



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 09:27 AM UTC

PDB ID : 4V7W / pdb_00004v7w
Title : Structure of the *Thermus thermophilus* ribosome complexed with chloramphenicol.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-16
Resolution : 3.00 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

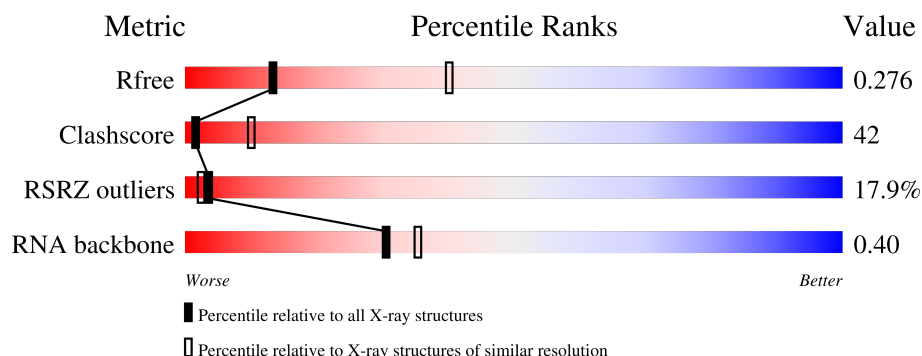
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	1522	18% 23% 61% 15%
1	CA	1522	13% 23% 61% 15%
2	AB	256	31% 28% 64% 8%
2	CB	256	19% 29% 62% 8%
3	AC	239	18% 33% 54% 13%
3	CC	239	16% 34% 53% 13%

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Mol	Chain	Length	Quality of chain
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	

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Mol	Chain	Length	Quality of chain
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	
28	B6	54	
28	D6	54	

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Mol	Chain	Length	Quality of chain
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
38	BI	148	
38	DI	148	
39	BN	140	
39	DN	140	
40	BO	122	
40	DO	122	
41	BP	150	

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Mol	Chain	Length	Quality of chain
41	DP	150	
42	BQ	141	
42	DQ	141	
43	BR	118	
43	DR	118	
44	BS	112	
44	DS	112	
45	BT	146	
45	DT	146	
46	BU	118	
46	DU	118	
47	BV	101	
47	DV	101	
48	BW	113	
48	DW	113	
49	BX	96	
49	DX	96	
50	BY	110	
50	DY	110	
51	BZ	206	
51	DZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	CA	1638	-	-	-	X
53	ZN	CD	301	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 277987 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	conflict	UNP P80374
CI	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	VAL	-	insertion	UNP Q5SHN3
AL	3	ALA	-	insertion	UNP Q5SHN3
AL	4	LEU	-	insertion	UNP Q5SHN3
CL	2	VAL	-	insertion	UNP Q5SHN3
CL	3	ALA	-	insertion	UNP Q5SHN3
CL	4	LEU	-	insertion	UNP Q5SHN3

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	CM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B4	32	Total	C	N	O	0	0	0
			157	93	32	32			
26	D4	32	Total	C	N	O	0	0	0
			157	93	32	32			

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			
31	DA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

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

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

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

- Molecule 38 is a protein called 50S ribosomal protein L9.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

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

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			
45	DT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

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

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	AA	56	Total	Mg	0	0
			56	56		
52	B1	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	BA	368	Total	Mg	0	0
			368	368		
52	BB	7	Total	Mg	0	0
			7	7		
52	BD	1	Total	Mg	0	0
			1	1		
52	BE	1	Total	Mg	0	0
			1	1		
52	BF	1	Total	Mg	0	0
			1	1		
52	BP	2	Total	Mg	0	0
			2	2		
52	BQ	2	Total	Mg	0	0
			2	2		
52	BR	2	Total	Mg	0	0
			2	2		
52	BU	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	CA	53	Total	Mg	0	0
			53	53		
52	D1	1	Total	Mg	0	0
			1	1		
52	D5	2	Total	Mg	0	0
			2	2		
52	DA	332	Total	Mg	0	0
			332	332		
52	DB	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
52	DD	1	Total Mg 1 1	0	0
52	DE	1	Total Mg 1 1	0	0
52	DF	1	Total Mg 1 1	0	0
52	DP	1	Total Mg 1 1	0	0
52	DQ	1	Total Mg 1 1	0	0
52	DR	1	Total Mg 1 1	0	0
52	DU	1	Total Mg 1 1	0	0
52	DX	1	Total Mg 1 1	0	0

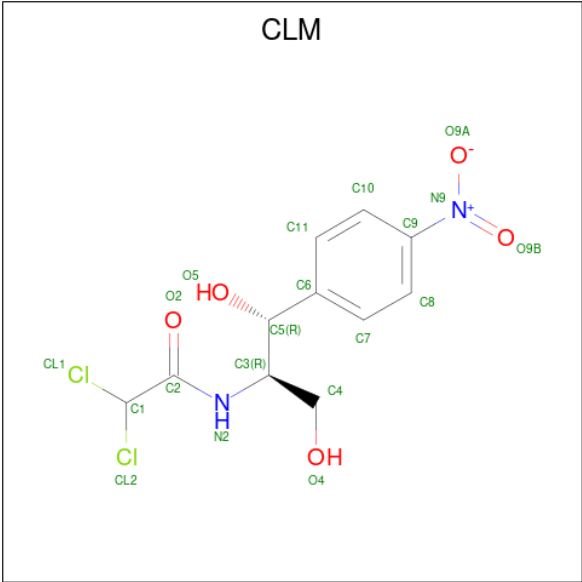
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BA	1	Total K 1 1	0	0
54	DA	1	Total K 1 1	0	0

- Molecule 55 is CHLORAMPHENICOL (CCD ID: CLM) (formula: C₁₁H₁₂Cl₂N₂O₅).

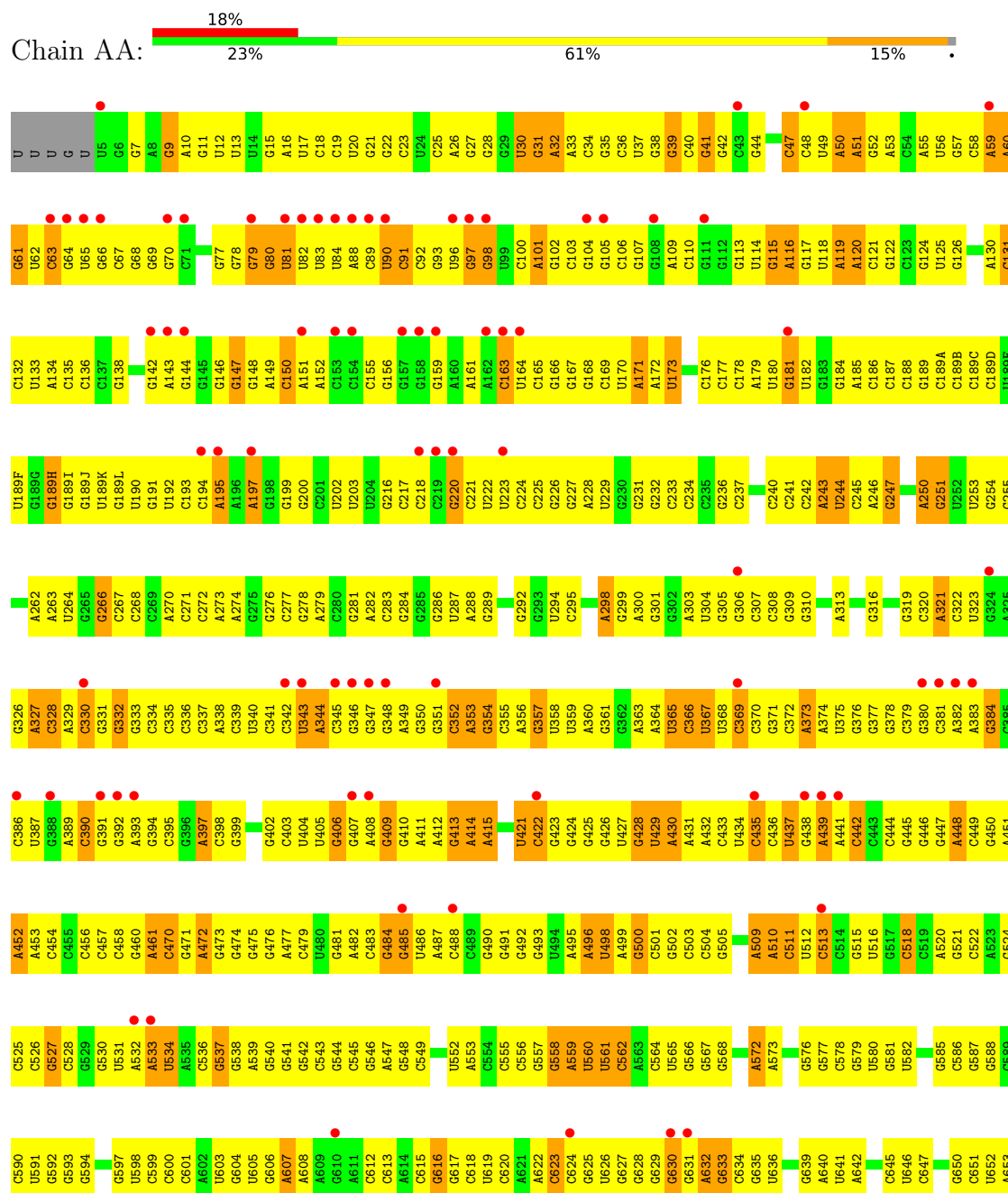


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	BA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
55	DA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

3 Residue-property plots

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

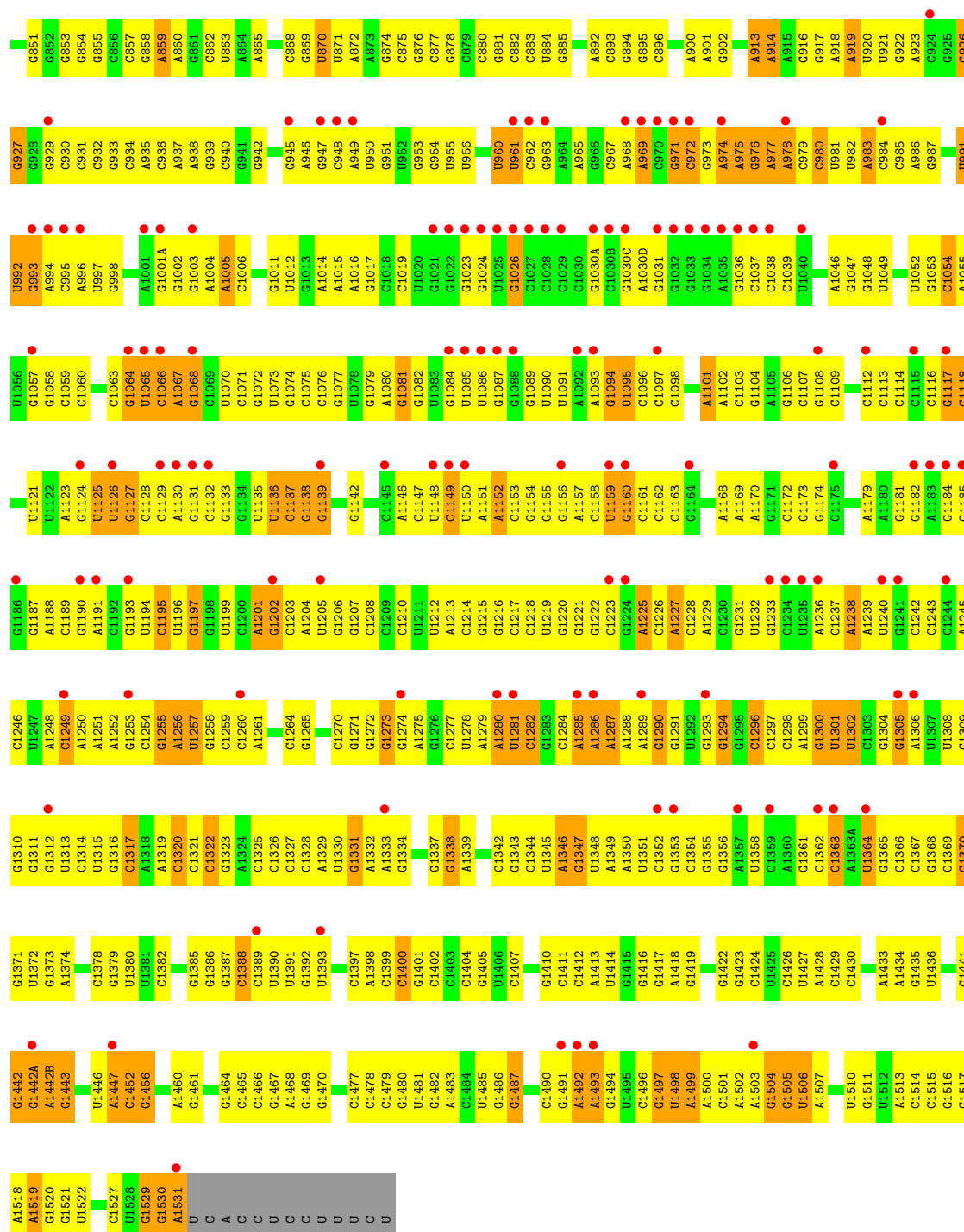
• Molecule 1: 16S rRNA

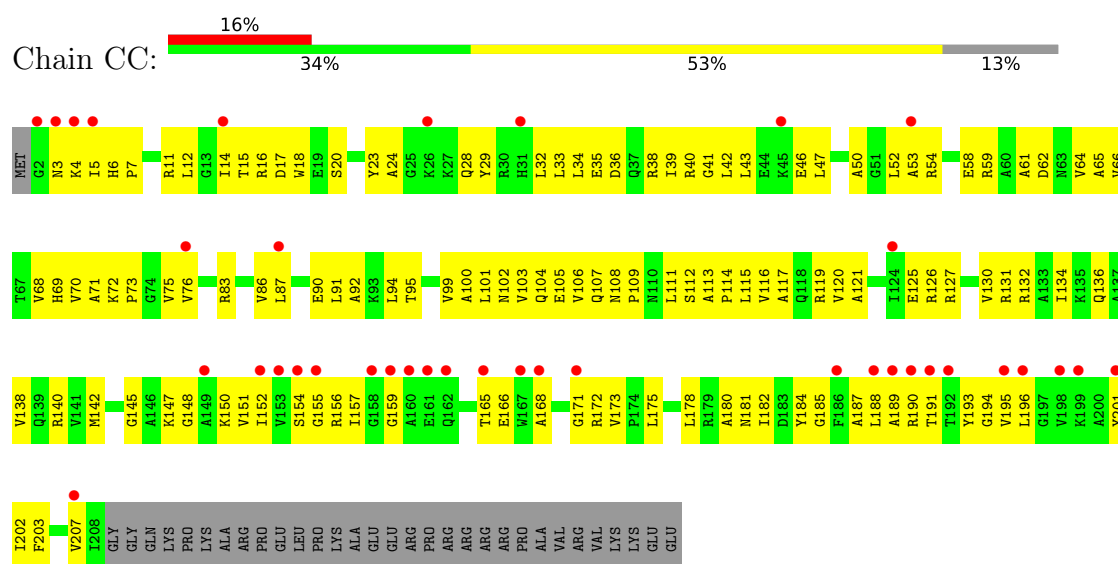


U1510	A1434	G1371	G1311	A1248	G1187	U1122	C1060	U1000	A937	A860	A781	C719	G654
G1511	G1435	U1372	G1312	C1249	A1188	A1123	C1063	A1001	A938	G861	A782	C720	A655
U1512	U1436	G1373	U1313	A1250	G1189	G1124	C1064	G1001A	G939	U863	C783	G721	C856
A1513	A1374	A1374	C1314	A1251	G1190	U1125	U1064	G1002	C940	U863	C784	A722	G657
C1514	G1441	A1375	U1315	A1252	A1191	U1126	U1065	G1003	G941	A864	G785	G723	U659
C1515	G1442	A1376	G1316	G1253	C1192	G1127	C1066	A1004	G942	A865	G786	G724	G660
G1516	G1443	A1377	C1317	C1254	G1193	C1128	A1067	A1005	G945	A866	A787	G725	G661
G1517	A1442A	A1378	A1318	G1255	U1194	C1129	C1068	C1006	G946	C868	U788	G726	G662
A1518	A1442B	G1379	A1319	U1257	C1195	A1130	C1069	C1007	G947	C869	U789	G727	G663
A1519	G1443	U1380	C1320	U1258	U1196	G1131	U1070	G1008	G948	U870	G790	A728	A663
G1520	U1446	U1381	C1321	C1259	G1197	C1132	C1071	C1008	U871	A872	G791	A729	G664
G1521	A1447	C1382	G1322	C1260	U1198	G1133	G1072	G1009	A949	A873	U792	G730	A665
U1522	G1452	C1382	G1323	C1260	U1199	G1134	U1073	U1012	U950	A874	U793	G731	A666
C1527	G1456	G1385	A1384	C1264	C1200	U1135	G1074	G1013	G951	G874	A794	G732	G667
U1528	A1460	G1386	C1325	C1264	A1201	U1136	C1075	A1014	U952	C875	A795	G733	G668
G1529	G1461	G1387	C1326	G1265	G1202	C1137	C1076	A1015	G953	C876	G796	G734	U669
G1530	C1388	C1388	C1327	G1266	C1203	G1138	G1077	A1016	G954	C877	G797	C735	G670
G1531	G1464	C1389	C1328	C1267	A1204	G1139	U1078	G1017	U955	C878	U804	C736	G671
U	C1465	U1390	A1329	G1270	U1205	G1140	G1079	C1018	U956	C879	C805	A737	U672
C	C1466	U1391	U1330	G1271	G1206	G1141	A1080	C1019	U960	C880	C806	C738	G673
A	G1467	G1392	G1331	G1272	G1207	G1142	U1081	U1020	U961	C881	A807	C739	G674
C	A1468	U1393	A1332	G1273	C1208	G1143	U1082	G1023	G962	C882	U740	A675	A676
C	G1469	A1394	A1333	G1274	G1209	G1144	U1083	G1024	G963	C883	G741	G742	A677
U	G1470	C1397	G1334	A1275	C1210	C1145	U1084	U1025	A964	C885	U743	G743	U678
C	G1471	A1398	C1335	G1276	U1212	A1146	U1085	G1026	A965	C886	A814	C744	C679
C	U1472	C1399	C1336	G1277	U1213	C1147	U1086	C1027	A966	C887	A815	C745	C680
U	A1473	C1400	G1337	U1278	A1214	U1148	G1087	C1028	C967	C893	A816	A746	C681
U	G1477	G1401	G1338	U1279	G1215	C1149	G1088	C1029	A968	C894	C817	A747	G682
U	C1478	C1402	A1339	A1280	A1151	U1150	U1089	C1030	A969	C895	C818	C748	G683
C	C1479	G1403	G1342	U1281	C1217	A1152	U1091	G1030A	C970	C896	C749	A684	A684
C	G1480	C1404	G1343	C1282	C1218	C1153	A1092	C1030B	G971	U900	U820	G750	G685
U	U1481	G1405	C1344	G1283	U1219	G1154	A1093	G1030C	C972	A901	G821	U751	U686
U	G1482	U1406	U1345	C1284	G1221	G1155	U1094	G1030D	A974	A753	G752	C754	A687
C	A1483	C1407	A1346	A1285	G1222	G1156	U1095	G1031	A975	A754	C826	C755	C688
C	C1484	G1408	G1347	A1286	C1223	A1157	C1096	G1034	A976	C827	U827	C689	C689
U	U1485	G1410	U1348	A1287	C1224	U1158	C1097	A1035	A977	A828	G829	G690	G691
U	G1486	C1411	A1349	A1288	G1225	U1159	C1098	G1036	A978	A913	C829	U692	U692
U	G1487	C1412	U1350	A1289	A1226	C1161	A1101	G1037	A979	A914	G830	G758	G693
C	U1490	A1413	C1352	G1291	A1227	G1162	A1102	C1038	C980	A915	U831	A759	A694
C	G1491	U1414	G1353	U1292	C1228	C1163	C1103	C1039	U981	G917	C832	G760	A695
C	A1492	G1415	C1354	G1293	A1229	A1168	G1104	U1040	U982	A918	U833	G761	A695
C	A1493	G1416	G1355	G1294	C1230	A1169	A1105	C1043	A983	U919	U835	G762	C701
C	G1494	G1417	G1356	G1295	G1231	A1170	G1106	U1043	C984	U921	G836	G763	A702
C	U1495	A1418	A1357	C1296	U1232	G1171	C1107	A1046	A985	G922	G764	G765	G703
C	G1496	G1419	C1358	C1297	G1233	G1172	C1108	G1047	A986	A923	A766	A766	A704
C	G1497	G1422	C1359	C1298	C1234	G1173	C1109	U1049	G988	C924	A767	U705	A706
C	U1498	G1423	A1360	A1299	U1235	G1174	A1110	G1050	C989	G925	A768	C707	C707
C	A1499	C1424	G1361	G1300	A1236	G1175	A1111	C1051	C990	G926	C770	C770	C708
C	A1500	U1425	C1362	U1301	C1237	G1176	C1112	G1052	G991	G927	G771	G771	G709
C	C1501	C1426	A1363A	C1302	A1238	U1179	C1113	U1052	U992	G928	G774	G774	G710
C	A1502	U1427	U1363A	G1303	A1239	A1180	G1114	G1053	G993	C930	G775	G775	G713
C	A1503	A1428	G1364	G1304	U1240	G1181	C1115	C1054	A994	C931	G776	G776	G714
C	G1504	C1429	A1305	G1305	G1241	G1182	G1116	U1055	C995	C932	A777	A777	A715
C	G1505	C1430	C1366	U1367	C1242	A1183	C1117	U1056	A996	G933	C856	C778	A716
C	U1506	C1431	C1367	U1367	C1243	A1184	C1118	G1057	U997	C934	C857	C779	A717
C	G1432	G1368	G1368	U1308	C1244	G1185	C1119	G1058	G998	A859	G718	G718	A718
C	A1507	G1370	G1370	G1310	A1245	G1186	U1121	C1059	C999	C936			

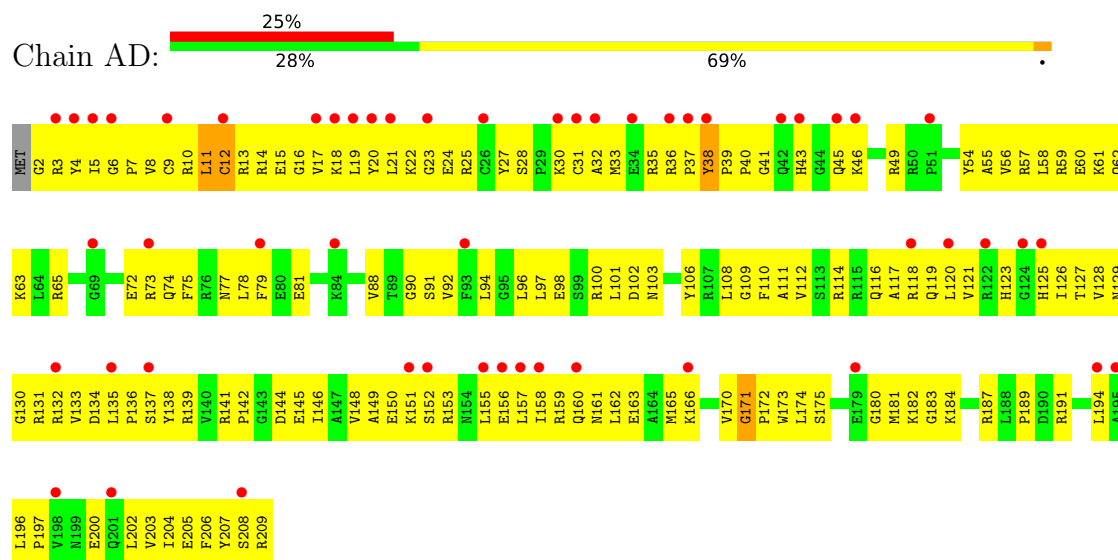
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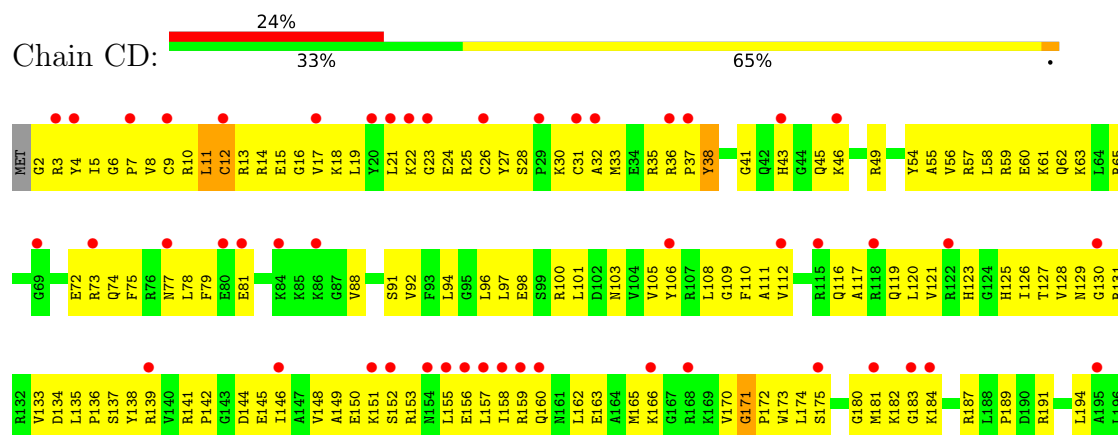




• Molecule 4: 30S ribosomal protein S4

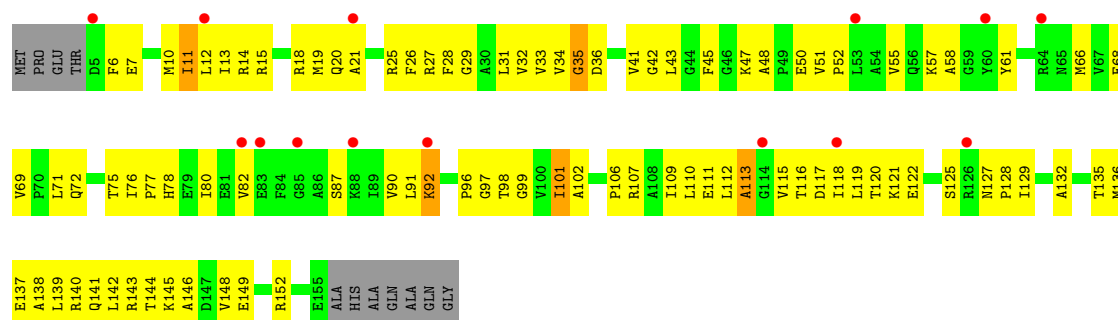


• Molecule 4: 30S ribosomal protein S4

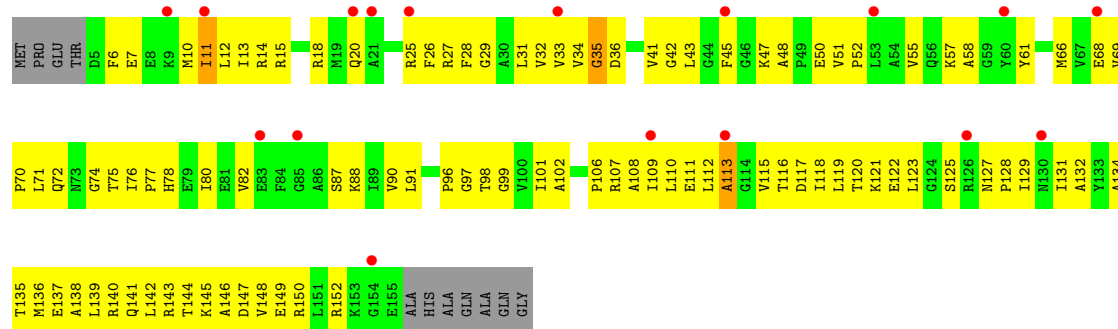




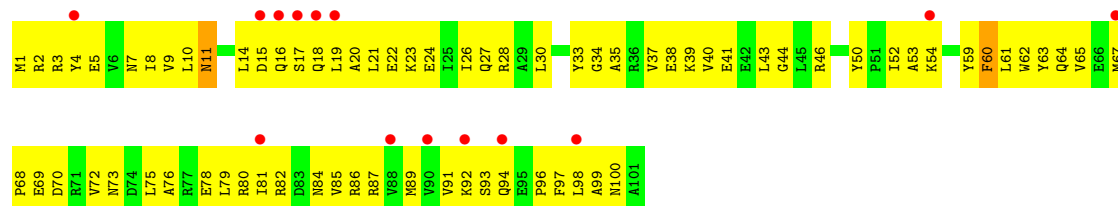
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

