



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:53 AM UTC

PDB ID : 4V7X / pdb_00004v7x
Title : Structure of the Thermus thermophilus ribosome complexed with erythromycin.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-17
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

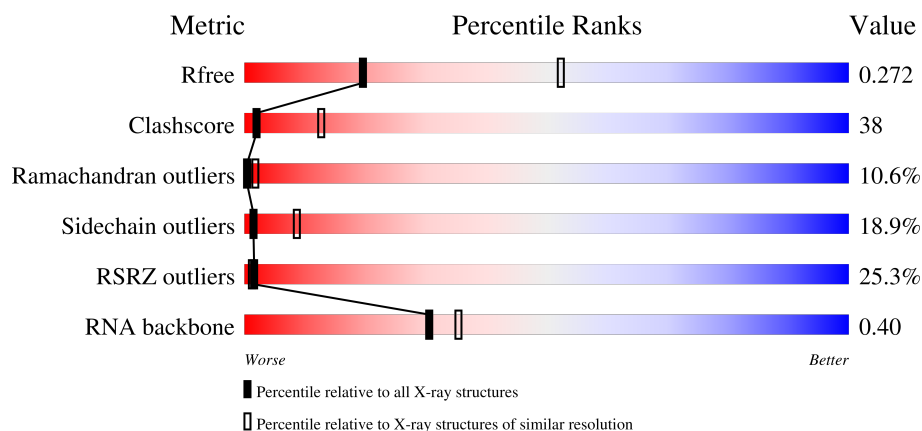
1 Overall quality at a glance

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)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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	25% 25% 58% 15% .
1	CA	1522	23% 26% 58% 15% .
2	AB	256	29% 31% 47% 13% . 8%
2	CB	256	33% 32% 46% 13% . 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	160	
5	CE	160	
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	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
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	

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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
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	

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Mol	Chain	Length	Quality of chain
40	DO	122	
41	BP	150	
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	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 278034 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	9	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	9	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	54	Total	Mg	0	0
			54	54		
52	B0	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	BA	362	Total	Mg	0	0
			362	362		
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	3	Total	Mg	0	0
			3	3		
52	BQ	2	Total	Mg	0	0
			2	2		
52	BR	1	Total	Mg	0	0
			1	1		
52	BU	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	CA	50	Total	Mg	0	0
			50	50		
52	D0	1	Total	Mg	0	0
			1	1		
52	D3	1	Total	Mg	0	0
			1	1		
52	D5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
52	D7	1	Total Mg 1 1	0	0
52	DA	328	Total Mg 328 328	0	0
52	DB	3	Total Mg 3 3	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

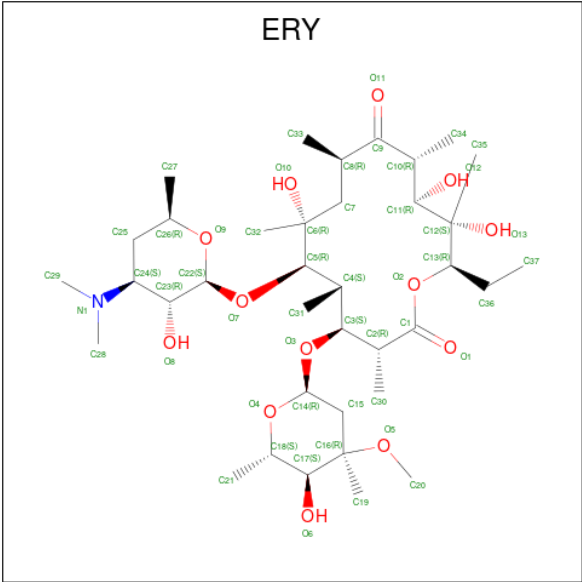
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

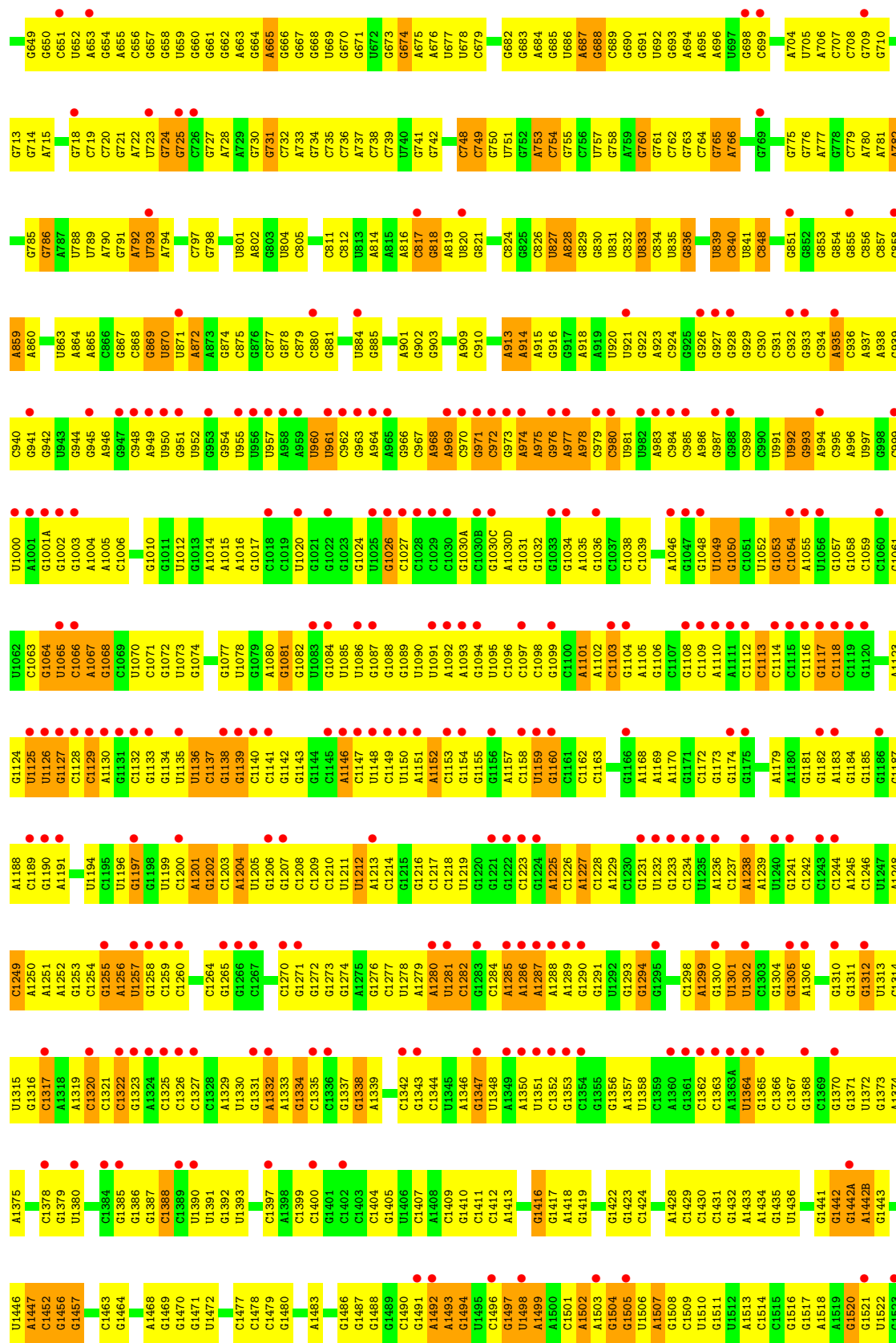
- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

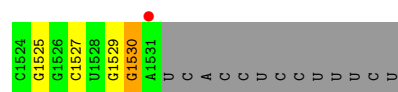
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BA	1	Total K 1 1	0	0
54	DA	1	Total K 1 1	0	0

- Molecule 55 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).

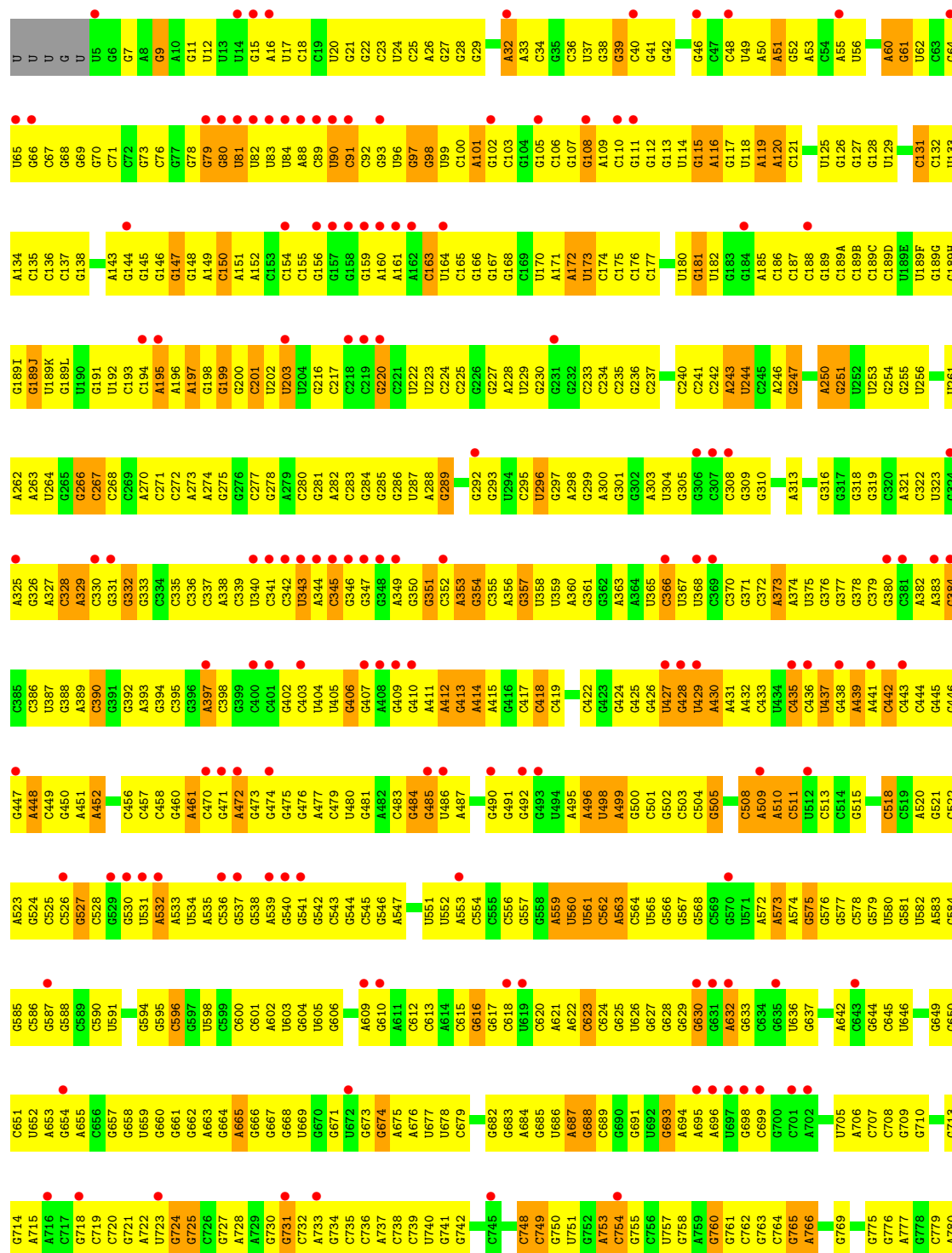


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			51	37	1	13		
55	DA	1	Total	C	N	O	0	0
			51	37	1	13		

