG	CA	3408	1/1	0.96	0.09	64,64,64,64	0
58	MG	BA	1757	1/1	0.96	0.12	38,38,38,38	0
58	MG	CA	3068	1/1	0.96	0.11	57,57,57,57	0
58	MG	CA	3214	1/1	0.96	0.14	40,40,40,40	0
58	MG	AA	3231	1/1	0.96	0.19	53,53,53,53	0
58	MG	AA	3813	1/1	0.96	0.25	54,54,54,54	0
58	MG	AA	3602	1/1	0.96	0.10	37,37,37,37	0
58	MG	CA	3218	1/1	0.96	0.33	54,54,54,54	0
58	MG	AA	3490	1/1	0.96	0.06	50,50,50,50	0
58	MG	AA	3412	1/1	0.96	0.10	43,43,43,43	0
58	MG	AA	3333	1/1	0.96	0.07	66,66,66,66	0
58	MG	CA	3422	1/1	0.96	0.12	55,55,55,55	0
58	MG	AA	3334	1/1	0.96	0.09	57,57,57,57	0
58	MG	AA	3495	1/1	0.96	0.10	59,59,59,59	0
58	MG	AA	3609	1/1	0.96	0.09	53,53,53,53	0
58	MG	CA	3078	1/1	0.96	0.08	47,47,47,47	0
58	MG	CA	3427	1/1	0.96	0.09	55,55,55,55	0
58	MG	BA	1769	1/1	0.96	0.06	58,58,58,58	0
58	MG	AB	3007	1/1	0.96	0.04	45,45,45,45	0
58	MG	BA	1772	1/1	0.96	0.11	56,56,56,56	0
58	MG	AA	3419	1/1	0.96	0.08	31,31,31,31	0
58	MG	CA	3083	1/1	0.96	0.16	90,90,90,90	0
58	MG	CA	3623	1/1	0.96	0.06	64,64,64,64	0
58	MG	AA	3499	1/1	0.96	0.07	51,51,51,51	1
58	MG	AA	3705	1/1	0.96	0.17	24,24,24,24	1
58	MG	BA	1776	1/1	0.96	0.06	61,61,61,61	0
58	MG	AA	3196	1/1	0.96	0.17	52,52,52,52	0
58	MG	CA	3438	1/1	0.96	0.07	46,46,46,46	0
58	MG	CA	3439	1/1	0.96	0.06	38,38,38,38	0
58	MG	BA	1645	1/1	0.96	0.06	58,58,58,58	0
58	MG	AA	3504	1/1	0.96	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3709	1/1	0.96	0.14	29,29,29,29	1
58	MG	AA	3505	1/1	0.96	0.05	31,31,31,31	0
58	MG	AA	3615	1/1	0.96	0.06	35,35,35,35	1
58	MG	AA	3423	1/1	0.96	0.06	22,22,22,22	0
58	MG	CA	3448	1/1	0.96	0.08	43,43,43,43	0
58	MG	DA	1714	1/1	0.96	0.06	51,51,51,51	0
58	MG	AA	3121	1/1	0.96	0.13	70,70,70,70	0
58	MG	CA	3451	1/1	0.96	0.10	63,63,63,63	0
58	MG	AA	3145	1/1	0.96	0.12	33,33,33,33	0
58	MG	AA	3619	1/1	0.96	0.06	42,42,42,42	0
58	MG	AA	3513	1/1	0.96	0.07	35,35,35,35	0
58	MG	CA	3647	1/1	0.96	0.05	66,66,66,66	0
58	MG	CA	3250	1/1	0.96	0.07	52,52,52,52	0
58	MG	AA	3004	1/1	0.96	0.07	25,25,25,25	0
58	MG	AA	3724	1/1	0.96	0.11	40,40,40,40	0
58	MG	BA	1657	1/1	0.96	0.15	69,69,69,69	0
58	MG	AA	3429	1/1	0.96	0.10	41,41,41,41	0
58	MG	CA	3104	1/1	0.96	0.07	48,48,48,48	0
58	MG	AA	3090	1/1	0.96	0.16	30,30,30,30	1
58	MG	AA	3025	1/1	0.96	0.07	35,35,35,35	1
58	MG	AA	3522	1/1	0.96	0.11	28,28,28,28	0
58	MG	CA	3259	1/1	0.96	0.09	47,47,47,47	0
58	MG	AA	3240	1/1	0.96	0.16	30,30,30,30	0
58	MG	CA	3262	1/1	0.96	0.06	61,61,61,61	0
58	MG	AD	310	1/1	0.96	0.13	42,42,42,42	0
58	MG	BA	1798	1/1	0.96	0.07	70,70,70,70	0
58	MG	AA	3627	1/1	0.96	0.11	54,54,54,54	0
58	MG	AD	312	1/1	0.96	0.15	58,58,58,58	0
58	MG	CA	3479	1/1	0.96	0.12	46,46,46,46	0
58	MG	AA	3628	1/1	0.96	0.12	80,80,80,80	0
58	MG	DA	1741	1/1	0.96	0.08	78,78,78,78	0
58	MG	AA	3202	1/1	0.96	0.08	47,47,47,47	0
58	MG	AA	3149	1/1	0.96	0.12	62,62,62,62	0