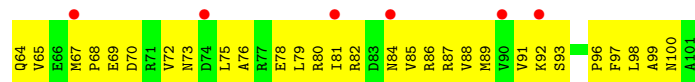


• Molecule 6: 30S ribosomal protein S6

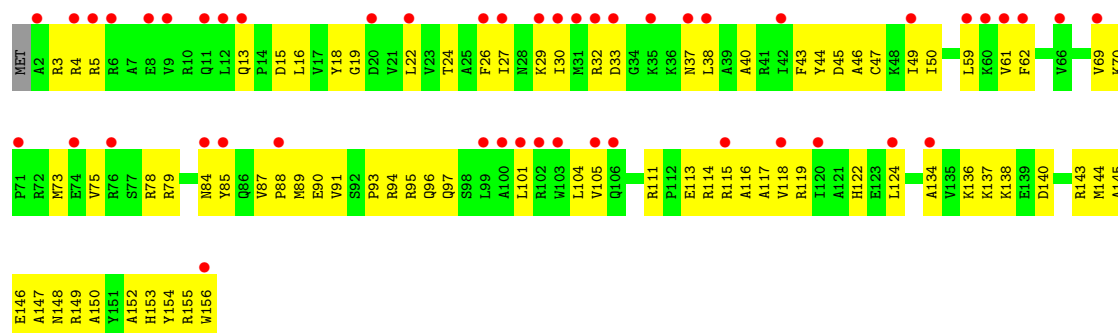


• Molecule 6: 30S ribosomal protein S6





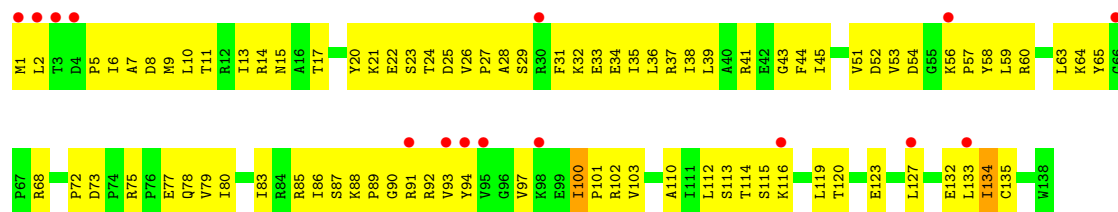
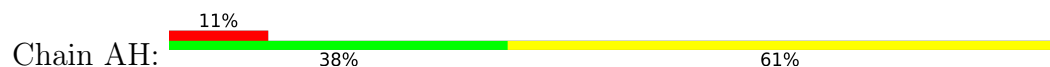
• Molecule 7: 30S ribosomal protein S7



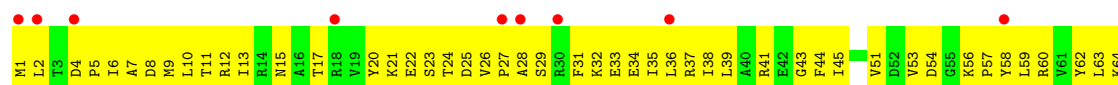
• Molecule 7: 30S ribosomal protein S7

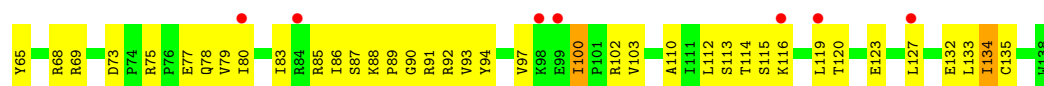


• Molecule 8: 30S ribosomal protein S8

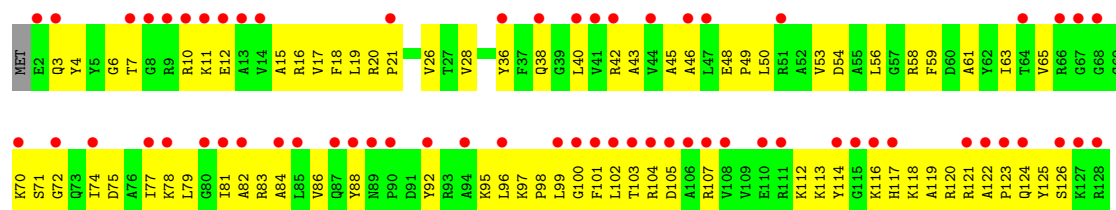


• Molecule 8: 30S ribosomal protein S8

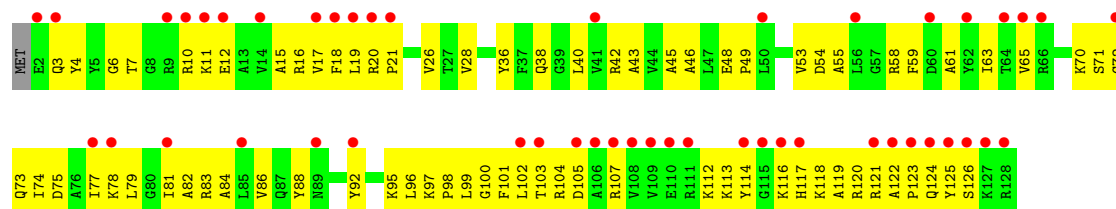
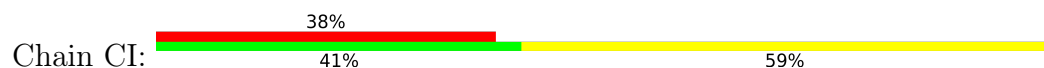




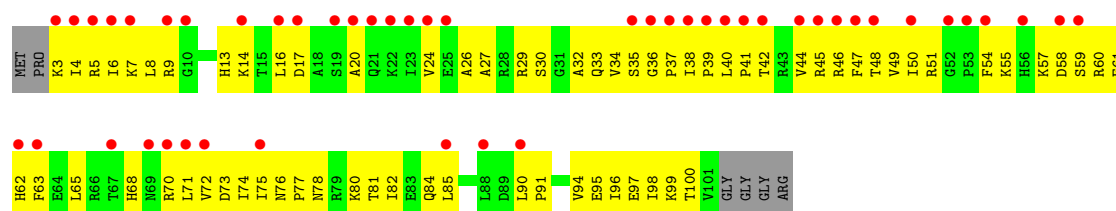
• Molecule 9: 30S ribosomal protein S9



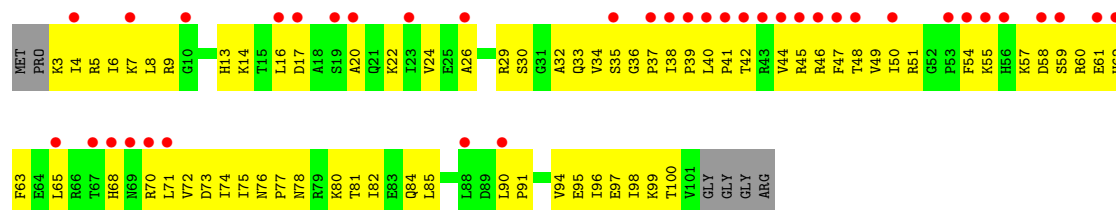
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

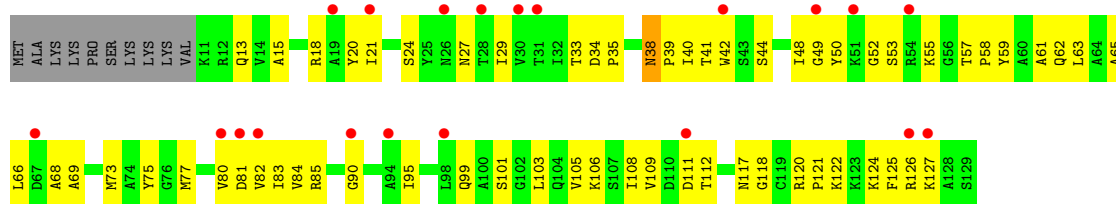


• Molecule 10: 30S ribosomal protein S10

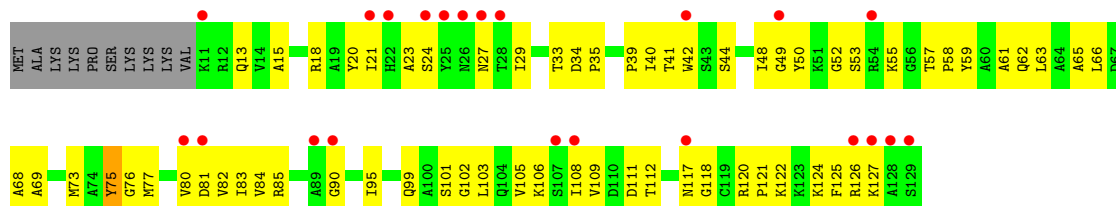
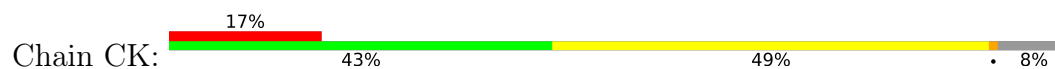


• Molecule 11: 30S ribosomal protein S11

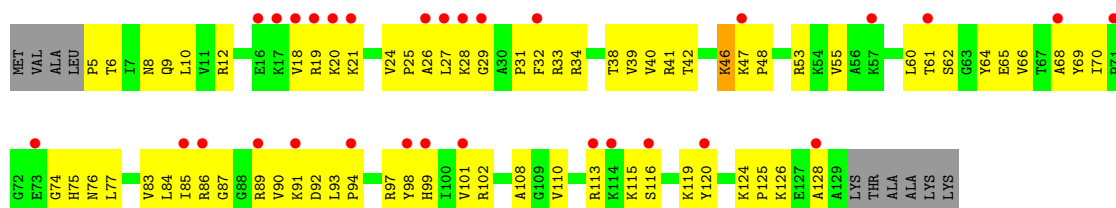
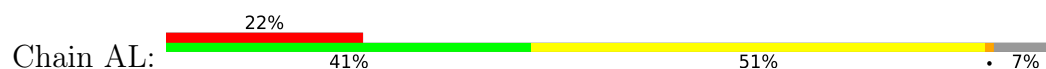




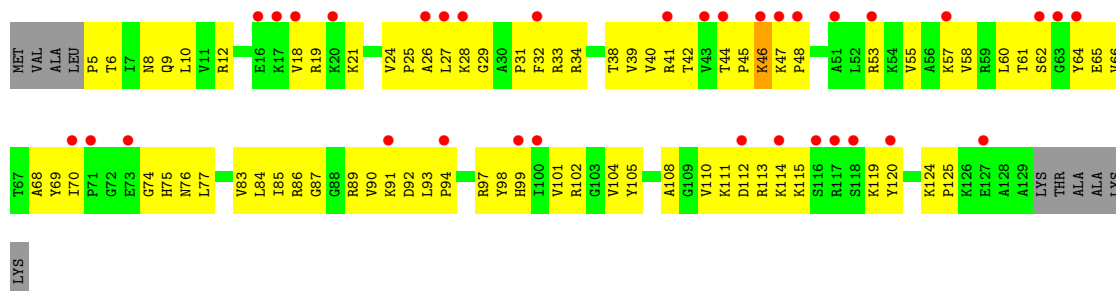
• Molecule 11: 30S ribosomal protein S11



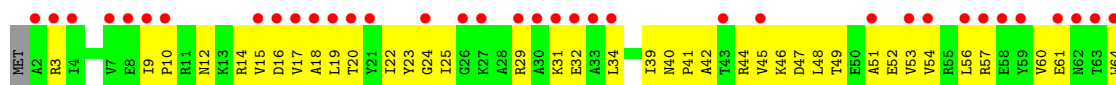
• Molecule 12: 30S ribosomal protein S12

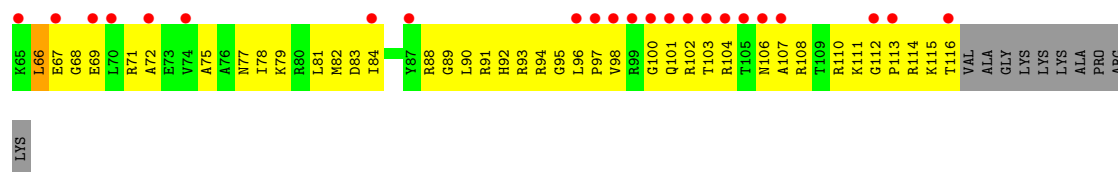


• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

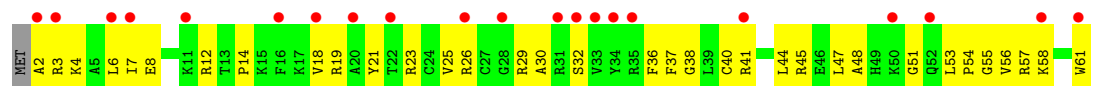
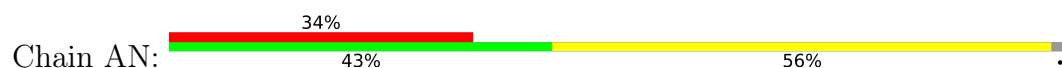




- Molecule 13: 30S ribosomal protein S13



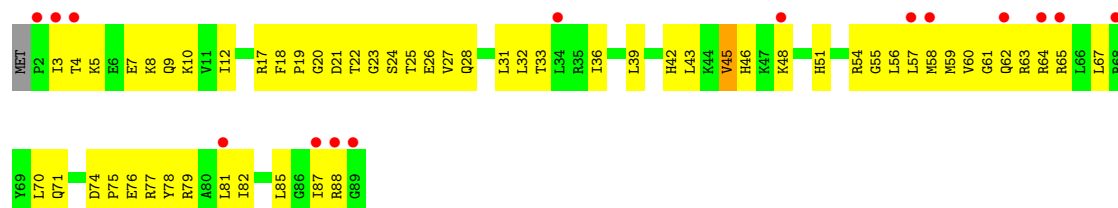
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

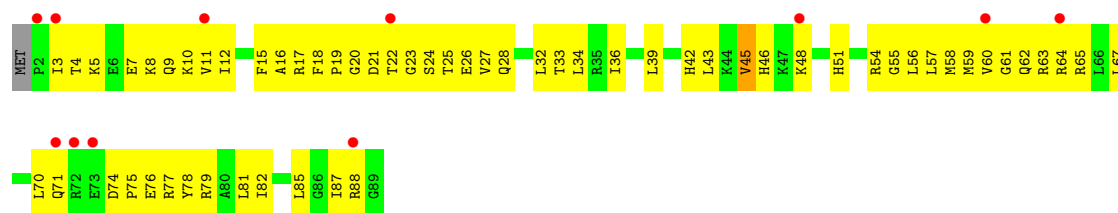


- Molecule 15: 30S ribosomal protein S15

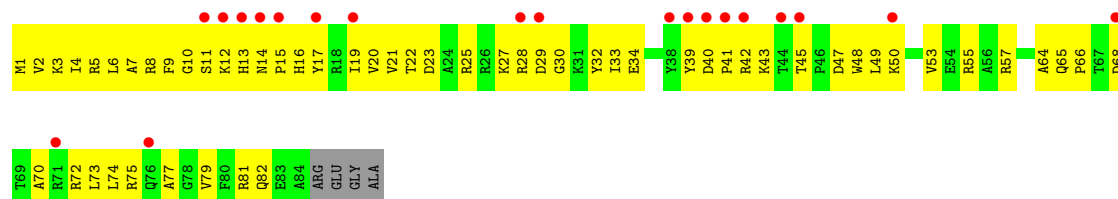


- Molecule 15: 30S ribosomal protein S15

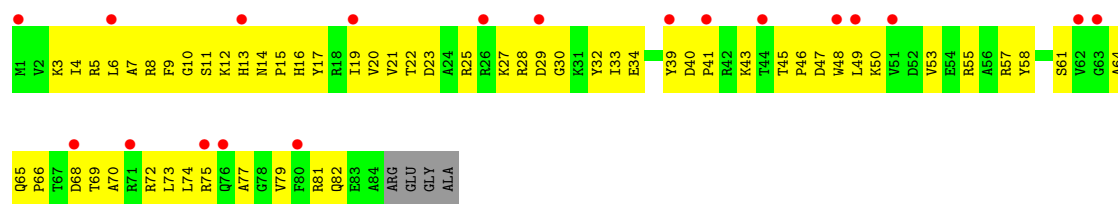




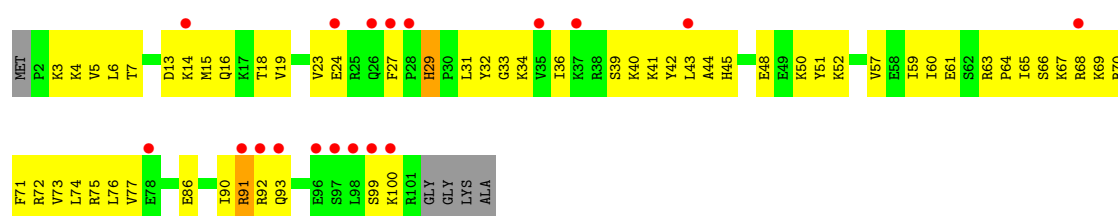
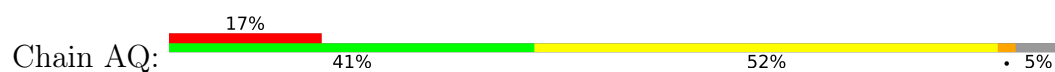
• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16



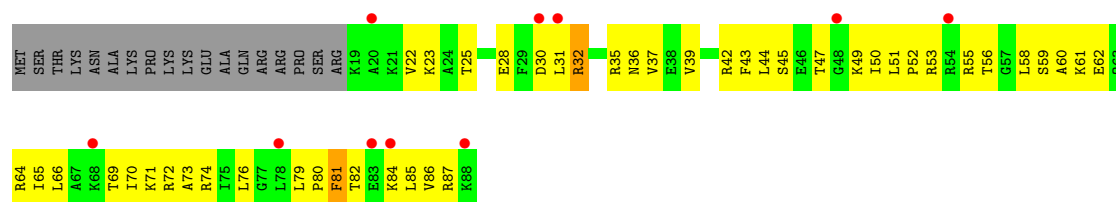
• Molecule 17: 30S ribosomal protein S17



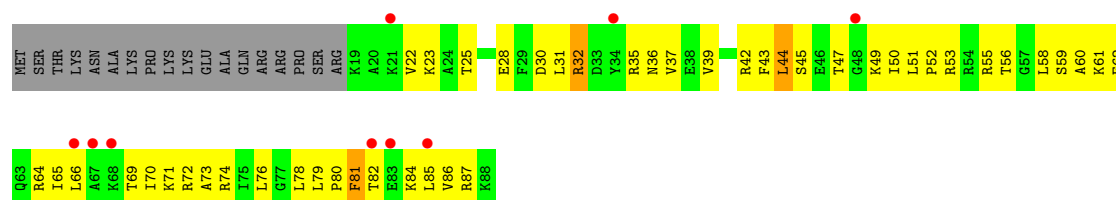
• Molecule 17: 30S ribosomal protein S17



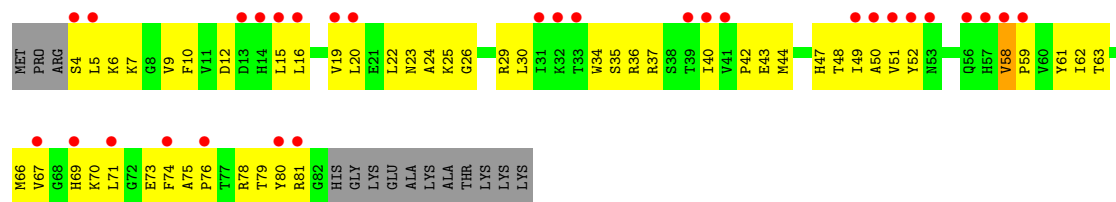
Chain AR:



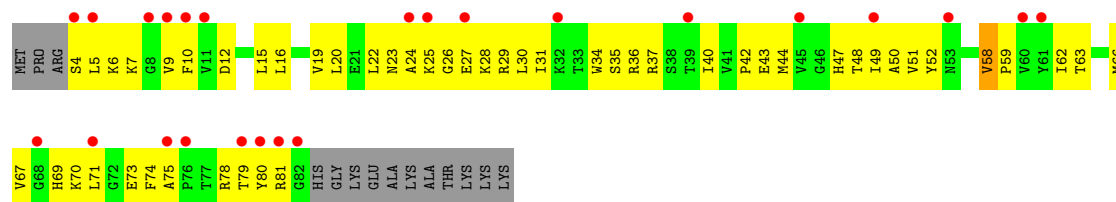
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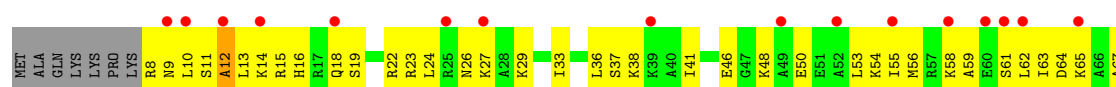
Chain AS:



Chain CS:

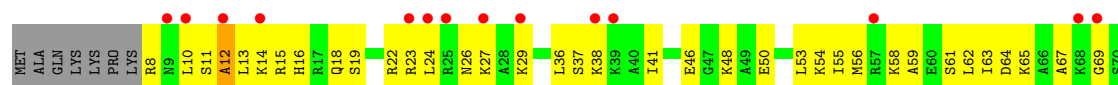


Chain AT:

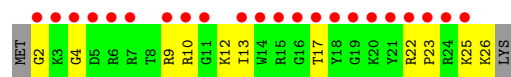
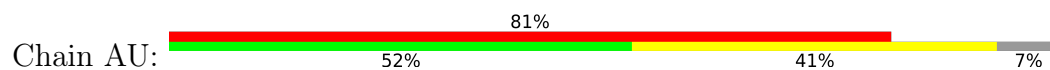




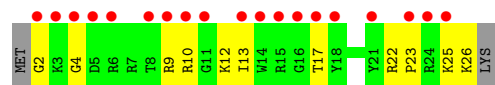
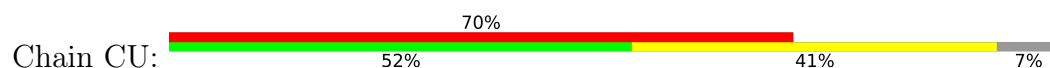
- Molecule 20: 30S ribosomal protein S20



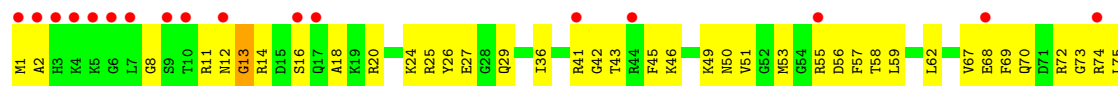
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



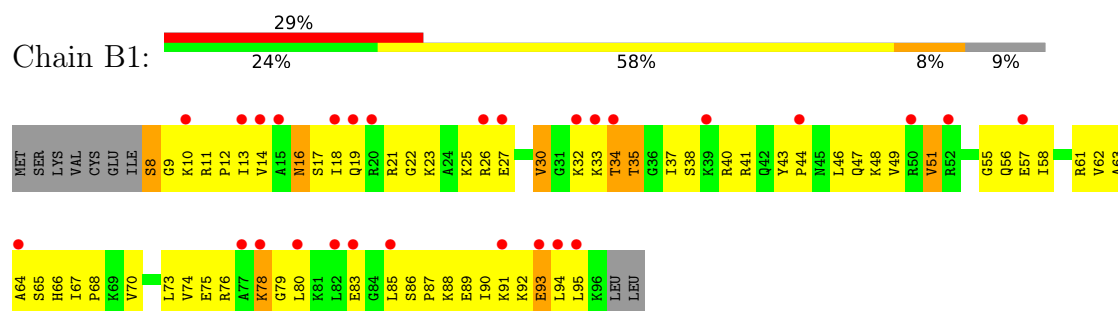
- Molecule 22: 50S ribosomal protein L27



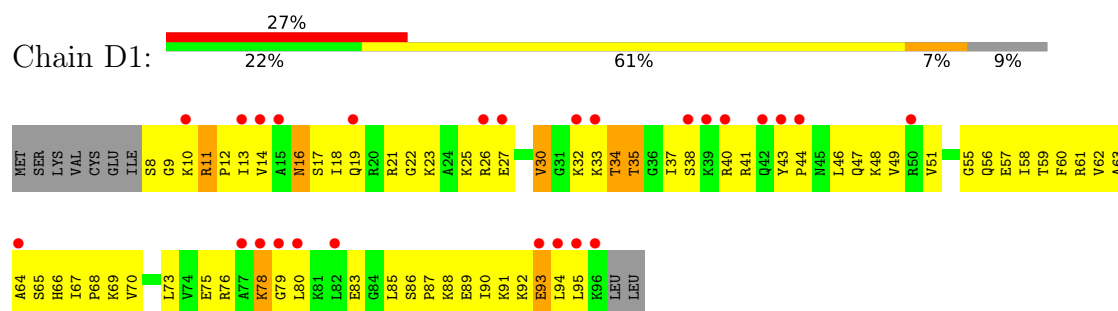
- Molecule 22: 50S ribosomal protein L27



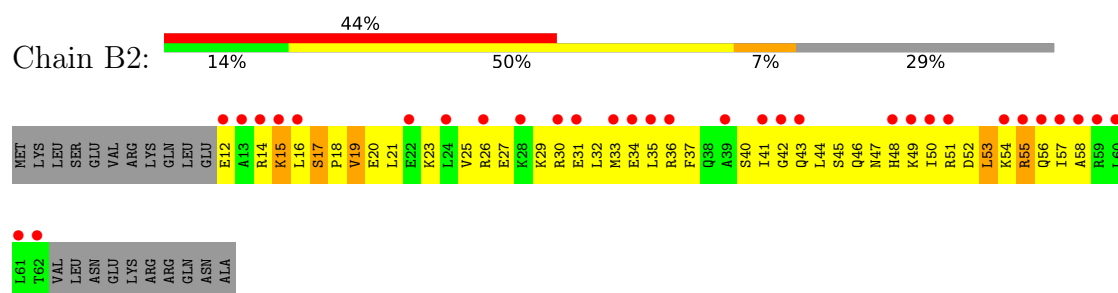
- Molecule 23: 50S ribosomal protein L28