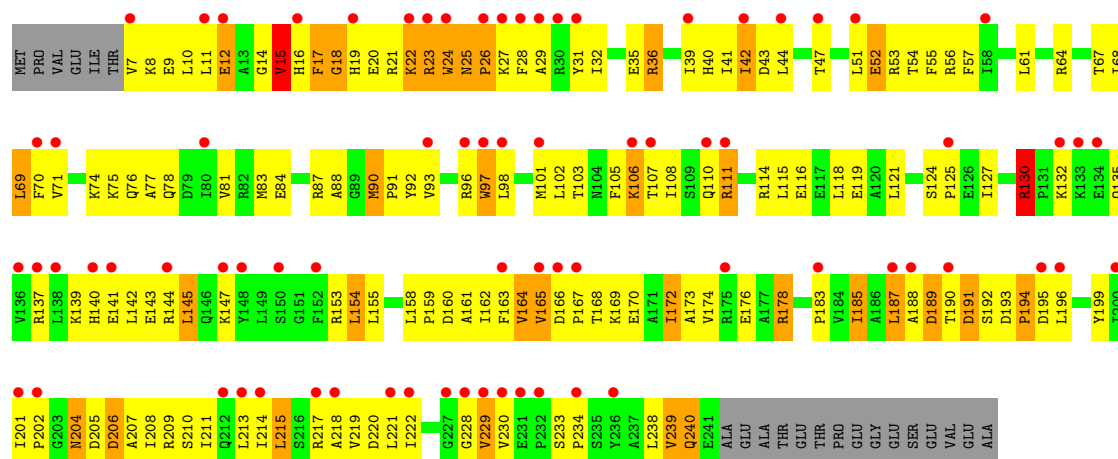




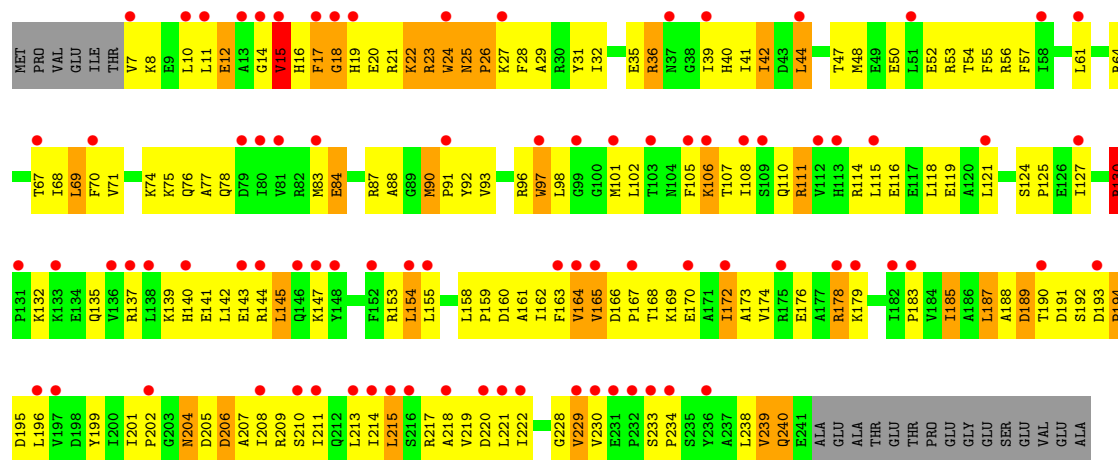
• Molecule 1: 16S rRNA



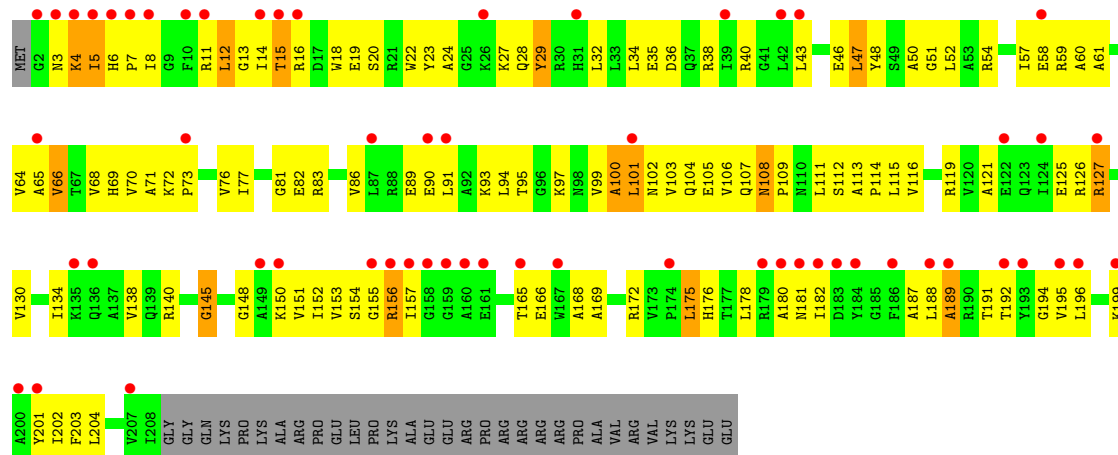




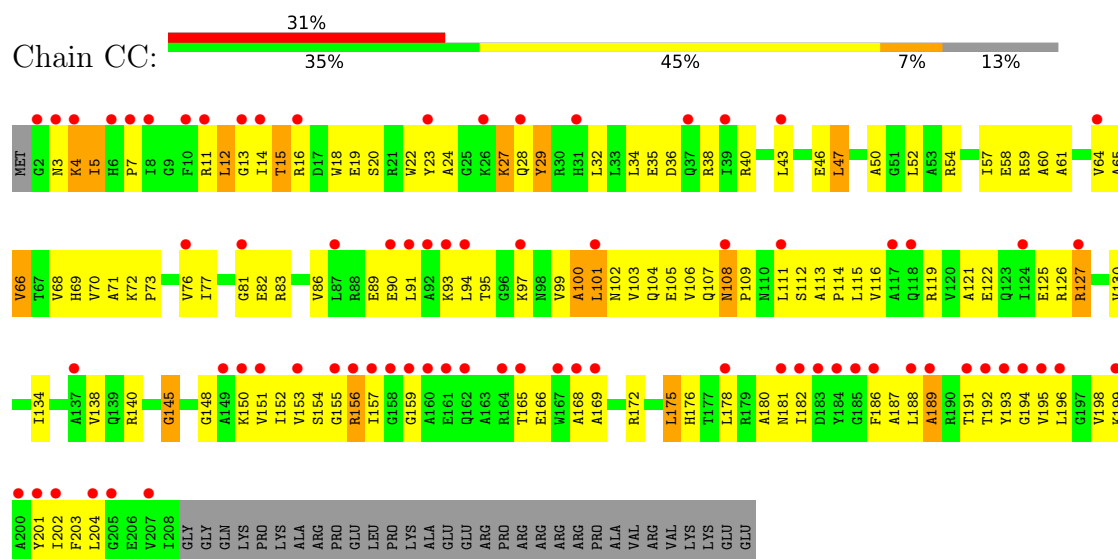
• Molecule 2: 30S ribosomal protein S2



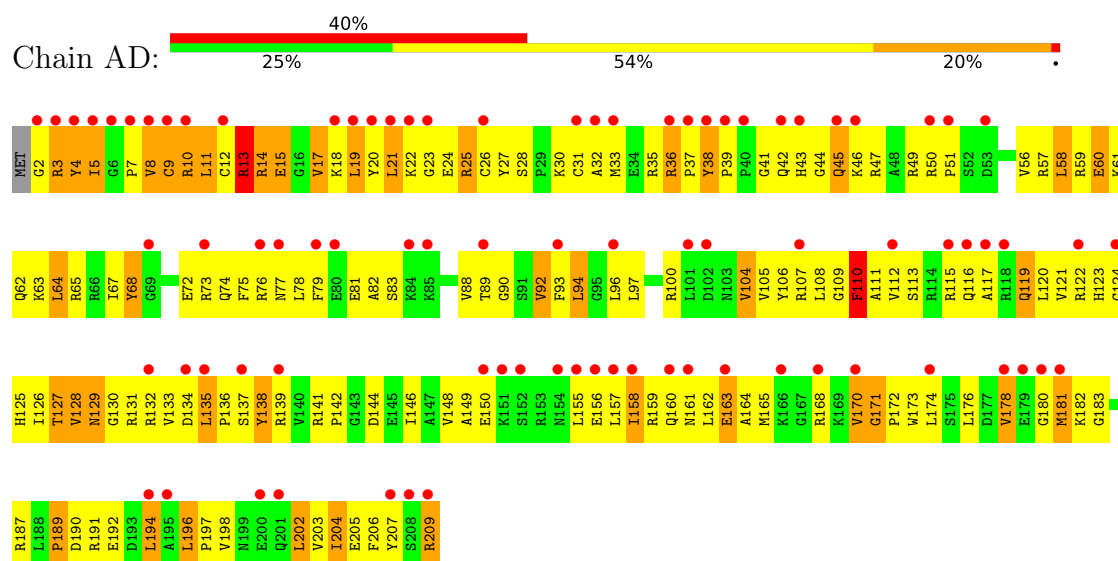
• Molecule 3: 30S ribosomal protein S3



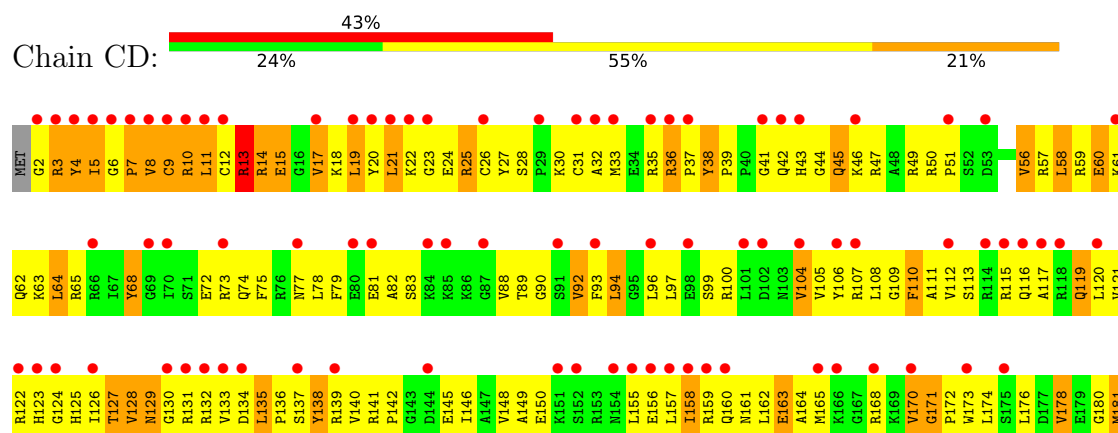
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

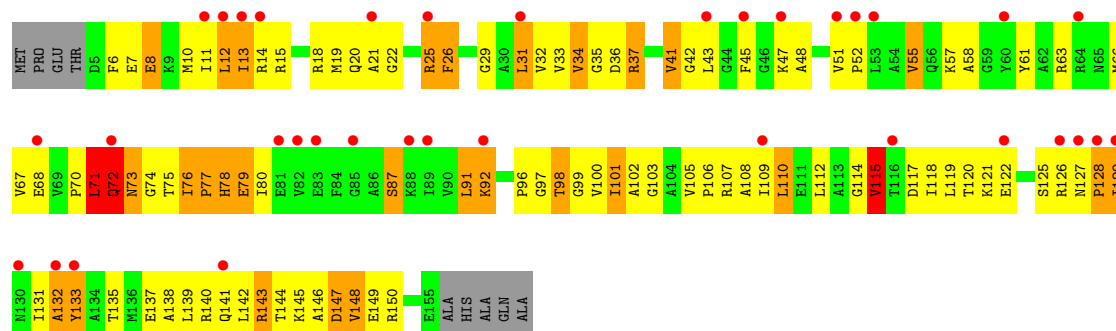


• Molecule 4: 30S ribosomal protein S4

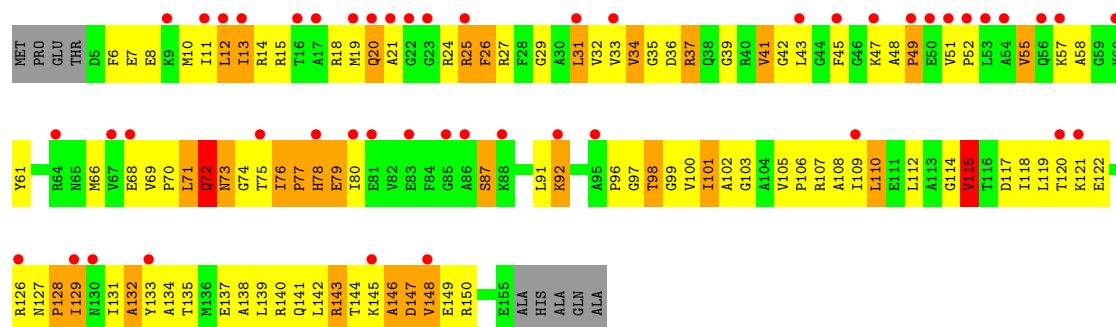




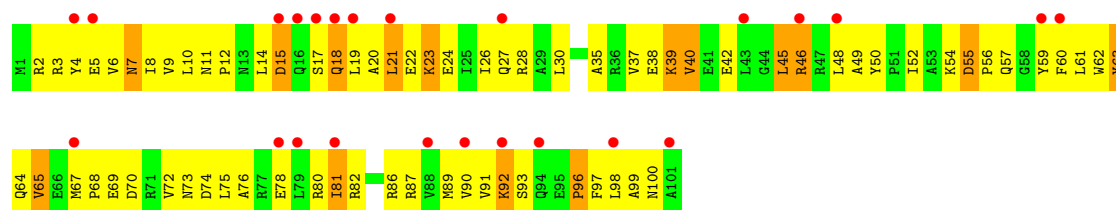
• Molecule 5: 30S ribosomal protein S5



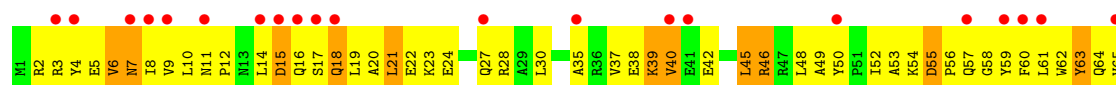
• Molecule 5: 30S ribosomal protein S5

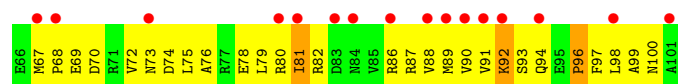


• Molecule 6: 30S ribosomal protein S6

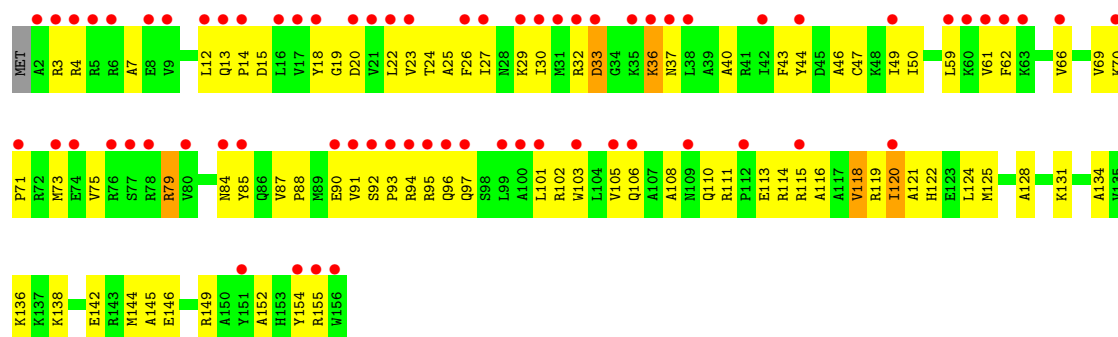


• Molecule 6: 30S ribosomal protein S6

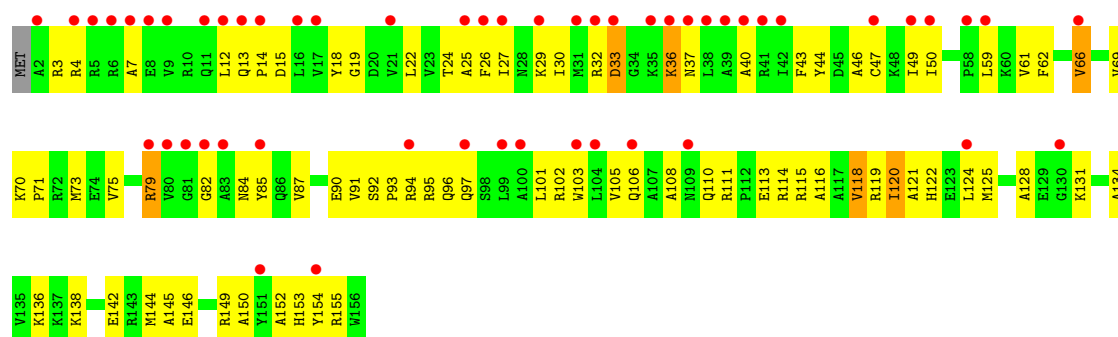




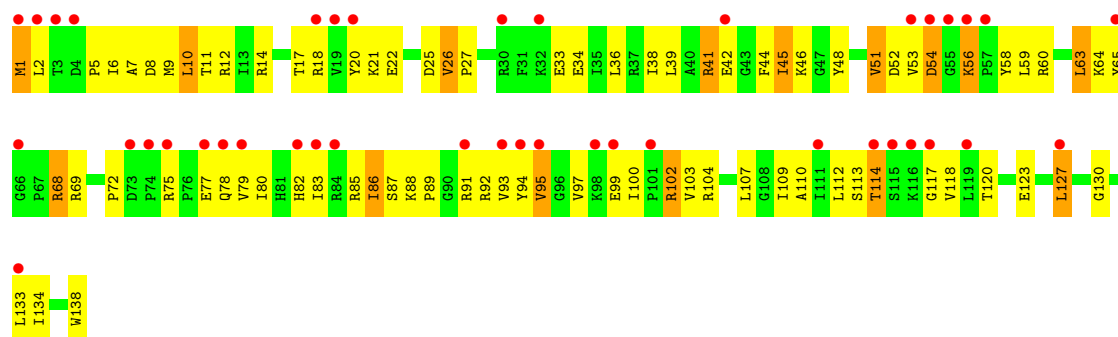
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7

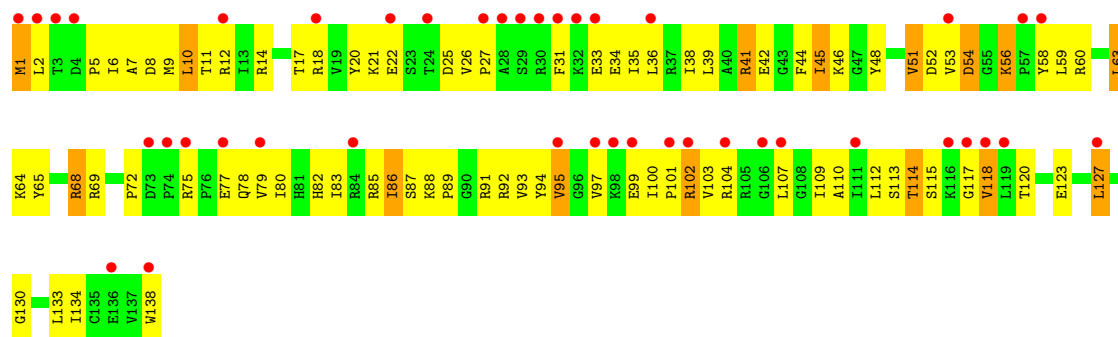


• Molecule 8: 30S ribosomal protein S8

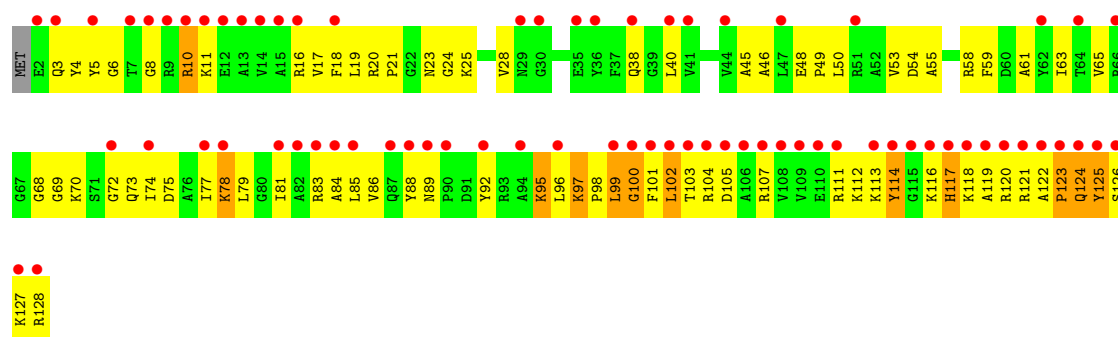


• Molecule 8: 30S ribosomal protein S8

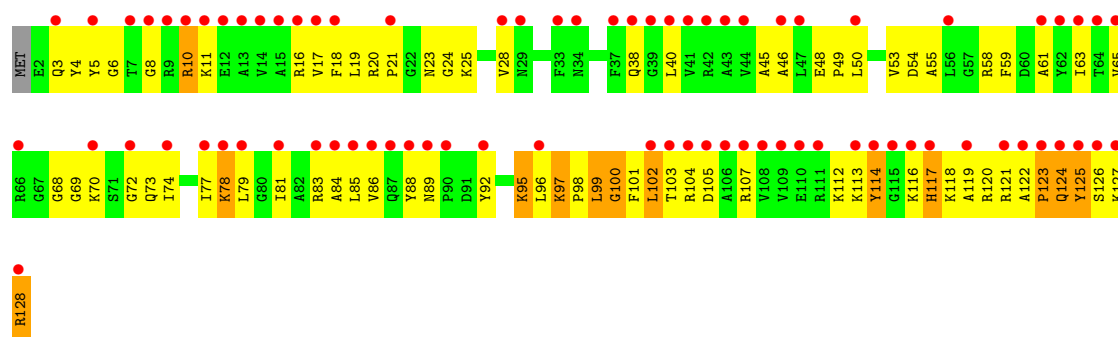




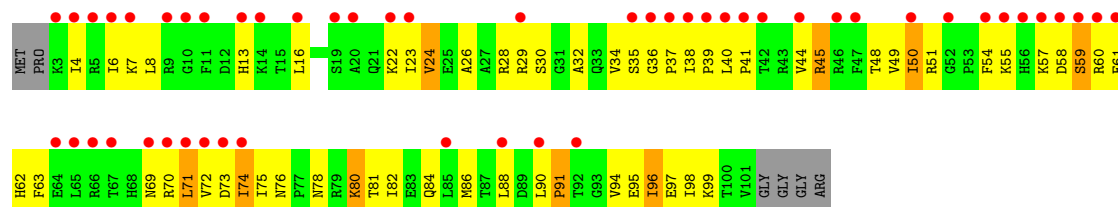
● Molecule 9: 30S ribosomal protein S9



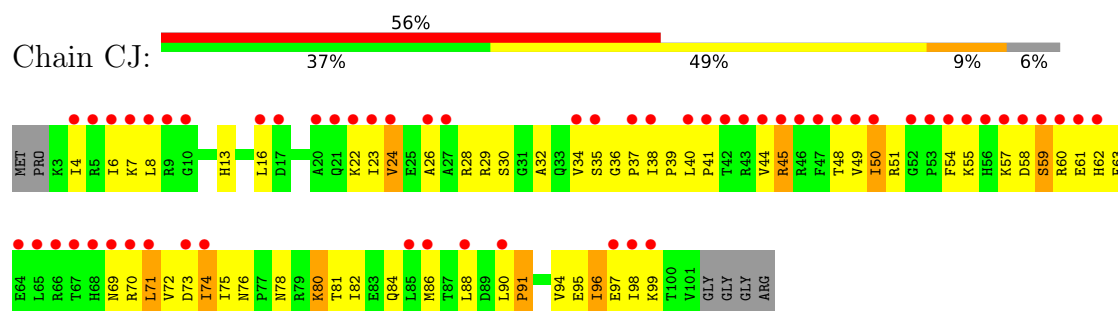
● Molecule 9: 30S ribosomal protein S9



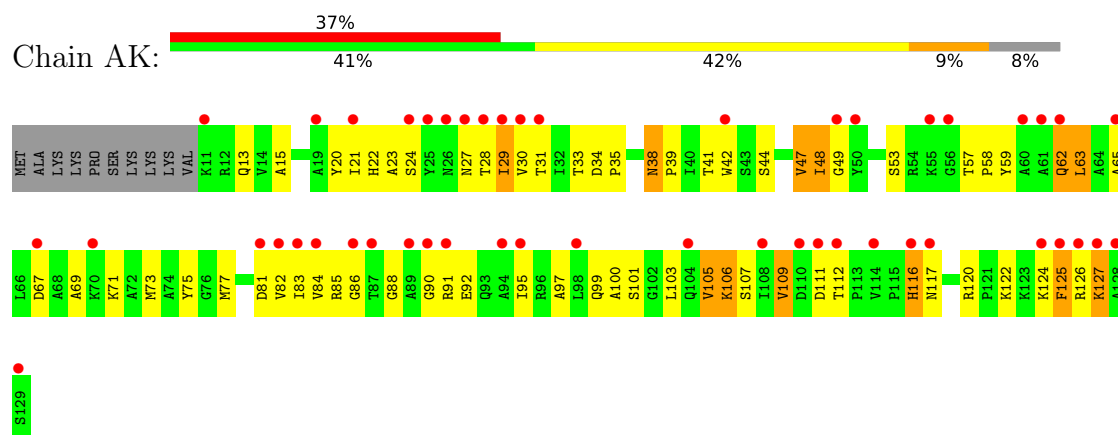
● Molecule 10: 30S ribosomal protein S10