58	MG	AA	3175	1/1	0.96	0.09	51,51,51,51	0
58	MG	CA	3276	1/1	0.96	0.16	50,50,50,50	0
58	MG	AF	302	1/1	0.96	0.14	40,40,40,40	0
58	MG	CA	3119	1/1	0.96	0.17	128,128,128,128	0
58	MG	AA	3048	1/1	0.96	0.06	34,34,34,34	0
58	MG	AF	306	1/1	0.96	0.12	50,50,50,50	0
58	MG	AA	3351	1/1	0.96	0.05	30,30,30,30	0
58	MG	AA	3740	1/1	0.96	0.07	45,45,45,45	0
58	MG	AA	3056	1/1	0.96	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3077	1/1	0.96	0.17	50,50,50,50	0
58	MG	AA	3444	1/1	0.96	0.08	63,63,63,63	0
58	MG	AA	3745	1/1	0.96	0.06	29,29,29,29	0
58	MG	AA	3746	1/1	0.96	0.08	64,64,64,64	0
58	MG	AA	3288	1/1	0.96	0.06	24,24,24,24	0
58	MG	AA	3550	1/1	0.96	0.09	47,47,47,47	0
58	MG	CA	3297	1/1	0.96	0.18	56,56,56,56	0
58	MG	AA	3180	1/1	0.96	0.16	94,94,94,94	0
58	MG	AQ	203	1/1	0.96	0.17	41,41,41,41	0
58	MG	CA	3504	1/1	0.96	0.08	62,62,62,62	0
58	MG	AR	201	1/1	0.96	0.12	37,37,37,37	1
58	MG	AR	202	1/1	0.96	0.07	32,32,32,32	0
58	MG	AA	3211	1/1	0.96	0.23	42,42,42,42	1
58	MG	AU	203	1/1	0.96	0.13	29,29,29,29	1
58	MG	AA	3554	1/1	0.96	0.06	49,49,49,49	0
58	MG	CP	202	1/1	0.96	0.15	71,71,71,71	0
58	MG	AA	3753	1/1	0.96	0.10	41,41,41,41	0
58	MG	AA	3064	1/1	0.96	0.05	29,29,29,29	0
58	MG	AV	206	1/1	0.96	0.14	38,38,38,38	0
58	MG	AA	3213	1/1	0.96	0.05	58,58,58,58	0
58	MG	CQ	204	1/1	0.96	0.08	61,61,61,61	0
58	MG	AW	3002	1/1	0.96	0.12	55,55,55,55	0
58	MG	CA	3144	1/1	0.96	0.22	67,67,67,67	0
58	MG	AA	3559	1/1	0.96	0.12	39,39,39,39	0
58	MG	AA	3006	1/1	0.96	0.16	52,52,52,52	0
58	MG	CW	201	1/1	0.96	0.09	39,39,39,39	0
58	MG	CA	3322	1/1	0.96	0.13	45,45,45,45	0
58	MG	C3	3001	1/1	0.96	0.10	69,69,69,69	0
58	MG	AP	201	1/1	0.97	0.24	65,65,65,65	0
58	MG	CA	3260	1/1	0.97	0.11	65,65,65,65	0
58	MG	AA	3508	1/1	0.97	0.16	49,49,49,49	0
58	MG	CA	3036	1/1	0.97	0.07	44,44,44,44	0
58	MG	CA	3417	1/1	0.97	0.10	37,37,37,37	0
58	MG	AA	3433	1/1	0.97	0.06	28,28,28,28	0
58	MG	CA	3264	1/1	0.97	0.09	59,59,59,59	0
58	MG	CA	3575	1/1	0.97	0.05	43,43,43,43	1
58	MG	CA	3266	1/1	0.97	0.12	69,69,69,69	0
58	MG	AQ	202	1/1	0.97	0.10	31,31,31,31	0
58	MG	AA	3141	1/1	0.97	0.09	40,40,40,40	0
58	MG	AA	3684	1/1	0.97	0.05	29,29,29,29	0
58	MG	AA	3435	1/1	0.97	0.05	20,20,20,20	0
58	MG	BA	1764	1/1	0.97	0.05	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3035	1/1	0.97	0.08	57,57,57,57	0
58	MG	CA	3274	1/1	0.97	0.05	50,50,50,50	1
58	MG	AU	202	1/1	0.97	0.08	44,44,44,44	0
58	MG	AA	3687	1/1	0.97	0.05	45,45,45,45	0
58	MG	AA	3234	1/1	0.97	0.07	30,30,30,30	1
58	MG	AA	3608	1/1	0.97	0.07	73,73,73,73	0
58	MG	AA	3169	1/1	0.97	0.08	39,39,39,39	0
58	MG	CA	3281	1/1	0.97	0.08	51,51,51,51	0
58	MG	CA	3282	1/1	0.97	0.05	50,50,50,50	0
58	MG	BA	1771	1/1	0.97	0.11	63,63,63,63	0
58	MG	CA	3160	1/1	0.97	0.07	42,42,42,42	0
58	MG	CA	3437	1/1	0.97	0.05	48,48,48,48	0