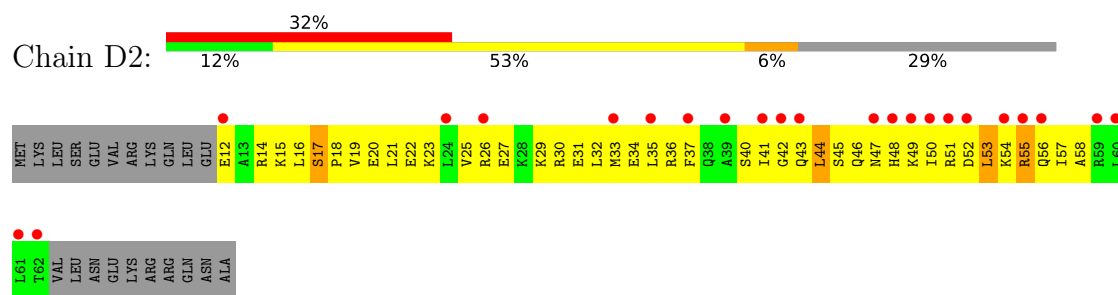
- Molecule 23: 50S ribosomal protein L28



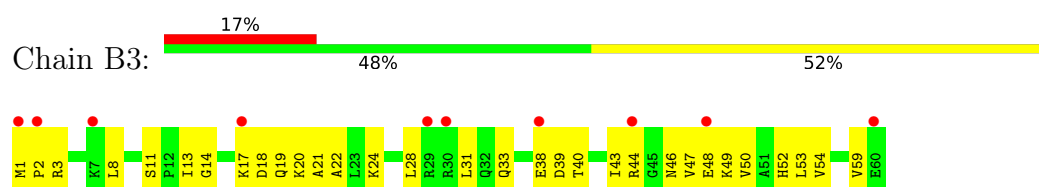
- Molecule 24: 50S ribosomal protein L29



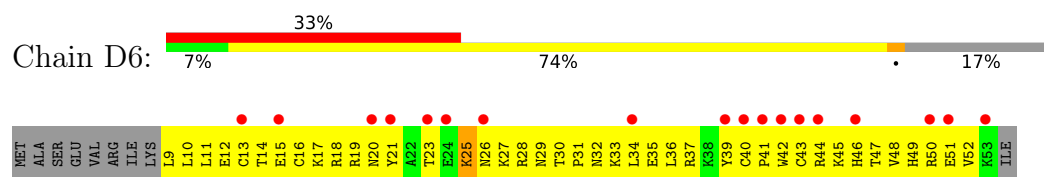
- Molecule 24: 50S ribosomal protein L29



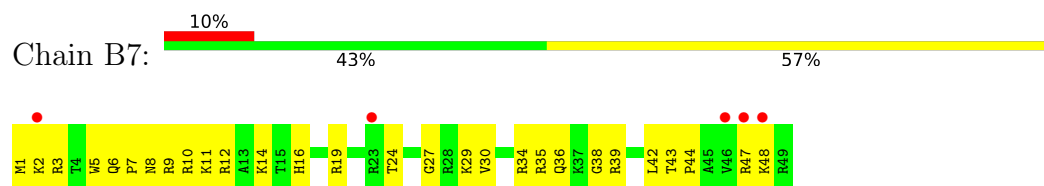
- Molecule 25: 50S ribosomal protein L30



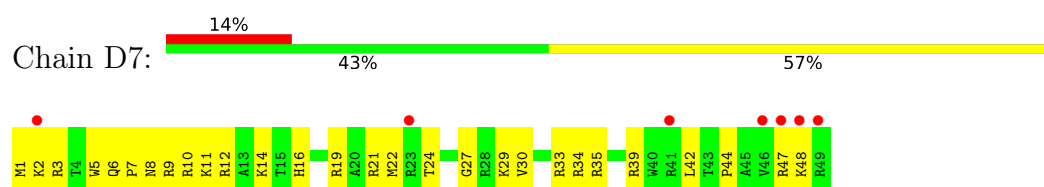
- Molecule 28: 50S ribosomal protein L33



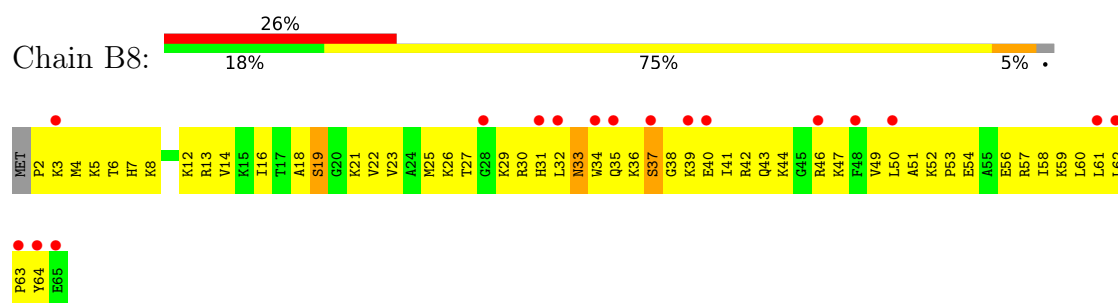
- Molecule 29: 50S ribosomal protein L34



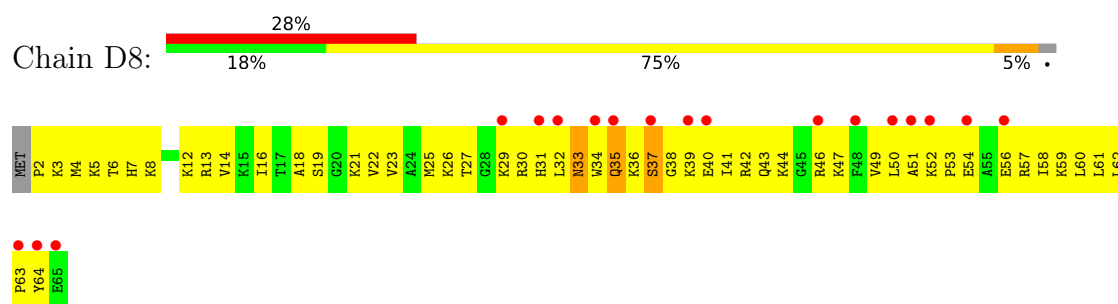
- Molecule 29: 50S ribosomal protein L34



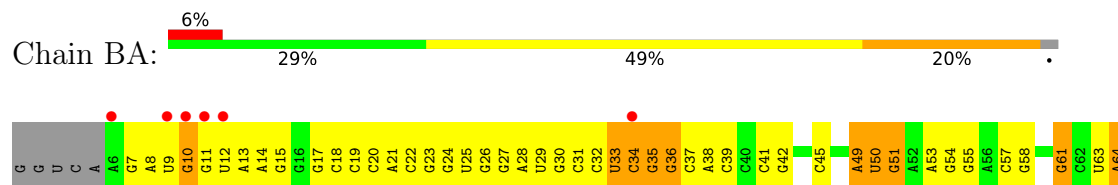
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

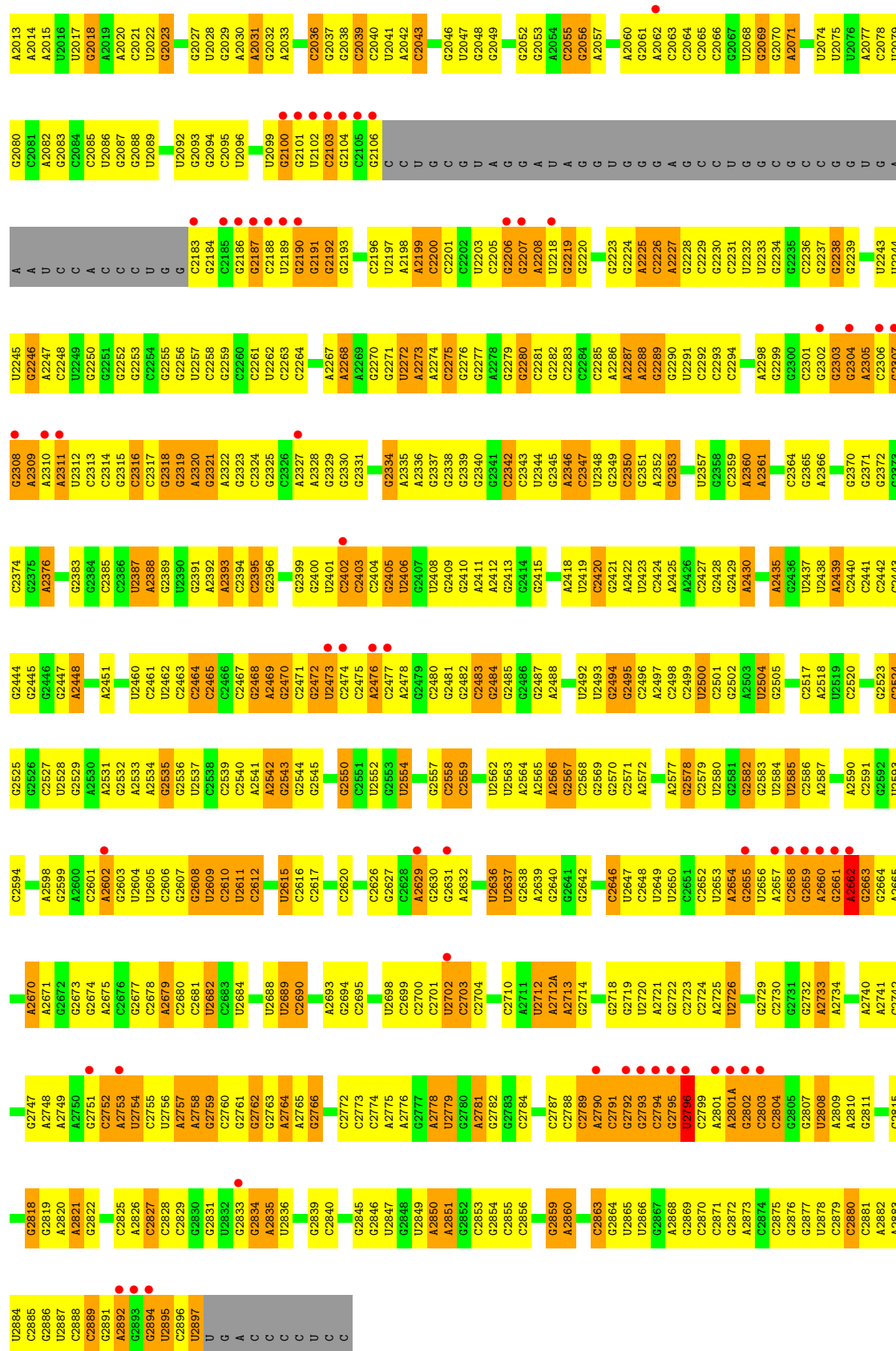


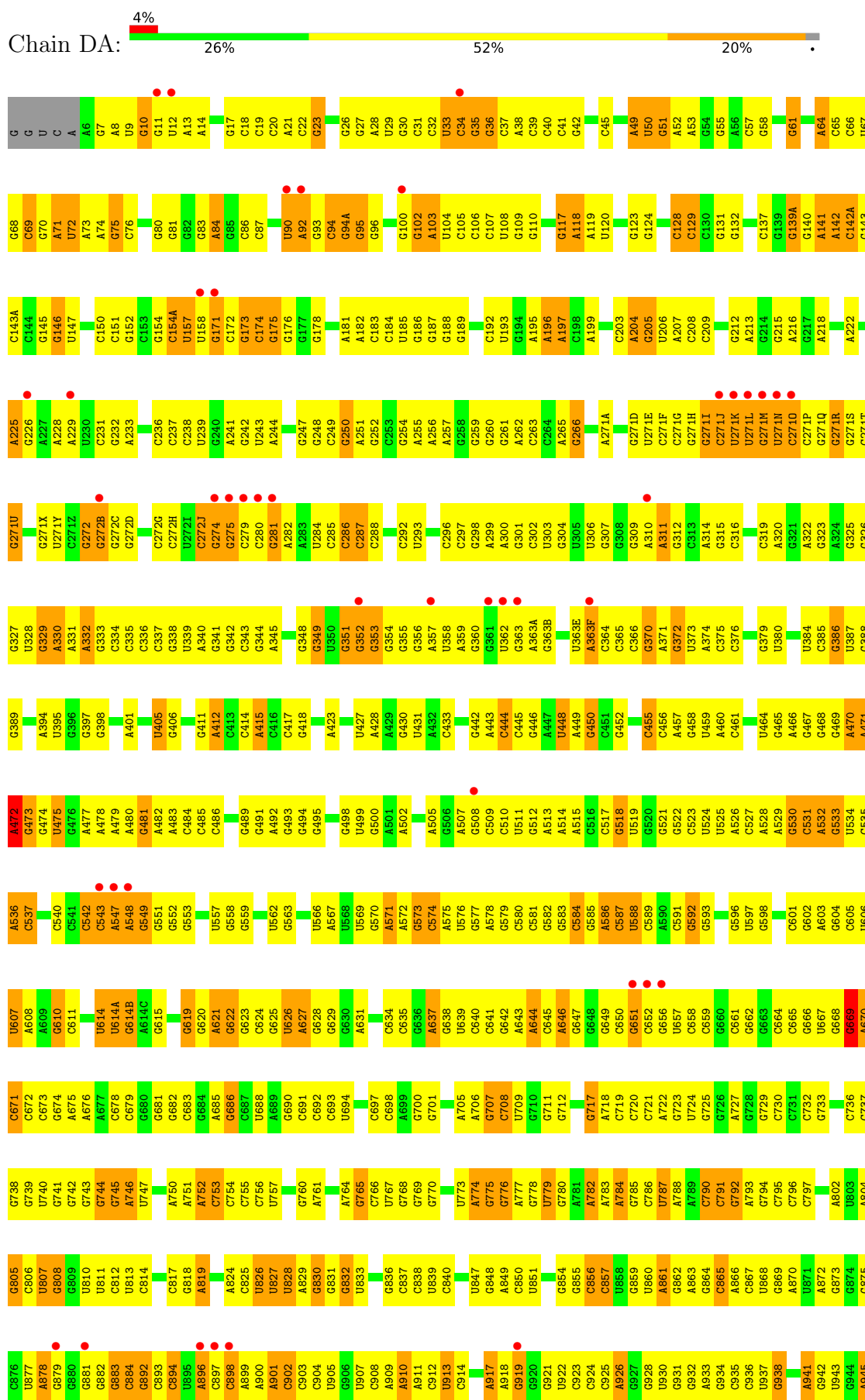
- Molecule 31: 23S ribosomal RNA





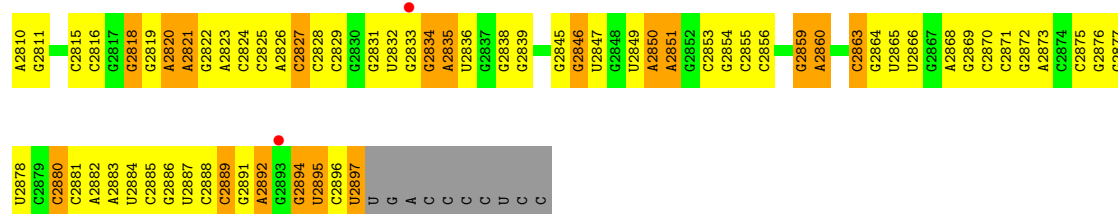
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A1938	U1864	G1792	U1706	C1640	A1570	A1496	G1435	A1365	U1292	A1220	A1143	A1027
	G1865	C1793		A1641	A1571	U1497	G1436	A1366	U1293	C1221	G1144	A1028
U1942	C1866	U1794	C1711	G1642		C1498	C1437	A1367	U1294	C1221A		A1029
U1943	A1876	C1795	G1712	G1643	G1577	C1499	U1438	G1368				G1030
	A1877	U1796	U1713	C1644	U1578	G1500	A1439	G1369	G1295	C1224		
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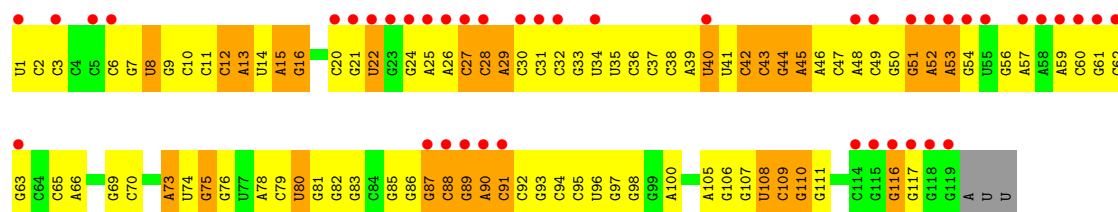
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	A2670	C2597	A2530	C2464	G2396	A2328	U2266	G2192	C2103	C2038	A1969	
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A2749	G2673	A2600	A2533	C2467	U2401	G2331	A2269		G2106	U2041	A1972	A1901
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G2751	G2677	G2606	G2536	G2469	C2403	A2333	U2271		U	C2043	C1974	G1903
C2752	C2678	C2607	U2537	A2470	C2404	G2334	U2272		C	C2044	G1980	G1904
A2753	A2679	C2608	G2538	C2471	G2405	A2335	A2273		G	G2045	C1981	C1905
G2755	G2680	G2609	C2539	G2472	U2406	G2336	A2274		C	G2046	G1982	G1906
U2756	C2681	U2609	C2540	U2473	G2407	G2337	G2275		G	U2047	C1983	
A2757	U2682	C2610	C2541	C2474	G2408	G2338	G2276		U	G2048	C1984	C1909
G2758		U2611	A2541	C2475	U2409	G2339	G2277		A	G2049	C1985	G1910
U2759	U2687	U2612	G2542	A2476	G2410	G2340	A2278		G	G2052	G1987	A1912
G2760	U2688	G2613	G2543	C2477	A2411	G2341	G2279		A	G2053	C1988	A1913
G2761	U2689	U2614	G2544	A2478	A2412	C2342	A2280		U	A2054	C1989	A1914
	C2690	A2614	G2545	G2479	G2413	C2343	U2218		A	G2055	C1990	U1915
G2762		U2615	G2550	C2480	G2414	U2344	G2282		G	G2056	U1991	A1916
G2763	A2693	C2616	C2551	G2481	G2415	G2345	C2283		G	A2057	G1992	U1917
A2764	G2694	C2617	U2552	C2482	C2416	A2346	C2284		G		U1993	U1918
A2765	C2695	G2617	G2553	G2483	G2417	C2347	C2285		U	G2060	C1994	A1918
G2766			U2554	G2484	C2418	U2348	A2286		G	G2061	G1997	G1922
	U2698	C2620		G2485	U2419	G2349	A2287		G	A2062	G1998	U1923
G2772	C2699	C2626	G2557	G2486	C2420	C2350	A2288		A	C2063	C1924	C1924
C2773	C2700	G2627		G2487	G2421	C2351	G2289		G	C2064	C1999	C1925
G2774	C2628	A2629	C2558		G2422	A2352	G2290		G	C2065	G2000	U1926
A2775	U2702	C2630	C2559	U2492	A2422	C2353	U2291		C	C2066	A2001	A1927
G2776	C2703	G2630	C2560	U2493	U2423	G2354	C2292		U	G2067	G2002	A1928
G2777	C2704	C2631	A2561	G2494	C2424		C2293		G	U2068	G2006	G1929
A2778		A2632	U2562	G2495	A2425	U2357			G	A2069	C2006	G1930
U2779	C2710		U2563	C2496	A2426	G2358	A2298		G	A2071	G2009	G1934
G2780	A2711	U2636	U2564	A2497	C2426	C2359	G2299		U	U2074	G2010	G1935
A2781	U2712	U2637	A2565	C2498	G2428	A2360	G2300		A	U2075	G2012	A1936
G2782	A2712A	C2638	A2566	C2499	G2429	A2361	C2301		G	U2076	G2013	A1937
G2783	A2713	A2639	G2567	U2500	A2430		G2302		C	U2077	A2014	A1938
C2784	G2714	G2640	G2568	C2501	A2433	C2364	G2303		G	A2078	A2015	C1942
	G2715	G2641	G2569	G2502	A2434	G2365	A2304		U	C2078	U2016	U1943
C2787	U2716	G2642		A2503	A2435	A2366	A2305		A	G2080	U2017	U1944
C2788	G2717		A2572	G2504		G2370	G2306		A	C2081	G1945	G1945
G2789	G2718	G2645	C2575	U2506	U2438	G2371	G2307		U	A2082	U2018	U1946
A2790	U2719	C2646	G2576	C2507	A2439		G2308		C	G2082	A2019	G1947
C2791	U2720	U2647	A2577	G2508	C2440	C2374	A2309		U	C2083	C2020	G1948
G2792	A2721	C2648	G2578		C2441	G2375	A2310		C	C2084	C2021	G1949
G2793	G2722	U2649	C2579	U2511	C2442	A2376	U2249		A	C2085	U2022	
C2794	C2723	U2650	U2580	C2512	C2443	A2377	G2250		C	U2086	G2023	A1952
G2795	C2724	C2651	G2581		G2444	A2378	G2251		C	G2087	G2024	A1953
U2796	A2725	U2652	G2582	C2515	G2445		G2252		C	G2088	G2025	G1954
C2799	U2726	U2653	G2583	G2516	G2446	G2383	G2253		C	U2089	C2026	U1955
A2801		A2654	U2584	C2517	G2447	G2384	C2254		U		G2027	U1956
G2801A	G2729	C2655	U2585	A2518	A2448	C2385	G2255		G	U2092	G2028	C1957
C2802	C2730	U2656	A2586	U2519	U2449	G2386	G2256		G	G2093	G2029	
C2803	A2657	C2587	C2587	C2520	A2450	U2387	U2257			C2183	A2030	
C2804	G2732	U2658	A2587	C2521	A2451	A2388	G2258			G2184	G2095	
G2805	A2733	C2659		U2522		A2389	G2259			C2185	A2031	C1962
G2807	A2734	C2660	A2590	G2523		U2390	G2260			U2096	G2032	U1963
U2808		G2591	G2591	G2523			G2261					G1964
A2809	A2738	A2662	G2592	G2524		G2391	G2323					