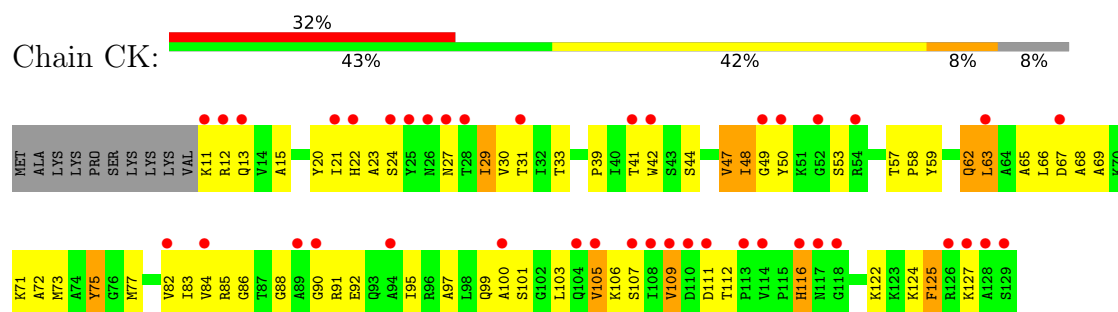
● Molecule 10: 30S ribosomal protein S10



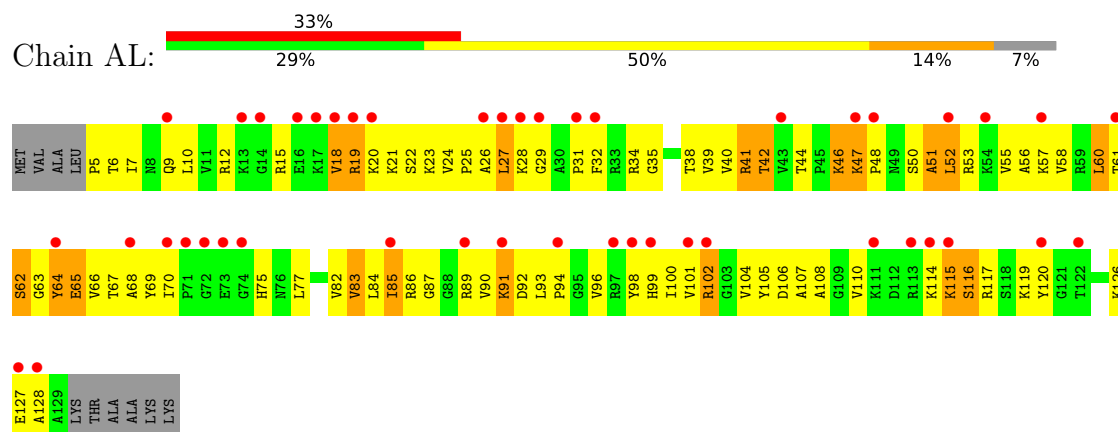
● Molecule 11: 30S ribosomal protein S11



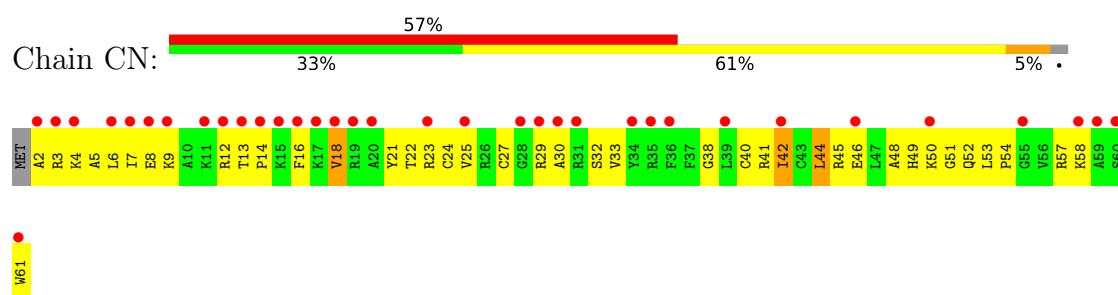
● Molecule 11: 30S ribosomal protein S11



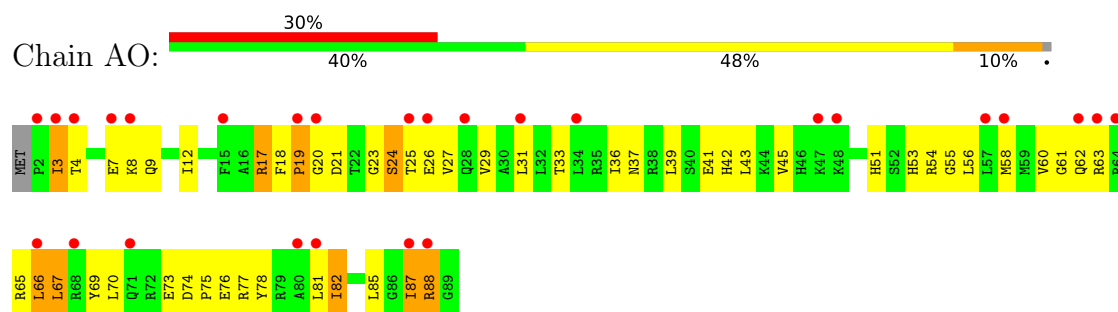
● Molecule 12: 30S ribosomal protein S12



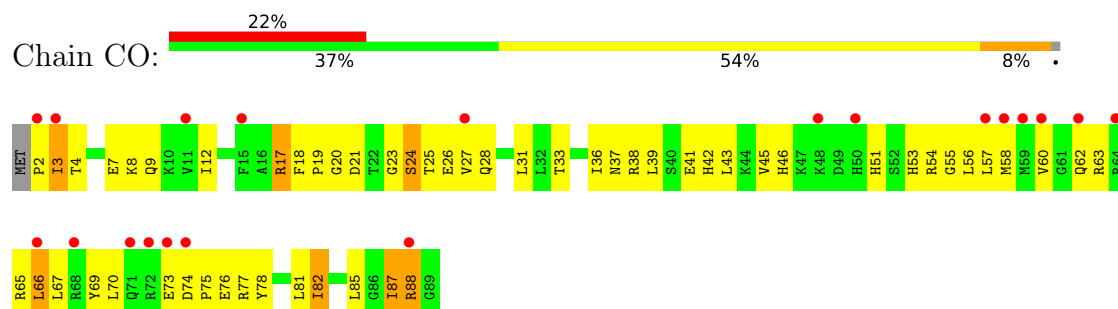
- Molecule 14: 30S ribosomal protein S14



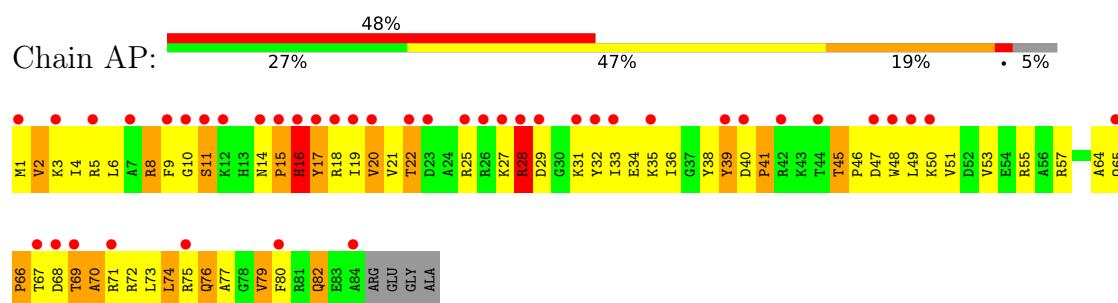
• Molecule 15: 30S ribosomal protein S15



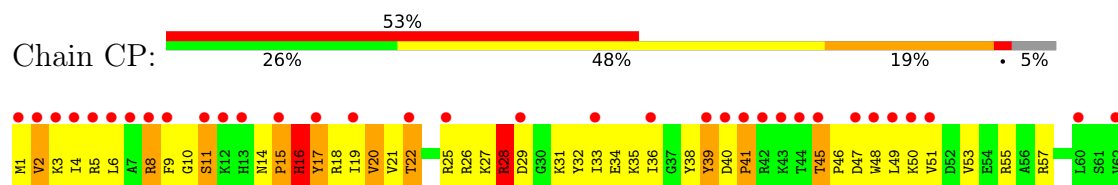
• Molecule 15: 30S ribosomal protein S15



• Molecule 16: 30S ribosomal protein S16

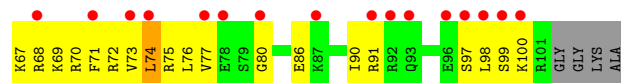


• Molecule 16: 30S ribosomal protein S16

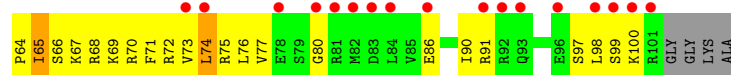
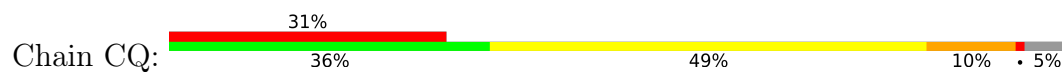




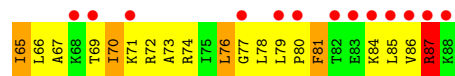
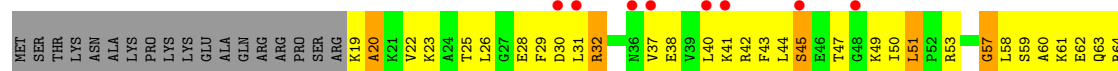
- Molecule 17: 30S ribosomal protein S17



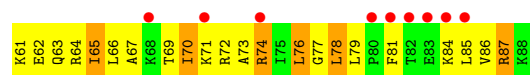
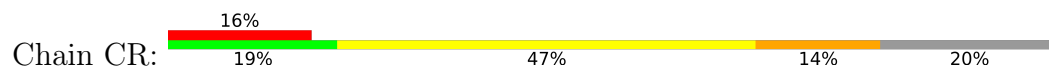
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

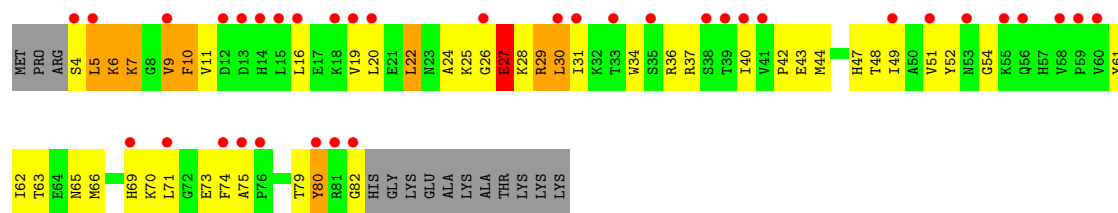


- Molecule 18: 30S ribosomal protein S18

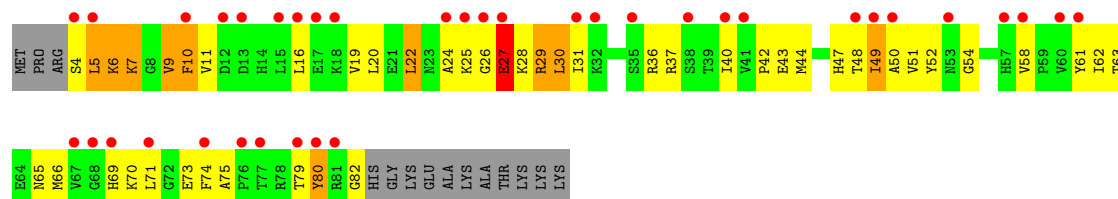


- Molecule 19: 30S ribosomal protein S19

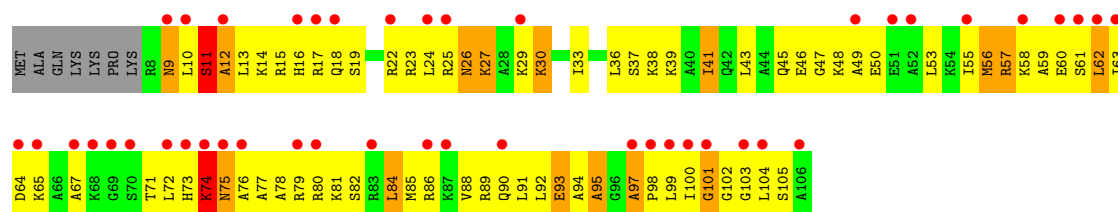




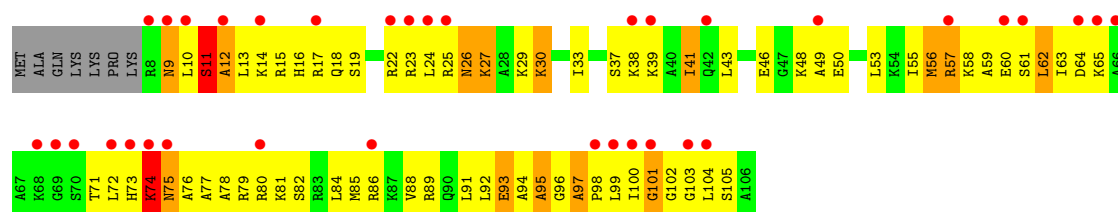
• Molecule 19: 30S ribosomal protein S19



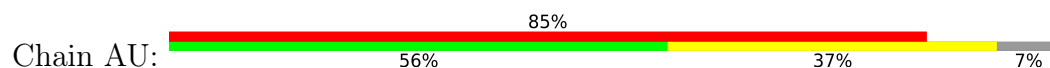
• Molecule 20: 30S ribosomal protein S20



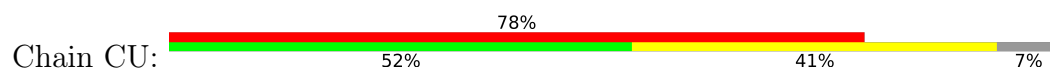
• Molecule 20: 30S ribosomal protein S20



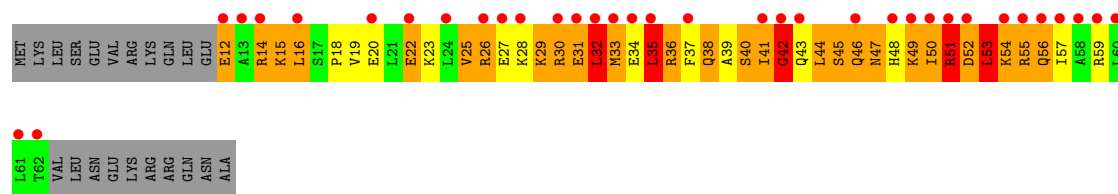
• Molecule 21: 30S ribosomal protein Thx



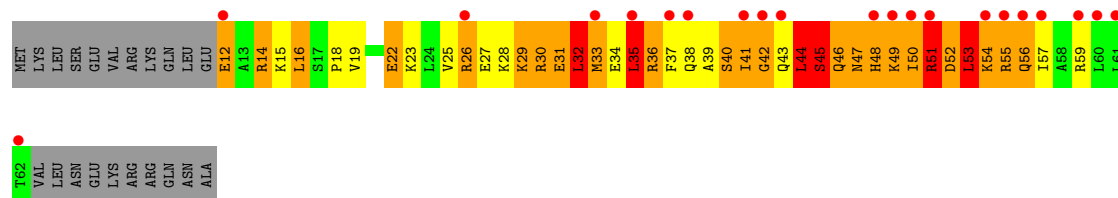
• Molecule 21: 30S ribosomal protein Thx



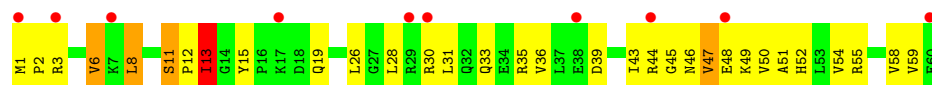




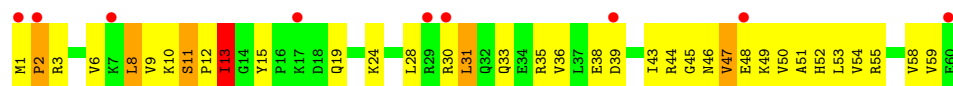
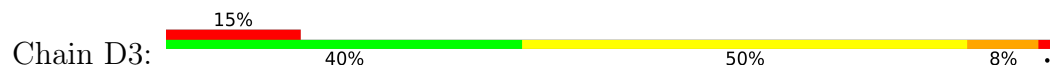
• Molecule 24: 50S ribosomal protein L29