58	MG	AA	3005	1/1	0.97	0.06	62,62,62,62	0
58	MG	AA	3072	1/1	0.97	0.04	26,26,26,26	0
58	MG	AA	3787	1/1	0.97	0.08	53,53,53,53	0
58	MG	CA	3288	1/1	0.97	0.06	54,54,54,54	0
58	MG	AA	3039	1/1	0.97	0.07	39,39,39,39	1
58	MG	CA	3055	1/1	0.97	0.15	39,39,39,39	0
58	MG	CA	3445	1/1	0.97	0.12	40,40,40,40	0
58	MG	AA	3523	1/1	0.97	0.07	30,30,30,30	0
58	MG	AA	3318	1/1	0.97	0.10	51,51,51,51	1
58	MG	AA	3792	1/1	0.97	0.12	45,45,45,45	0
58	MG	CA	3296	1/1	0.97	0.08	42,42,42,42	0
58	MG	AA	3119	1/1	0.97	0.08	40,40,40,40	1
58	MG	CA	3170	1/1	0.97	0.16	47,47,47,47	0
58	MG	AA	3020	1/1	0.97	0.05	25,25,25,25	0
58	MG	CA	3455	1/1	0.97	0.14	47,47,47,47	0
58	MG	AA	3532	1/1	0.97	0.11	25,25,25,25	0
58	MG	CA	3457	1/1	0.97	0.09	47,47,47,47	0
58	MG	CA	3458	1/1	0.97	0.06	49,49,49,49	0
58	MG	CA	3459	1/1	0.97	0.07	48,48,48,48	0
58	MG	AA	3533	1/1	0.97	0.07	22,22,22,22	0
58	MG	CA	3461	1/1	0.97	0.07	43,43,43,43	0
58	MG	CA	3462	1/1	0.97	0.08	49,49,49,49	0
58	MG	AA	3535	1/1	0.97	0.03	15,15,15,15	0
58	MG	AA	3322	1/1	0.97	0.04	32,32,32,32	1
58	MG	DA	1670	1/1	0.97	0.06	75,75,75,75	0
58	MG	AA	3011	1/1	0.97	0.04	40,40,40,40	0
58	MG	CA	3305	1/1	0.97	0.07	62,62,62,62	0
58	MG	AA	3800	1/1	0.97	0.04	30,30,30,30	0
58	MG	CA	3307	1/1	0.97	0.13	52,52,52,52	0
58	MG	AA	3541	1/1	0.97	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1788	1/1	0.97	0.10	66,66,66,66	0
58	MG	CA	3627	1/1	0.97	0.08	63,63,63,63	0
58	MG	AA	3374	1/1	0.97	0.07	18,18,18,18	0
58	MG	CA	3630	1/1	0.97	0.09	63,63,63,63	0
58	MG	DA	1680	1/1	0.97	0.09	62,62,62,62	0
58	MG	AA	3325	1/1	0.97	0.06	66,66,66,66	0
58	MG	DA	1682	1/1	0.97	0.14	47,47,47,47	0
58	MG	CA	3632	1/1	0.97	0.06	79,79,79,79	0
58	MG	CA	3182	1/1	0.97	0.14	27,27,27,27	0
58	MG	AA	3377	1/1	0.97	0.05	20,20,20,20	0
58	MG	CA	3317	1/1	0.97	0.05	44,44,44,44	0
58	MG	A7	103	1/1	0.97	0.07	49,49,49,49	0
58	MG	CA	3321	1/1	0.97	0.05	31,31,31,31	0
58	MG	AA	3043	1/1	0.97	0.11	31,31,31,31	0
58	MG	CA	3639	1/1	0.97	0.12	55,55,55,55	0
58	MG	AA	3453	1/1	0.97	0.13	56,56,56,56	0
58	MG	AA	3150	1/1	0.97	0.10	15,15,15,15	0
58	MG	AA	3210	1/1	0.97	0.12	24,24,24,24	1
58	MG	AA	3552	1/1	0.97	0.07	63,63,63,63	0
58	MG	AA	3810	1/1	0.97	0.07	54,54,54,54	0
58	MG	AA	3631	1/1	0.97	0.07	46,46,46,46	0
58	MG	CA	3486	1/1	0.97	0.15	69,69,69,69	0
58	MG	CA	3487	1/1	0.97	0.11	70,70,70,70	0
58	MG	CA	3648	1/1	0.97	0.13	53,53,53,53	0
58	MG	CA	3329	1/1	0.97	0.07	29,29,29,29	0
58	MG	AA	3717	1/1	0.97	0.12	47,47,47,47	0
58	MG	CA	3652	1/1	0.97	0.07	53,53,53,53	0
58	MG	CA	3193	1/1	0.97	0.07	64,64,64,64	0
58	MG	AA	3179	1/1	0.97	0.11	71,71,71,71	0
58	MG	AA	3719	1/1	0.97	0.06	58,58,58,58	0
58	MG	AA	3384	1/1	0.97	0.06	34,34,34,34	0
58	MG	AA	3044	1/1	0.97	0.10	34,34,34,34	0
58	MG	AA	3557	1/1	0.97	0.05	19,19,19,19	0
58	MG	CA	3496	1/1	0.97	0.09	63,63,63,63	0