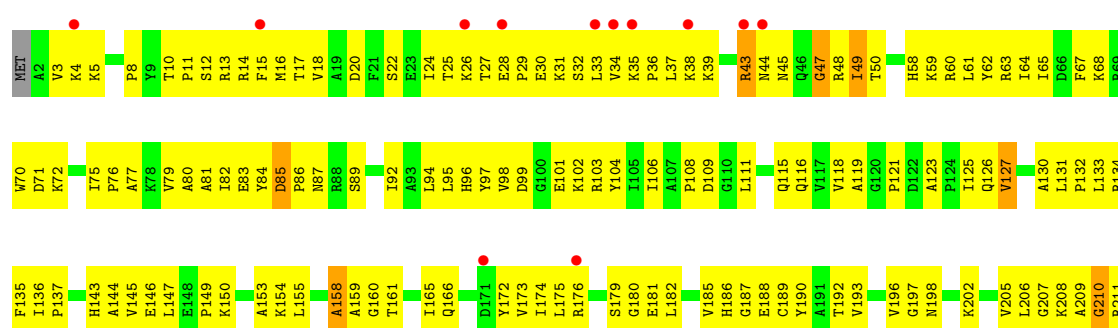
• Molecule 32: 5S ribosomal RNA



• Molecule 32: 5S ribosomal RNA

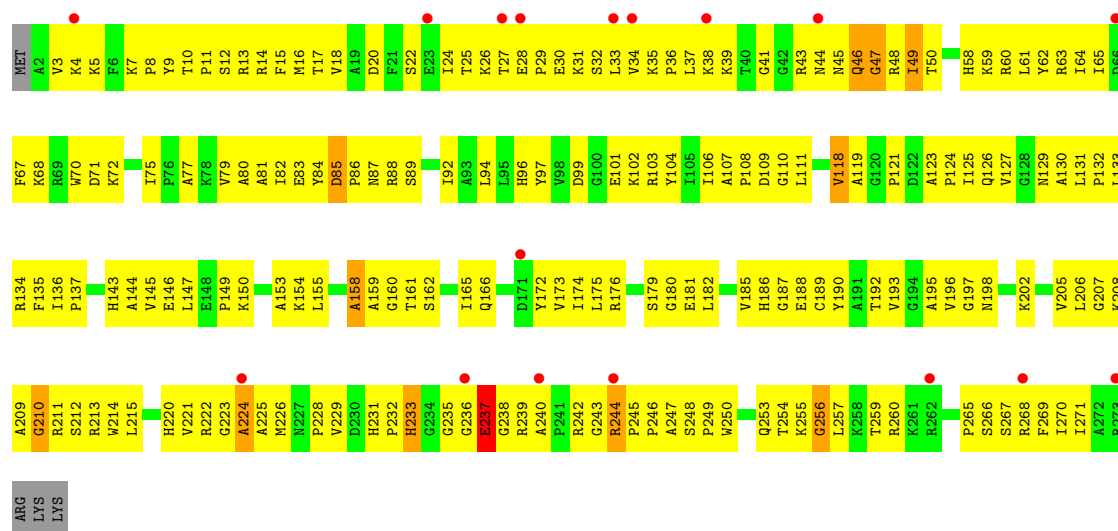


• Molecule 33: 50S ribosomal protein L2

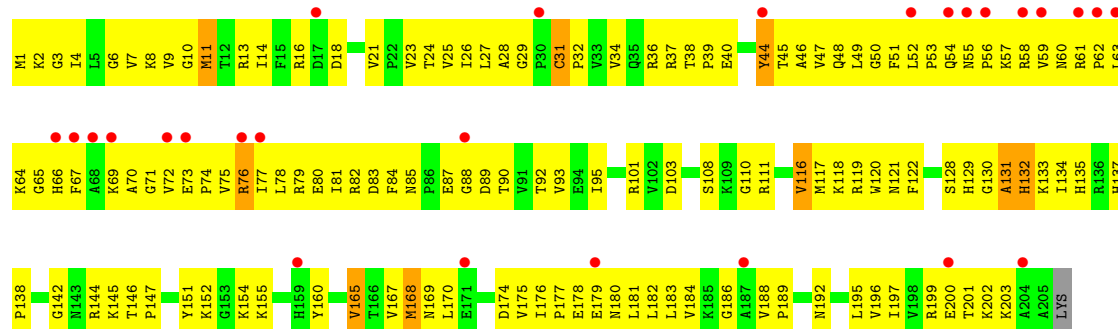


• Molecule 33: 50S ribosomal protein L2

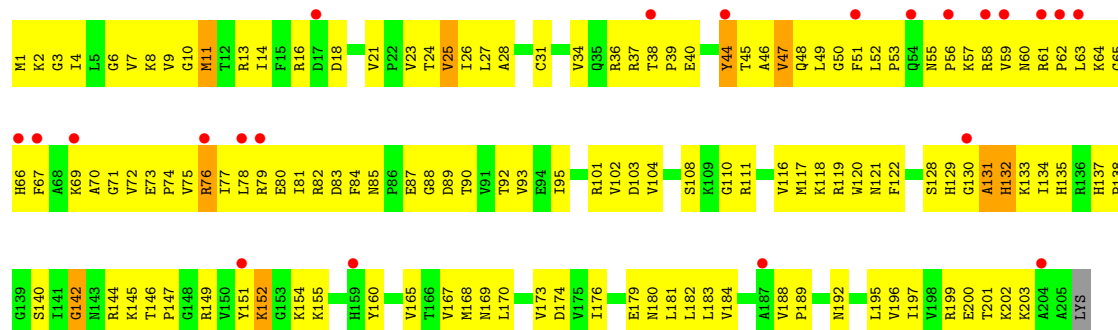




• Molecule 34: 50S ribosomal protein L3

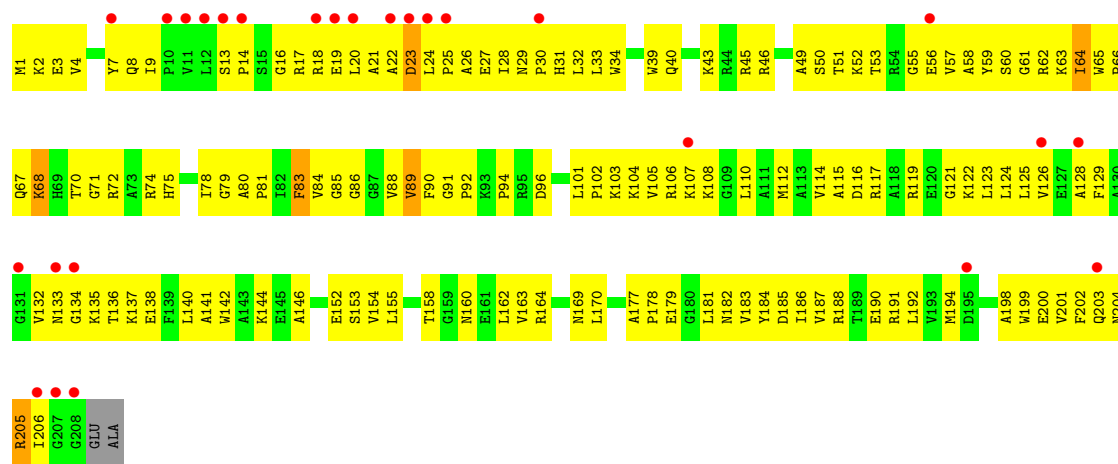


• Molecule 34: 50S ribosomal protein L3

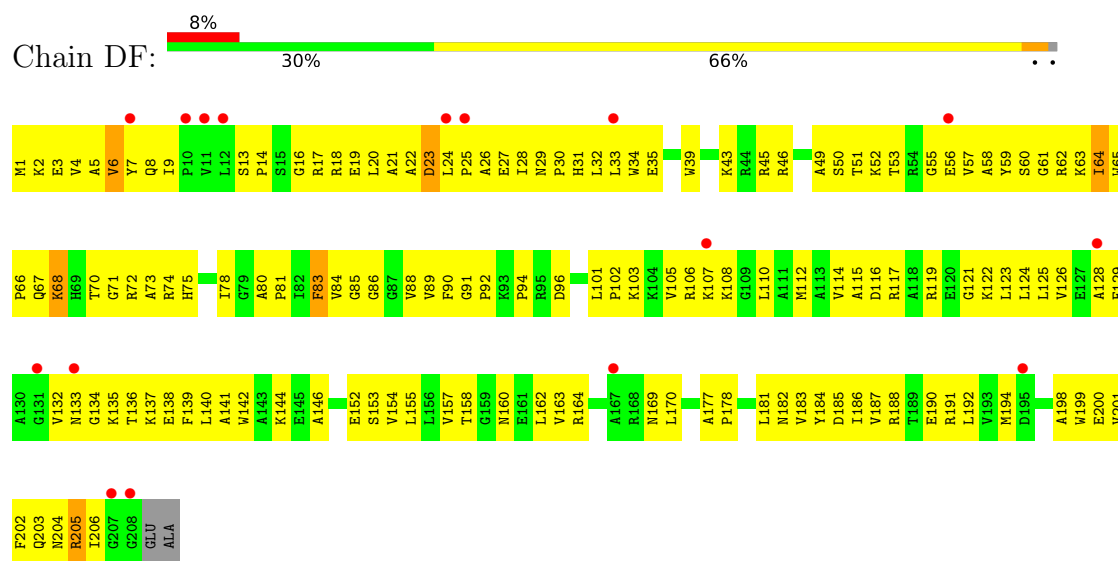


• Molecule 35: 50S ribosomal protein L4

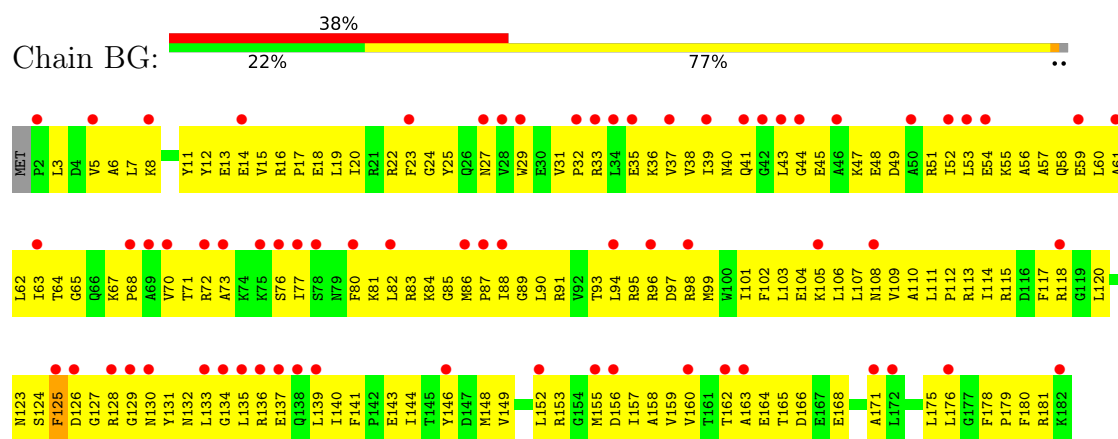




• Molecule 35: 50S ribosomal protein L4



• Molecule 36: 50S ribosomal protein L5

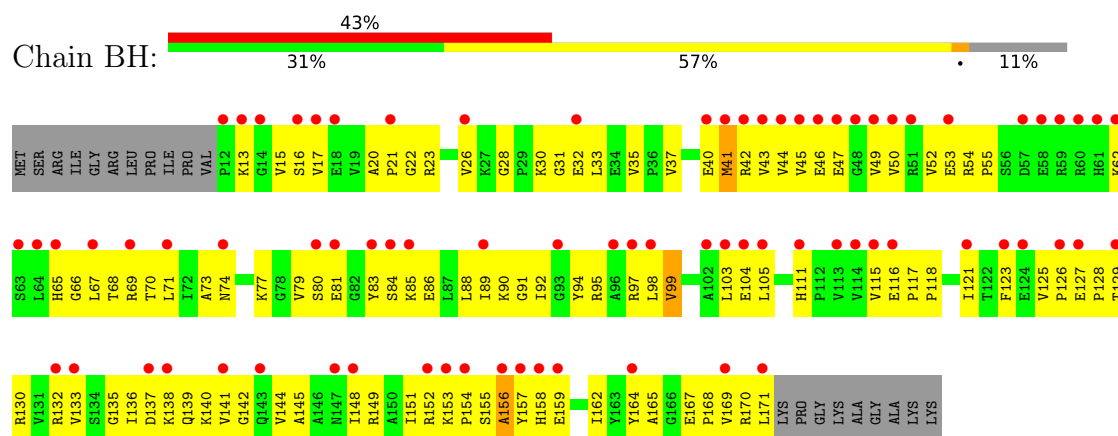


• Molecule 36: 50S ribosomal protein L5

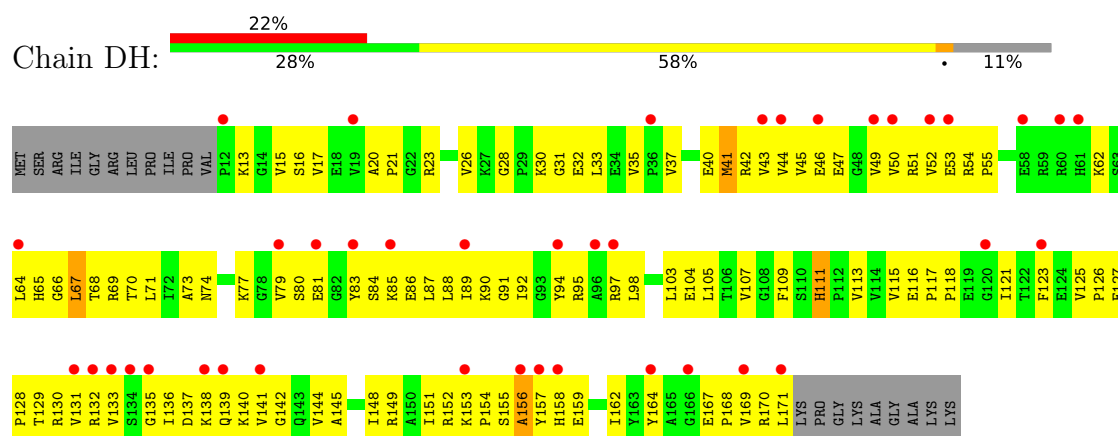




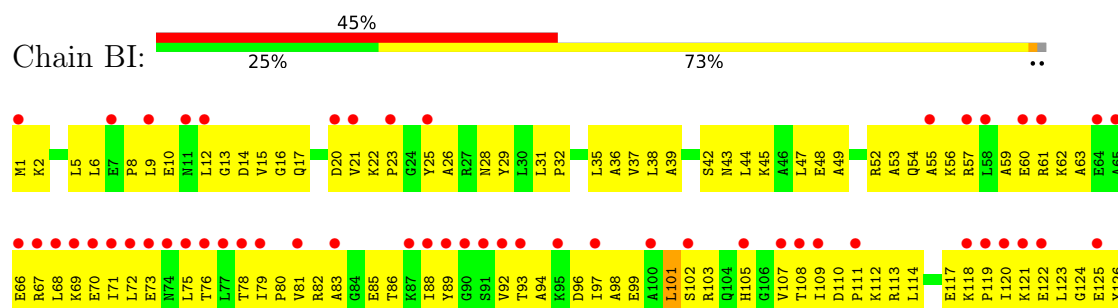
- Molecule 37: 50S ribosomal protein L6

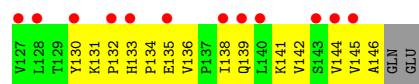


- Molecule 37: 50S ribosomal protein L6

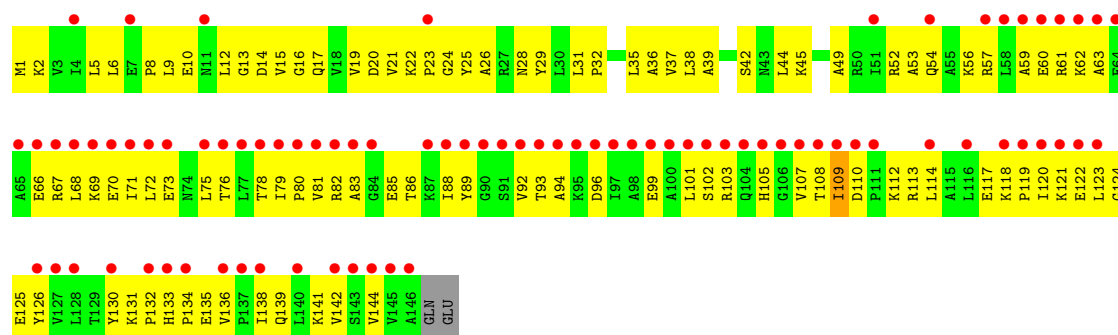


- Molecule 38: 50S ribosomal protein L9





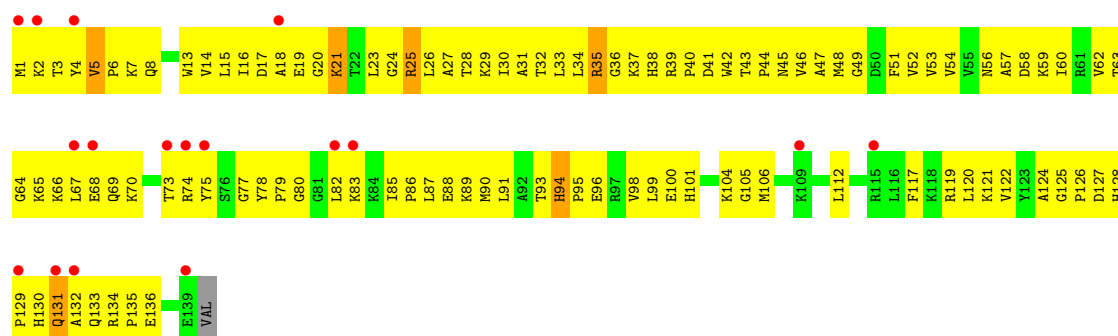
• Molecule 38: 50S ribosomal protein L9



• Molecule 39: 50S ribosomal protein L13



• Molecule 39: 50S ribosomal protein L13

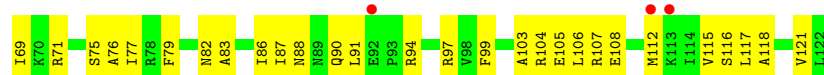
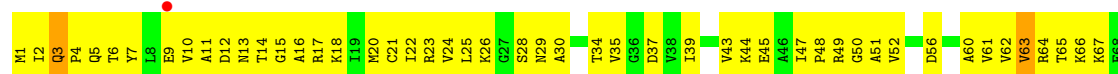


• Molecule 40: 50S ribosomal protein L14

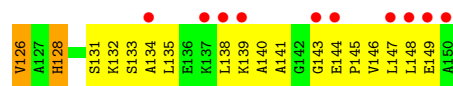
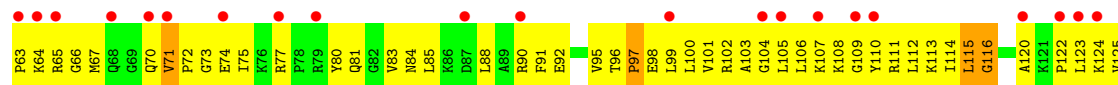
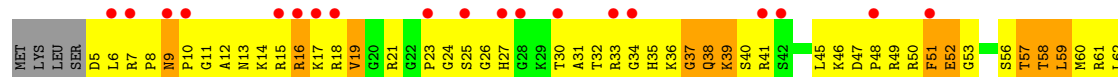




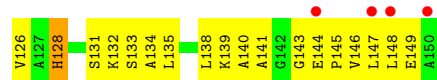
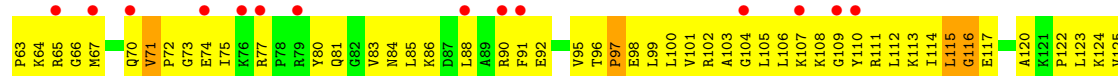
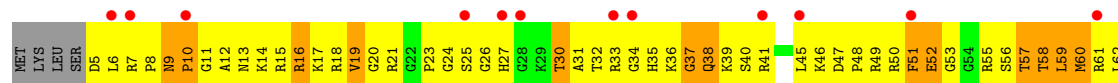
• Molecule 40: 50S ribosomal protein L14



• Molecule 41: 50S ribosomal protein L15

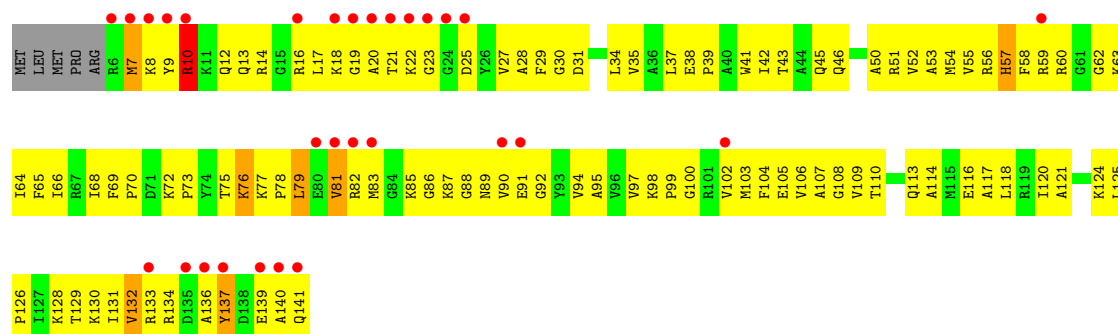


• Molecule 41: 50S ribosomal protein L15



• Molecule 42: 50S ribosomal protein L16

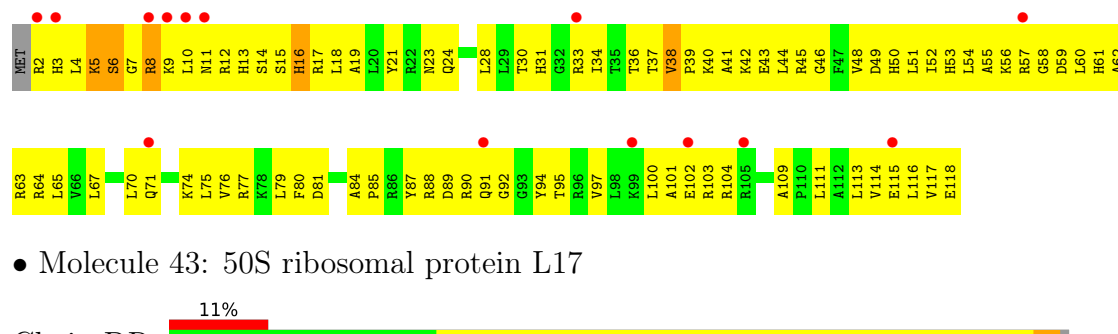




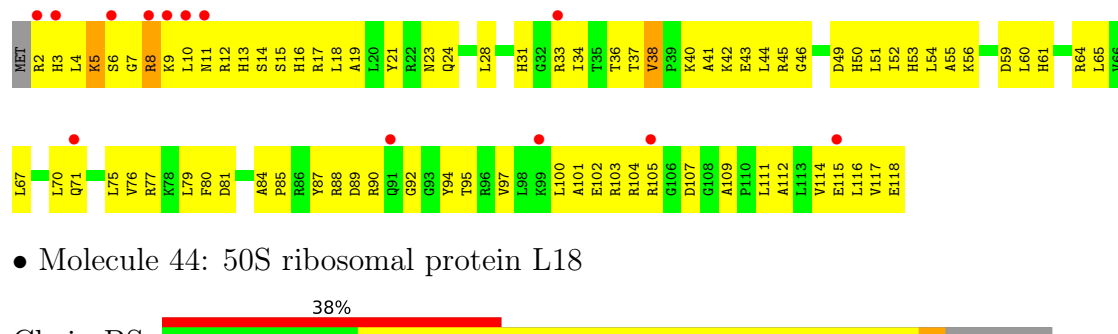
• Molecule 42: 50S ribosomal protein L16



• Molecule 43: 50S ribosomal protein L17

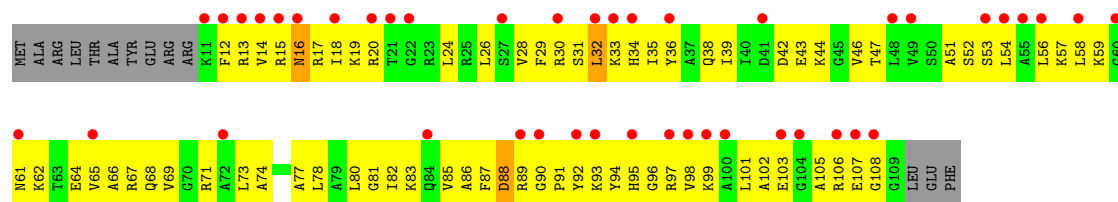


• Molecule 43: 50S ribosomal protein L17

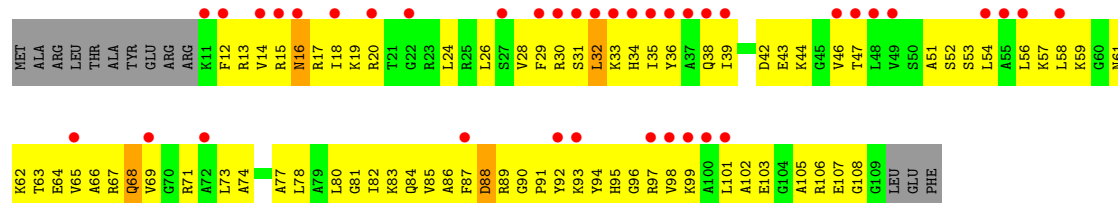


• Molecule 44: 50S ribosomal protein L18

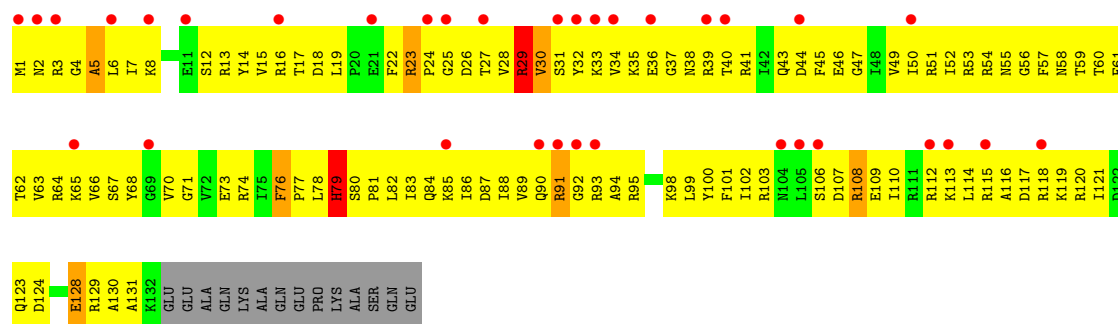




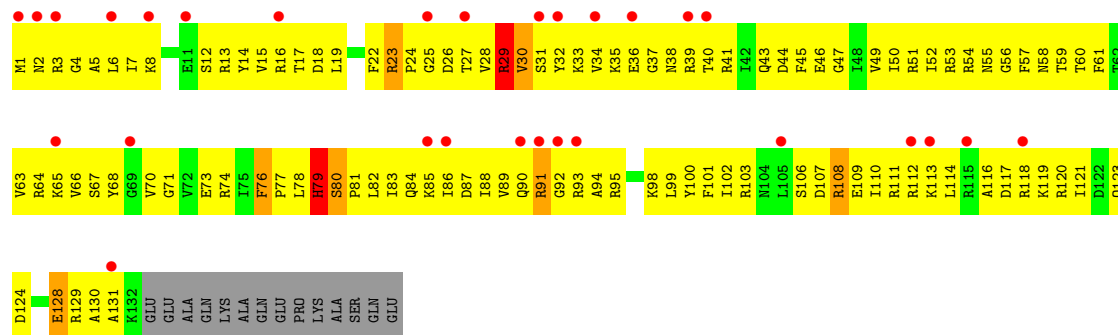
• Molecule 44: 50S ribosomal protein L18



• Molecule 45: 50S ribosomal protein L19

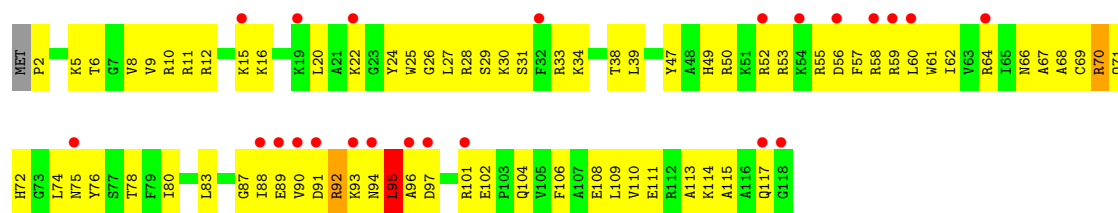


• Molecule 45: 50S ribosomal protein L19

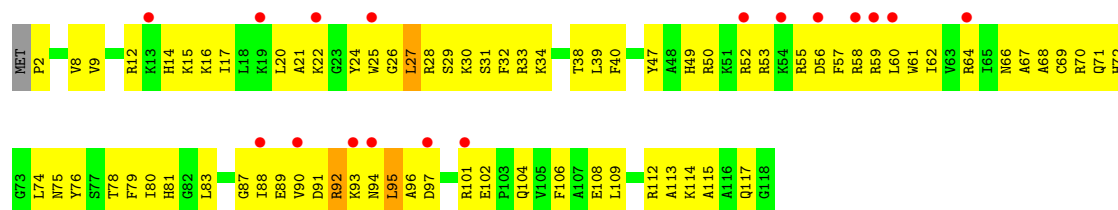


• Molecule 46: 50S ribosomal protein L20

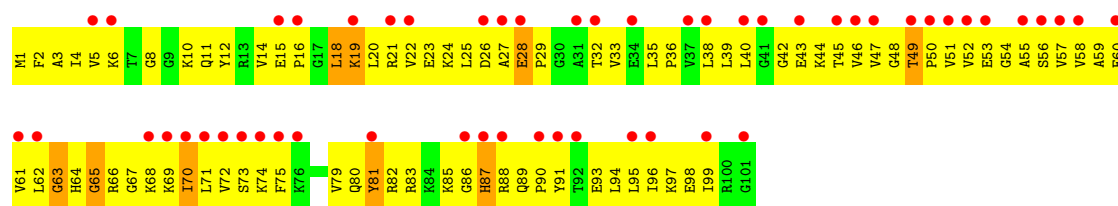




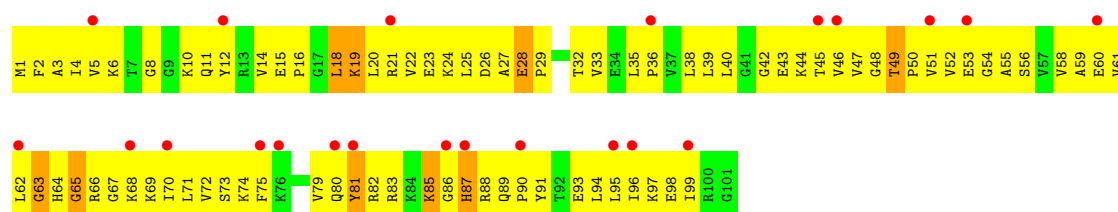
• Molecule 46: 50S ribosomal protein L20



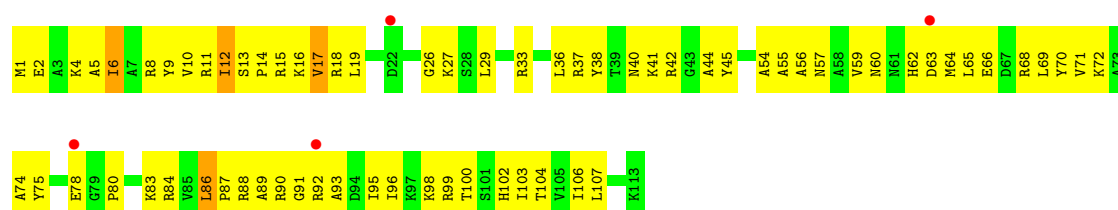
• Molecule 47: 50S ribosomal protein L21