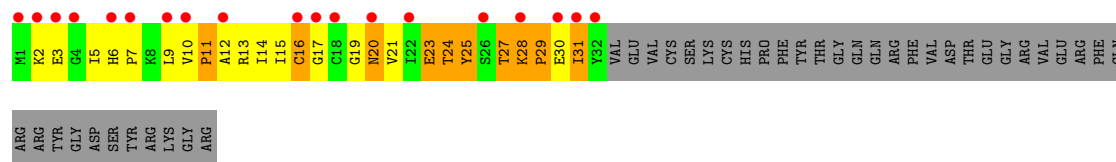
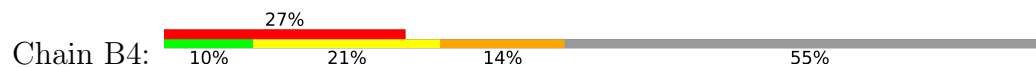
• Molecule 25: 50S ribosomal protein L30



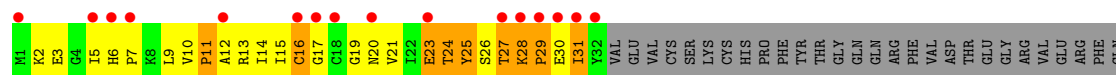
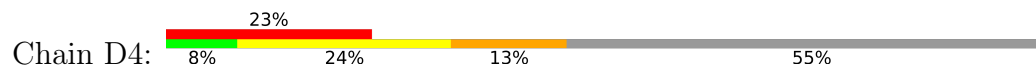
• Molecule 25: 50S ribosomal protein L30



• Molecule 26: 50S ribosomal protein L31

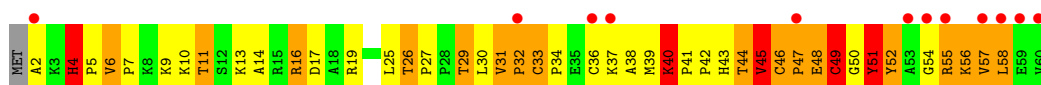
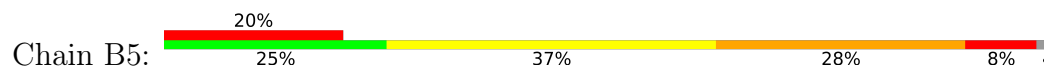


• Molecule 26: 50S ribosomal protein L31

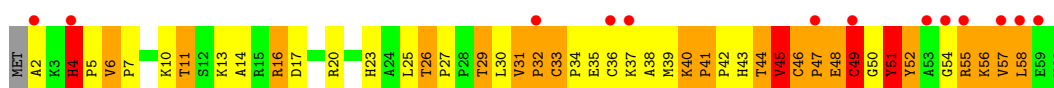
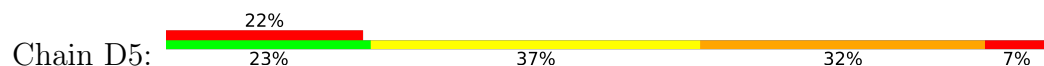


ARG
ARG
TYR
GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 27: 50S ribosomal protein L32



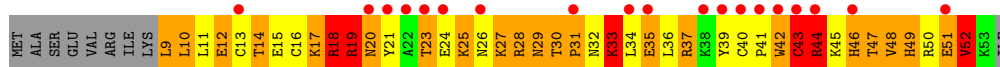
• Molecule 27: 50S ribosomal protein L32



• Molecule 28: 50S ribosomal protein L33



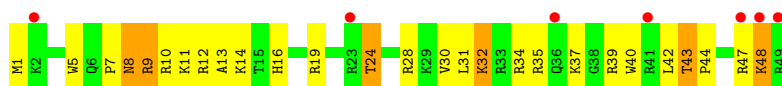
• Molecule 28: 50S ribosomal protein L33



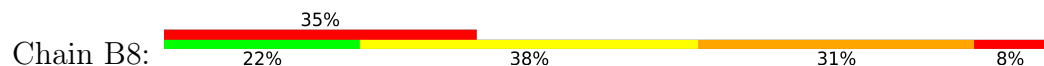
• Molecule 29: 50S ribosomal protein L34

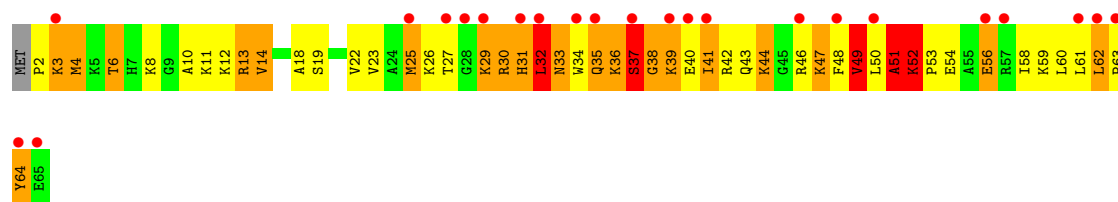


• Molecule 29: 50S ribosomal protein L34

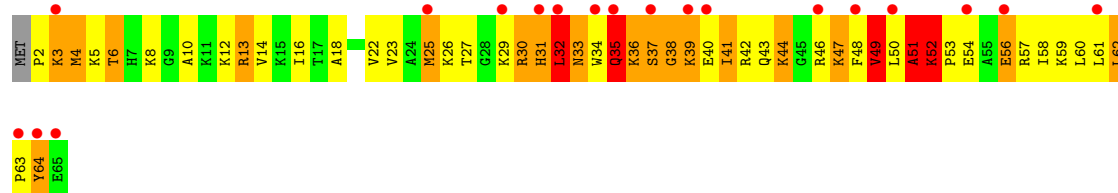
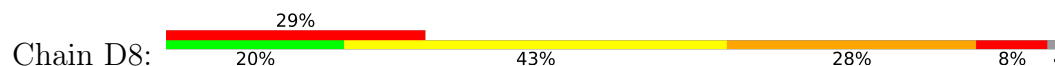