58	MG	CA	3338	1/1	0.97	0.11	63,63,63,63	0
58	MG	AA	3637	1/1	0.97	0.05	45,45,45,45	0
58	MG	AA	3104	1/1	0.97	0.06	28,28,28,28	0
58	MG	AA	3285	1/1	0.97	0.06	45,45,45,45	0
58	MG	BA	1613	1/1	0.97	0.09	31,31,31,31	0
58	MG	AA	3395	1/1	0.97	0.08	18,18,18,18	0
58	MG	AA	3641	1/1	0.97	0.08	41,41,41,41	0
58	MG	AA	3397	1/1	0.97	0.05	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3562	1/1	0.97	0.05	48,48,48,48	1
58	MG	AA	3401	1/1	0.97	0.06	33,33,33,33	0
58	MG	AA	3125	1/1	0.97	0.10	23,23,23,23	1
58	MG	AA	3287	1/1	0.97	0.13	47,47,47,47	0
58	MG	AA	3567	1/1	0.97	0.06	51,51,51,51	0
58	MG	CA	3510	1/1	0.97	0.06	65,65,65,65	0
58	MG	CA	3354	1/1	0.97	0.07	61,61,61,61	0
58	MG	AA	3154	1/1	0.97	0.13	46,46,46,46	0
58	MG	AA	3470	1/1	0.97	0.05	29,29,29,29	0
58	MG	CA	3102	1/1	0.97	0.06	56,56,56,56	0
58	MG	AA	3471	1/1	0.97	0.09	34,34,34,34	0
58	MG	AA	3408	1/1	0.97	0.04	20,20,20,20	0
58	MG	AA	3574	1/1	0.97	0.06	30,30,30,30	1
58	MG	CA	3519	1/1	0.97	0.10	79,79,79,79	0
58	MG	AA	3253	1/1	0.97	0.15	29,29,29,29	1
58	MG	AA	3046	1/1	0.97	0.07	34,34,34,34	0
58	MG	AA	3156	1/1	0.97	0.13	33,33,33,33	1
58	MG	AA	3047	1/1	0.97	0.12	34,34,34,34	0
58	MG	AA	3482	1/1	0.97	0.09	65,65,65,65	0
58	MG	CA	3369	1/1	0.97	0.06	59,59,59,59	0
58	MG	AA	3417	1/1	0.97	0.06	25,25,25,25	0
58	MG	AA	3418	1/1	0.97	0.07	43,43,43,43	0
58	MG	AA	3189	1/1	0.97	0.08	40,40,40,40	0
58	MG	CA	3529	1/1	0.97	0.06	57,57,57,57	0
58	MG	BA	1729	1/1	0.97	0.05	45,45,45,45	0
58	MG	BA	1730	1/1	0.97	0.06	52,52,52,52	0
58	MG	AA	3488	1/1	0.97	0.05	20,20,20,20	0
58	MG	AA	3757	1/1	0.97	0.05	55,55,55,55	0
58	MG	AA	3420	1/1	0.97	0.12	26,26,26,26	0
58	MG	AA	3666	1/1	0.97	0.05	64,64,64,64	0
58	MG	AA	3084	1/1	0.97	0.08	32,32,32,32	0
58	MG	AA	3023	1/1	0.97	0.16	33,33,33,33	1
58	MG	AA	3001	1/1	0.97	0.06	37,37,37,37	0
58	MG	CA	3124	1/1	0.97	0.17	48,48,48,48	0
58	MG	CA	3238	1/1	0.97	0.09	59,59,59,59	0
58	MG	CU	201	1/1	0.97	0.18	64,64,64,64	0
58	MG	CA	3390	1/1	0.97	0.03	64,64,64,64	0
58	MG	CA	3011	1/1	0.97	0.07	47,47,47,47	0
58	MG	AA	3031	1/1	0.97	0.11	10,10,10,10	1
58	MG	AF	303	1/1	0.97	0.09	41,41,41,41	1
58	MG	CA	3242	1/1	0.97	0.04	41,41,41,41	0
58	MG	AA	3593	1/1	0.97	0.05	25,25,25,25	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3427	1/1	0.97	0.04	33,33,33,33	0
58	MG	AA	3009	1/1	0.97	0.04	24,24,24,24	0
58	MG	DA	1601	1/1	0.97	0.09	61,61,61,61	0
58	MG	AA	3034	1/1	0.97	0.10	57,57,57,57	0
58	MG	BA	1746	1/1	0.97	0.04	37,37,37,37	0
58	MG	AA	3768	1/1	0.97	0.16	99,99,99,99	0
58	MG	CA	3022	1/1	0.97	0.12	38,38,38,38	0
58	MG	CA	3554	1/1	0.97	0.11	67,67,67,67	0
58	MG	AA	3502	1/1	0.97	0.06	51,51,51,51	1
58	MG	AA	3303	1/1	0.97	0.11	56,56,56,56	0
58	MG	AA	3053	1/1	0.97	0.07	14,14,14,14	0
58	MG	AA	3069	1/1	0.97	0.06	34,34,34,34	0
58	MG	AN	3002	1/1	0.97	0.09	27,27,27,27	0