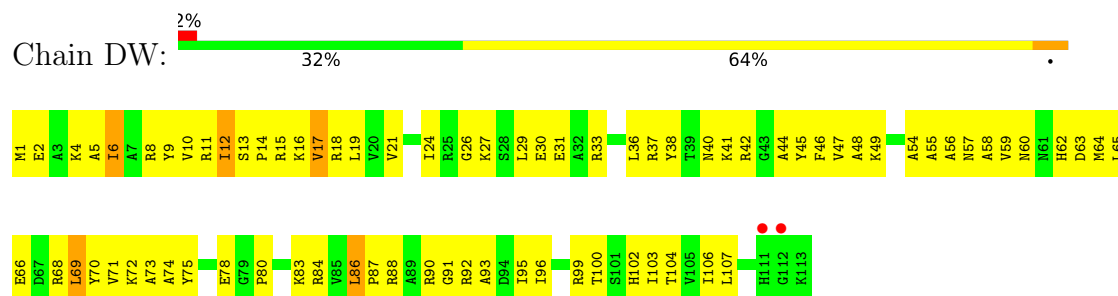
• Molecule 47: 50S ribosomal protein L21



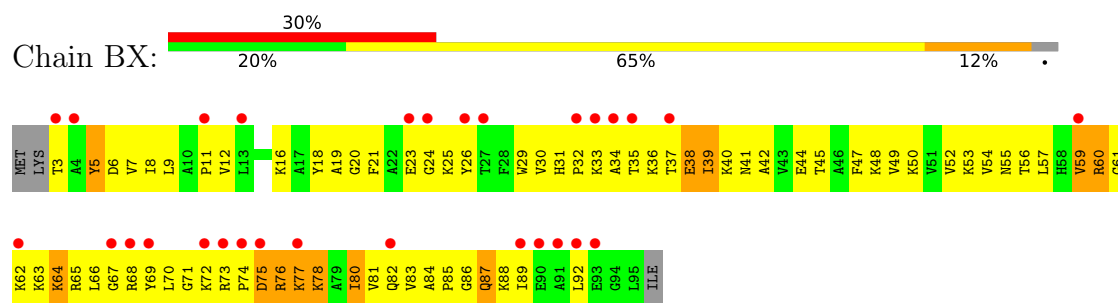
• Molecule 48: 50S ribosomal protein L22



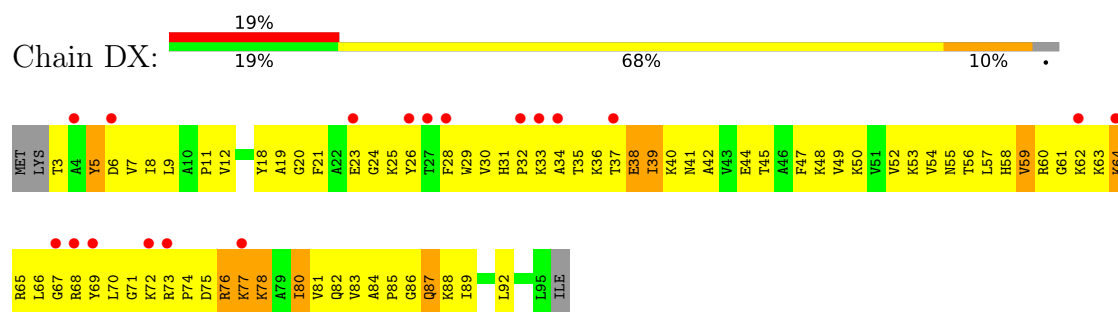
- Molecule 48: 50S ribosomal protein L22



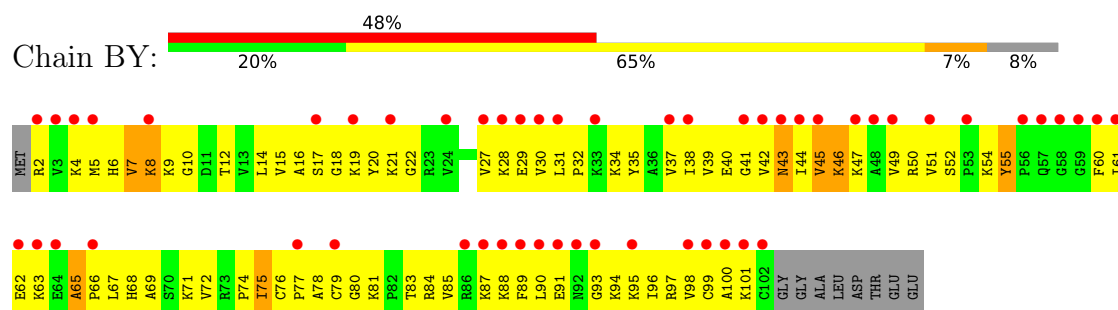
- Molecule 49: 50S ribosomal protein L23



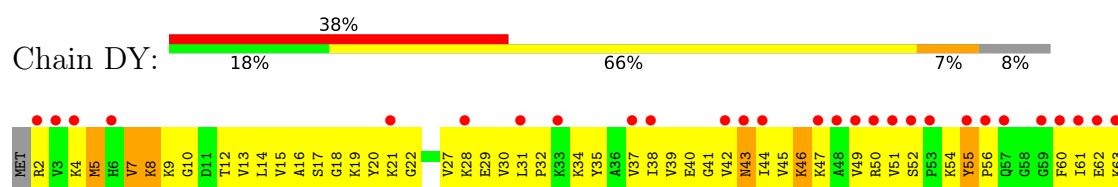
- Molecule 49: 50S ribosomal protein L23

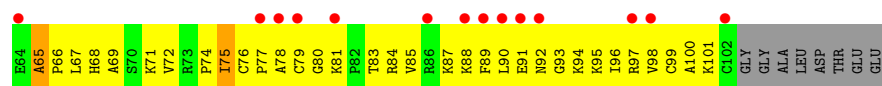


- Molecule 50: 50S ribosomal protein L24

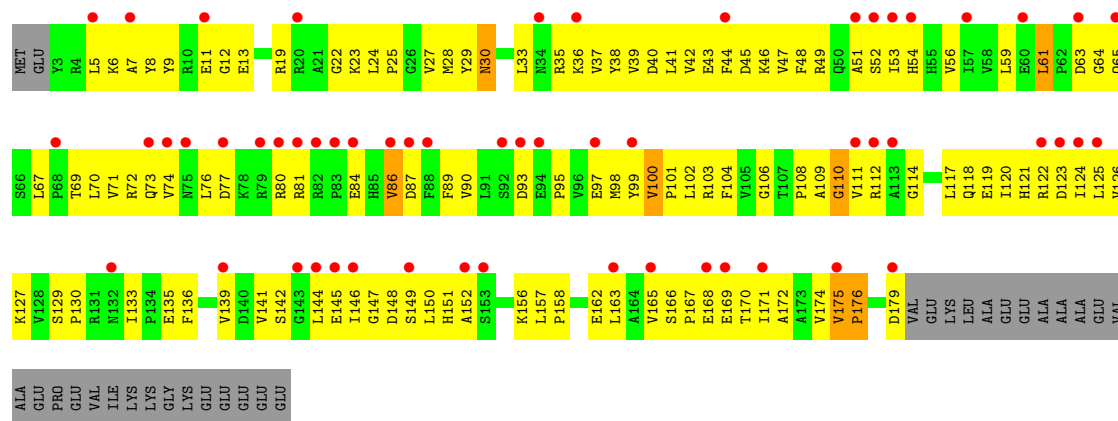


- Molecule 50: 50S ribosomal protein L24

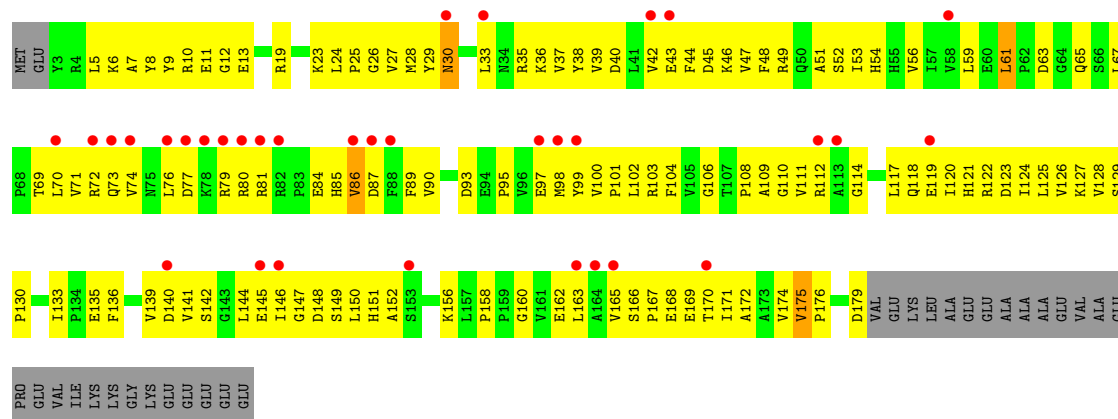




• Molecule 51: 50S ribosomal protein L25



• Molecule 51: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.18Å 448.40Å 621.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.00 49.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.57-3.00) 98.5 (49.57-3.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.244 , 0.281 0.243 , 0.276	Depositor DCC
R_{free} test set	57196 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 105.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	277987	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: MG, CLM, ZN, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.31	0/36190	0.40	0/56486
1	CA	0.31	0/36190	0.40	0/56486
2	AB	0.38	0/1936	0.84	1/2611 (0.0%)
2	CB	0.37	0/1936	0.83	1/2611 (0.0%)
3	AC	0.36	0/1637	0.77	1/2207 (0.0%)
3	CC	0.35	0/1637	0.76	1/2207 (0.0%)
4	AD	0.44	0/1733	0.90	6/2318 (0.3%)
4	CD	0.45	0/1733	0.91	6/2318 (0.3%)
5	AE	0.50	0/1163	0.96	6/1566 (0.4%)
5	CE	0.50	0/1163	0.96	3/1566 (0.2%)
6	AF	0.47	0/856	0.95	3/1154 (0.3%)
6	CF	0.44	0/856	0.93	0/1154
7	AG	0.35	0/1276	0.77	0/1709
7	CG	0.34	0/1276	0.77	0/1709
8	AH	0.44	0/1136	0.92	5/1527 (0.3%)
8	CH	0.42	0/1136	0.90	6/1527 (0.4%)
9	AI	0.32	0/1028	0.75	0/1375
9	CI	0.33	0/1028	0.75	0/1375
10	AJ	0.38	0/808	0.84	0/1087
10	CJ	0.37	0/808	0.84	0/1087
11	AK	0.44	0/900	0.90	3/1213 (0.2%)
11	CK	0.46	0/900	0.89	2/1213 (0.2%)
12	AL	0.52	0/987	0.98	2/1322 (0.2%)
12	CL	0.54	0/987	0.98	2/1322 (0.2%)
13	AM	0.35	0/928	0.84	1/1238 (0.1%)
13	CM	0.34	0/928	0.84	2/1238 (0.2%)
14	AN	0.32	0/501	0.76	0/664
14	CN	0.33	0/501	0.75	0/664
15	AO	0.49	0/745	0.85	1/992 (0.1%)
15	CO	0.45	0/745	0.85	1/992 (0.1%)
16	AP	0.44	0/717	0.90	1/965 (0.1%)
16	CP	0.47	0/717	0.93	1/965 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	0/837	0.89	3/1119 (0.3%)
17	CQ	0.45	0/837	0.92	3/1119 (0.3%)
18	AR	0.45	0/579	0.96	2/768 (0.3%)
18	CR	0.43	0/579	0.96	3/768 (0.4%)
19	AS	0.38	0/643	0.76	1/867 (0.1%)
19	CS	0.37	0/643	0.76	1/867 (0.1%)
20	AT	0.48	0/765	0.90	3/1007 (0.3%)
20	CT	0.50	0/765	0.92	2/1007 (0.2%)
21	AU	0.35	0/213	0.70	0/279
21	CU	0.36	0/213	0.74	0/279
22	B0	0.69	0/658	1.08	4/878 (0.5%)
22	D0	0.59	0/658	1.05	2/878 (0.2%)
23	B1	1.06	4/700 (0.6%)	1.42	11/931 (1.2%)
23	D1	0.96	3/700 (0.4%)	1.37	13/931 (1.4%)
24	B2	0.91	1/423 (0.2%)	1.28	4/560 (0.7%)
24	D2	0.67	0/423	1.21	4/560 (0.7%)
25	B3	0.83	0/473	1.04	0/636
25	D3	0.66	0/473	1.04	0/636
26	B4	0.49	0/156	1.52	3/215 (1.4%)
26	D4	0.51	0/156	1.46	2/215 (0.9%)
27	B5	0.99	0/473	1.79	10/639 (1.6%)
27	D5	0.89	1/473 (0.2%)	1.70	10/639 (1.6%)
28	B6	1.01	0/387	1.41	3/517 (0.6%)
28	D6	0.85	0/387	1.31	1/517 (0.2%)
29	B7	0.81	0/427	1.22	2/563 (0.4%)
29	D7	0.76	0/427	1.15	2/563 (0.4%)
30	B8	0.95	0/516	1.37	4/681 (0.6%)
30	D8	0.78	0/516	1.32	4/681 (0.6%)
31	BA	0.59	4/65745 (0.0%)	0.54	8/102639 (0.0%)
31	DA	0.49	3/65745 (0.0%)	0.54	9/102639 (0.0%)
32	BB	0.48	0/2853	0.46	0/4451
32	DB	0.39	0/2853	0.45	0/4451
33	BD	0.85	1/2155 (0.0%)	1.24	15/2907 (0.5%)
33	DD	0.78	0/2155	1.23	19/2907 (0.7%)
34	BE	0.81	1/1597 (0.1%)	1.22	9/2155 (0.4%)
34	DE	0.71	0/1597	1.18	10/2155 (0.5%)
35	BF	0.80	0/1659	1.12	8/2246 (0.4%)
35	DF	0.65	0/1659	1.11	7/2246 (0.3%)
36	BG	0.45	0/1498	0.90	2/2013 (0.1%)
36	DG	0.39	0/1498	0.89	3/2013 (0.1%)
37	BH	0.76	0/1246	1.16	7/1684 (0.4%)
37	DH	0.53	0/1246	1.11	7/1684 (0.4%)
38	BI	0.54	0/1147	0.90	1/1553 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.56	0/1147	0.90	2/1553 (0.1%)
39	BN	0.88	0/1132	1.29	13/1527 (0.9%)
39	DN	0.70	0/1132	1.21	8/1527 (0.5%)
40	BO	0.74	0/943	1.16	8/1269 (0.6%)
40	DO	0.64	0/943	1.10	5/1269 (0.4%)
41	BP	0.91	0/1131	1.43	15/1504 (1.0%)
41	DP	0.75	0/1131	1.39	18/1504 (1.2%)
42	BQ	0.86	2/1100 (0.2%)	1.24	8/1470 (0.5%)
42	DQ	0.76	1/1100 (0.1%)	1.22	10/1470 (0.7%)
43	BR	0.93	3/974 (0.3%)	1.11	3/1302 (0.2%)
43	DR	0.72	0/974	1.06	2/1302 (0.2%)
44	BS	0.65	0/779	1.04	3/1038 (0.3%)
44	DS	0.51	0/779	1.00	4/1038 (0.4%)
45	BT	0.78	1/1114 (0.1%)	1.38	18/1488 (1.2%)
45	DT	0.68	1/1114 (0.1%)	1.37	16/1488 (1.1%)
46	BU	0.92	0/975	1.12	5/1297 (0.4%)
46	DU	0.66	0/975	1.07	5/1297 (0.4%)
47	BV	0.91	1/789 (0.1%)	1.37	8/1054 (0.8%)
47	DV	0.72	0/789	1.28	9/1054 (0.9%)
48	BW	0.90	0/907	1.15	7/1216 (0.6%)
48	DW	0.75	1/907 (0.1%)	1.13	6/1216 (0.5%)
49	BX	0.92	0/740	1.41	15/995 (1.5%)
49	DX	0.81	0/740	1.38	13/995 (1.3%)
50	BY	0.94	2/789 (0.3%)	1.42	13/1053 (1.2%)
50	DY	0.78	0/789	1.36	13/1053 (1.2%)
51	BZ	0.65	0/1436	1.06	12/1951 (0.6%)
51	DZ	0.53	0/1436	1.03	8/1951 (0.4%)
All	All	0.53	30/301000 (0.0%)	0.70	504/449812 (0.1%)

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
23	B1	0	1
23	D1	0	1
24	B2	0	1
24	D2	0	1
27	B5	0	1
27	D5	0	1
28	B6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	BA	19	0
31	DA	19	0
33	BD	0	3
33	DD	0	3
34	BE	0	2
34	DE	0	2
37	BH	0	1
37	DH	0	1
41	BP	0	5
41	DP	0	4
42	BQ	0	1
42	DQ	0	1
43	BR	0	2
43	DR	0	2
44	BS	0	1
44	DS	0	1
45	BT	0	2
45	DT	0	2
46	BU	0	1
47	BV	0	3
47	DV	0	3
49	BX	0	4
49	DX	0	4
All	All	38	55

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	BR	38	VAL	CA-CB	-8.80	1.49	1.54
31	BA	669	G	C4'-C3'	-8.28	1.40	1.53
50	BY	45	VAL	CA-CB	7.98	1.67	1.54
31	DA	669	G	C4'-C3'	-7.57	1.41	1.53
31	BA	1300	U	C4'-C3'	-7.25	1.42	1.53

The worst 5 of 504 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B5	46	CYS	CA-C-N	18.37	142.80	119.84
27	B5	46	CYS	C-N-CA	18.37	142.80	119.84
27	D5	46	CYS	CA-C-N	16.94	141.01	119.84
27	D5	46	CYS	C-N-CA	16.94	141.01	119.84
34	BE	186	GLY	N-CA-C	13.98	124.53	111.67

5 of 38 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	100	G	C1'
31	BA	472	A	C3'
31	BA	669	G	C3',C1',C4'
31	BA	945	A	C1'
31	BA	1300	U	C3',C1',C4'

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
24	B2	55	ARG	Peptide
27	B5	51	TYR	Peptide
28	B6	47	THR	Peptide
33	BD	47	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1593	0
1	CA	32329	0	16318	1560	0
2	AB	1901	0	1951	222	0
2	CB	1901	0	1951	219	0
3	AC	1613	0	1677	124	0
3	CC	1613	0	1677	126	0
4	AD	1703	0	1765	206	0
4	CD	1703	0	1764	206	0
5	AE	1147	0	1207	106	0
5	CE	1147	0	1207	109	0
6	AF	843	0	857	101	0
6	CF	843	0	857	101	0
7	AG	1257	0	1296	79	0
7	CG	1257	0	1296	77	0
8	AH	1116	0	1177	105	0
8	CH	1116	0	1177	105	0
9	AI	1011	0	1042	110	0
9	CI	1011	0	1042	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	105	0
10	CJ	795	0	840	105	0
11	AK	885	0	904	66	0
11	CK	885	0	904	71	0
12	AL	971	0	1057	104	0
12	CL	971	0	1057	106	0
13	AM	921	0	976	91	0
13	CM	921	0	976	94	0
14	AN	492	0	530	47	0
14	CN	492	0	529	46	0
15	AO	734	0	771	79	0
15	CO	734	0	771	84	0
16	AP	701	0	720	97	0
16	CP	701	0	720	102	0
17	AQ	824	0	891	70	0
17	CQ	824	0	891	59	0
18	AR	574	0	644	78	0
18	CR	574	0	644	78	0
19	AS	630	0	652	56	0
19	CS	630	0	652	56	0
20	AT	763	0	861	91	0
20	CT	763	0	861	81	0
21	AU	209	0	221	9	0
21	CU	209	0	221	9	0
22	B0	650	0	654	57	0
22	D0	650	0	654	59	0
23	B1	693	0	764	149	0
23	D1	693	0	764	144	0
24	B2	421	0	461	126	0
24	D2	421	0	461	127	0
25	B3	468	0	523	34	0
25	D3	468	0	523	43	0
26	B4	157	0	69	20	0
26	D4	157	0	69	22	0
27	B5	459	0	480	98	0
27	D5	459	0	480	93	0
28	B6	381	0	390	104	0
28	D6	381	0	390	102	0
29	B7	419	0	467	38	0
29	D7	419	0	467	41	0
30	B8	508	0	576	163	0
30	D8	508	0	576	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29590	2619	0
31	DA	58698	0	29591	2787	0
32	BB	2551	0	1295	144	0
32	DB	2551	0	1295	157	0
33	BD	2105	0	2182	339	0
33	DD	2105	0	2182	350	0
34	BE	1564	0	1629	253	0
34	DE	1564	0	1629	260	0
35	BF	1624	0	1677	198	0
35	DF	1624	0	1677	201	0
36	BG	1474	0	1534	200	0
36	DG	1474	0	1534	193	0
37	BH	1223	0	1282	169	0
37	DH	1223	0	1282	164	0
38	BI	1132	0	1218	126	0
38	DI	1132	0	1218	128	0
39	BN	1105	0	1180	228	0
39	DN	1105	0	1180	239	0
40	BO	933	0	996	81	0
40	DO	933	0	996	89	0
41	BP	1114	0	1187	311	0
41	DP	1114	0	1187	298	0
42	BQ	1080	0	1127	181	0
42	DQ	1080	0	1127	193	0
43	BR	960	0	1021	138	0
43	DR	960	0	1021	132	0
44	BS	771	0	832	152	0
44	DS	771	0	832	145	0
45	BT	1100	0	1164	217	0
45	DT	1100	0	1164	202	0
46	BU	958	0	1015	150	0
46	DU	958	0	1015	158	0
47	BV	779	0	851	232	0
47	DV	779	0	851	233	0
48	BW	896	0	953	82	0
48	DW	896	0	953	91	0
49	BX	726	0	778	173	0
49	DX	726	0	778	168	0
50	BY	776	0	870	180	0
50	DY	776	0	870	181	0
51	BZ	1404	0	1432	158	0
51	DZ	1404	0	1432	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	56	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	BA	368	0	0	0	0
52	BB	7	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	2	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	2	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	53	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	DA	332	0	0	0	0
52	DB	4	0	0	0	0
52	DD	1	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	2	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	20	0	10	0	0
55	DA	20	0	10	0	0
All	All	277987	0	189127	19544	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 42.

The worst 5 of 19544 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)
27:B5:46:CYS:SG	27:B5:47:PRO:HD2	1.78	1.22
31:BA:1899:G:H22	31:BA:1902:C:N4	1.41	1.18
30:B8:32:LEU:CB	30:B8:35:GLN:H	1.57	1.17
32:DB:20:C:H2'	32:DB:21:G:H5''	1.25	1.17
41:BP:141:ALA:HB3	25:D3:1:MET:SD	1.86	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	282 (18%)	31 (2%)
1	CA	1503/1522 (98%)	285 (18%)	31 (2%)
31	BA	2723/2787 (97%)	717 (26%)	70 (2%)
31	DA	2723/2787 (97%)	712 (26%)	69 (2%)
32	BB	118/122 (96%)	34 (28%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	1 (0%)
All	All	8688/8862 (98%)	2065 (23%)	203 (2%)

5 of 2065 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	30	U
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 203 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	509	A
31	DA	472	A
31	DA	2791	C
1	CA	748	C
1	CA	1493	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 853 ligands modelled in this entry, 851 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	CLM	BA	3370	54	20,20,20	1.28	1 (5%)	23,27,27	0.91	0
55	CLM	DA	3334	54	20,20,20	1.29	1 (5%)	23,27,27	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CLM	BA	3370	54	-	0/20/22/22	0/1/1/1
55	CLM	DA	3334	54	-	0/20/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3334	CLM	C9-N9	-4.35	1.34	1.45
55	BA	3370	CLM	C9-N9	-4.33	1.34	1.45

There are no bond angle outliers.

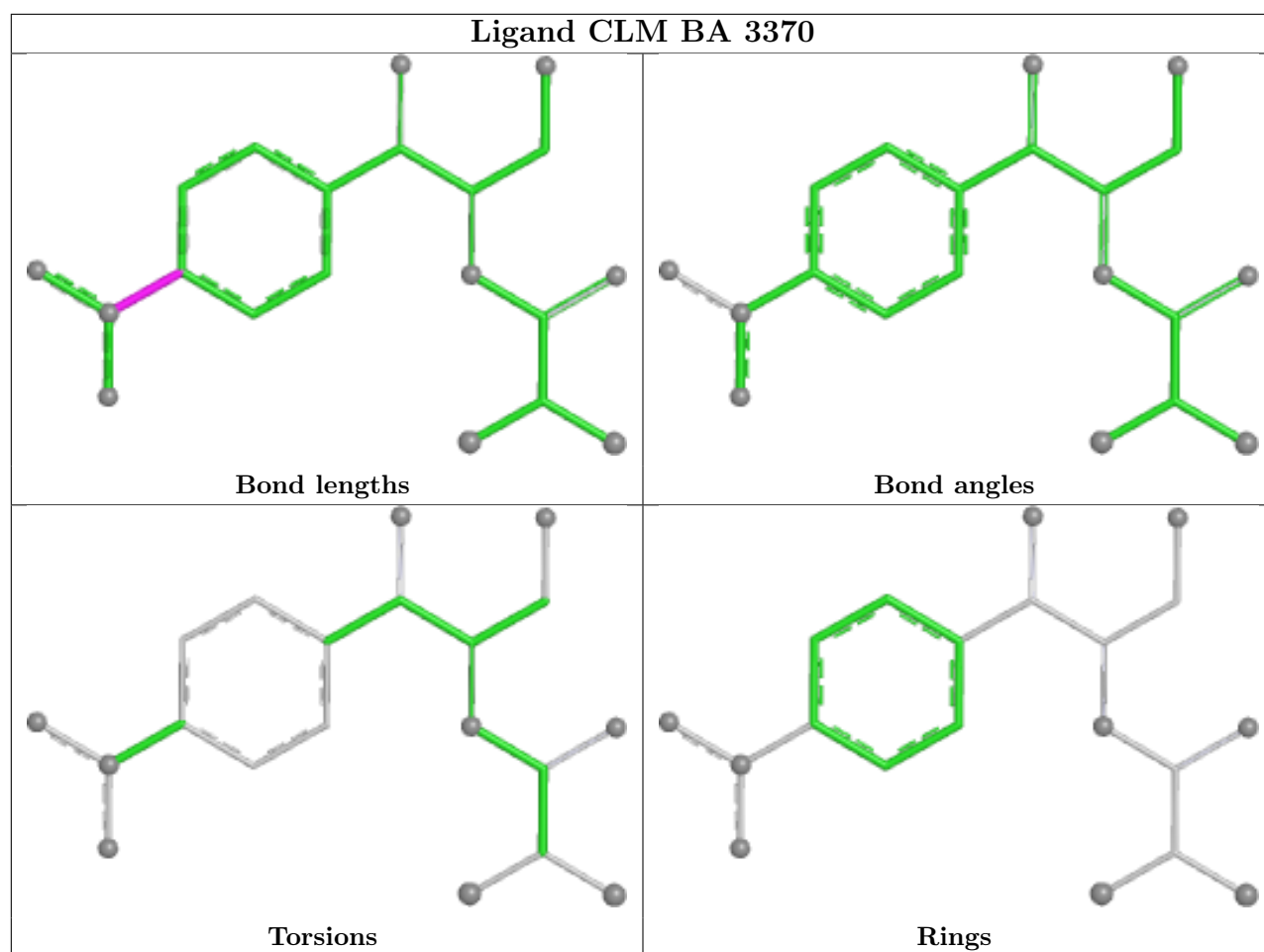
There are no chirality outliers.