• Molecule 30: 50S ribosomal protein L35

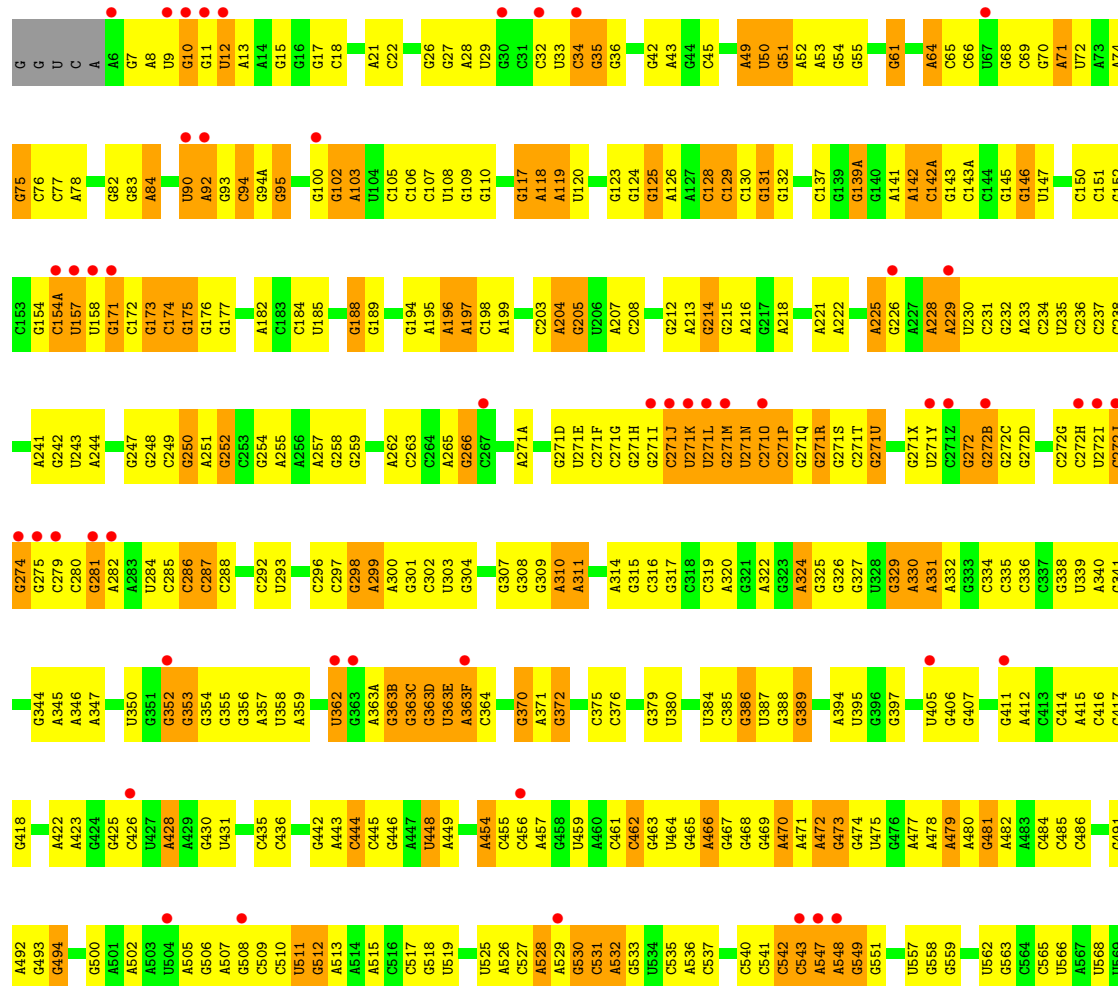




• Molecule 30: 50S ribosomal protein L35

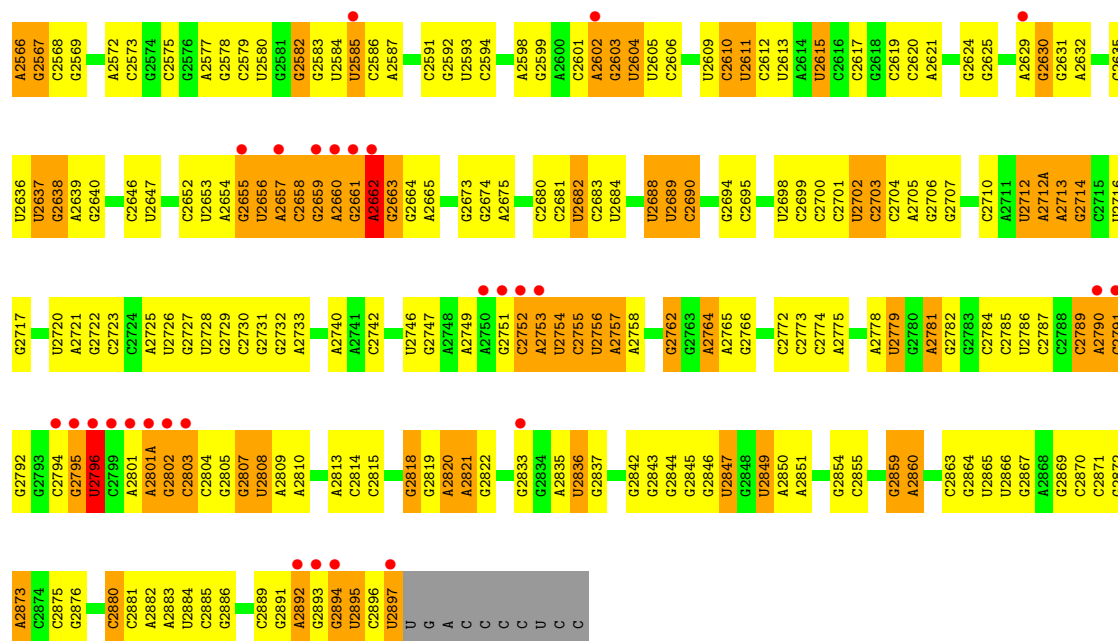


• Molecule 31: 23S ribosomal RNA

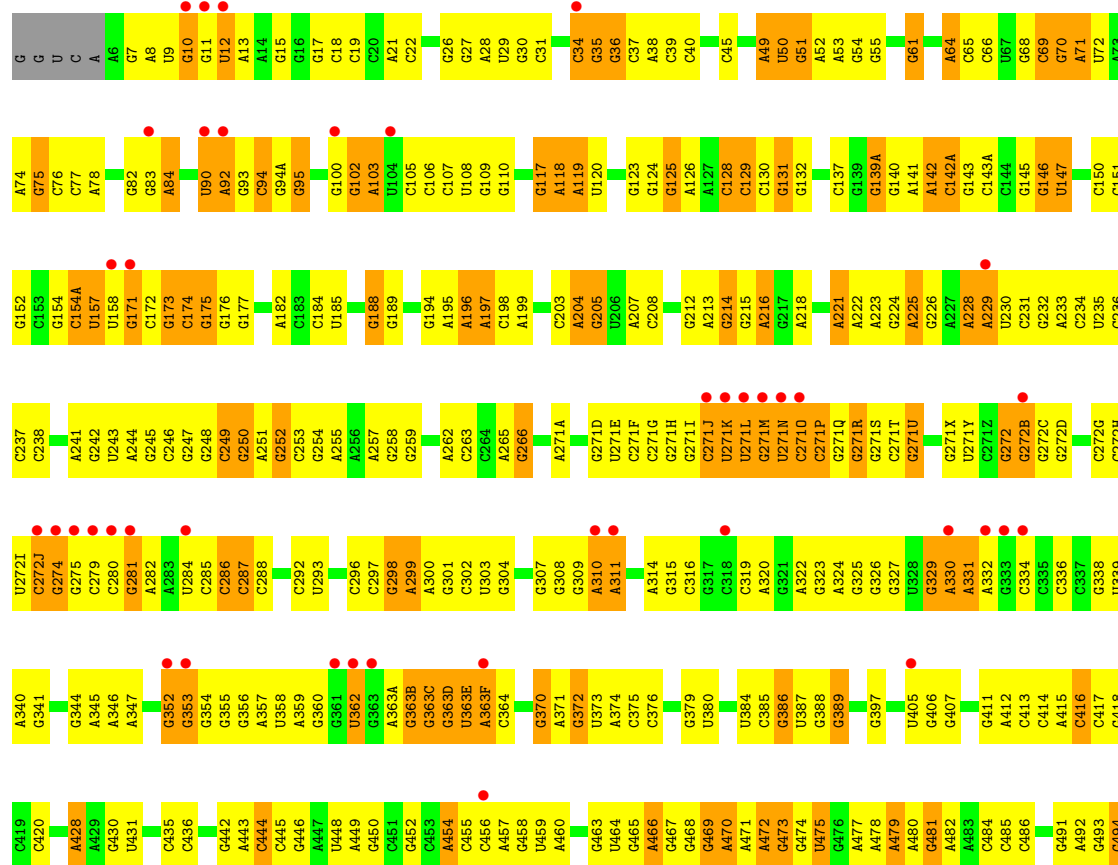


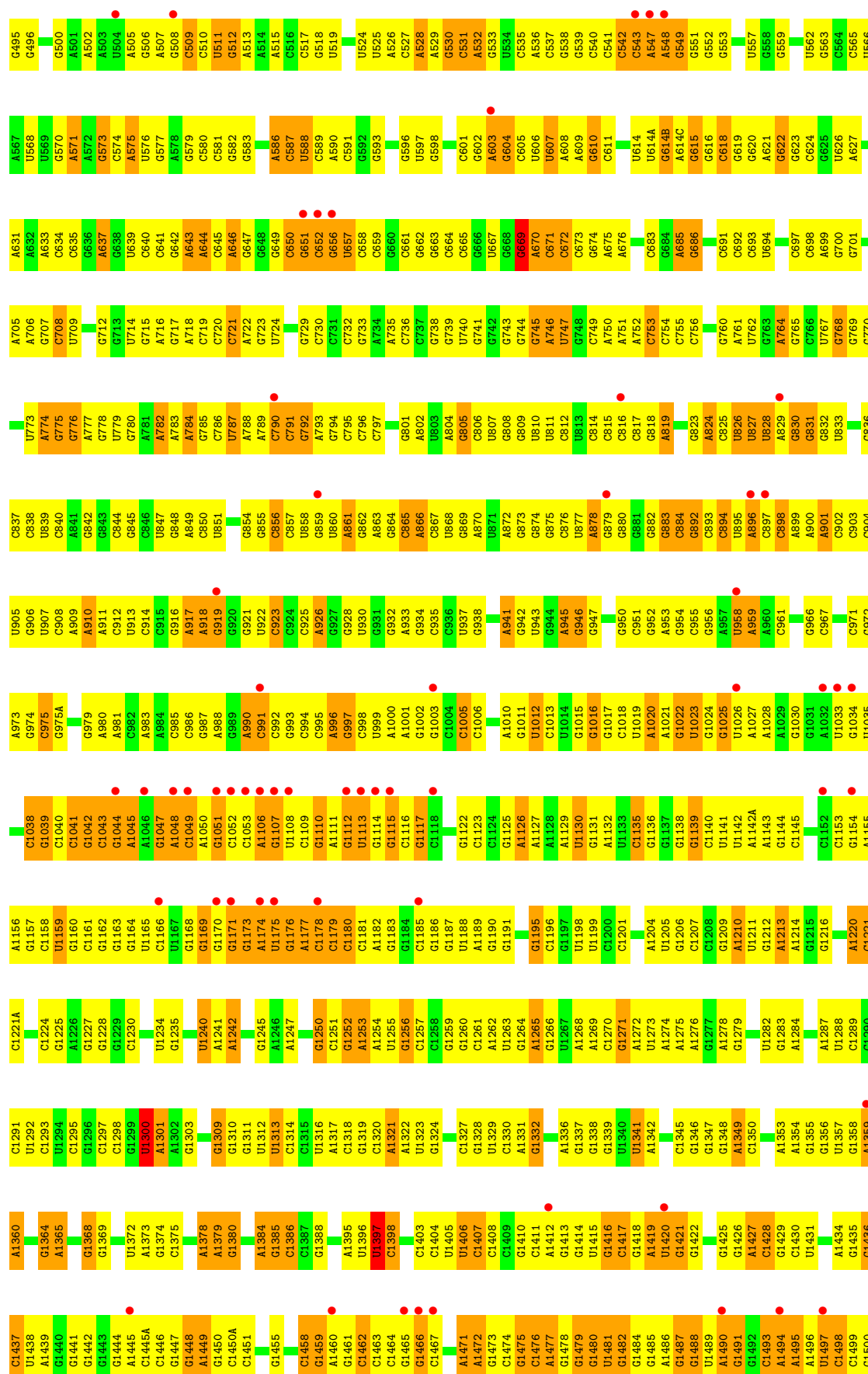
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G1418	A1419	A1420	G1421	G1425	G1426	A1427	G1428	G1429	C1430	U1431	A1434	A1435	G1436	G1437	U1438	A1439	G1440	G1441	G1442	G1443	G1444	A1445	A1446	G1447	G1448	A1449	G1450	C1451	G1455	C1458	G1459	A1460	G1461	G1462	C1463	G1464	G1465	A1466	C1467	C1468	A1469	C1530	C1531	C1532	G1533	C1543	A1544	A1545	C1546	C1547	C1548	C1549	C1550	C1551					
C1330	A1331	G1332	G1339	U1340	G1341	A1342	G1345	G1348	A1349	A1353	A1354	G1355	G1356	U1357	G1358	A1359	A1360	G1364	A1365	G1368	U1369	G1372	A1373	A1378	U1379	G1380	A1384	G1385	C1386	C1387	G1388	A1395	U1396	U1397	C1398	G1403	C1404	U1405	U1406	C1407	G1408	C1409	G1410	C1411	A1412	G1413	G1416	G1417	G1418	G1419	G1420	G1421							
G1256	C1257	A1262	U1263	G1264	A1265	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1274	A1275	G1276	G1277	A1278	G1279	U1282	G1283	A1284	A1287	U1288	C1289	G1290	C1291	U1292	A1293	C1298	G1299	U1300	A1301	A1302	G1303	G1309	G1310	G1311	U1312	C1313	C1314	A1317	G1318	G1319	C1320	A1321	A1322	U1323	G1324	C1327	U1329								
A1177	C1178	C1180	C1181	A1182	G1183	G1184	C1185	G1186	A1187	U1188	A1189	G1190	G1191	G1195	G1196	C1201	A1204	U1205	G1206	G1209	A1210	A1211	U1212	G1213	A1214	G1216	A1220	C1221	A1221A	G1224	G1225	A1226	G1227	U1234	G1235	G1239	U1240	A1241	A1242	G1245	A1246	A1247	G1250	C1251	G1252	A1253	U1255												
G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	G1116	G1117	C1118	G1119	G1122	C1123	G1124	G1125	A1126	A1127	A1129	A1129	U1130	G1131	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	A1142A	A1143	G1144	C1153	G1154	A1155	U1156	G1157	U1158	G1159	C1161	G1162	G1163	G1164	U1165	C1166	U1167	G1168	G1169	G1170	G1171	G1173	U1174	U1175	G1176				
A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	G1003	C1004	C1005	C1006	A1010	G1011	U1012	C1013	U1014	G1015	G1016	U1019	A1020	A1021	A1022	G1023	U1024	C1025	U1026	A1027	A1028	A1029	G1030	U1033	G1034	U1035	C1038	G1039	A1040	C1041	G1042	C1043	G1044	A1045	C1046	U1047	A1048	A1049	A1050	C1051	C1052	G1053	A1054	A1055			
G854	G855	G856	C857	U858	G859	U860	A861	A862	A863	G864	G865	A866	C867	U868	C869	A870	U871	A872	G873	U874	G875	C876	U877	A878	G879	C880	G881	G882	G883	C884	C882	C893	U894	A895	A896	C897	C898	A899	A900	A901	C902	C903	C904	U905	G906	U907	C908	A909	A910	A911	C912	U913	A914	C915	G916	A917	C918	G919	
U787	A788	A789	C790	C791	G792	A793	G794	C795	C796	C797	G801	A802	U803	A804	G805	C806	U807	G808	G809	U810	U811	G812	U813	C814	C817	G818	A819	G823	A824	C825	U826	U827	U828	A829	G830	G831	G832	U833	C834	A835	G836	C837	C838	U839	C840	A841	G842	U843	G844	G845	C846	U847	C848	A849	C850	G851			
A716	G717	A718	C719	C720	C721	A722	G723	U724	A727	G728	G729	C730	G731	C732	U740	G741	G742	G743	G744	G745	U746	U747	A750	A751	A752	C753	C754	C755	C756	G760	A761	U762	G763	A764	G765	C766	U767	G769	G770	U773	A774	G775	G776	A777	U778	U779	G780	A781	A782	C783	A784	C786							
A637	G638	U639	C640	C641	G642	A643	A644	C645	A646	G647	G648	C649	C650	G651	U652	G656	U657	C658	C659	G660	G661	G662	G663	C664	U667	G668	C669	A670	C671	C672	C673	A675	U676	C683	G684	A685	G686	C691	C692	C693	U694	G695	G696	A699	G700	G701	A705	A706	C707	C708	U709	G715							
G570	A571	A572	G573	C574	A575	U576	G577	A578	G579	C580	C581	G582	G583	A586	C587	U588	C589	A590	C591	G592	G593	G596	U597	G598	C601	G602	A603	G604	C605	U606	U607	A608	A609	G610	C611	U614	G614B	G615	C618	G619	G620	A621	G622	U626	A627	A631	C634	C635	G636										