58	MG	DZ	702	1/1	0.97	0.11	57,57,57,57	0
58	MG	BA	1753	1/1	0.97	0.07	58,58,58,58	0
60	SF4	BD	501	8/8	0.97	0.04	80,80,80,80	0
60	SF4	DD	501	8/8	0.97	0.05	90,90,90,90	1
58	MG	AN	3003	1/1	0.97	0.06	47,47,47,47	0
58	MG	CA	3410	1/1	0.97	0.06	31,31,31,31	0
62	GDP	BZ	704	28/28	0.97	0.06	53,53,53,53	1
58	MG	AA	3506	1/1	0.97	0.07	32,32,32,32	0
58	MG	CA	3471	1/1	0.98	0.08	45,45,45,45	0
58	MG	AA	3101	1/1	0.98	0.17	52,52,52,52	0
58	MG	AA	3742	1/1	0.98	0.08	82,82,82,82	0
58	MG	CA	3211	1/1	0.98	0.10	40,40,40,40	0
58	MG	AA	3497	1/1	0.98	0.04	46,46,46,46	0
58	MG	CA	3337	1/1	0.98	0.06	41,41,41,41	0
58	MG	AA	3187	1/1	0.98	0.13	32,32,32,32	0
58	MG	AB	3020	1/1	0.98	0.10	55,55,55,55	0
58	MG	AA	3500	1/1	0.98	0.05	47,47,47,47	0
58	MG	AB	3022	1/1	0.98	0.03	58,58,58,58	0
58	MG	AA	3296	1/1	0.98	0.04	17,17,17,17	0
58	MG	CA	3345	1/1	0.98	0.07	38,38,38,38	0
58	MG	AA	3130	1/1	0.98	0.06	37,37,37,37	0
58	MG	CA	3219	1/1	0.98	0.10	31,31,31,31	0
58	MG	DA	1654	1/1	0.98	0.03	30,30,30,30	0
58	MG	CA	3108	1/1	0.98	0.13	60,60,60,60	0
58	MG	AA	3659	1/1	0.98	0.06	14,14,14,14	0
58	MG	AA	3225	1/1	0.98	0.06	27,27,27,27	1
58	MG	AA	3379	1/1	0.98	0.05	30,30,30,30	0
58	MG	AA	3584	1/1	0.98	0.06	65,65,65,65	0
58	MG	CA	3629	1/1	0.98	0.06	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3380	1/1	0.98	0.04	15,15,15,15	0
58	MG	AA	3754	1/1	0.98	0.03	29,29,29,29	0
58	MG	AA	3507	1/1	0.98	0.06	14,14,14,14	0
58	MG	AA	3587	1/1	0.98	0.09	53,53,53,53	0
58	MG	AA	3588	1/1	0.98	0.08	38,38,38,38	0
58	MG	CA	3359	1/1	0.98	0.10	42,42,42,42	0
58	MG	CA	3007	1/1	0.98	0.04	28,28,28,28	0
58	MG	AA	3337	1/1	0.98	0.03	10,10,10,10	0
58	MG	AA	3131	1/1	0.98	0.13	55,55,55,55	0
58	MG	AA	3022	1/1	0.98	0.03	9,9,9,9	0
58	MG	CA	3364	1/1	0.98	0.09	29,29,29,29	0
58	MG	CA	3234	1/1	0.98	0.14	54,54,54,54	0
58	MG	AA	3160	1/1	0.98	0.07	57,57,57,57	0
58	MG	AA	3251	1/1	0.98	0.07	42,42,42,42	0
58	MG	AE	305	1/1	0.98	0.07	30,30,30,30	0
58	MG	AA	3387	1/1	0.98	0.03	17,17,17,17	0
58	MG	CA	3370	1/1	0.98	0.06	47,47,47,47	0
58	MG	AA	3389	1/1	0.98	0.06	17,17,17,17	0
58	MG	AA	3275	1/1	0.98	0.12	47,47,47,47	1
58	MG	AA	3304	1/1	0.98	0.10	30,30,30,30	0
58	MG	BA	1745	1/1	0.98	0.05	52,52,52,52	0
58	MG	CA	3511	1/1	0.98	0.06	68,68,68,68	0
58	MG	CA	3019	1/1	0.98	0.05	28,28,28,28	0
58	MG	CA	3377	1/1	0.98	0.05	80,80,80,80	0
58	MG	AF	305	1/1	0.98	0.15	41,41,41,41	0
58	MG	CA	3021	1/1	0.98	0.04	29,29,29,29	0
58	MG	AA	3346	1/1	0.98	0.07	46,46,46,46	0
58	MG	DA	1688	1/1	0.98	0.08	66,66,66,66	0
58	MG	CA	3658	1/1	0.98	0.07	50,50,50,50	0
58	MG	CA	3381	1/1	0.98	0.05	38,38,38,38	0
58	MG	CA	3023	1/1	0.98	0.10	46,46,46,46	0
58	MG	AA	3396	1/1	0.98	0.03	22,22,22,22	0
58	MG	CA	3249	1/1	0.98	0.06	46,46,46,46	0
58	MG	AA	3276	1/1	0.98	0.14	47,47,47,47	1
58	MG	AA	3400	1/1	0.98	0.11	39,39,39,39	0