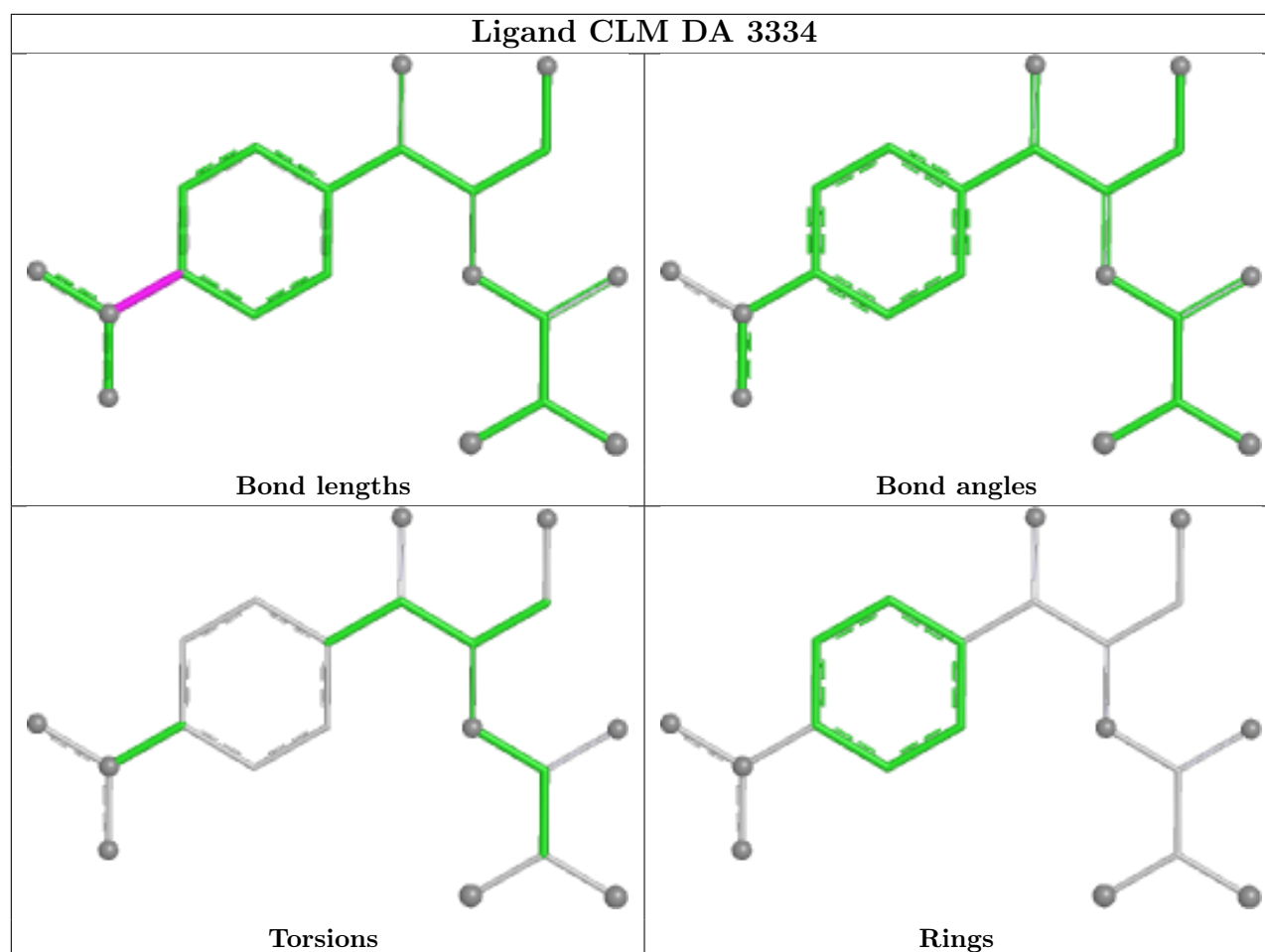
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
36	BG	1
36	DG	1
28	B6	1
28	D6	1
9	AI	1
47	BV	1
9	CI	1

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Mol	Chain	Number of breaks
47	DV	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	5.35
1	AM	69:GLU	C	70:LEU	N	5.34
1	BG	112:PRO	C	113:ARG	N	4.53
1	DG	112:PRO	C	113:ARG	N	4.53
1	CM	112:GLY	C	113:PRO	N	4.49

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	1.07	272 (18%) 3 2	42, 106, 199, 201	0
1	CA	1504/1522 (98%)	0.98	196 (13%) 7 4	46, 105, 198, 201	0
2	AB	235/256 (91%)	1.68	80 (34%) 1 1	83, 146, 188, 195	0
2	CB	235/256 (91%)	1.32	49 (20%) 2 2	84, 149, 187, 196	0
3	AC	207/239 (86%)	1.41	44 (21%) 2 1	97, 158, 187, 194	0
3	CC	207/239 (86%)	1.27	38 (18%) 3 2	98, 160, 187, 194	0
4	AD	208/209 (99%)	1.37	52 (25%) 2 1	72, 112, 165, 186	0
4	CD	208/209 (99%)	1.37	50 (24%) 2 1	70, 111, 164, 185	0
5	AE	151/162 (93%)	0.80	14 (9%) 14 7	59, 97, 151, 194	0
5	CE	151/162 (93%)	0.97	17 (11%) 10 6	64, 98, 153, 194	0
6	AF	101/101 (100%)	1.14	14 (13%) 6 4	66, 111, 160, 183	0
6	CF	101/101 (100%)	1.18	15 (14%) 5 3	67, 113, 160, 188	0
7	AG	155/156 (99%)	1.62	48 (30%) 1 1	124, 172, 192, 197	0
7	CG	155/156 (99%)	1.43	38 (24%) 2 1	125, 172, 192, 198	0
8	AH	138/138 (100%)	0.92	15 (10%) 10 6	67, 102, 147, 162	0
8	CH	138/138 (100%)	1.02	16 (11%) 9 5	66, 102, 147, 163	0
9	AI	127/128 (99%)	2.08	64 (50%) 0 0	125, 179, 196, 199	0
9	CI	127/128 (99%)	1.91	48 (37%) 1 1	126, 180, 197, 199	0
10	AJ	99/105 (94%)	2.22	48 (48%) 0 0	122, 175, 196, 198	0
10	CJ	99/105 (94%)	1.96	39 (39%) 1 1	121, 176, 197, 199	0
11	AK	119/129 (92%)	1.12	20 (16%) 4 3	63, 105, 164, 188	0
11	CK	119/129 (92%)	1.34	22 (18%) 3 2	65, 104, 168, 191	0
12	AL	125/135 (92%)	1.27	30 (24%) 2 1	57, 89, 154, 198	0
12	CL	125/135 (92%)	1.41	34 (27%) 1 1	55, 89, 158, 198	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	2.26	59 (51%)	0	0	136, 190, 198, 200	0
13	CM	115/126 (91%)	1.97	48 (41%)	0	1	136, 188, 197, 199	0
14	AN	60/61 (98%)	1.72	21 (35%)	1	1	113, 167, 193, 196	0
14	CN	60/61 (98%)	2.04	28 (46%)	0	0	112, 168, 191, 196	0
15	AO	88/89 (98%)	1.17	15 (17%)	4	3	59, 91, 149, 155	0
15	CO	88/89 (98%)	0.81	11 (12%)	8	5	63, 92, 150, 157	0
16	AP	84/88 (95%)	1.44	20 (23%)	2	1	77, 101, 161, 188	0
16	CP	84/88 (95%)	1.49	19 (22%)	2	1	78, 100, 154, 186	0
17	AQ	100/105 (95%)	1.13	18 (18%)	3	2	62, 93, 138, 158	0
17	CQ	100/105 (95%)	0.95	13 (13%)	7	4	59, 92, 140, 157	0
18	AR	70/88 (79%)	1.09	10 (14%)	6	3	73, 98, 167, 197	0
18	CR	70/88 (79%)	1.01	9 (12%)	7	5	74, 100, 167, 196	0
19	AS	79/93 (84%)	1.99	30 (37%)	1	1	142, 191, 198, 199	0
19	CS	79/93 (84%)	1.69	24 (30%)	1	1	142, 190, 198, 199	0
20	AT	99/106 (93%)	1.53	28 (28%)	1	1	73, 110, 157, 186	0
20	CT	99/106 (93%)	1.41	26 (26%)	1	1	74, 108, 156, 189	0
21	AU	25/27 (92%)	3.96	22 (88%)	0	0	138, 175, 193, 196	0
21	CU	25/27 (92%)	3.07	19 (76%)	0	0	135, 172, 193, 195	0
22	B0	85/85 (100%)	1.04	18 (21%)	2	1	34, 59, 182, 197	0
22	D0	85/85 (100%)	0.90	12 (14%)	6	4	40, 64, 178, 197	0
23	B1	89/98 (90%)	1.61	28 (31%)	1	1	37, 64, 140, 187	0
23	D1	89/98 (90%)	1.34	26 (29%)	1	1	40, 66, 142, 191	0
24	B2	51/72 (70%)	2.77	32 (62%)	0	0	49, 87, 184, 193	0
24	D2	51/72 (70%)	2.12	23 (45%)	0	0	50, 91, 183, 195	0
25	B3	60/60 (100%)	0.84	10 (16%)	4	3	36, 56, 132, 180	0
25	D3	60/60 (100%)	0.72	7 (11%)	9	5	42, 61, 138, 178	0
26	B4	32/71 (45%)	2.38	17 (53%)	0	0	109, 156, 186, 191	0
26	D4	32/71 (45%)	2.01	12 (37%)	1	1	112, 161, 188, 195	0
27	B5	59/60 (98%)	0.99	10 (16%)	4	3	25, 47, 180, 195	0
27	D5	59/60 (98%)	0.52	9 (15%)	5	3	28, 50, 184, 195	0
28	B6	45/54 (83%)	2.37	23 (51%)	0	0	36, 70, 133, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	1.81	18 (40%)	1 1	42, 74, 138, 184	0
29	B7	49/49 (100%)	0.20	5 (10%)	12 6	26, 33, 117, 170	0
29	D7	49/49 (100%)	0.36	7 (14%)	6 3	27, 37, 118, 170	0
30	B8	64/65 (98%)	1.64	17 (26%)	1 1	34, 57, 138, 181	0
30	D8	64/65 (98%)	1.38	18 (28%)	1 1	38, 59, 139, 183	0
31	BA	2725/2787 (97%)	0.02	160 (5%)	28 14	26, 46, 145, 201	0
31	DA	2725/2787 (97%)	-0.00	122 (4%)	38 20	27, 51, 148, 201	0
32	BB	119/122 (97%)	1.47	39 (32%)	1 1	39, 91, 140, 185	0
32	DB	119/122 (97%)	1.57	43 (36%)	1 1	48, 95, 154, 190	0
33	BD	272/276 (98%)	0.31	19 (6%)	22 12	27, 47, 100, 177	0
33	DD	272/276 (98%)	0.33	17 (6%)	26 13	29, 50, 104, 181	0
34	BE	205/206 (99%)	0.64	27 (13%)	7 4	25, 52, 145, 189	0
34	DE	205/206 (99%)	0.62	22 (10%)	11 6	29, 56, 142, 189	0
35	BF	208/210 (99%)	0.64	26 (12%)	8 5	24, 58, 180, 197	0
35	DF	208/210 (99%)	0.55	16 (7%)	19 10	27, 63, 178, 197	0
36	BG	181/182 (99%)	1.95	69 (38%)	1 1	87, 144, 189, 199	0
36	DG	181/182 (99%)	1.94	67 (37%)	1 1	91, 153, 193, 199	0
37	BH	160/180 (88%)	2.37	78 (48%)	0 0	62, 102, 150, 193	0
37	DH	160/180 (88%)	1.39	40 (25%)	2 1	70, 110, 157, 195	0
38	BI	146/148 (98%)	2.04	66 (45%)	0 0	52, 143, 185, 195	0
38	DI	146/148 (98%)	2.79	82 (56%)	0 0	56, 156, 188, 198	0
39	BN	139/140 (99%)	1.28	36 (25%)	1 1	32, 60, 140, 187	0
39	DN	139/140 (99%)	0.72	17 (12%)	8 5	38, 65, 142, 188	0
40	BO	122/122 (100%)	0.15	3 (2%)	58 35	32, 52, 105, 141	0
40	DO	122/122 (100%)	0.18	4 (3%)	49 28	35, 55, 111, 146	0
41	BP	146/150 (97%)	1.66	50 (34%)	1 1	22, 79, 148, 199	0
41	DP	146/150 (97%)	1.29	30 (20%)	2 2	27, 81, 150, 198	0
42	BQ	136/141 (96%)	1.25	29 (21%)	2 1	39, 64, 150, 189	0
42	DQ	136/141 (96%)	1.06	20 (14%)	6 3	43, 69, 149, 190	0
43	BR	117/118 (99%)	0.40	14 (11%)	9 5	28, 44, 113, 143	0
43	DR	117/118 (99%)	0.35	13 (11%)	10 6	30, 49, 115, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	1.99	43 (43%)	0	1	53, 98, 141, 178	0
44	DS	99/112 (88%)	1.90	39 (39%)	1	1	63, 103, 146, 180	0
45	BT	132/146 (90%)	1.38	34 (25%)	1	1	42, 73, 157, 191	0
45	DT	132/146 (90%)	1.09	29 (21%)	2	1	46, 77, 159, 194	0
46	BU	117/118 (99%)	0.88	23 (19%)	3	2	23, 50, 114, 190	0
46	DU	117/118 (99%)	0.69	17 (14%)	6	3	32, 56, 119, 193	0
47	BV	101/101 (100%)	2.41	53 (52%)	0	0	32, 91, 171, 194	0
47	DV	101/101 (100%)	1.42	22 (21%)	2	1	35, 97, 169, 195	0
48	BW	113/113 (100%)	0.09	4 (3%)	47	27	28, 40, 101, 168	0
48	DW	113/113 (100%)	0.01	2 (1%)	67	44	31, 43, 106, 175	0
49	BX	93/96 (96%)	1.52	29 (31%)	1	1	36, 65, 142, 184	0
49	DX	93/96 (96%)	1.16	18 (19%)	3	2	42, 69, 147, 185	0
50	BY	101/110 (91%)	2.57	53 (52%)	0	0	39, 91, 191, 199	0
50	DY	101/110 (91%)	2.03	42 (41%)	0	1	40, 96, 191, 198	0
51	BZ	177/206 (85%)	1.62	57 (32%)	1	1	56, 100, 150, 175	0
51	DZ	177/206 (85%)	1.20	33 (18%)	3	2	63, 103, 153, 179	0
All	All	20064/20922 (95%)	0.90	3582 (17%)	3	2	22, 84, 190, 201	0