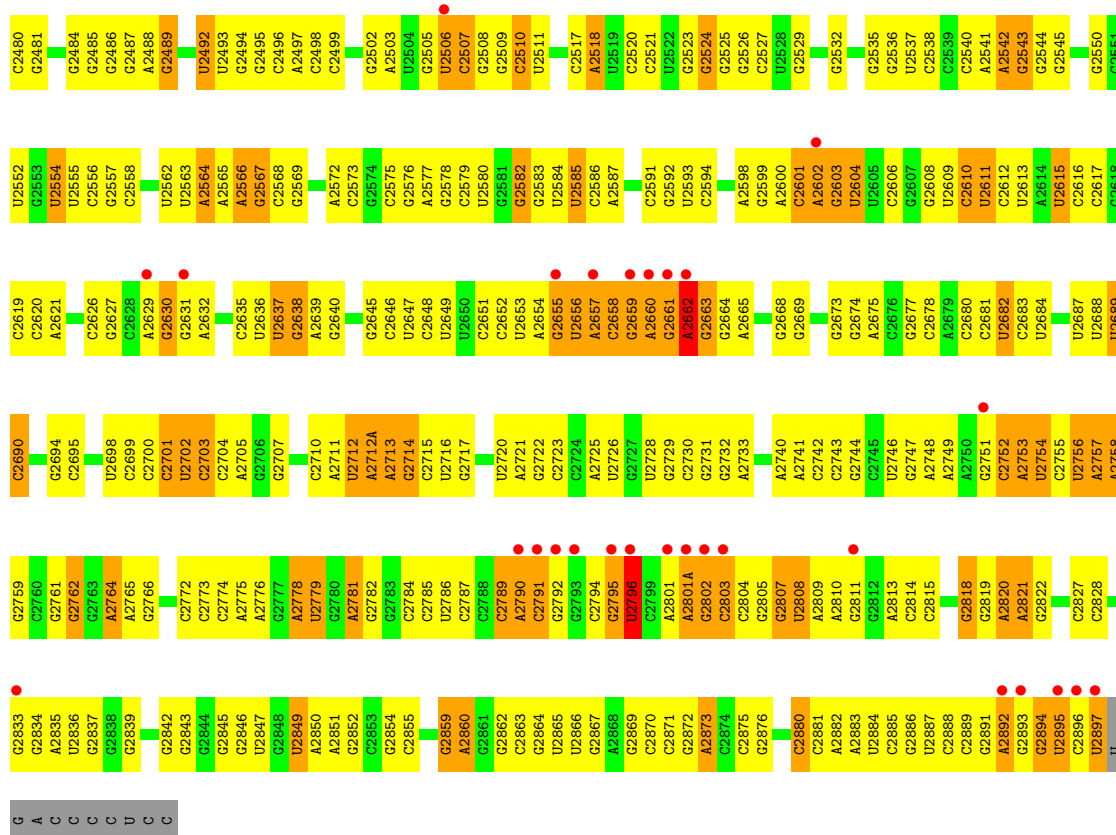


• Molecule 31: 23S ribosomal RNA

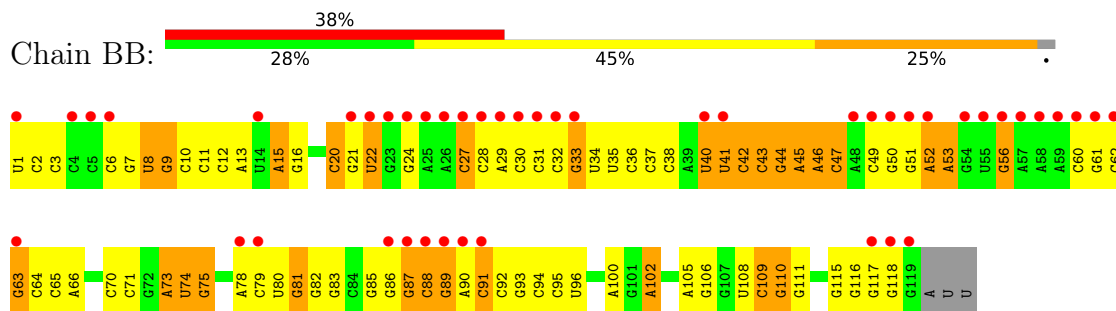




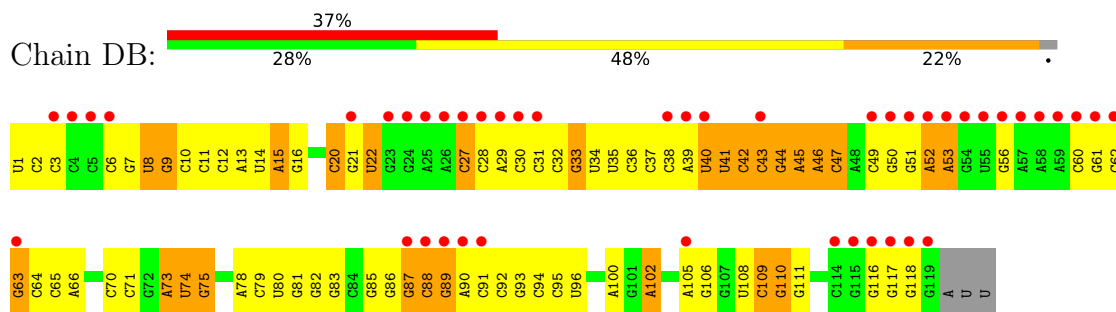




• Molecule 32: 5S ribosomal RNA

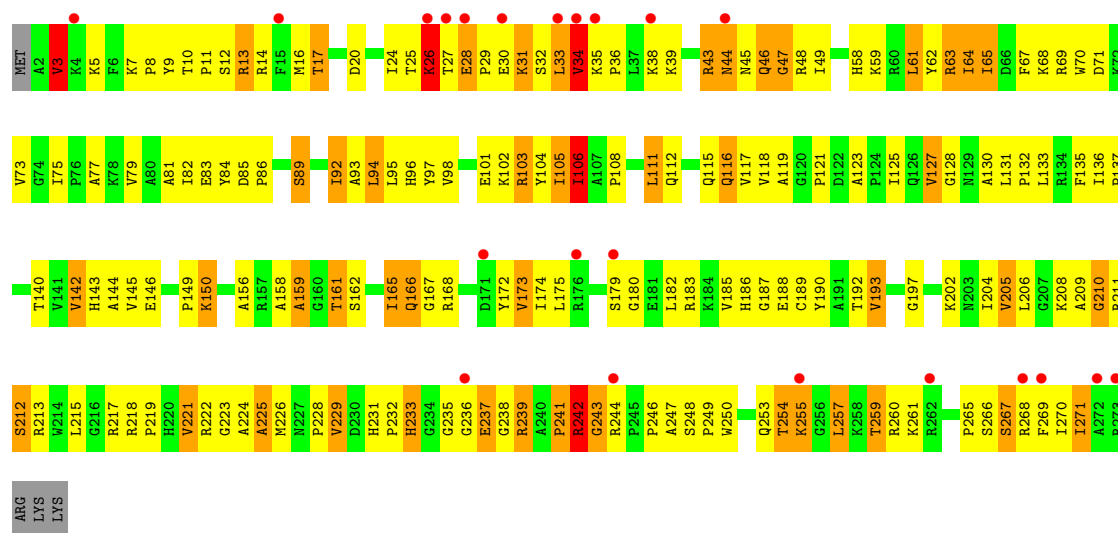


• Molecule 32: 5S ribosomal RNA

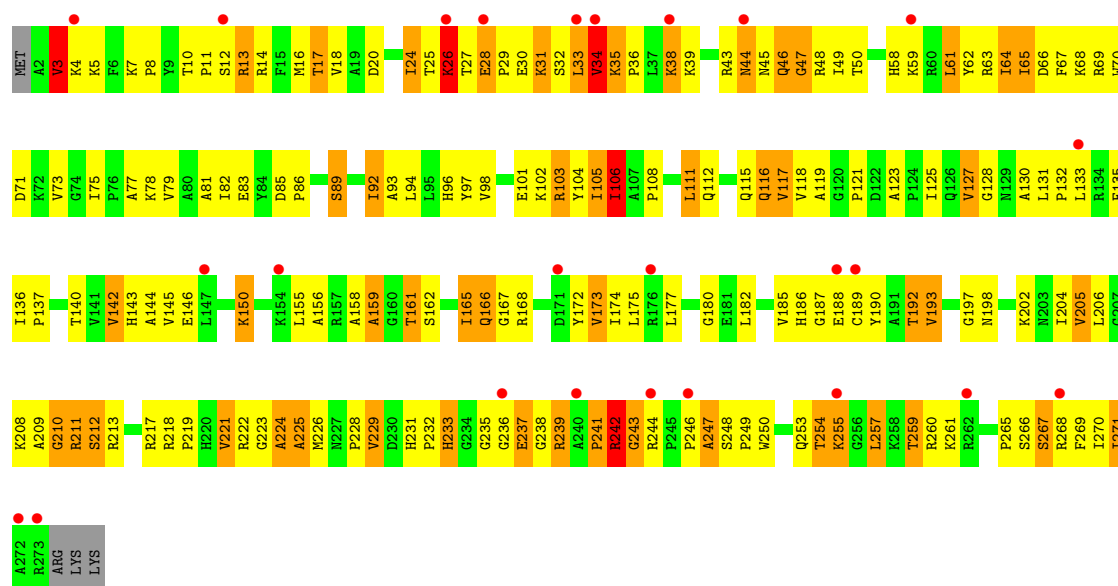


• Molecule 33: 50S ribosomal protein L2

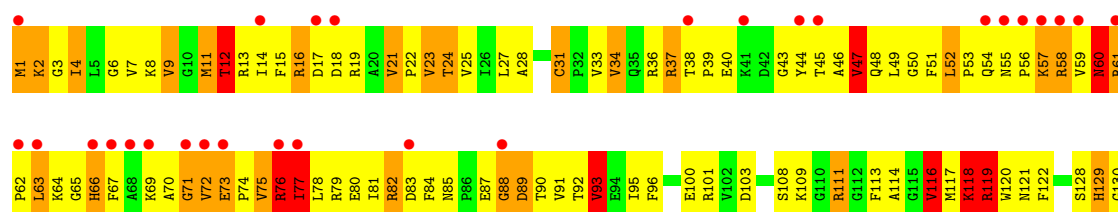


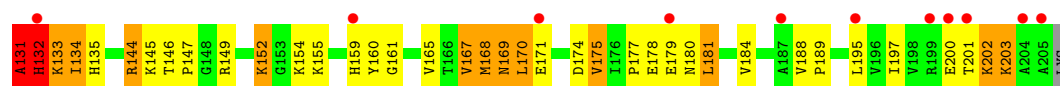


• Molecule 33: 50S ribosomal protein L2

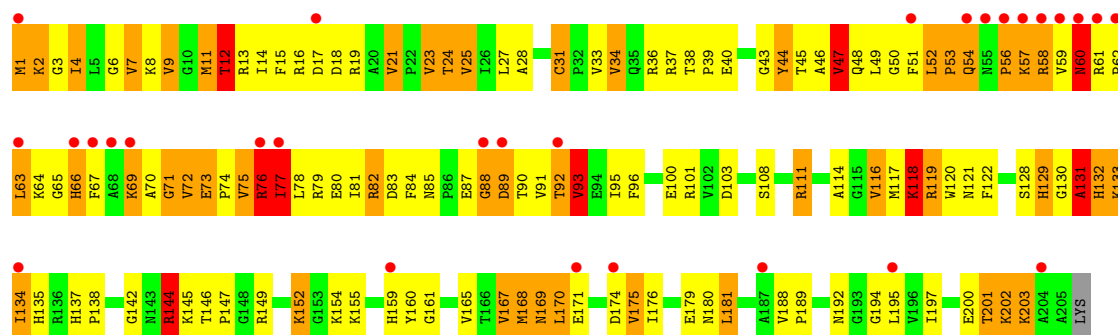


• Molecule 34: 50S ribosomal protein L3

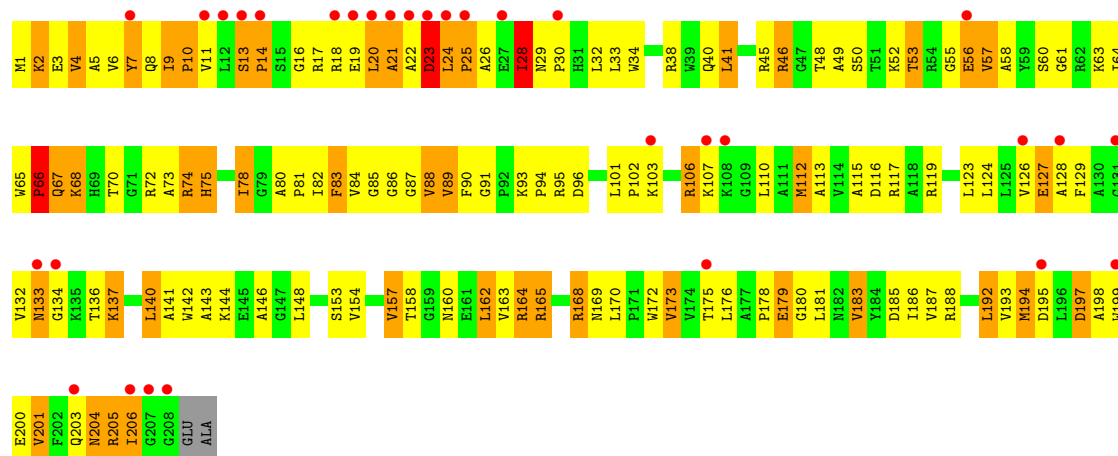




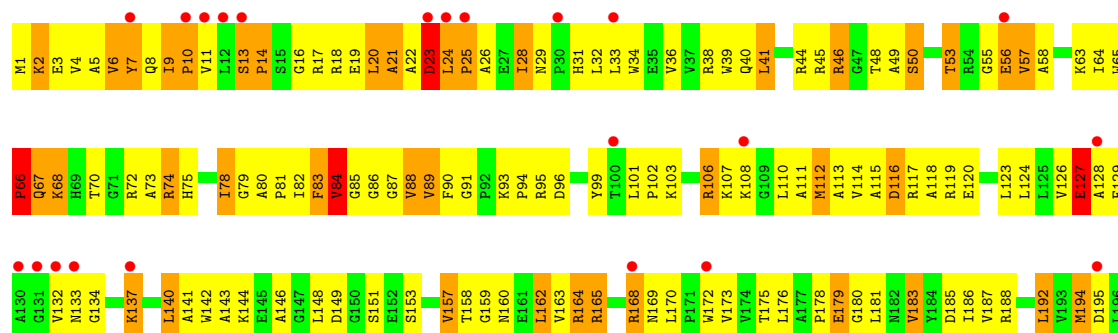
• Molecule 34: 50S ribosomal protein L3



• Molecule 35: 50S ribosomal protein L4

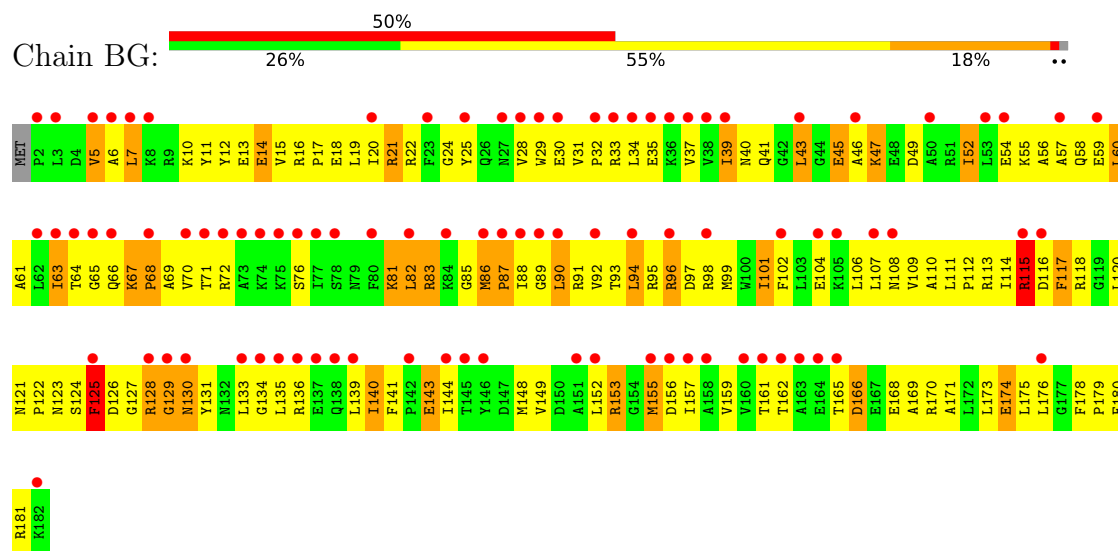


• Molecule 35: 50S ribosomal protein L4

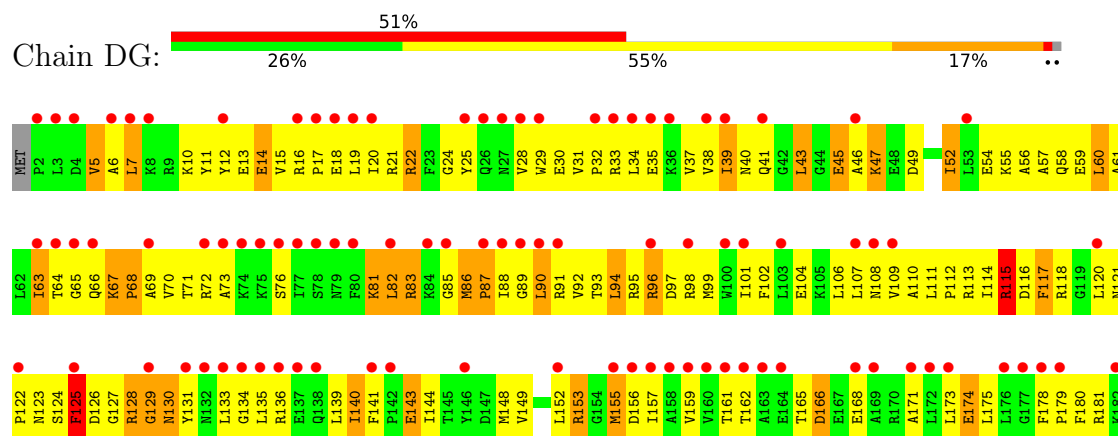




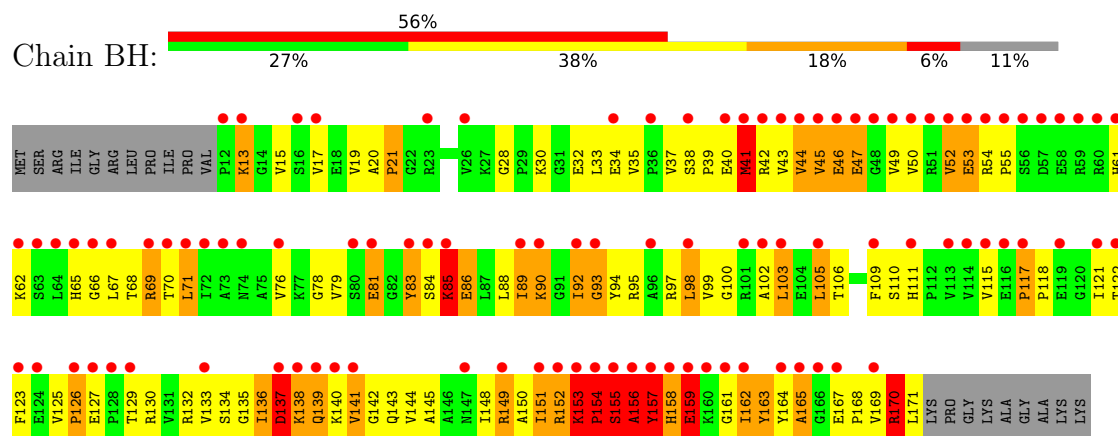
• Molecule 36: 50S ribosomal protein L5



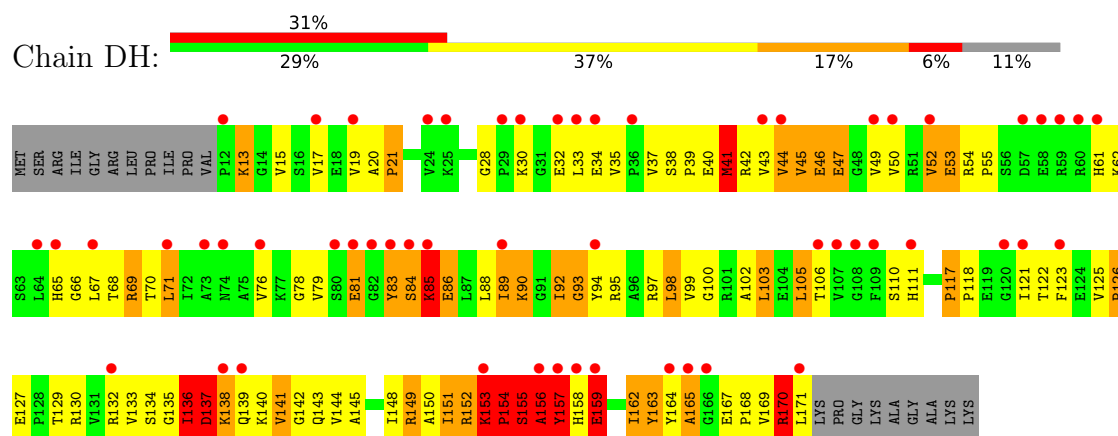
• Molecule 36: 50S ribosomal protein L5



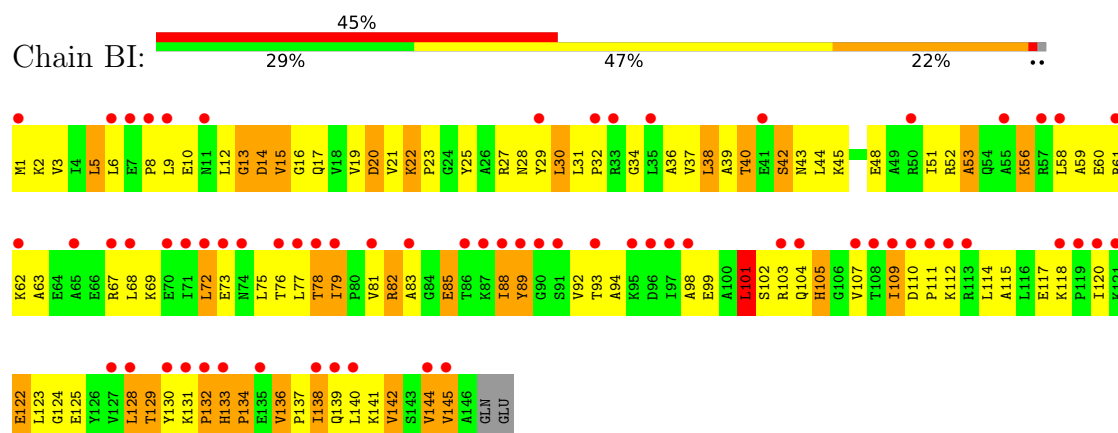
• Molecule 37: 50S ribosomal protein L6



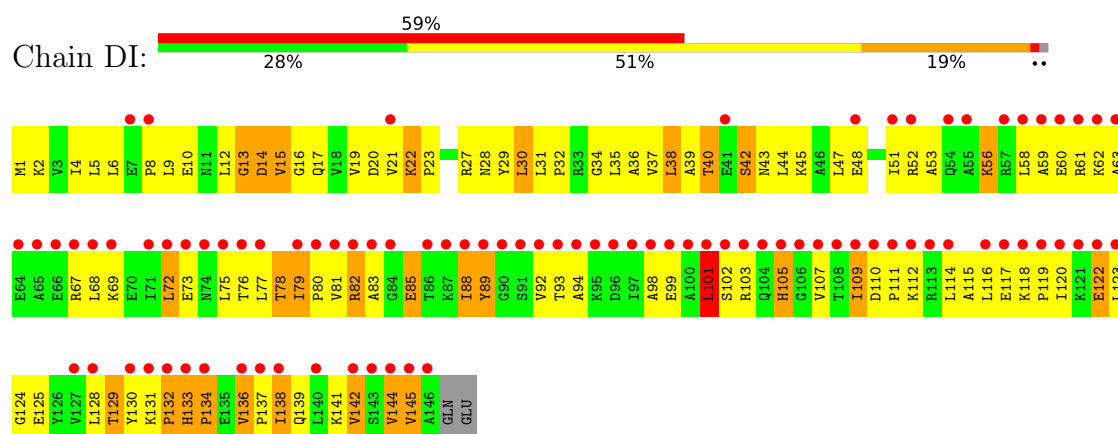
- Molecule 37: 50S ribosomal protein L6



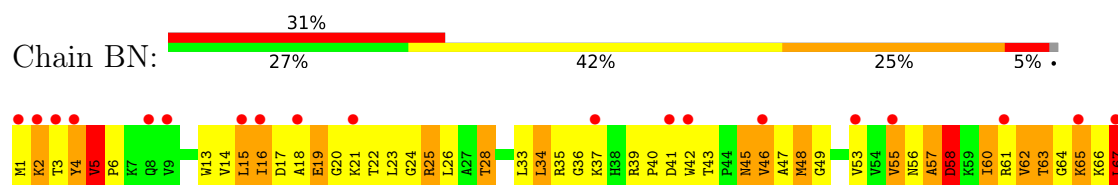
- Molecule 38: 50S ribosomal protein L9



- Molecule 38: 50S ribosomal protein L9

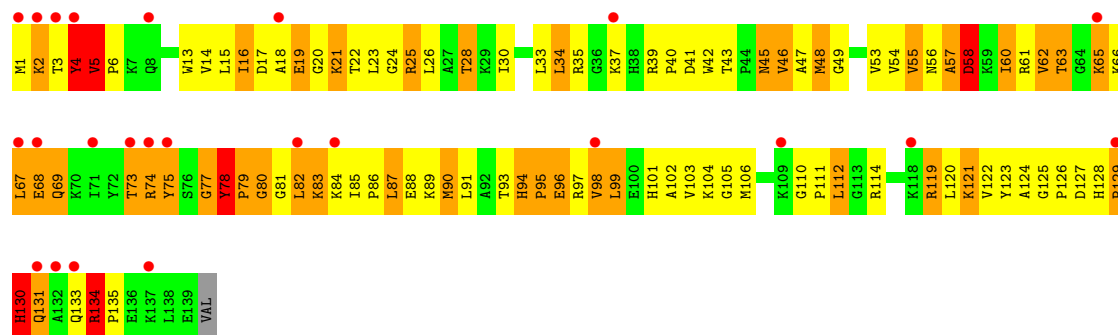


- Molecule 39: 50S ribosomal protein L13

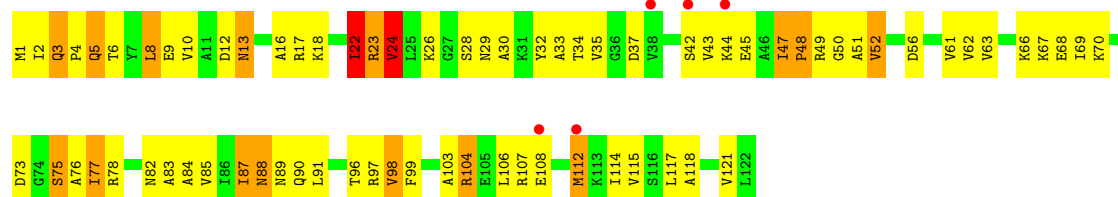




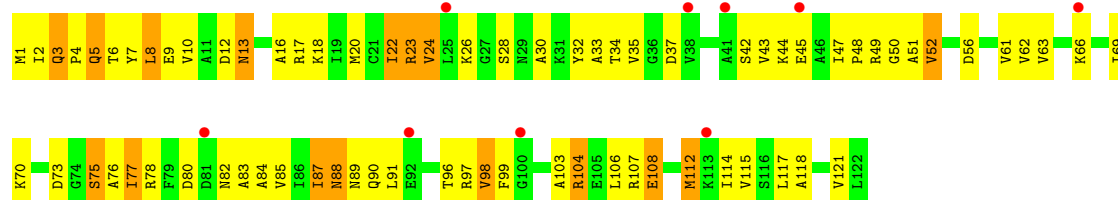
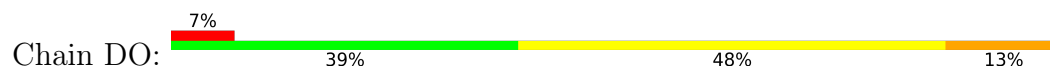
• Molecule 39: 50S ribosomal protein L13



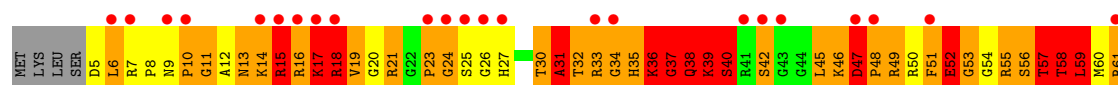
• Molecule 40: 50S ribosomal protein L14

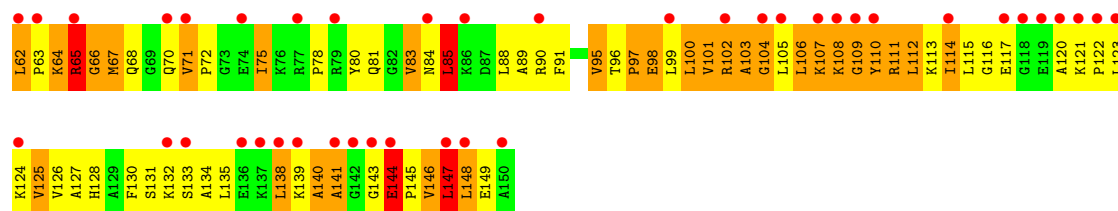


• Molecule 40: 50S ribosomal protein L14

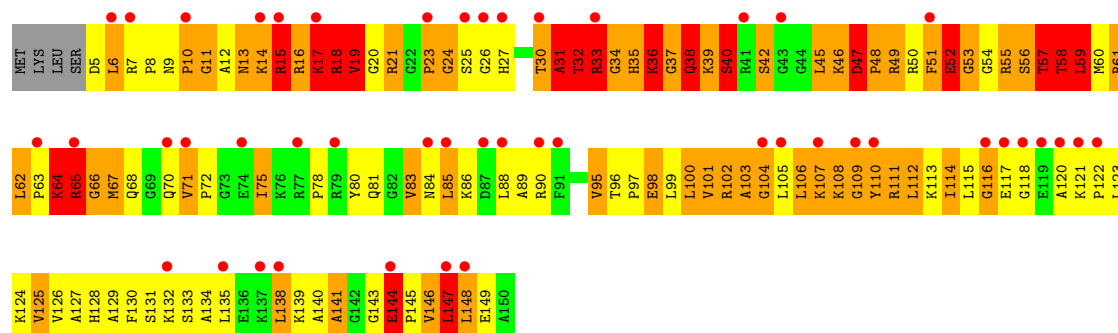


• Molecule 41: 50S ribosomal protein L15

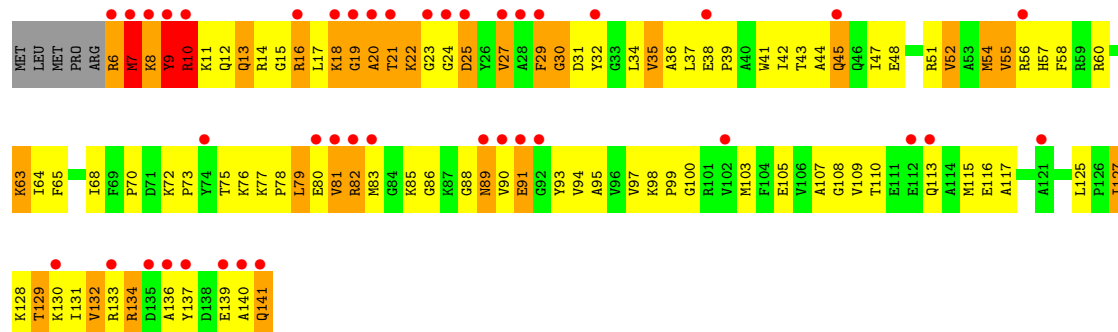




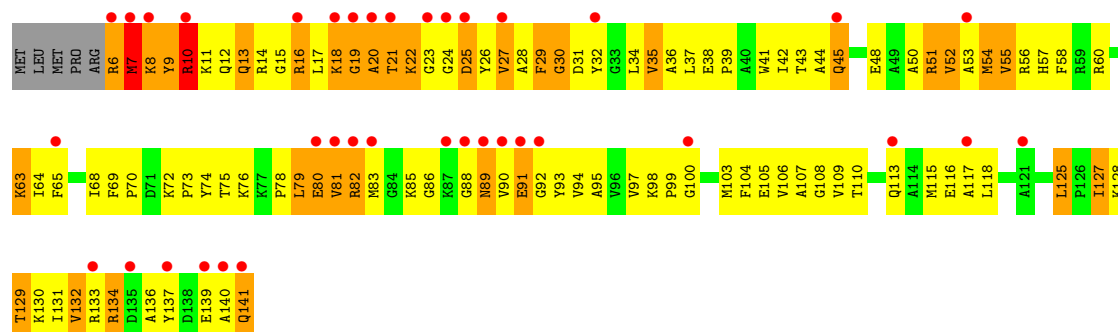
• Molecule 41: 50S ribosomal protein L15