58	MG	AA	3527	1/1	0.98	0.07	26,26,26,26	0
58	MG	AA	3528	1/1	0.98	0.05	28,28,28,28	0
58	MG	AA	3529	1/1	0.98	0.07	16,16,16,16	0
58	MG	AA	3530	1/1	0.98	0.04	53,53,53,53	0
58	MG	AA	3306	1/1	0.98	0.09	47,47,47,47	0
58	MG	AA	3402	1/1	0.98	0.10	33,33,33,33	0
58	MG	AA	3033	1/1	0.98	0.16	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3534	1/1	0.98	0.06	27,27,27,27	0
58	MG	CA	3146	1/1	0.98	0.06	60,60,60,60	0
58	MG	AP	202	1/1	0.98	0.10	28,28,28,28	1
58	MG	AA	3350	1/1	0.98	0.09	31,31,31,31	0
58	MG	AA	3536	1/1	0.98	0.03	35,35,35,35	0
58	MG	AA	3134	1/1	0.98	0.20	59,59,59,59	1
58	MG	CA	3041	1/1	0.98	0.17	31,31,31,31	0
58	MG	CA	3403	1/1	0.98	0.05	91,91,91,91	0
58	MG	CD	303	1/1	0.98	0.17	37,37,37,37	0
58	MG	AA	3082	1/1	0.98	0.15	23,23,23,23	1
58	MG	AA	3693	1/1	0.98	0.07	48,48,48,48	0
58	MG	AA	3539	1/1	0.98	0.03	28,28,28,28	0
58	MG	AA	3540	1/1	0.98	0.04	29,29,29,29	0
58	MG	DA	1717	1/1	0.98	0.08	52,52,52,52	0
58	MG	AA	3410	1/1	0.98	0.06	30,30,30,30	0
58	MG	DA	1719	1/1	0.98	0.06	74,74,74,74	0
58	MG	AA	3542	1/1	0.98	0.08	63,63,63,63	0
58	MG	AU	204	1/1	0.98	0.18	62,62,62,62	0
58	MG	AA	3089	1/1	0.98	0.11	47,47,47,47	1
58	MG	AA	3544	1/1	0.98	0.05	16,16,16,16	0
58	MG	AV	203	1/1	0.98	0.09	40,40,40,40	0
58	MG	AV	204	1/1	0.98	0.06	38,38,38,38	0
58	MG	CA	3279	1/1	0.98	0.03	34,34,34,34	0
58	MG	CA	3550	1/1	0.98	0.08	33,33,33,33	0
58	MG	AA	3545	1/1	0.98	0.05	51,51,51,51	1
58	MG	AA	3097	1/1	0.98	0.09	26,26,26,26	0
58	MG	AA	3257	1/1	0.98	0.03	14,14,14,14	0
58	MG	AA	3469	1/1	0.98	0.06	43,43,43,43	0
58	MG	AA	3315	1/1	0.98	0.10	34,34,34,34	0
58	MG	AA	3357	1/1	0.98	0.06	27,27,27,27	0
58	MG	AA	3707	1/1	0.98	0.16	29,29,29,29	1
58	MG	AA	3474	1/1	0.98	0.09	53,53,53,53	0
58	MG	CA	3559	1/1	0.98	0.08	52,52,52,52	1
58	MG	AA	3083	1/1	0.98	0.10	38,38,38,38	1
58	MG	CA	3289	1/1	0.98	0.10	42,42,42,42	0
58	MG	AA	3359	1/1	0.98	0.05	51,51,51,51	0
58	MG	CA	3291	1/1	0.98	0.05	27,27,27,27	0
58	MG	BA	1682	1/1	0.98	0.03	53,53,53,53	0
58	MG	CA	3566	1/1	0.98	0.04	41,41,41,41	0
58	MG	CA	3064	1/1	0.98	0.06	43,43,43,43	0
58	MG	AA	3478	1/1	0.98	0.05	40,40,40,40	0
58	MG	DA	1745	1/1	0.98	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3555	1/1	0.98	0.06	38,38,38,38	0
58	MG	AA	3126	1/1	0.98	0.15	50,50,50,50	0
58	MG	AA	3421	1/1	0.98	0.10	12,12,12,12	0
58	MG	AA	3217	1/1	0.98	0.04	6,6,6,6	0
58	MG	AA	3716	1/1	0.98	0.04	57,57,57,57	0
58	MG	AA	3238	1/1	0.98	0.10	61,61,61,61	0
58	MG	CA	3576	1/1	0.98	0.04	36,36,36,36	0
58	MG	A5	103	1/1	0.98	0.07	45,45,45,45	0
58	MG	AA	3483	1/1	0.98	0.04	43,43,43,43	1
58	MG	AA	3218	1/1	0.98	0.11	38,38,38,38	0
58	MG	AA	3003	1/1	0.98	0.03	20,20,20,20	0
58	MG	A7	102	1/1	0.98	0.06	38,38,38,38	0
58	MG	AA	3721	1/1	0.98	0.05	10,10,10,10	0
58	MG	AA	3323	1/1	0.98	0.03	22,22,22,22	0
58	MG	CA	3308	1/1	0.98	0.04	41,41,41,41	0