The worst 5 of 3582 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	BQ	140	ALA	19.8
39	BN	68	GLU	16.5
38	DI	100	ALA	15.8
42	BQ	141	GLN	14.4
38	DI	97	ILE	13.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
52	MG	BA	3317	1/1	0.61	0.21	53,53,53,53	0
52	MG	BA	3098	1/1	0.69	0.29	59,59,59,59	0
52	MG	DA	3236	1/1	0.69	0.30	71,71,71,71	0
52	MG	BA	3154	1/1	0.71	0.34	77,77,77,77	0
52	MG	DA	3167	1/1	0.72	0.27	63,63,63,63	0
52	MG	BA	3150	1/1	0.72	0.21	40,40,40,40	0
52	MG	CA	1627	1/1	0.74	0.31	81,81,81,81	0
52	MG	DA	3069	1/1	0.74	0.21	63,63,63,63	0
52	MG	BA	3363	1/1	0.74	0.19	54,54,54,54	0
52	MG	CA	1626	1/1	0.74	0.32	68,68,68,68	0
52	MG	AA	1649	1/1	0.75	0.28	76,76,76,76	0
52	MG	DA	3153	1/1	0.75	0.38	73,73,73,73	0
52	MG	AA	1643	1/1	0.77	0.28	66,66,66,66	0
52	MG	DA	3074	1/1	0.77	0.24	54,54,54,54	0
52	MG	DA	3124	1/1	0.77	0.14	49,49,49,49	0
54	K	BA	3369	1/1	0.77	0.10	41,41,41,41	0
52	MG	DA	3331	1/1	0.78	0.31	67,67,67,67	0
52	MG	AA	1624	1/1	0.79	0.34	59,59,59,59	0
52	MG	BA	3127	1/1	0.79	0.23	44,44,44,44	0
52	MG	CA	1611	1/1	0.79	0.28	76,76,76,76	0
52	MG	BA	3163	1/1	0.79	0.19	53,53,53,53	0
52	MG	BA	3299	1/1	0.79	0.17	37,37,37,37	0
52	MG	DA	3175	1/1	0.79	0.22	51,51,51,51	0
52	MG	CA	1630	1/1	0.79	0.33	66,66,66,66	0
52	MG	DA	3297	1/1	0.79	0.18	55,55,55,55	0
52	MG	CA	1638	1/1	0.79	0.41	64,64,64,64	0
52	MG	DA	3015	1/1	0.79	0.26	52,52,52,52	0
52	MG	DA	3072	1/1	0.80	0.43	71,71,71,71	0
52	MG	CA	1642	1/1	0.80	0.34	71,71,71,71	0
52	MG	DA	3265	1/1	0.80	0.15	38,38,38,38	0
52	MG	CA	1651	1/1	0.80	0.25	51,51,51,51	0
52	MG	BA	3368	1/1	0.80	0.20	60,60,60,60	0
52	MG	CA	1615	1/1	0.80	0.26	64,64,64,64	0
52	MG	BA	3111	1/1	0.81	0.36	41,41,41,41	0
52	MG	BA	3338	1/1	0.81	0.15	50,50,50,50	0
52	MG	DA	3133	1/1	0.81	0.23	55,55,55,55	0
52	MG	BA	3166	1/1	0.81	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	CA	1637	1/1	0.81	0.23	65,65,65,65	0
52	MG	BA	3367	1/1	0.81	0.18	47,47,47,47	0
52	MG	DA	3195	1/1	0.81	0.12	36,36,36,36	0
52	MG	DA	3223	1/1	0.81	0.26	37,37,37,37	0
52	MG	BA	3181	1/1	0.81	0.16	32,32,32,32	0
52	MG	BA	3292	1/1	0.81	0.11	41,41,41,41	0
52	MG	DA	3284	1/1	0.81	0.20	49,49,49,49	0
52	MG	CA	1613	1/1	0.81	0.24	58,58,58,58	0
52	MG	DA	3299	1/1	0.81	0.09	41,41,41,41	0
52	MG	DA	3323	1/1	0.81	0.35	62,62,62,62	0
52	MG	AA	1637	1/1	0.81	0.39	51,51,51,51	0
52	MG	CA	1625	1/1	0.81	0.26	59,59,59,59	0
54	K	DA	3333	1/1	0.81	0.20	62,62,62,62	0
52	MG	BA	3180	1/1	0.82	0.32	46,46,46,46	0
52	MG	AA	1654	1/1	0.82	0.27	64,64,64,64	0
52	MG	BA	3177	1/1	0.82	0.42	67,67,67,67	0
52	MG	CA	1610	1/1	0.82	0.18	66,66,66,66	0
52	MG	DA	3041	1/1	0.82	0.23	29,29,29,29	0
52	MG	DU	201	1/1	0.82	0.19	60,60,60,60	0
52	MG	DA	3068	1/1	0.82	0.18	57,57,57,57	0
52	MG	DA	3280	1/1	0.82	0.29	70,70,70,70	0
52	MG	DA	3110	1/1	0.83	0.32	50,50,50,50	0
52	MG	DA	3242	1/1	0.83	0.14	35,35,35,35	0
52	MG	AA	1644	1/1	0.83	0.23	68,68,68,68	0
52	MG	BA	3004	1/1	0.83	0.20	14,14,14,14	0
52	MG	AA	1638	1/1	0.83	0.28	69,69,69,69	0
52	MG	DA	3289	1/1	0.83	0.15	53,53,53,53	0
52	MG	DA	3164	1/1	0.83	0.26	41,41,41,41	0
52	MG	BA	3186	1/1	0.83	0.18	38,38,38,38	0
52	MG	DA	3301	1/1	0.83	0.10	15,15,15,15	0
52	MG	DA	3309	1/1	0.83	0.31	66,66,66,66	0
52	MG	BA	3362	1/1	0.83	0.26	50,50,50,50	0
52	MG	BA	3246	1/1	0.83	0.11	40,40,40,40	0
52	MG	DA	3197	1/1	0.83	0.27	46,46,46,46	0
52	MG	CA	1618	1/1	0.83	0.29	58,58,58,58	0
52	MG	DA	3227	1/1	0.83	0.16	47,47,47,47	0
52	MG	BA	3328	1/1	0.84	0.14	27,27,27,27	0
52	MG	DA	3159	1/1	0.84	0.18	40,40,40,40	0
52	MG	BA	3123	1/1	0.84	0.27	40,40,40,40	0
52	MG	BA	3343	1/1	0.84	0.25	40,40,40,40	0
52	MG	BA	3298	1/1	0.84	0.13	41,41,41,41	0
52	MG	BA	3286	1/1	0.84	0.24	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3316	1/1	0.84	0.23	41,41,41,41	0
52	MG	DA	3005	1/1	0.84	0.14	49,49,49,49	0
52	MG	DA	3310	1/1	0.84	0.35	56,56,56,56	0
52	MG	DA	3127	1/1	0.84	0.11	33,33,33,33	0
52	MG	DA	3232	1/1	0.84	0.36	63,63,63,63	0
52	MG	DQ	201	1/1	0.84	0.20	42,42,42,42	0
52	MG	BA	3289	1/1	0.84	0.16	44,44,44,44	0
52	MG	DA	3145	1/1	0.84	0.30	40,40,40,40	0
52	MG	DA	3264	1/1	0.84	0.13	58,58,58,58	0
52	MG	CA	1652	1/1	0.85	0.17	61,61,61,61	0
52	MG	AA	1648	1/1	0.85	0.21	80,80,80,80	0
52	MG	BA	3234	1/1	0.85	0.07	16,16,16,16	0
52	MG	DA	3292	1/1	0.85	0.15	52,52,52,52	0
52	MG	BA	3240	1/1	0.85	0.21	50,50,50,50	0
52	MG	AA	1613	1/1	0.85	0.23	62,62,62,62	0
52	MG	AA	1650	1/1	0.85	0.23	49,49,49,49	0
52	MG	BA	3170	1/1	0.85	0.28	36,36,36,36	0
52	MG	AA	1606	1/1	0.85	0.28	86,86,86,86	0
52	MG	DA	3090	1/1	0.85	0.26	33,33,33,33	0
52	MG	BA	3296	1/1	0.85	0.09	36,36,36,36	0
52	MG	AA	1609	1/1	0.85	0.26	52,52,52,52	0
52	MG	CA	1606	1/1	0.85	0.34	52,52,52,52	0
52	MG	CA	1608	1/1	0.85	0.23	68,68,68,68	0
52	MG	BA	3151	1/1	0.85	0.14	47,47,47,47	0
55	CLM	DA	3334	20/20	0.85	0.27	90,90,90,90	0
52	MG	BA	3160	1/1	0.86	0.18	41,41,41,41	0
52	MG	DA	3274	1/1	0.86	0.21	71,71,71,71	0
52	MG	DA	3149	1/1	0.86	0.37	54,54,54,54	0
52	MG	AA	1656	1/1	0.86	0.17	62,62,62,62	0
52	MG	BA	3209	1/1	0.86	0.16	36,36,36,36	0
52	MG	DA	3290	1/1	0.86	0.20	55,55,55,55	0
52	MG	BA	3128	1/1	0.86	0.28	45,45,45,45	0
52	MG	BA	3167	1/1	0.86	0.19	51,51,51,51	0
52	MG	CA	1631	1/1	0.86	0.16	71,71,71,71	0
52	MG	BA	3116	1/1	0.86	0.08	41,41,41,41	0
52	MG	DA	3304	1/1	0.86	0.28	63,63,63,63	0
52	MG	BA	3176	1/1	0.86	0.16	58,58,58,58	0
52	MG	BA	3122	1/1	0.86	0.21	37,37,37,37	0
52	MG	DA	3116	1/1	0.86	0.22	45,45,45,45	0
52	MG	DA	3326	1/1	0.86	0.13	49,49,49,49	0
52	MG	BA	3108	1/1	0.86	0.11	31,31,31,31	0
52	MG	CA	1617	1/1	0.86	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3132	1/1	0.86	0.40	53,53,53,53	0
52	MG	DA	3251	1/1	0.86	0.13	72,72,72,72	0
52	MG	DA	3259	1/1	0.86	0.22	79,79,79,79	0
52	MG	D5	102	1/1	0.86	0.16	58,58,58,58	0
52	MG	BA	3221	1/1	0.87	0.24	31,31,31,31	0
52	MG	DA	3136	1/1	0.87	0.18	48,48,48,48	0
52	MG	DA	3140	1/1	0.87	0.30	42,42,42,42	0
52	MG	DA	3270	1/1	0.87	0.35	55,55,55,55	0
52	MG	AA	1604	1/1	0.87	0.21	62,62,62,62	0
52	MG	AA	1612	1/1	0.87	0.30	56,56,56,56	0
52	MG	BA	3072	1/1	0.87	0.27	41,41,41,41	0
52	MG	DA	3157	1/1	0.87	0.16	48,48,48,48	0
52	MG	BA	3254	1/1	0.87	0.25	34,34,34,34	0
52	MG	CA	1632	1/1	0.87	0.20	56,56,56,56	0
52	MG	DA	3293	1/1	0.87	0.28	54,54,54,54	0
52	MG	CA	1635	1/1	0.87	0.24	73,73,73,73	0
52	MG	DA	3077	1/1	0.87	0.21	38,38,38,38	0
52	MG	DA	3178	1/1	0.87	0.20	30,30,30,30	0
52	MG	DA	3191	1/1	0.87	0.13	38,38,38,38	0
52	MG	DA	3088	1/1	0.87	0.21	40,40,40,40	0
52	MG	BA	3263	1/1	0.87	0.13	29,29,29,29	0
52	MG	DA	3312	1/1	0.87	0.21	45,45,45,45	0
52	MG	DA	3096	1/1	0.87	0.29	61,61,61,61	0
52	MG	DA	3224	1/1	0.87	0.23	41,41,41,41	0
52	MG	BA	3329	1/1	0.87	0.21	49,49,49,49	0
52	MG	DA	3332	1/1	0.87	0.31	69,69,69,69	0
52	MG	BA	3171	1/1	0.87	0.26	35,35,35,35	0
52	MG	BA	3197	1/1	0.87	0.19	27,27,27,27	0
52	MG	BA	3358	1/1	0.87	0.26	59,59,59,59	0
52	MG	DA	3249	1/1	0.87	0.17	48,48,48,48	0
52	MG	AA	1608	1/1	0.87	0.39	70,70,70,70	0
52	MG	BA	3314	1/1	0.88	0.14	41,41,41,41	0
52	MG	CA	1641	1/1	0.88	0.21	45,45,45,45	0
52	MG	AA	1607	1/1	0.88	0.26	47,47,47,47	0
52	MG	DA	3261	1/1	0.88	0.07	51,51,51,51	0
52	MG	AA	1605	1/1	0.88	0.25	71,71,71,71	0
52	MG	BA	3320	1/1	0.88	0.27	52,52,52,52	0
52	MG	BA	3039	1/1	0.88	0.26	37,37,37,37	0
52	MG	BA	3284	1/1	0.88	0.28	39,39,39,39	0
52	MG	BA	3188	1/1	0.88	0.17	36,36,36,36	0
52	MG	DA	3024	1/1	0.88	0.24	47,47,47,47	0
52	MG	DA	3028	1/1	0.88	0.34	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3131	1/1	0.88	0.29	45,45,45,45	0
52	MG	DA	3047	1/1	0.88	0.27	33,33,33,33	0
52	MG	DA	3165	1/1	0.88	0.13	38,38,38,38	0
52	MG	DA	3067	1/1	0.88	0.09	35,35,35,35	0
52	MG	CA	1621	1/1	0.88	0.36	50,50,50,50	0
52	MG	BA	3113	1/1	0.88	0.22	26,26,26,26	0
52	MG	BA	3041	1/1	0.88	0.25	24,24,24,24	0
52	MG	DA	3305	1/1	0.88	0.25	46,46,46,46	0
52	MG	BA	3152	1/1	0.88	0.18	49,49,49,49	0
52	MG	CA	1629	1/1	0.88	0.13	57,57,57,57	0
52	MG	BA	3366	1/1	0.88	0.21	52,52,52,52	0
52	MG	AA	1642	1/1	0.88	0.20	46,46,46,46	0
52	MG	BA	3301	1/1	0.88	0.24	36,36,36,36	0
52	MG	DA	3228	1/1	0.88	0.14	38,38,38,38	0
52	MG	BB	205	1/1	0.88	0.10	59,59,59,59	0
52	MG	BR	202	1/1	0.88	0.19	31,31,31,31	0
52	MG	DA	3237	1/1	0.88	0.24	57,57,57,57	0
52	MG	DA	3239	1/1	0.88	0.22	41,41,41,41	0
52	MG	DA	3241	1/1	0.88	0.20	54,54,54,54	0
52	MG	DA	3122	1/1	0.88	0.27	40,40,40,40	0
52	MG	BA	3218	1/1	0.89	0.18	30,30,30,30	0
52	MG	BA	3120	1/1	0.89	0.24	25,25,25,25	0
52	MG	DA	3245	1/1	0.89	0.21	65,65,65,65	0
52	MG	BA	3344	1/1	0.89	0.15	56,56,56,56	0
52	MG	DA	3008	1/1	0.89	0.15	33,33,33,33	0
52	MG	DA	3139	1/1	0.89	0.27	43,43,43,43	0
52	MG	DA	3014	1/1	0.89	0.41	71,71,71,71	0
52	MG	BA	3349	1/1	0.89	0.32	65,65,65,65	0
52	MG	CA	1620	1/1	0.89	0.25	45,45,45,45	0
52	MG	AA	1628	1/1	0.89	0.28	70,70,70,70	0
52	MG	BA	3093	1/1	0.89	0.46	50,50,50,50	0
52	MG	AA	1655	1/1	0.89	0.19	45,45,45,45	0
52	MG	DA	3160	1/1	0.89	0.28	51,51,51,51	0
52	MG	DA	3161	1/1	0.89	0.09	44,44,44,44	0
52	MG	BA	3365	1/1	0.89	0.13	43,43,43,43	0
52	MG	BA	3308	1/1	0.89	0.21	45,45,45,45	0
52	MG	AA	1629	1/1	0.89	0.13	49,49,49,49	0
52	MG	DA	3295	1/1	0.89	0.39	73,73,73,73	0
52	MG	DA	3070	1/1	0.89	0.22	35,35,35,35	0
52	MG	DA	3176	1/1	0.89	0.23	66,66,66,66	0
52	MG	AA	1616	1/1	0.89	0.18	57,57,57,57	0
52	MG	DA	3184	1/1	0.89	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3281	1/1	0.89	0.16	41,41,41,41	0
52	MG	CA	1634	1/1	0.89	0.16	47,47,47,47	0
52	MG	AA	1625	1/1	0.89	0.30	40,40,40,40	0
52	MG	DA	3207	1/1	0.89	0.34	54,54,54,54	0
52	MG	DA	3318	1/1	0.89	0.12	43,43,43,43	0
52	MG	DA	3319	1/1	0.89	0.14	55,55,55,55	0
52	MG	DA	3214	1/1	0.89	0.20	39,39,39,39	0
52	MG	DA	3325	1/1	0.89	0.26	46,46,46,46	0
52	MG	CA	1604	1/1	0.89	0.23	67,67,67,67	0
52	MG	DA	3329	1/1	0.89	0.17	51,51,51,51	0
52	MG	BA	3325	1/1	0.89	0.27	53,53,53,53	0
52	MG	DA	3103	1/1	0.89	0.14	33,33,33,33	0
52	MG	DA	3109	1/1	0.89	0.19	48,48,48,48	0
52	MG	BA	3327	1/1	0.89	0.24	48,48,48,48	0
52	MG	DX	101	1/1	0.89	0.07	45,45,45,45	0
52	MG	BA	3207	1/1	0.89	0.13	32,32,32,32	0
52	MG	CA	1643	1/1	0.89	0.21	42,42,42,42	0
55	CLM	BA	3370	20/20	0.89	0.24	90,90,90,90	0
52	MG	AA	1627	1/1	0.89	0.18	60,60,60,60	0
52	MG	BA	3064	1/1	0.90	0.27	41,41,41,41	0
52	MG	DA	3081	1/1	0.90	0.16	24,24,24,24	0
52	MG	AA	1651	1/1	0.90	0.17	45,45,45,45	0
52	MG	BA	3245	1/1	0.90	0.33	52,52,52,52	0
52	MG	DA	3094	1/1	0.90	0.26	38,38,38,38	0
52	MG	BA	3075	1/1	0.90	0.26	38,38,38,38	0
52	MG	DA	3101	1/1	0.90	0.17	34,34,34,34	0
52	MG	BA	3249	1/1	0.90	0.22	54,54,54,54	0
52	MG	BA	3250	1/1	0.90	0.19	48,48,48,48	0
52	MG	BA	3086	1/1	0.90	0.25	27,27,27,27	0
52	MG	BA	3347	1/1	0.90	0.24	47,47,47,47	0
52	MG	DA	3121	1/1	0.90	0.25	49,49,49,49	0
52	MG	BA	3255	1/1	0.90	0.27	54,54,54,54	0
52	MG	BA	3355	1/1	0.90	0.15	51,51,51,51	0
52	MG	BA	3356	1/1	0.90	0.12	60,60,60,60	0
52	MG	DA	3131	1/1	0.90	0.34	55,55,55,55	0
52	MG	DA	3271	1/1	0.90	0.35	56,56,56,56	0
52	MG	BA	3173	1/1	0.90	0.29	50,50,50,50	0
52	MG	BA	3360	1/1	0.90	0.30	48,48,48,48	0
52	MG	DA	3282	1/1	0.90	0.17	61,61,61,61	0
52	MG	BA	3266	1/1	0.90	0.26	37,37,37,37	0
52	MG	BA	3090	1/1	0.90	0.15	14,14,14,14	0
52	MG	CA	1646	1/1	0.90	0.43	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	AA	1630	1/1	0.90	0.24	49,49,49,49	0
52	MG	BA	3178	1/1	0.90	0.21	32,32,32,32	0
52	MG	D1	101	1/1	0.90	0.21	47,47,47,47	0
52	MG	BA	3141	1/1	0.90	0.14	47,47,47,47	0
52	MG	DA	3158	1/1	0.90	0.11	33,33,33,33	0
52	MG	BA	3148	1/1	0.90	0.14	23,23,23,23	0
52	MG	DA	3302	1/1	0.90	0.18	39,39,39,39	0
52	MG	BA	3293	1/1	0.90	0.19	47,47,47,47	0
52	MG	BA	3182	1/1	0.90	0.21	37,37,37,37	0
52	MG	DA	3163	1/1	0.90	0.21	30,30,30,30	0
52	MG	AA	1632	1/1	0.90	0.25	51,51,51,51	0
52	MG	BA	3102	1/1	0.90	0.16	38,38,38,38	0
52	MG	DA	3316	1/1	0.90	0.16	62,62,62,62	0
52	MG	DA	3025	1/1	0.90	0.28	46,46,46,46	0
52	MG	AA	1645	1/1	0.90	0.23	61,61,61,61	0
52	MG	DA	3037	1/1	0.90	0.27	33,33,33,33	0
52	MG	DA	3040	1/1	0.90	0.42	58,58,58,58	0
52	MG	BA	3199	1/1	0.90	0.27	42,42,42,42	0
52	MG	AA	1621	1/1	0.90	0.19	37,37,37,37	0
52	MG	DA	3193	1/1	0.90	0.24	40,40,40,40	0
52	MG	CA	1612	1/1	0.90	0.16	48,48,48,48	0
52	MG	DB	204	1/1	0.90	0.25	37,37,37,37	0
52	MG	BA	3315	1/1	0.90	0.24	43,43,43,43	0
52	MG	DA	3200	1/1	0.90	0.13	37,37,37,37	0
52	MG	BA	3155	1/1	0.90	0.20	39,39,39,39	0
52	MG	AA	1615	1/1	0.90	0.11	35,35,35,35	0
52	MG	DA	3222	1/1	0.90	0.23	41,41,41,41	0
52	MG	AA	1620	1/1	0.90	0.34	52,52,52,52	0
52	MG	BA	3321	1/1	0.90	0.14	33,33,33,33	0
52	MG	DA	3051	1/1	0.91	0.24	29,29,29,29	0
52	MG	BA	3014	1/1	0.91	0.31	30,30,30,30	0
52	MG	BA	3310	1/1	0.91	0.13	31,31,31,31	0
52	MG	BA	3312	1/1	0.91	0.10	41,41,41,41	0
52	MG	AA	1622	1/1	0.91	0.17	40,40,40,40	0
52	MG	BA	3235	1/1	0.91	0.21	38,38,38,38	0
52	MG	DA	3220	1/1	0.91	0.15	40,40,40,40	0
52	MG	AA	1640	1/1	0.91	0.12	60,60,60,60	0
52	MG	DA	3075	1/1	0.91	0.25	38,38,38,38	0
52	MG	BA	3119	1/1	0.91	0.26	34,34,34,34	0
52	MG	DA	3079	1/1	0.91	0.17	36,36,36,36	0
52	MG	BA	3048	1/1	0.91	0.25	22,22,22,22	0
52	MG	DA	3082	1/1	0.91	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3056	1/1	0.91	0.05	20,20,20,20	0
52	MG	CA	1623	1/1	0.91	0.19	50,50,50,50	0
52	MG	DA	3092	1/1	0.91	0.34	47,47,47,47	0
52	MG	BA	3323	1/1	0.91	0.20	42,42,42,42	0
52	MG	DA	3095	1/1	0.91	0.16	47,47,47,47	0
52	MG	DA	3244	1/1	0.91	0.17	36,36,36,36	0
52	MG	BA	3324	1/1	0.91	0.11	53,53,53,53	0
52	MG	DA	3248	1/1	0.91	0.11	33,33,33,33	0
52	MG	DA	3098	1/1	0.91	0.25	34,34,34,34	0
52	MG	AA	1614	1/1	0.91	0.20	47,47,47,47	0
52	MG	DA	3253	1/1	0.91	0.09	32,32,32,32	0
52	MG	BA	3251	1/1	0.91	0.18	40,40,40,40	0
52	MG	BA	3124	1/1	0.91	0.29	39,39,39,39	0
52	MG	AA	1634	1/1	0.91	0.36	51,51,51,51	0
52	MG	DA	3114	1/1	0.91	0.21	46,46,46,46	0
52	MG	DA	3269	1/1	0.91	0.19	61,61,61,61	0
52	MG	BA	3336	1/1	0.91	0.15	49,49,49,49	0
52	MG	DA	3117	1/1	0.91	0.21	54,54,54,54	0
52	MG	BA	3258	1/1	0.91	0.06	21,21,21,21	0
52	MG	BA	3260	1/1	0.91	0.11	13,13,13,13	0
52	MG	DA	3281	1/1	0.91	0.22	63,63,63,63	0
52	MG	CA	1636	1/1	0.91	0.09	77,77,77,77	0
52	MG	BA	3074	1/1	0.91	0.22	48,48,48,48	0
52	MG	DA	3288	1/1	0.91	0.10	42,42,42,42	0
52	MG	BA	3129	1/1	0.91	0.14	33,33,33,33	0
52	MG	CA	1639	1/1	0.91	0.27	50,50,50,50	0
52	MG	BA	3270	1/1	0.91	0.12	26,26,26,26	0
52	MG	BA	3271	1/1	0.91	0.26	53,53,53,53	0
52	MG	BA	3272	1/1	0.91	0.24	36,36,36,36	0
52	MG	BA	3279	1/1	0.91	0.13	39,39,39,39	0
52	MG	AA	1635	1/1	0.91	0.08	53,53,53,53	0
52	MG	AA	1618	1/1	0.91	0.12	53,53,53,53	0
52	MG	DA	3150	1/1	0.91	0.28	32,32,32,32	0
52	MG	AA	1646	1/1	0.91	0.10	48,48,48,48	0
52	MG	DA	3156	1/1	0.91	0.16	51,51,51,51	0
52	MG	BA	3364	1/1	0.91	0.16	64,64,64,64	0
52	MG	DA	3004	1/1	0.91	0.16	19,19,19,19	0
52	MG	B1	101	1/1	0.91	0.14	25,25,25,25	0
52	MG	BA	3096	1/1	0.91	0.15	16,16,16,16	0
52	MG	B5	102	1/1	0.91	0.18	44,44,44,44	0
52	MG	BA	3294	1/1	0.91	0.24	40,40,40,40	0
52	MG	DA	3020	1/1	0.91	0.32	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BB	203	1/1	0.91	0.08	55,55,55,55	0
52	MG	BA	3203	1/1	0.91	0.15	47,47,47,47	0
52	MG	DA	3170	1/1	0.91	0.11	42,42,42,42	0
52	MG	DA	3330	1/1	0.91	0.24	53,53,53,53	0
52	MG	DA	3173	1/1	0.91	0.30	57,57,57,57	0
52	MG	DA	3174	1/1	0.91	0.20	54,54,54,54	0
52	MG	DB	201	1/1	0.91	0.46	57,57,57,57	0
52	MG	DB	203	1/1	0.91	0.08	73,73,73,73	0
52	MG	BF	301	1/1	0.91	0.11	43,43,43,43	0
52	MG	BA	3003	1/1	0.91	0.21	44,44,44,44	0
52	MG	AA	1647	1/1	0.91	0.20	46,46,46,46	0
52	MG	BA	3159	1/1	0.91	0.25	52,52,52,52	0
52	MG	DA	3187	1/1	0.91	0.27	44,44,44,44	0
52	MG	DA	3188	1/1	0.91	0.34	43,43,43,43	0
52	MG	BA	3305	1/1	0.91	0.17	54,54,54,54	0
52	MG	DA	3192	1/1	0.91	0.29	36,36,36,36	0
52	MG	AA	1601	1/1	0.92	0.19	50,50,50,50	0
52	MG	BA	3230	1/1	0.92	0.28	37,37,37,37	0
52	MG	BA	3287	1/1	0.92	0.09	27,27,27,27	0
52	MG	DA	3031	1/1	0.92	0.15	51,51,51,51	0
52	MG	BA	3288	1/1	0.92	0.18	46,46,46,46	0
52	MG	DA	3038	1/1	0.92	0.24	25,25,25,25	0
52	MG	BA	3339	1/1	0.92	0.14	31,31,31,31	0
52	MG	BA	3341	1/1	0.92	0.16	66,66,66,66	0
52	MG	DA	3142	1/1	0.92	0.26	32,32,32,32	0
52	MG	DA	3143	1/1	0.92	0.14	40,40,40,40	0
52	MG	DA	3252	1/1	0.92	0.23	57,57,57,57	0
52	MG	DA	3045	1/1	0.92	0.24	30,30,30,30	0
52	MG	DA	3254	1/1	0.92	0.20	46,46,46,46	0
52	MG	DA	3258	1/1	0.92	0.14	38,38,38,38	0
52	MG	DA	3148	1/1	0.92	0.28	51,51,51,51	0
52	MG	BA	3059	1/1	0.92	0.19	25,25,25,25	0
52	MG	BA	3022	1/1	0.92	0.12	37,37,37,37	0
52	MG	DA	3056	1/1	0.92	0.16	24,24,24,24	0
52	MG	DA	3267	1/1	0.92	0.19	46,46,46,46	0
52	MG	DA	3155	1/1	0.92	0.08	41,41,41,41	0
52	MG	DA	3058	1/1	0.92	0.19	42,42,42,42	0
52	MG	BA	3345	1/1	0.92	0.20	43,43,43,43	0
52	MG	BA	3067	1/1	0.92	0.17	28,28,28,28	0
52	MG	BA	3348	1/1	0.92	0.21	34,34,34,34	0
52	MG	BA	3244	1/1	0.92	0.16	50,50,50,50	0
52	MG	BA	3103	1/1	0.92	0.21	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3143	1/1	0.92	0.23	29,29,29,29	0
52	MG	DA	3287	1/1	0.92	0.37	61,61,61,61	0
52	MG	BA	3104	1/1	0.92	0.08	22,22,22,22	0
52	MG	BA	3359	1/1	0.92	0.14	39,39,39,39	0
52	MG	BA	3105	1/1	0.92	0.22	19,19,19,19	0
52	MG	DA	3080	1/1	0.92	0.29	30,30,30,30	0
52	MG	BA	3068	1/1	0.92	0.26	35,35,35,35	0
52	MG	BA	3025	1/1	0.92	0.12	29,29,29,29	0
52	MG	DA	3085	1/1	0.92	0.12	19,19,19,19	0
52	MG	BA	3309	1/1	0.92	0.32	49,49,49,49	0
52	MG	DA	3089	1/1	0.92	0.25	31,31,31,31	0
52	MG	DA	3180	1/1	0.92	0.07	38,38,38,38	0
52	MG	DA	3181	1/1	0.92	0.24	29,29,29,29	0
52	MG	BA	3187	1/1	0.92	0.23	33,33,33,33	0
52	MG	DA	3308	1/1	0.92	0.16	43,43,43,43	0
52	MG	BA	3031	1/1	0.92	0.18	39,39,39,39	0
52	MG	BA	3189	1/1	0.92	0.21	46,46,46,46	0
52	MG	AA	1611	1/1	0.92	0.14	72,72,72,72	0
52	MG	BA	3077	1/1	0.92	0.22	20,20,20,20	0
52	MG	BA	3268	1/1	0.92	0.23	38,38,38,38	0
52	MG	BA	3318	1/1	0.92	0.19	34,34,34,34	0
52	MG	BP	201	1/1	0.92	0.20	35,35,35,35	0
52	MG	DA	3198	1/1	0.92	0.18	37,37,37,37	0
52	MG	DA	3108	1/1	0.92	0.27	39,39,39,39	0
52	MG	DA	3202	1/1	0.92	0.24	46,46,46,46	0
52	MG	BA	3079	1/1	0.92	0.17	36,36,36,36	0
52	MG	DA	3210	1/1	0.92	0.08	46,46,46,46	0
52	MG	BA	3083	1/1	0.92	0.27	34,34,34,34	0
52	MG	DA	3215	1/1	0.92	0.16	27,27,27,27	0
52	MG	DA	3216	1/1	0.92	0.30	45,45,45,45	0
52	MG	DA	3111	1/1	0.92	0.33	39,39,39,39	0
52	MG	DF	301	1/1	0.92	0.21	53,53,53,53	0
52	MG	DP	201	1/1	0.92	0.11	19,19,19,19	0
52	MG	DA	3221	1/1	0.92	0.25	43,43,43,43	0
52	MG	AA	1639	1/1	0.92	0.30	48,48,48,48	0
52	MG	CA	1607	1/1	0.92	0.32	46,46,46,46	0
52	MG	BA	3276	1/1	0.92	0.23	35,35,35,35	0
52	MG	BA	3215	1/1	0.92	0.08	10,10,10,10	0
52	MG	BA	3007	1/1	0.92	0.22	40,40,40,40	0
52	MG	DA	3123	1/1	0.92	0.07	38,38,38,38	0
52	MG	BA	3225	1/1	0.93	0.21	32,32,32,32	0
52	MG	DA	3240	1/1	0.93	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3227	1/1	0.93	0.22	22,22,22,22	0
52	MG	BA	3118	1/1	0.93	0.16	38,38,38,38	0
52	MG	BA	3303	1/1	0.93	0.18	37,37,37,37	0
52	MG	BA	3304	1/1	0.93	0.27	49,49,49,49	0
52	MG	DA	3247	1/1	0.93	0.13	37,37,37,37	0
52	MG	BA	3231	1/1	0.93	0.11	26,26,26,26	0
52	MG	DA	3029	1/1	0.93	0.15	43,43,43,43	0
52	MG	BA	3232	1/1	0.93	0.20	27,27,27,27	0
52	MG	DA	3032	1/1	0.93	0.18	31,31,31,31	0