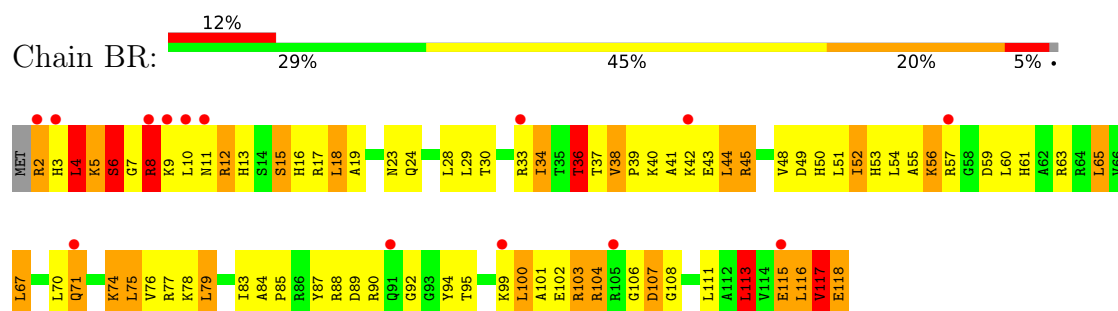
• Molecule 42: 50S ribosomal protein L16



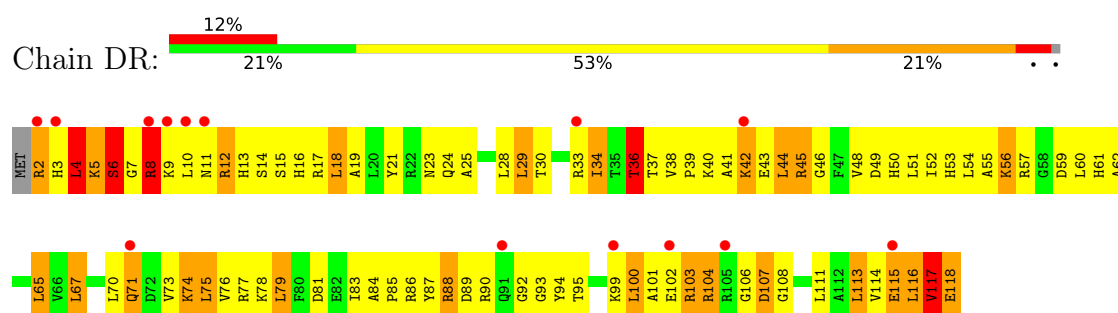
• Molecule 42: 50S ribosomal protein L16



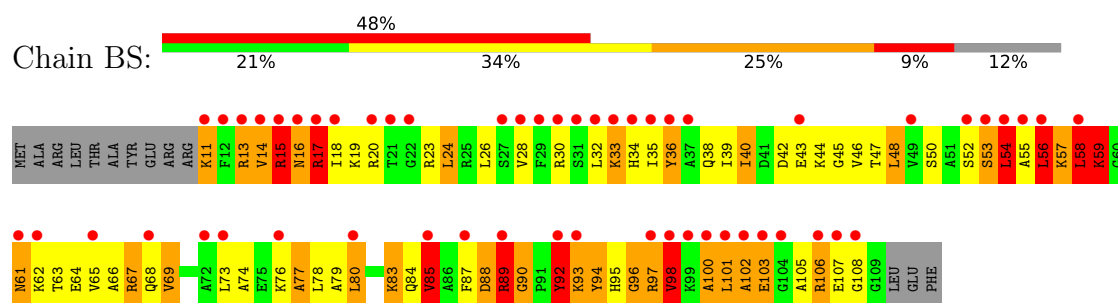
- Molecule 43: 50S ribosomal protein L17



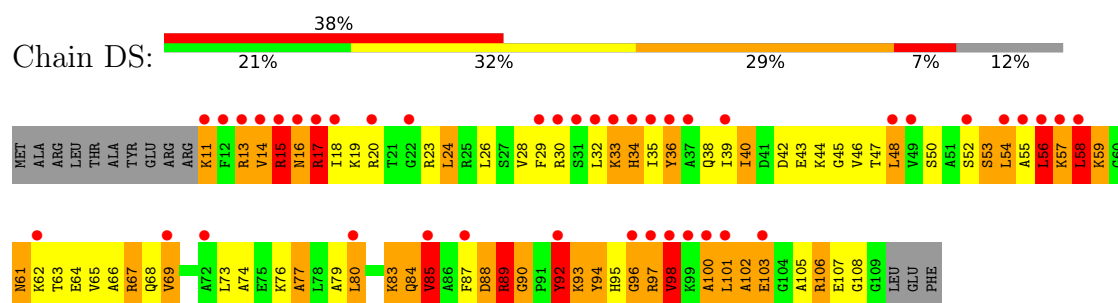
- Molecule 43: 50S ribosomal protein L17



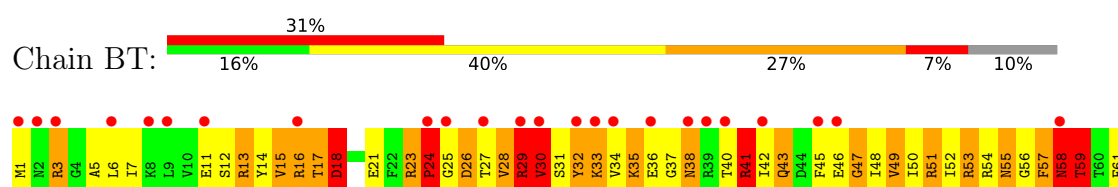
- Molecule 44: 50S ribosomal protein L18

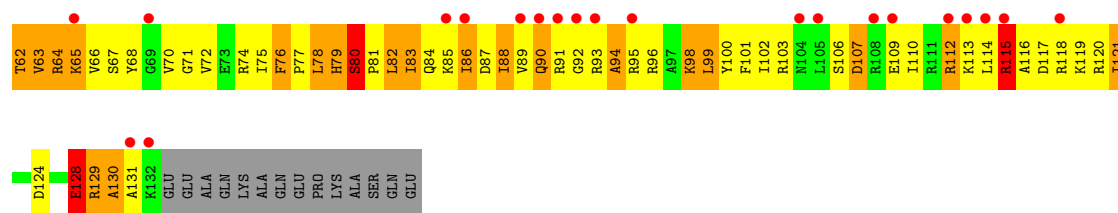


- Molecule 44: 50S ribosomal protein L18

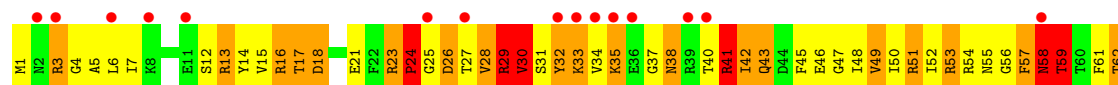
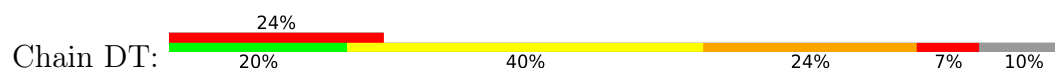


- Molecule 45: 50S ribosomal protein L19

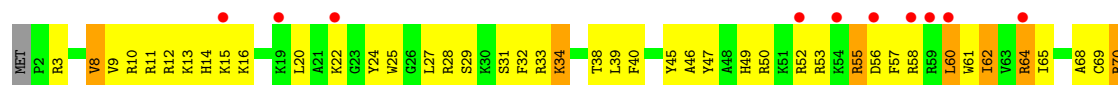




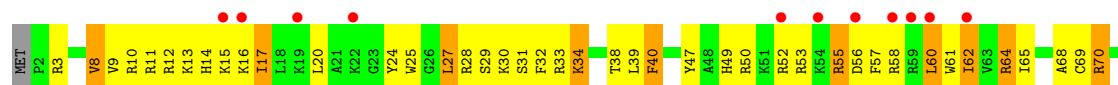
• Molecule 45: 50S ribosomal protein L19



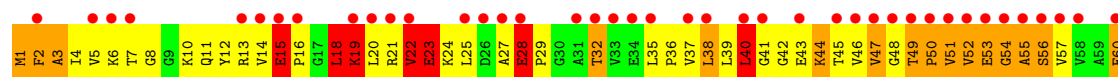
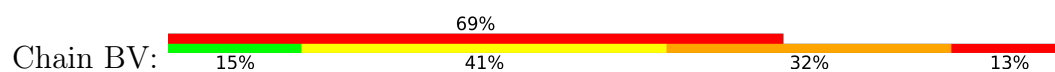
• Molecule 46: 50S ribosomal protein L20

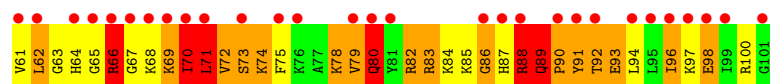


• Molecule 46: 50S ribosomal protein L20

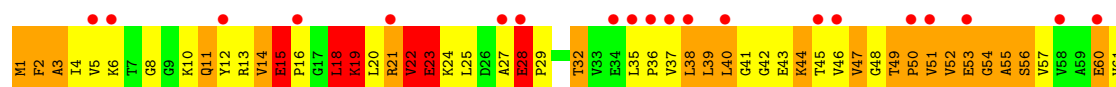


• Molecule 47: 50S ribosomal protein L21

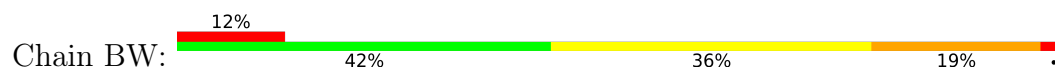




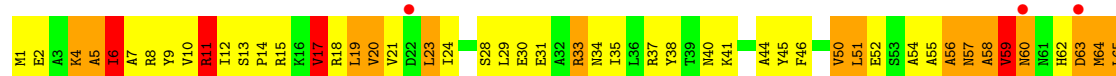
• Molecule 47: 50S ribosomal protein L21



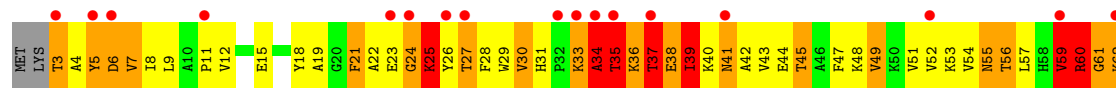
• Molecule 48: 50S ribosomal protein L22



• Molecule 48: 50S ribosomal protein L22

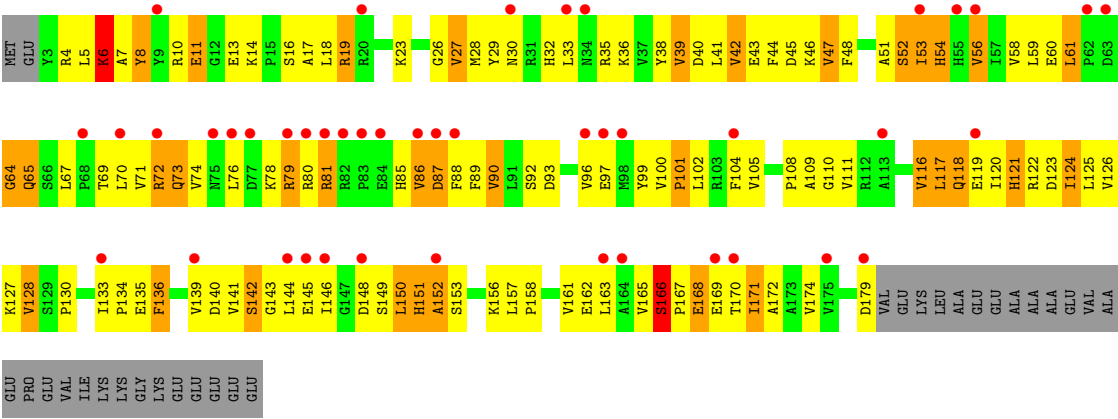


• Molecule 49: 50S ribosomal protein L23



• Molecule 49: 50S ribosomal protein L23





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.47Å 447.96Å 620.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 3.00 49.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.61-3.00) 99.7 (49.61-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.278 0.239 , 0.272	Depositor DCC
R_{free} test set	57802 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 101.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	278034	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: ERY, MG, K, ZN