58	MG	A7	105	1/1	0.98	0.06	43,43,43,43	0
58	MG	AA	3085	1/1	0.98	0.09	53,53,53,53	0
58	MG	DA	1764	1/1	0.98	0.04	55,55,55,55	0
58	MG	CA	3587	1/1	0.98	0.03	34,34,34,34	0
58	MG	DA	1617	1/1	0.98	0.10	48,48,48,48	0
58	MG	CA	3311	1/1	0.98	0.07	48,48,48,48	0
58	MG	CA	3450	1/1	0.98	0.05	48,48,48,48	0
58	MG	AA	3815	1/1	0.98	0.05	29,29,29,29	1
58	MG	A8	5002	1/1	0.98	0.06	31,31,31,31	0
58	MG	AA	3565	1/1	0.98	0.07	29,29,29,29	0
58	MG	AA	3170	1/1	0.98	0.08	53,53,53,53	0
58	MG	AA	3643	1/1	0.98	0.08	49,49,49,49	0
58	MG	CA	3318	1/1	0.98	0.05	33,33,33,33	0
58	MG	AA	3243	1/1	0.98	0.10	24,24,24,24	1
58	MG	AA	3568	1/1	0.98	0.07	16,16,16,16	0
58	MG	AA	3369	1/1	0.98	0.08	27,27,27,27	0
58	MG	AA	3327	1/1	0.98	0.03	13,13,13,13	0
58	MG	AA	3293	1/1	0.98	0.11	32,32,32,32	0
58	MG	AA	3572	1/1	0.98	0.03	32,32,32,32	0
59	ZN	A4	501	1/1	0.98	0.04	137,137,137,137	0
59	ZN	BN	501	1/1	0.98	0.05	123,123,123,123	0
58	MG	CA	3092	1/1	0.98	0.07	70,70,70,70	0
59	ZN	DN	501	1/1	0.98	0.05	129,129,129,129	0
58	MG	AA	3650	1/1	0.98	0.04	60,60,60,60	0
58	MG	AB	3011	1/1	0.98	0.06	30,30,30,30	0
58	MG	AB	3012	1/1	0.98	0.08	29,29,29,29	1
58	MG	AB	3013	1/1	0.98	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3494	1/1	0.98	0.09	50,50,50,50	0
58	MG	AA	3331	1/1	0.98	0.12	34,34,34,34	0
58	MG	AA	3521	1/1	0.99	0.05	29,29,29,29	0
58	MG	CA	3320	1/1	0.99	0.05	30,30,30,30	0
58	MG	AA	3038	1/1	0.99	0.05	11,11,11,11	0
58	MG	CA	3028	1/1	0.99	0.18	35,35,35,35	1
58	MG	CA	3029	1/1	0.99	0.06	33,33,33,33	0
58	MG	AA	3328	1/1	0.99	0.03	18,18,18,18	0
58	MG	AA	3524	1/1	0.99	0.05	28,28,28,28	0
58	MG	AA	3413	1/1	0.99	0.03	20,20,20,20	0
58	MG	CA	3265	1/1	0.99	0.04	40,40,40,40	0
58	MG	AA	3329	1/1	0.99	0.05	17,17,17,17	0
58	MG	AA	3012	1/1	0.99	0.06	34,34,34,34	0
58	MG	AA	3485	1/1	0.99	0.04	14,14,14,14	0
58	MG	AA	3749	1/1	0.99	0.03	14,14,14,14	0
58	MG	CA	3270	1/1	0.99	0.08	35,35,35,35	0
58	MG	AA	3416	1/1	0.99	0.04	30,30,30,30	0
58	MG	AA	3700	1/1	0.99	0.08	35,35,35,35	0
58	MG	AA	3314	1/1	0.99	0.11	28,28,28,28	0
58	MG	AA	3388	1/1	0.99	0.05	25,25,25,25	0
58	MG	CA	3617	1/1	0.99	0.04	31,31,31,31	0
58	MG	AA	3289	1/1	0.99	0.03	27,27,27,27	0
58	MG	AA	3074	1/1	0.99	0.09	15,15,15,15	0
58	MG	CA	3339	1/1	0.99	0.03	34,34,34,34	0
58	MG	AA	3075	1/1	0.99	0.03	9,9,9,9	0
58	MG	BA	1760	1/1	0.99	0.02	57,57,57,57	0
58	MG	CA	3342	1/1	0.99	0.07	45,45,45,45	0
58	MG	AA	3392	1/1	0.99	0.04	42,42,42,42	0
58	MG	AA	3393	1/1	0.99	0.07	21,21,21,21	0
58	MG	AA	3394	1/1	0.99	0.07	27,27,27,27	0
58	MG	AA	3425	1/1	0.99	0.07	18,18,18,18	0
58	MG	CA	3415	1/1	0.99	0.03	31,31,31,31	1
58	MG	AA	3040	1/1	0.99	0.14	40,40,40,40	1
58	MG	AA	3459	1/1	0.99	0.04	18,18,18,18	0
58	MG	AA	3498	1/1	0.99	0.04	37,37,37,37	0
58	MG	AA	3583	1/1	0.99	0.02	13,13,13,13	0