52	MG	DA	3035	1/1	0.93	0.22	31,31,31,31	0
52	MG	CA	1601	1/1	0.93	0.17	61,61,61,61	0
52	MG	DA	3256	1/1	0.93	0.20	46,46,46,46	0
52	MG	BA	3052	1/1	0.93	0.23	23,23,23,23	0
52	MG	BA	3169	1/1	0.93	0.27	33,33,33,33	0
52	MG	BA	3236	1/1	0.93	0.15	31,31,31,31	0
52	MG	DA	3152	1/1	0.93	0.16	36,36,36,36	0
52	MG	BA	3313	1/1	0.93	0.30	56,56,56,56	0
52	MG	DA	3266	1/1	0.93	0.28	45,45,45,45	0
52	MG	BA	3237	1/1	0.93	0.31	42,42,42,42	0
52	MG	DA	3268	1/1	0.93	0.24	63,63,63,63	0
52	MG	DA	3048	1/1	0.93	0.24	30,30,30,30	0
52	MG	DA	3049	1/1	0.93	0.26	42,42,42,42	0
52	MG	BA	3009	1/1	0.93	0.40	38,38,38,38	0
52	MG	AA	1631	1/1	0.93	0.27	52,52,52,52	0
52	MG	BA	3061	1/1	0.93	0.25	35,35,35,35	0
52	MG	DA	3063	1/1	0.93	0.22	38,38,38,38	0
52	MG	DA	3065	1/1	0.93	0.12	30,30,30,30	0
52	MG	DA	3283	1/1	0.93	0.29	52,52,52,52	0
52	MG	BA	3094	1/1	0.93	0.25	30,30,30,30	0
52	MG	DA	3285	1/1	0.93	0.06	33,33,33,33	0
52	MG	BA	3095	1/1	0.93	0.20	38,38,38,38	0
52	MG	BA	3062	1/1	0.93	0.15	30,30,30,30	0
52	MG	BA	3018	1/1	0.93	0.17	27,27,27,27	0
52	MG	DA	3071	1/1	0.93	0.29	31,31,31,31	0
52	MG	DA	3291	1/1	0.93	0.11	36,36,36,36	0
52	MG	BA	3101	1/1	0.93	0.18	24,24,24,24	0
52	MG	BA	3138	1/1	0.93	0.16	4,4,4,4	0
52	MG	BA	3184	1/1	0.93	0.17	40,40,40,40	0
52	MG	AA	1653	1/1	0.93	0.15	46,46,46,46	0
52	MG	BA	3001	1/1	0.93	0.16	36,36,36,36	0
52	MG	DA	3300	1/1	0.93	0.29	54,54,54,54	0
52	MG	BA	3145	1/1	0.93	0.23	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3183	1/1	0.93	0.26	35,35,35,35	0
52	MG	BA	3071	1/1	0.93	0.13	22,22,22,22	0
52	MG	BA	3191	1/1	0.93	0.26	19,19,19,19	0
52	MG	DA	3307	1/1	0.93	0.12	42,42,42,42	0
52	MG	DA	3084	1/1	0.93	0.19	31,31,31,31	0
52	MG	BA	3192	1/1	0.93	0.18	17,17,17,17	0
52	MG	BA	3194	1/1	0.93	0.22	30,30,30,30	0
52	MG	AA	1626	1/1	0.93	0.20	46,46,46,46	0
52	MG	DA	3313	1/1	0.93	0.26	48,48,48,48	0
52	MG	DA	3314	1/1	0.93	0.20	40,40,40,40	0
52	MG	AA	1636	1/1	0.93	0.27	47,47,47,47	0
52	MG	BA	3280	1/1	0.93	0.24	41,41,41,41	0
52	MG	BA	3202	1/1	0.93	0.27	35,35,35,35	0
52	MG	DA	3320	1/1	0.93	0.08	31,31,31,31	0
52	MG	DA	3322	1/1	0.93	0.24	45,45,45,45	0
52	MG	BA	3283	1/1	0.93	0.22	50,50,50,50	0
52	MG	BA	3350	1/1	0.93	0.33	54,54,54,54	0
52	MG	BA	3110	1/1	0.93	0.29	27,27,27,27	0
52	MG	BA	3204	1/1	0.93	0.16	36,36,36,36	0
52	MG	DA	3211	1/1	0.93	0.27	50,50,50,50	0
52	MG	BA	3005	1/1	0.93	0.17	26,26,26,26	0
52	MG	CA	1647	1/1	0.93	0.14	49,49,49,49	0
52	MG	CA	1649	1/1	0.93	0.31	55,55,55,55	0
52	MG	BA	3047	1/1	0.93	0.20	22,22,22,22	0
52	MG	BA	3211	1/1	0.93	0.12	30,30,30,30	0
52	MG	DD	301	1/1	0.93	0.13	32,32,32,32	0
52	MG	BA	3290	1/1	0.93	0.30	40,40,40,40	0
52	MG	DA	3115	1/1	0.93	0.19	47,47,47,47	0
52	MG	BA	3115	1/1	0.93	0.22	34,34,34,34	0
52	MG	DR	201	1/1	0.93	0.07	34,34,34,34	0
52	MG	BA	3217	1/1	0.93	0.20	34,34,34,34	0
52	MG	DA	3119	1/1	0.93	0.15	36,36,36,36	0
52	MG	AA	1633	1/1	0.93	0.10	42,42,42,42	0
52	MG	DA	3233	1/1	0.93	0.24	51,51,51,51	0
52	MG	BA	3117	1/1	0.93	0.26	50,50,50,50	0
52	MG	DA	3009	1/1	0.93	0.30	47,47,47,47	0
52	MG	BA	3196	1/1	0.94	0.20	26,26,26,26	0
52	MG	DA	3255	1/1	0.94	0.20	49,49,49,49	0
52	MG	BA	3228	1/1	0.94	0.16	27,27,27,27	0
52	MG	DA	3027	1/1	0.94	0.32	36,36,36,36	0
52	MG	BA	3229	1/1	0.94	0.20	26,26,26,26	0
52	MG	DA	3260	1/1	0.94	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3093	1/1	0.94	0.21	44,44,44,44	0
52	MG	DA	3262	1/1	0.94	0.28	60,60,60,60	0
52	MG	DA	3263	1/1	0.94	0.23	65,65,65,65	0
52	MG	DA	3168	1/1	0.94	0.29	32,32,32,32	0
52	MG	DA	3169	1/1	0.94	0.32	45,45,45,45	0
52	MG	CA	1628	1/1	0.94	0.18	50,50,50,50	0
52	MG	DA	3172	1/1	0.94	0.10	48,48,48,48	0
52	MG	BA	3259	1/1	0.94	0.14	40,40,40,40	0
52	MG	AA	1617	1/1	0.94	0.20	57,57,57,57	0
52	MG	DA	3033	1/1	0.94	0.12	31,31,31,31	0
52	MG	BA	3198	1/1	0.94	0.37	62,62,62,62	0
52	MG	DA	3177	1/1	0.94	0.10	37,37,37,37	0
52	MG	DA	3275	1/1	0.94	0.20	51,51,51,51	0
52	MG	DA	3278	1/1	0.94	0.28	54,54,54,54	0
52	MG	DA	3279	1/1	0.94	0.15	44,44,44,44	0
52	MG	BA	3264	1/1	0.94	0.08	11,11,11,11	0
52	MG	DA	3179	1/1	0.94	0.14	29,29,29,29	0
52	MG	DA	3105	1/1	0.94	0.11	39,39,39,39	0
52	MG	AA	1619	1/1	0.94	0.23	44,44,44,44	0
52	MG	DA	3039	1/1	0.94	0.22	48,48,48,48	0
52	MG	BB	206	1/1	0.94	0.31	48,48,48,48	0
52	MG	DA	3185	1/1	0.94	0.26	49,49,49,49	0
52	MG	DA	3186	1/1	0.94	0.18	42,42,42,42	0
52	MG	BB	207	1/1	0.94	0.15	58,58,58,58	0
52	MG	DA	3113	1/1	0.94	0.06	59,59,59,59	0
52	MG	DA	3043	1/1	0.94	0.20	49,49,49,49	0
52	MG	BA	3267	1/1	0.94	0.12	41,41,41,41	0
52	MG	BA	3049	1/1	0.94	0.26	23,23,23,23	0
52	MG	BA	3010	1/1	0.94	0.29	37,37,37,37	0
52	MG	CA	1640	1/1	0.94	0.09	53,53,53,53	0
52	MG	DA	3120	1/1	0.94	0.22	36,36,36,36	0
52	MG	BA	3342	1/1	0.94	0.25	69,69,69,69	0
52	MG	DA	3201	1/1	0.94	0.16	43,43,43,43	0
52	MG	CA	1603	1/1	0.94	0.31	32,32,32,32	0
52	MG	DA	3203	1/1	0.94	0.18	38,38,38,38	0
52	MG	BA	3135	1/1	0.94	0.23	30,30,30,30	0
52	MG	DA	3306	1/1	0.94	0.20	54,54,54,54	0
52	MG	DA	3208	1/1	0.94	0.13	34,34,34,34	0
52	MG	DA	3059	1/1	0.94	0.19	24,24,24,24	0
52	MG	DA	3126	1/1	0.94	0.10	36,36,36,36	0
52	MG	DA	3060	1/1	0.94	0.19	46,46,46,46	0
52	MG	DA	3128	1/1	0.94	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3129	1/1	0.94	0.14	36,36,36,36	0
52	MG	DA	3219	1/1	0.94	0.21	25,25,25,25	0
52	MG	BA	3307	1/1	0.94	0.26	38,38,38,38	0
52	MG	BA	3026	1/1	0.94	0.15	45,45,45,45	0
52	MG	CA	1648	1/1	0.94	0.24	53,53,53,53	0
52	MG	BA	3238	1/1	0.94	0.27	43,43,43,43	0
52	MG	DA	3137	1/1	0.94	0.20	69,69,69,69	0
52	MG	DA	3226	1/1	0.94	0.16	55,55,55,55	0
52	MG	CA	1650	1/1	0.94	0.15	45,45,45,45	0
52	MG	BA	3140	1/1	0.94	0.22	44,44,44,44	0
52	MG	DA	3141	1/1	0.94	0.29	35,35,35,35	0
52	MG	BA	3058	1/1	0.94	0.16	30,30,30,30	0
52	MG	BA	3027	1/1	0.94	0.29	25,25,25,25	0
52	MG	BA	3351	1/1	0.94	0.10	48,48,48,48	0
52	MG	BA	3282	1/1	0.94	0.15	46,46,46,46	0
52	MG	DB	202	1/1	0.94	0.29	60,60,60,60	0
52	MG	BA	3028	1/1	0.94	0.42	24,24,24,24	0
52	MG	DA	3078	1/1	0.94	0.21	31,31,31,31	0
52	MG	DA	3151	1/1	0.94	0.19	40,40,40,40	0
52	MG	DA	3243	1/1	0.94	0.20	56,56,56,56	0
52	MG	BA	3247	1/1	0.94	0.15	35,35,35,35	0
52	MG	BA	3012	1/1	0.94	0.23	38,38,38,38	0
52	MG	DA	3010	1/1	0.94	0.20	35,35,35,35	0
52	MG	BA	3006	1/1	0.94	0.32	33,33,33,33	0
52	MG	DA	3083	1/1	0.94	0.21	37,37,37,37	0
52	MG	DA	3250	1/1	0.94	0.16	56,56,56,56	0
52	MG	BA	3016	1/1	0.94	0.09	11,11,11,11	0
52	MG	CA	1624	1/1	0.94	0.16	50,50,50,50	0
52	MG	DA	3086	1/1	0.94	0.16	34,34,34,34	0
52	MG	BA	3302	1/1	0.95	0.17	31,31,31,31	0
52	MG	BA	3216	1/1	0.95	0.24	35,35,35,35	0
52	MG	BA	3257	1/1	0.95	0.05	35,35,35,35	0
52	MG	DA	3066	1/1	0.95	0.16	29,29,29,29	0
52	MG	BA	3146	1/1	0.95	0.23	33,33,33,33	0
52	MG	BA	3361	1/1	0.95	0.23	52,52,52,52	0
52	MG	BA	3306	1/1	0.95	0.27	35,35,35,35	0
52	MG	BA	3054	1/1	0.95	0.12	48,48,48,48	0
52	MG	DA	3257	1/1	0.95	0.20	46,46,46,46	0
52	MG	BA	3219	1/1	0.95	0.27	24,24,24,24	0
52	MG	BA	3262	1/1	0.95	0.12	30,30,30,30	0
52	MG	BA	3220	1/1	0.95	0.23	22,22,22,22	0
52	MG	BA	3311	1/1	0.95	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3076	1/1	0.95	0.17	23,23,23,23	0
52	MG	CA	1645	1/1	0.95	0.20	45,45,45,45	0
52	MG	BA	3038	1/1	0.95	0.25	17,17,17,17	0
52	MG	DA	3166	1/1	0.95	0.20	64,64,64,64	0
52	MG	BA	3223	1/1	0.95	0.28	25,25,25,25	0
52	MG	BA	3099	1/1	0.95	0.19	34,34,34,34	0
52	MG	BA	3121	1/1	0.95	0.17	34,34,34,34	0
52	MG	BA	3100	1/1	0.95	0.18	23,23,23,23	0
52	MG	BD	301	1/1	0.95	0.15	25,25,25,25	0
52	MG	BE	301	1/1	0.95	0.20	16,16,16,16	0
52	MG	CA	1653	1/1	0.95	0.16	47,47,47,47	0
52	MG	BA	3008	1/1	0.95	0.20	27,27,27,27	0
52	MG	DA	3087	1/1	0.95	0.11	24,24,24,24	0
52	MG	BA	3076	1/1	0.95	0.18	21,21,21,21	0
52	MG	DA	3001	1/1	0.95	0.12	45,45,45,45	0
52	MG	BP	202	1/1	0.95	0.05	0,0,0,0	0
52	MG	BQ	201	1/1	0.95	0.05	18,18,18,18	0
52	MG	DA	3007	1/1	0.95	0.12	48,48,48,48	0
52	MG	BQ	202	1/1	0.95	0.23	37,37,37,37	0
52	MG	BA	3040	1/1	0.95	0.20	37,37,37,37	0
52	MG	BA	3278	1/1	0.95	0.06	31,31,31,31	0
52	MG	BA	3322	1/1	0.95	0.19	41,41,41,41	0
52	MG	DA	3099	1/1	0.95	0.29	34,34,34,34	0
52	MG	DA	3100	1/1	0.95	0.18	35,35,35,35	0
52	MG	BA	3161	1/1	0.95	0.21	32,32,32,32	0
52	MG	DA	3016	1/1	0.95	0.16	29,29,29,29	0
52	MG	DA	3018	1/1	0.95	0.16	29,29,29,29	0
52	MG	BA	3233	1/1	0.95	0.15	20,20,20,20	0
52	MG	DA	3021	1/1	0.95	0.15	38,38,38,38	0
52	MG	DA	3298	1/1	0.95	0.26	59,59,59,59	0
52	MG	BA	3193	1/1	0.95	0.12	46,46,46,46	0
52	MG	BA	3002	1/1	0.95	0.24	23,23,23,23	0
52	MG	DA	3026	1/1	0.95	0.19	55,55,55,55	0
52	MG	CA	1609	1/1	0.95	0.32	41,41,41,41	0
52	MG	BA	3164	1/1	0.95	0.14	33,33,33,33	0
52	MG	DA	3206	1/1	0.95	0.25	45,45,45,45	0
52	MG	BA	3043	1/1	0.95	0.12	32,32,32,32	0
52	MG	BA	3332	1/1	0.95	0.07	35,35,35,35	0
52	MG	BA	3023	1/1	0.95	0.14	13,13,13,13	0
52	MG	CA	1614	1/1	0.95	0.27	57,57,57,57	0
52	MG	BA	3087	1/1	0.95	0.16	10,10,10,10	0
52	MG	CA	1616	1/1	0.95	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3241	1/1	0.95	0.15	44,44,44,44	0
52	MG	DA	3217	1/1	0.95	0.17	36,36,36,36	0
52	MG	DA	3315	1/1	0.95	0.12	43,43,43,43	0
52	MG	BA	3089	1/1	0.95	0.12	15,15,15,15	0
52	MG	DA	3317	1/1	0.95	0.09	48,48,48,48	0
52	MG	DA	3125	1/1	0.95	0.08	33,33,33,33	0
52	MG	AA	1603	1/1	0.95	0.31	43,43,43,43	0
52	MG	BA	3032	1/1	0.95	0.20	15,15,15,15	0
52	MG	DA	3321	1/1	0.95	0.13	41,41,41,41	0
52	MG	DA	3042	1/1	0.95	0.14	29,29,29,29	0
52	MG	BA	3205	1/1	0.95	0.15	34,34,34,34	0
52	MG	DA	3225	1/1	0.95	0.07	37,37,37,37	0
52	MG	DA	3130	1/1	0.95	0.15	53,53,53,53	0
52	MG	DA	3328	1/1	0.95	0.30	61,61,61,61	0
52	MG	BA	3174	1/1	0.95	0.17	29,29,29,29	0
52	MG	BA	3346	1/1	0.95	0.18	63,63,63,63	0
52	MG	DA	3229	1/1	0.95	0.26	36,36,36,36	0
52	MG	DA	3230	1/1	0.95	0.08	25,25,25,25	0
52	MG	BA	3295	1/1	0.95	0.11	35,35,35,35	0
52	MG	DA	3134	1/1	0.95	0.26	28,28,28,28	0
52	MG	DA	3235	1/1	0.95	0.21	48,48,48,48	0
52	MG	DA	3135	1/1	0.95	0.33	39,39,39,39	0
52	MG	BA	3142	1/1	0.95	0.23	26,26,26,26	0
52	MG	DA	3238	1/1	0.95	0.08	36,36,36,36	0
52	MG	DA	3050	1/1	0.95	0.15	33,33,33,33	0
52	MG	BA	3297	1/1	0.95	0.17	31,31,31,31	0
52	MG	DA	3052	1/1	0.95	0.19	36,36,36,36	0
52	MG	DA	3054	1/1	0.95	0.20	55,55,55,55	0
52	MG	BA	3070	1/1	0.95	0.24	24,24,24,24	0
52	MG	DA	3057	1/1	0.95	0.21	32,32,32,32	0
52	MG	BA	3253	1/1	0.95	0.08	17,17,17,17	0
52	MG	DA	3147	1/1	0.95	0.16	43,43,43,43	0
52	MG	BA	3036	1/1	0.95	0.16	8,8,8,8	0
52	MG	BA	3252	1/1	0.96	0.14	50,50,50,50	0
52	MG	BU	201	1/1	0.96	0.18	25,25,25,25	0
52	MG	BX	101	1/1	0.96	0.06	21,21,21,21	0
52	MG	DA	3194	1/1	0.96	0.09	22,22,22,22	0
52	MG	DA	3061	1/1	0.96	0.20	34,34,34,34	0
52	MG	DA	3272	1/1	0.96	0.26	47,47,47,47	0
52	MG	DA	3062	1/1	0.96	0.09	24,24,24,24	0
52	MG	BA	3337	1/1	0.96	0.20	32,32,32,32	0
52	MG	DA	3276	1/1	0.96	0.20	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3277	1/1	0.96	0.14	38,38,38,38	0
52	MG	DA	3064	1/1	0.96	0.14	44,44,44,44	0
52	MG	BA	3033	1/1	0.96	0.09	18,18,18,18	0
52	MG	BA	3183	1/1	0.96	0.15	43,43,43,43	0
52	MG	CA	1605	1/1	0.96	0.17	68,68,68,68	0
52	MG	D5	101	1/1	0.96	0.19	30,30,30,30	0
52	MG	BA	3034	1/1	0.96	0.18	45,45,45,45	0
52	MG	BA	3156	1/1	0.96	0.21	12,12,12,12	0
52	MG	DA	3209	1/1	0.96	0.19	51,51,51,51	0
52	MG	DA	3003	1/1	0.96	0.28	39,39,39,39	0
52	MG	BA	3092	1/1	0.96	0.23	19,19,19,19	0
52	MG	DA	3212	1/1	0.96	0.09	33,33,33,33	0
52	MG	DA	3138	1/1	0.96	0.24	31,31,31,31	0
52	MG	BA	3300	1/1	0.96	0.23	45,45,45,45	0
52	MG	DA	3006	1/1	0.96	0.31	38,38,38,38	0
52	MG	AA	1652	1/1	0.96	0.30	44,44,44,44	0
52	MG	BA	3226	1/1	0.96	0.03	14,14,14,14	0
52	MG	BA	3134	1/1	0.96	0.14	36,36,36,36	0
52	MG	DA	3144	1/1	0.96	0.20	43,43,43,43	0
52	MG	BA	3190	1/1	0.96	0.22	36,36,36,36	0
52	MG	DA	3011	1/1	0.96	0.23	27,27,27,27	0
52	MG	BA	3162	1/1	0.96	0.12	45,45,45,45	0
52	MG	BA	3265	1/1	0.96	0.26	43,43,43,43	0
52	MG	AA	1602	1/1	0.96	0.22	32,32,32,32	0
52	MG	BA	3354	1/1	0.96	0.12	40,40,40,40	0
52	MG	BA	3136	1/1	0.96	0.24	22,22,22,22	0
52	MG	CA	1619	1/1	0.96	0.34	40,40,40,40	0
52	MG	BA	3165	1/1	0.96	0.11	26,26,26,26	0
52	MG	DA	3231	1/1	0.96	0.24	54,54,54,54	0
52	MG	BA	3357	1/1	0.96	0.26	44,44,44,44	0
52	MG	DA	3311	1/1	0.96	0.13	29,29,29,29	0
52	MG	BA	3114	1/1	0.96	0.26	21,21,21,21	0
52	MG	DA	3234	1/1	0.96	0.26	60,60,60,60	0
52	MG	AA	1641	1/1	0.96	0.14	64,64,64,64	0
52	MG	BA	3066	1/1	0.96	0.23	34,34,34,34	0
52	MG	BA	3097	1/1	0.96	0.17	32,32,32,32	0
52	MG	BA	3078	1/1	0.96	0.20	22,22,22,22	0
52	MG	DA	3162	1/1	0.96	0.20	50,50,50,50	0
52	MG	BA	3144	1/1	0.96	0.29	29,29,29,29	0
52	MG	BA	3024	1/1	0.96	0.14	20,20,20,20	0
52	MG	BA	3175	1/1	0.96	0.18	43,43,43,43	0
52	MG	BA	3242	1/1	0.96	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3319	1/1	0.96	0.20	46,46,46,46	0
52	MG	DA	3324	1/1	0.96	0.04	38,38,38,38	0
52	MG	CA	1633	1/1	0.96	0.31	50,50,50,50	0
52	MG	DA	3246	1/1	0.96	0.08	43,43,43,43	0
52	MG	DA	3327	1/1	0.96	0.06	41,41,41,41	0
52	MG	DA	3102	1/1	0.96	0.29	24,24,24,24	0
52	MG	BA	3243	1/1	0.96	0.07	30,30,30,30	0
52	MG	DA	3171	1/1	0.96	0.12	26,26,26,26	0
52	MG	AA	1623	1/1	0.96	0.27	31,31,31,31	0
52	MG	DA	3107	1/1	0.96	0.27	15,15,15,15	0
52	MG	BB	204	1/1	0.96	0.23	41,41,41,41	0
52	MG	BA	3084	1/1	0.96	0.09	5,5,5,5	0
52	MG	DA	3044	1/1	0.96	0.19	35,35,35,35	0
52	MG	BA	3069	1/1	0.96	0.11	26,26,26,26	0
52	MG	DA	3112	1/1	0.96	0.12	28,28,28,28	0
52	MG	DE	301	1/1	0.96	0.16	31,31,31,31	0
52	MG	BA	3213	1/1	0.96	0.15	17,17,17,17	0
52	MG	BA	3248	1/1	0.96	0.25	33,33,33,33	0
52	MG	BA	3326	1/1	0.96	0.16	40,40,40,40	0
52	MG	DA	3182	1/1	0.96	0.15	41,41,41,41	0
52	MG	BA	3179	1/1	0.96	0.21	25,25,25,25	0
52	MG	BA	3291	1/1	0.96	0.17	54,54,54,54	0
52	MG	CA	1644	1/1	0.96	0.20	43,43,43,43	0
52	MG	BA	3057	1/1	0.96	0.10	37,37,37,37	0
52	MG	BA	3088	1/1	0.96	0.12	33,33,33,33	0
52	MG	BA	3335	1/1	0.96	0.21	57,57,57,57	0
52	MG	DA	3205	1/1	0.97	0.22	39,39,39,39	0
52	MG	CA	1622	1/1	0.97	0.23	46,46,46,46	0
52	MG	DA	3017	1/1	0.97	0.29	37,37,37,37	0
52	MG	BA	3037	1/1	0.97	0.16	1,1,1,1	0
52	MG	BA	3132	1/1	0.97	0.11	15,15,15,15	0
52	MG	BA	3274	1/1	0.97	0.18	33,33,33,33	0
52	MG	DA	3023	1/1	0.97	0.20	27,27,27,27	0
52	MG	BA	3106	1/1	0.97	0.19	37,37,37,37	0
52	MG	DA	3213	1/1	0.97	0.18	26,26,26,26	0
52	MG	BA	3107	1/1	0.97	0.12	7,7,7,7	0
52	MG	DA	3146	1/1	0.97	0.20	37,37,37,37	0
52	MG	BA	3050	1/1	0.97	0.18	21,21,21,21	0
52	MG	BA	3239	1/1	0.97	0.11	32,32,32,32	0
52	MG	DA	3218	1/1	0.97	0.17	24,24,24,24	0
52	MG	BA	3200	1/1	0.97	0.20	12,12,12,12	0
52	MG	BA	3137	1/1	0.97	0.25	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3030	1/1	0.97	0.15	37,37,37,37	0
52	MG	BA	3051	1/1	0.97	0.23	19,19,19,19	0
52	MG	AA	1610	1/1	0.97	0.18	33,33,33,33	0
52	MG	DA	3296	1/1	0.97	0.18	45,45,45,45	0
52	MG	DA	3154	1/1	0.97	0.20	51,51,51,51	0
52	MG	DA	3091	1/1	0.97	0.18	11,11,11,11	0
52	MG	BA	3285	1/1	0.97	0.18	35,35,35,35	0
52	MG	DA	3034	1/1	0.97	0.21	38,38,38,38	0
52	MG	BA	3172	1/1	0.97	0.24	18,18,18,18	0
52	MG	DA	3036	1/1	0.97	0.14	12,12,12,12	0
52	MG	DA	3303	1/1	0.97	0.21	43,43,43,43	0
52	MG	BA	3206	1/1	0.97	0.21	29,29,29,29	0
52	MG	DA	3097	1/1	0.97	0.20	30,30,30,30	0
52	MG	BA	3112	1/1	0.97	0.05	14,14,14,14	0
52	MG	BA	3208	1/1	0.97	0.12	17,17,17,17	0
52	MG	BA	3053	1/1	0.97	0.15	6,6,6,6	0
52	MG	BA	3330	1/1	0.97	0.27	48,48,48,48	0
52	MG	BA	3091	1/1	0.97	0.17	14,14,14,14	0
52	MG	BA	3333	1/1	0.97	0.27	50,50,50,50	0
52	MG	BA	3334	1/1	0.97	0.21	39,39,39,39	0
52	MG	BA	3029	1/1	0.97	0.16	25,25,25,25	0
52	MG	DA	3046	1/1	0.97	0.25	34,34,34,34	0
52	MG	BA	3015	1/1	0.97	0.19	29,29,29,29	0
52	MG	BA	3073	1/1	0.97	0.11	7,7,7,7	0
52	MG	B5	101	1/1	0.97	0.17	28,28,28,28	0
52	MG	BA	3149	1/1	0.97	0.06	8,8,8,8	0
52	MG	CA	1602	1/1	0.97	0.17	40,40,40,40	0
52	MG	BA	3340	1/1	0.97	0.14	39,39,39,39	0
52	MG	BA	3017	1/1	0.97	0.27	27,27,27,27	0
52	MG	DA	3055	1/1	0.97	0.26	34,34,34,34	0
52	MG	BA	3256	1/1	0.97	0.04	24,24,24,24	0
52	MG	DA	3118	1/1	0.97	0.19	43,43,43,43	0
52	MG	BA	3044	1/1	0.97	0.15	9,9,9,9	0
52	MG	BA	3046	1/1	0.97	0.17	24,24,24,24	0
52	MG	BA	3153	1/1	0.97	0.27	34,34,34,34	0
52	MG	BA	3185	1/1	0.97	0.27	45,45,45,45	0
52	MG	BA	3261	1/1	0.97	0.12	27,27,27,27	0
52	MG	BA	3013	1/1	0.97	0.11	7,7,7,7	0
52	MG	BA	3063	1/1	0.97	0.33	45,45,45,45	0
52	MG	BA	3080	1/1	0.97	0.28	14,14,14,14	0
52	MG	DA	3190	1/1	0.97	0.26	43,43,43,43	0
52	MG	BA	3158	1/1	0.97	0.11	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3352	1/1	0.97	0.17	51,51,51,51	0
52	MG	BA	3353	1/1	0.97	0.17	31,31,31,31	0
52	MG	BA	3126	1/1	0.97	0.13	29,29,29,29	0
52	MG	BA	3021	1/1	0.97	0.18	19,19,19,19	0
52	MG	DA	3196	1/1	0.97	0.22	33,33,33,33	0
52	MG	BA	3065	1/1	0.97	0.15	28,28,28,28	0
52	MG	DA	3012	1/1	0.97	0.20	26,26,26,26	0
52	MG	DA	3199	1/1	0.97	0.20	43,43,43,43	0
52	MG	DA	3013	1/1	0.97	0.14	10,10,10,10	0
52	MG	DA	3073	1/1	0.97	0.16	27,27,27,27	0
53	ZN	AD	301	1/1	0.97	0.19	109,109,109,109	0
53	ZN	CD	301	1/1	0.97	0.19	107,107,107,107	0
52	MG	BA	3269	1/1	0.97	0.14	34,34,34,34	0
52	MG	BA	3085	1/1	0.97	0.13	9,9,9,9	0
52	MG	DA	3273	1/1	0.97	0.06	39,39,39,39	0
52	MG	DA	3204	1/1	0.97	0.20	42,42,42,42	0
52	MG	BA	3019	1/1	0.98	0.22	13,13,13,13	0
52	MG	BA	3224	1/1	0.98	0.11	27,27,27,27	0
52	MG	BA	3020	1/1	0.98	0.13	8,8,8,8	0
52	MG	DA	3002	1/1	0.98	0.29	22,22,22,22	0
52	MG	BB	201	1/1	0.98	0.29	35,35,35,35	0
52	MG	DA	3294	1/1	0.98	0.05	46,46,46,46	0
52	MG	BB	202	1/1	0.98	0.16	27,27,27,27	0
52	MG	BA	3139	1/1	0.98	0.33	30,30,30,30	0
52	MG	BA	3042	1/1	0.98	0.14	7,7,7,7	0
52	MG	BA	3011	1/1	0.98	0.21	17,17,17,17	0
52	MG	BA	3210	1/1	0.98	0.27	29,29,29,29	0
52	MG	BA	3130	1/1	0.98	0.07	36,36,36,36	0
52	MG	BA	3212	1/1	0.98	0.12	30,30,30,30	0
52	MG	BA	3331	1/1	0.98	0.17	37,37,37,37	0
52	MG	BA	3055	1/1	0.98	0.21	19,19,19,19	0
52	MG	BA	3157	1/1	0.98	0.13	13,13,13,13	0
52	MG	BA	3081	1/1	0.98	0.14	7,7,7,7	0
52	MG	BA	3133	1/1	0.98	0.12	25,25,25,25	0
52	MG	BA	3201	1/1	0.98	0.28	31,31,31,31	0
52	MG	BR	201	1/1	0.98	0.14	7,7,7,7	0
52	MG	BA	3273	1/1	0.98	0.04	3,3,3,3	0
52	MG	BA	3082	1/1	0.98	0.12	6,6,6,6	0
52	MG	DA	3104	1/1	0.98	0.36	41,41,41,41	0
52	MG	BA	3275	1/1	0.98	0.21	29,29,29,29	0
52	MG	DA	3022	1/1	0.98	0.09	38,38,38,38	0
52	MG	BA	3035	1/1	0.98	0.13	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	ZN	AN	101	1/1	0.98	0.04	144,144,144,144	0
52	MG	BA	3277	1/1	0.98	0.04	10,10,10,10	0
52	MG	BA	3125	1/1	0.98	0.18	18,18,18,18	0
52	MG	DA	3286	1/1	0.98	0.17	43,43,43,43	0
52	MG	DA	3053	1/1	0.98	0.14	21,21,21,21	0
52	MG	BA	3222	1/1	0.98	0.20	20,20,20,20	0
52	MG	BA	3109	1/1	0.99	0.21	40,40,40,40	0
52	MG	BA	3030	1/1	0.99	0.12	17,17,17,17	0
52	MG	DA	3189	1/1	0.99	0.13	42,42,42,42	0
52	MG	BA	3147	1/1	0.99	0.14	28,28,28,28	0
52	MG	DA	3019	1/1	0.99	0.27	25,25,25,25	0
52	MG	BA	3168	1/1	0.99	0.17	21,21,21,21	0
52	MG	BA	3214	1/1	0.99	0.13	23,23,23,23	0
53	ZN	CN	101	1/1	0.99	0.05	136,136,136,136	0
52	MG	BA	3045	1/1	0.99	0.17	14,14,14,14	0
52	MG	BA	3060	1/1	0.99	0.21	31,31,31,31	0
52	MG	BA	3195	1/1	0.99	0.12	49,49,49,49	0
52	MG	DA	3106	1/1	0.99	0.24	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.