58	MG	CA	3560	1/1	0.99	0.02	36,36,36,36	0
58	MG	AA	3188	1/1	0.99	0.06	13,13,13,13	0
58	MG	AA	3207	1/1	0.99	0.07	22,22,22,22	1
58	MG	AA	3399	1/1	0.99	0.02	18,18,18,18	0
58	MG	AA	3228	1/1	0.99	0.06	51,51,51,51	0
58	MG	AA	3308	1/1	0.99	0.03	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3356	1/1	0.99	0.04	57,57,57,57	0
58	MG	AA	3376	1/1	0.99	0.05	19,19,19,19	0
58	MG	AA	3675	1/1	0.99	0.05	38,38,38,38	0
58	MG	AA	3403	1/1	0.99	0.04	28,28,28,28	0
58	MG	AA	3723	1/1	0.99	0.05	21,21,21,21	0
58	MG	DA	1758	1/1	0.99	0.12	71,71,71,71	0
58	MG	AA	3340	1/1	0.99	0.08	59,59,59,59	0
58	MG	CA	3572	1/1	0.99	0.05	54,54,54,54	0
58	MG	AA	3140	1/1	0.99	0.06	50,50,50,50	0
58	MG	AA	3776	1/1	0.99	0.02	40,40,40,40	0
58	MG	AA	3635	1/1	0.99	0.03	23,23,23,23	0
58	MG	AA	3727	1/1	0.99	0.04	49,49,49,49	0
58	MG	DA	1611	1/1	0.99	0.03	38,38,38,38	0
58	MG	CA	3650	1/1	0.99	0.14	27,27,27,27	0
58	MG	AA	3509	1/1	0.99	0.06	49,49,49,49	0
58	MG	AA	3342	1/1	0.99	0.06	5,5,5,5	0
58	MG	AA	3730	1/1	0.99	0.09	30,30,30,30	0
58	MG	AA	3407	1/1	0.99	0.04	49,49,49,49	0
58	MG	AA	3045	1/1	0.99	0.09	43,43,43,43	0
58	MG	AA	3475	1/1	0.99	0.04	62,62,62,62	0
58	MG	CA	3372	1/1	0.99	0.03	42,42,42,42	0
58	MG	AA	3734	1/1	0.99	0.05	22,22,22,22	0
58	MG	DA	1621	1/1	0.99	0.08	44,44,44,44	0
58	MG	CA	3443	1/1	0.99	0.02	36,36,36,36	0
58	MG	DA	1699	1/1	0.99	0.06	75,75,75,75	0
58	MG	BA	1734	1/1	0.99	0.03	71,71,71,71	0
58	MG	AA	3515	1/1	0.99	0.04	20,20,20,20	0
58	MG	BA	1681	1/1	0.99	0.07	36,36,36,36	0
58	MG	AA	3439	1/1	0.99	0.12	17,17,17,17	0
58	MG	CA	3312	1/1	0.99	0.04	51,51,51,51	0
58	MG	AA	3440	1/1	0.99	0.10	31,31,31,31	0
58	MG	AA	3409	1/1	0.99	0.08	45,45,45,45	0
58	MG	AA	3037	1/1	0.99	0.04	45,45,45,45	0
58	MG	CA	3382	1/1	0.99	0.04	40,40,40,40	0
58	MG	CA	3453	1/1	0.99	0.04	39,39,39,39	0
58	MG	AA	3791	1/1	0.99	0.08	16,16,16,16	0
58	MG	AA	3520	1/1	0.99	0.04	38,38,38,38	0
58	MG	A0	101	1/1	0.99	0.03	43,43,43,43	0
58	MG	AE	303	1/1	1.00	0.07	18,18,18,18	0
59	ZN	AY	501	1/1	1.00	0.01	65,65,65,65	0
58	MG	AA	3472	1/1	1.00	0.03	24,24,24,24	0
59	ZN	A5	104	1/1	1.00	0.01	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	A6	102	1/1	1.00	0.02	46,46,46,46	0
59	ZN	A9	501	1/1	1.00	0.01	42,42,42,42	0
58	MG	AA	3473	1/1	1.00	0.03	15,15,15,15	0
59	ZN	CY	501	1/1	1.00	0.02	93,93,93,93	0
58	MG	AA	3398	1/1	1.00	0.01	15,15,15,15	0
59	ZN	C5	102	1/1	1.00	0.03	68,68,68,68	0
59	ZN	C6	501	1/1	1.00	0.02	61,61,61,61	0
59	ZN	C9	501	1/1	1.00	0.03	94,94,94,94	0
58	MG	AA	3465	1/1	1.00	0.04	39,39,39,39	0
58	MG	AA	3722	1/1	1.00	0.02	18,18,18,18	0
58	MG	AA	3514	1/1	1.00	0.03	18,18,18,18	0
58	MG	CA	3383	1/1	1.00	0.07	44,44,44,44	0
58	MG	AA	3320	1/1	1.00	0.06	24,24,24,24	0
58	MG	AA	3501	1/1	1.00	0.02	24,24,24,24	0
58	MG	AA	3385	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.