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	0.29	0/36190	0.39	0/56486
1	CA	0.29	0/36190	0.38	0/56486
2	AB	0.36	0/1936	0.82	4/2611 (0.2%)
2	CB	0.36	0/1936	0.82	3/2611 (0.1%)
3	AC	0.36	0/1637	0.82	1/2207 (0.0%)
3	CC	0.35	0/1637	0.81	1/2207 (0.0%)
4	AD	0.43	0/1733	0.91	4/2318 (0.2%)
4	CD	0.44	0/1733	0.91	5/2318 (0.2%)
5	AE	0.43	0/1163	0.87	5/1566 (0.3%)
5	CE	0.41	0/1163	0.88	5/1566 (0.3%)
6	AF	0.43	0/856	0.87	0/1154
6	CF	0.39	0/856	0.89	1/1154 (0.1%)
7	AG	0.34	0/1276	0.78	0/1709
7	CG	0.33	0/1276	0.78	0/1709
8	AH	0.42	0/1136	0.89	3/1527 (0.2%)
8	CH	0.40	0/1136	0.89	3/1527 (0.2%)
9	AI	0.33	0/1028	0.76	2/1375 (0.1%)
9	CI	0.33	0/1028	0.73	2/1375 (0.1%)
10	AJ	0.40	0/808	0.82	0/1087
10	CJ	0.40	0/808	0.83	0/1087
11	AK	0.43	0/900	0.88	3/1213 (0.2%)
11	CK	0.42	0/900	0.87	2/1213 (0.2%)
12	AL	0.52	0/987	0.98	3/1322 (0.2%)
12	CL	0.54	0/987	0.98	4/1322 (0.3%)
13	AM	0.35	0/928	0.81	4/1238 (0.3%)
13	CM	0.36	0/928	0.80	4/1238 (0.3%)
14	AN	0.33	0/501	0.74	0/664
14	CN	0.33	0/501	0.74	0/664
15	AO	0.45	0/745	0.81	0/992
15	CO	0.43	0/745	0.79	0/992
16	AP	0.41	0/717	0.85	2/965 (0.2%)
16	CP	0.43	0/717	0.86	2/965 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.39	0/837	0.85	2/1119 (0.2%)
17	CQ	0.39	0/837	0.86	2/1119 (0.2%)
18	AR	0.44	0/579	0.96	4/768 (0.5%)
18	CR	0.40	0/579	0.93	3/768 (0.4%)
19	AS	0.37	0/643	0.72	0/867
19	CS	0.36	0/643	0.72	0/867
20	AT	0.45	0/765	0.90	3/1007 (0.3%)
20	CT	0.47	0/765	0.90	3/1007 (0.3%)
21	AU	0.36	0/213	0.71	0/279
21	CU	0.36	0/213	0.72	0/279
22	B0	0.68	0/658	1.08	4/878 (0.5%)
22	D0	0.58	0/658	1.06	3/878 (0.3%)
23	B1	1.06	3/700 (0.4%)	1.52	16/931 (1.7%)
23	D1	0.98	2/700 (0.3%)	1.46	14/931 (1.5%)
24	B2	0.92	1/423 (0.2%)	1.24	4/560 (0.7%)
24	D2	0.71	0/423	1.18	3/560 (0.5%)
25	B3	0.80	0/473	1.16	3/636 (0.5%)
25	D3	0.58	0/473	1.15	3/636 (0.5%)
26	B4	0.44	0/156	1.28	2/215 (0.9%)
26	D4	0.44	0/156	1.36	3/215 (1.4%)
27	B5	1.04	1/473 (0.2%)	1.79	13/639 (2.0%)
27	D5	0.94	1/473 (0.2%)	1.77	14/639 (2.2%)
28	B6	0.95	0/387	1.30	2/517 (0.4%)
28	D6	0.83	0/387	1.22	1/517 (0.2%)
29	B7	0.83	1/427 (0.2%)	1.04	0/563
29	D7	0.78	0/427	1.07	0/563
30	B8	0.96	0/516	1.56	12/681 (1.8%)
30	D8	0.84	0/516	1.52	10/681 (1.5%)
31	BA	0.59	4/65745 (0.0%)	0.54	11/102639 (0.0%)
31	DA	0.50	4/65745 (0.0%)	0.54	13/102639 (0.0%)
32	BB	0.46	0/2853	0.46	0/4451
32	DB	0.39	0/2853	0.46	0/4451
33	BD	0.84	0/2155	1.23	10/2907 (0.3%)
33	DD	0.75	0/2155	1.22	13/2907 (0.4%)
34	BE	0.81	0/1597	1.21	12/2155 (0.6%)
34	DE	0.69	0/1597	1.17	10/2155 (0.5%)
35	BF	0.79	0/1659	1.13	10/2246 (0.4%)
35	DF	0.64	0/1659	1.14	12/2246 (0.5%)
36	BG	0.41	0/1498	0.88	4/2013 (0.2%)
36	DG	0.37	0/1498	0.86	4/2013 (0.2%)
37	BH	0.79	0/1246	1.16	10/1684 (0.6%)
37	DH	0.53	0/1246	1.09	8/1684 (0.5%)
38	BI	0.50	0/1147	0.93	5/1553 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.53	0/1147	0.93	5/1553 (0.3%)
39	BN	0.91	0/1132	1.31	10/1527 (0.7%)
39	DN	0.68	0/1132	1.28	9/1527 (0.6%)
40	BO	0.76	1/943 (0.1%)	1.13	4/1269 (0.3%)
40	DO	0.64	0/943	1.08	3/1269 (0.2%)
41	BP	0.95	3/1131 (0.3%)	1.47	19/1504 (1.3%)
41	DP	0.83	2/1131 (0.2%)	1.43	17/1504 (1.1%)
42	BQ	0.88	1/1100 (0.1%)	1.21	9/1470 (0.6%)
42	DQ	0.79	1/1100 (0.1%)	1.18	6/1470 (0.4%)
43	BR	0.88	1/974 (0.1%)	1.16	7/1302 (0.5%)
43	DR	0.73	0/974	1.14	4/1302 (0.3%)
44	BS	0.69	0/779	1.08	5/1038 (0.5%)
44	DS	0.56	0/779	1.06	4/1038 (0.4%)
45	BT	0.80	1/1114 (0.1%)	1.36	15/1488 (1.0%)
45	DT	0.69	1/1114 (0.1%)	1.32	14/1488 (0.9%)
46	BU	0.96	0/975	1.15	6/1297 (0.5%)
46	DU	0.68	0/975	1.11	8/1297 (0.6%)
47	BV	1.01	2/790 (0.3%)	1.34	15/1057 (1.4%)
47	DV	0.77	1/790 (0.1%)	1.26	12/1057 (1.1%)
48	BW	0.93	0/907	1.18	6/1216 (0.5%)
48	DW	0.79	1/907 (0.1%)	1.17	4/1216 (0.3%)
49	BX	0.97	0/740	1.39	12/995 (1.2%)
49	DX	0.86	0/740	1.37	12/995 (1.2%)
50	BY	0.92	1/789 (0.1%)	1.38	10/1053 (0.9%)
50	DY	0.75	0/789	1.33	10/1053 (0.9%)
51	BZ	0.63	0/1436	1.01	10/1951 (0.5%)
51	DZ	0.51	0/1436	0.98	4/1951 (0.2%)
All	All	0.53	33/301002 (0.0%)	0.70	549/449818 (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
27	B5	0	1
27	D5	0	1
30	B8	0	1
30	D8	0	1
31	BA	21	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	DA	21	0
33	BD	0	2
33	DD	0	2
34	BE	0	2
34	DE	0	2
37	BH	0	2
37	DH	0	2
41	BP	0	5
41	DP	0	3
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	1
45	DT	0	1
46	BU	0	1
46	DU	0	1
47	BV	0	1
47	DV	0	1
49	BX	0	5
49	DX	0	5
All	All	42	50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	BV	80	GLN	CA-C	9.71	1.65	1.52
31	BA	669	G	C4'-C3'	-8.32	1.40	1.53
47	DV	80	GLN	CA-C	7.81	1.63	1.52
31	BA	1300	U	C4'-C3'	-7.73	1.41	1.53
31	DA	669	G	C4'-C3'	-7.50	1.42	1.53

The worst 5 of 549 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D5	4	HIS	CA-C-N	-14.31	106.47	120.21
27	D5	4	HIS	C-N-CA	-14.31	106.47	120.21
27	B5	4	HIS	CA-C-N	-12.66	108.06	120.21
27	B5	4	HIS	C-N-CA	-12.66	108.06	120.21
41	BP	59	LEU	N-CA-C	-12.41	94.53	113.02

5 of 42 chirality outliers are listed below:

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

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
27	B5	51	TYR	Peptide
30	B8	51	ALA	Peptide
33	BD	197	GLY	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	1465	0
1	CA	32329	0	16318	1446	0
2	AB	1901	0	1951	196	0
2	CB	1901	0	1951	193	0
3	AC	1613	0	1677	123	0
3	CC	1613	0	1677	130	0
4	AD	1703	0	1763	198	0
4	CD	1703	0	1764	200	0
5	AE	1147	0	1207	106	0
5	CE	1147	0	1207	111	0
6	AF	843	0	857	96	0
6	CF	843	0	857	99	0
7	AG	1257	0	1296	72	0
7	CG	1257	0	1296	77	0
8	AH	1116	0	1177	98	0
8	CH	1116	0	1177	99	0
9	AI	1011	0	1042	102	0
9	CI	1011	0	1042	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	89	0
10	CJ	795	0	840	85	0
11	AK	885	0	904	60	0
11	CK	885	0	904	67	0
12	AL	971	0	1057	105	0
12	CL	971	0	1057	106	0
13	AM	921	0	976	84	0
13	CM	921	0	976	85	0
14	AN	492	0	530	44	0
14	CN	492	0	530	43	0
15	AO	734	0	771	53	0
15	CO	734	0	771	52	0
16	AP	701	0	720	82	0
16	CP	701	0	720	82	0
17	AQ	824	0	891	62	0
17	CQ	824	0	891	57	0
18	AR	574	0	644	63	0
18	CR	574	0	644	63	0
19	AS	630	0	652	41	0
19	CS	630	0	652	43	0
20	AT	763	0	861	94	0
20	CT	763	0	861	92	0
21	AU	209	0	221	9	0
21	CU	209	0	221	10	0
22	B0	650	0	654	58	0
22	D0	650	0	654	60	0
23	B1	693	0	764	142	0
23	D1	693	0	764	139	0
24	B2	421	0	461	124	0
24	D2	421	0	461	126	0
25	B3	468	0	523	32	0
25	D3	468	0	523	52	0
26	B4	157	0	69	21	0
26	D4	157	0	69	17	0
27	B5	459	0	480	89	0
27	D5	459	0	480	83	0
28	B6	381	0	390	87	0
28	D6	381	0	390	89	0
29	B7	419	0	467	29	0
29	D7	419	0	467	32	0
30	B8	508	0	576	140	0
30	D8	508	0	576	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29591	2323	0
31	DA	58698	0	29590	2546	0
32	BB	2551	0	1295	128	0
32	DB	2551	0	1295	142	0
33	BD	2105	0	2182	310	0
33	DD	2105	0	2182	319	0
34	BE	1564	0	1629	213	0
34	DE	1564	0	1629	223	0
35	BF	1624	0	1677	171	0
35	DF	1624	0	1677	188	0
36	BG	1474	0	1534	157	0
36	DG	1474	0	1534	157	0
37	BH	1223	0	1282	154	0
37	DH	1223	0	1282	151	0
38	BI	1132	0	1218	126	0
38	DI	1132	0	1218	124	0
39	BN	1105	0	1180	184	0
39	DN	1105	0	1180	189	0
40	BO	933	0	996	76	0
40	DO	933	0	996	70	0
41	BP	1114	0	1187	265	0
41	DP	1114	0	1187	252	0
42	BQ	1080	0	1127	159	0
42	DQ	1080	0	1127	168	0
43	BR	960	0	1021	111	0
43	DR	960	0	1021	128	0
44	BS	771	0	832	147	0
44	DS	771	0	832	149	0
45	BT	1100	0	1164	196	0
45	DT	1100	0	1164	192	0
46	BU	958	0	1015	136	0
46	DU	958	0	1015	132	0
47	BV	779	0	852	222	0
47	DV	779	0	852	221	0
48	BW	896	0	953	65	0
48	DW	896	0	953	76	0
49	BX	726	0	778	182	0
49	DX	726	0	778	182	0
50	BY	776	0	870	195	0
50	DY	776	0	870	197	0
51	BZ	1404	0	1432	158	0
51	DZ	1404	0	1432	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	54	0	0	0	0
52	B0	1	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	BA	362	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	3	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	1	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	50	0	0	0	0
52	D0	1	0	0	0	0
52	D3	1	0	0	0	0
52	D5	1	0	0	0	0
52	D7	1	0	0	0	0
52	DA	328	0	0	0	0
52	DB	3	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	0	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	51	0	67	1	0
55	DA	51	0	67	2	0
All	All	278034	0	189242	17771	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 38.

The worst 5 of 17771 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)
42:BQ:81:VAL:O	42:BQ:82:ARG:HD2	1.36	1.26
42:DQ:81:VAL:O	42:DQ:82:ARG:HD2	1.37	1.22
33:BD:35:LYS:HD2	33:BD:104:TYR:CD1	1.78	1.19
50:BY:95:LYS:HD3	50:BY:100:ALA:HB1	1.21	1.19
16:AP:28:ARG:HH11	16:AP:28:ARG:HG2	1.06	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	165 (71%)	51 (22%)	17 (7%)	1	4
2	CB	233/256 (91%)	165 (71%)	51 (22%)	17 (7%)	1	4
3	AC	205/239 (86%)	156 (76%)	35 (17%)	14 (7%)	1	5
3	CC	205/239 (86%)	156 (76%)	35 (17%)	14 (7%)	1	5
4	AD	206/209 (99%)	128 (62%)	59 (29%)	19 (9%)	0	2
4	CD	206/209 (99%)	128 (62%)	59 (29%)	19 (9%)	0	2
5	AE	149/160 (93%)	106 (71%)	31 (21%)	12 (8%)	1	3
5	CE	149/160 (93%)	104 (70%)	33 (22%)	12 (8%)	1	3
6	AF	99/101 (98%)	76 (77%)	18 (18%)	5 (5%)	1	10
6	CF	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	1	10
7	AG	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	4	23
7	CG	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	4	23
8	AH	136/138 (99%)	105 (77%)	24 (18%)	7 (5%)	1	10
8	CH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	1	10
9	AI	123/128 (96%)	93 (76%)	21 (17%)	9 (7%)	1	4
9	CI	123/128 (96%)	93 (76%)	21 (17%)	9 (7%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	2	13
10	CJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	2	13
11	AK	117/129 (91%)	92 (79%)	20 (17%)	5 (4%)	2	12
11	CK	117/129 (91%)	94 (80%)	18 (15%)	5 (4%)	2	12
12	AL	123/135 (91%)	85 (69%)	24 (20%)	14 (11%)	0	1
12	CL	123/135 (91%)	86 (70%)	23 (19%)	14 (11%)	0	1
13	AM	107/126 (85%)	85 (79%)	17 (16%)	5 (5%)	2	11
13	CM	107/126 (85%)	84 (78%)	18 (17%)	5 (5%)	2	11
14	AN	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	17
14	CN	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	17
15	AO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	3	16
15	CO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	16
16	AP	82/88 (93%)	49 (60%)	23 (28%)	10 (12%)	0	1
16	CP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	0	1
17	AQ	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	1	7
17	CQ	98/105 (93%)	76 (78%)	16 (16%)	6 (6%)	1	7
18	AR	68/88 (77%)	43 (63%)	21 (31%)	4 (6%)	1	7
18	CR	68/88 (77%)	40 (59%)	22 (32%)	6 (9%)	0	3
19	AS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	0	2
19	CS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	0	2
20	AT	97/106 (92%)	64 (66%)	25 (26%)	8 (8%)	0	3
20	CT	97/106 (92%)	61 (63%)	29 (30%)	7 (7%)	1	4
21	AU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	12
21	CU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	12
22	B0	83/85 (98%)	68 (82%)	11 (13%)	4 (5%)	2	11
22	D0	83/85 (98%)	70 (84%)	9 (11%)	4 (5%)	2	11
23	B1	87/98 (89%)	52 (60%)	17 (20%)	18 (21%)	0	0
23	D1	87/98 (89%)	52 (60%)	18 (21%)	17 (20%)	0	0
24	B2	49/72 (68%)	22 (45%)	17 (35%)	10 (20%)	0	0
24	D2	49/72 (68%)	24 (49%)	13 (26%)	12 (24%)	0	0
25	B3	58/60 (97%)	50 (86%)	6 (10%)	2 (3%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D3	58/60 (97%)	51 (88%)	4 (7%)	3 (5%)	1	9
26	B4	30/71 (42%)	4 (13%)	11 (37%)	15 (50%)	0	0
26	D4	30/71 (42%)	4 (13%)	11 (37%)	15 (50%)	0	0
27	B5	57/60 (95%)	41 (72%)	7 (12%)	9 (16%)	0	0
27	D5	57/60 (95%)	42 (74%)	6 (10%)	9 (16%)	0	0
28	B6	41/54 (76%)	21 (51%)	7 (17%)	13 (32%)	0	0
28	D6	41/54 (76%)	21 (51%)	7 (17%)	13 (32%)	0	0
29	B7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
30	B8	62/65 (95%)	42 (68%)	8 (13%)	12 (19%)	0	0
30	D8	62/65 (95%)	44 (71%)	6 (10%)	12 (19%)	0	0
33	BD	270/276 (98%)	217 (80%)	40 (15%)	13 (5%)	2	11
33	DD	270/276 (98%)	214 (79%)	42 (16%)	14 (5%)	1	9
34	BE	203/206 (98%)	153 (75%)	28 (14%)	22 (11%)	0	1
34	DE	203/206 (98%)	151 (74%)	29 (14%)	23 (11%)	0	1
35	BF	206/210 (98%)	155 (75%)	37 (18%)	14 (7%)	1	5
35	DF	206/210 (98%)	151 (73%)	42 (20%)	13 (6%)	1	6
36	BG	177/182 (97%)	123 (70%)	35 (20%)	19 (11%)	0	2
36	DG	177/182 (97%)	125 (71%)	32 (18%)	20 (11%)	0	1
37	BH	158/180 (88%)	103 (65%)	28 (18%)	27 (17%)	0	0
37	DH	158/180 (88%)	103 (65%)	30 (19%)	25 (16%)	0	0
38	BI	144/148 (97%)	89 (62%)	38 (26%)	17 (12%)	0	1
38	DI	144/148 (97%)	89 (62%)	39 (27%)	16 (11%)	0	1
39	BN	137/140 (98%)	96 (70%)	25 (18%)	16 (12%)	0	1
39	DN	137/140 (98%)	94 (69%)	26 (19%)	17 (12%)	0	1
40	BO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	4	23
40	DO	120/122 (98%)	103 (86%)	15 (12%)	2 (2%)	7	32
41	BP	144/150 (96%)	80 (56%)	23 (16%)	41 (28%)	0	0
41	DP	144/150 (96%)	80 (56%)	24 (17%)	40 (28%)	0	0
42	BQ	134/141 (95%)	95 (71%)	23 (17%)	16 (12%)	0	1
42	DQ	134/141 (95%)	94 (70%)	25 (19%)	15 (11%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BR	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	4
43	DR	115/118 (98%)	84 (73%)	21 (18%)	10 (9%)	0	3
44	BS	97/112 (87%)	54 (56%)	19 (20%)	24 (25%)	0	0
44	DS	97/112 (87%)	53 (55%)	21 (22%)	23 (24%)	0	0
45	BT	130/146 (89%)	93 (72%)	20 (15%)	17 (13%)	0	1
45	DT	130/146 (89%)	92 (71%)	22 (17%)	16 (12%)	0	1
46	BU	115/118 (98%)	90 (78%)	17 (15%)	8 (7%)	1	4
46	DU	115/118 (98%)	85 (74%)	22 (19%)	8 (7%)	1	4
47	BV	99/101 (98%)	57 (58%)	15 (15%)	27 (27%)	0	0
47	DV	99/101 (98%)	56 (57%)	15 (15%)	28 (28%)	0	0
48	BW	111/113 (98%)	88 (79%)	14 (13%)	9 (8%)	1	3
48	DW	111/113 (98%)	85 (77%)	18 (16%)	8 (7%)	1	4
49	BX	91/96 (95%)	52 (57%)	16 (18%)	23 (25%)	0	0
49	DX	91/96 (95%)	50 (55%)	18 (20%)	23 (25%)	0	0
50	BY	99/110 (90%)	49 (50%)	21 (21%)	29 (29%)	0	0
50	DY	99/110 (90%)	47 (48%)	23 (23%)	29 (29%)	0	0
51	BZ	175/206 (85%)	115 (66%)	44 (25%)	16 (9%)	0	2
51	DZ	175/206 (85%)	115 (66%)	41 (23%)	19 (11%)	0	1
All	All	11152/12056 (92%)	7925 (71%)	2047 (18%)	1180 (11%)	0	2

5 of 1180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	154	LEU
2	AB	165	VAL
2	AB	194	PRO
2	AB	195	ASP

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	175 (87%)	27 (13%)	4	18
2	CB	202/220 (92%)	175 (87%)	27 (13%)	4	18
3	AC	160/188 (85%)	153 (96%)	7 (4%)	25	60
3	CC	160/188 (85%)	153 (96%)	7 (4%)	25	60
4	AD	180/181 (99%)	148 (82%)	32 (18%)	2	10
4	CD	180/181 (99%)	149 (83%)	31 (17%)	2	11
5	AE	115/122 (94%)	93 (81%)	22 (19%)	1	8
5	CE	115/122 (94%)	93 (81%)	22 (19%)	1	8
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	21
6	CF	90/90 (100%)	80 (89%)	10 (11%)	6	25
7	AG	126/127 (99%)	121 (96%)	5 (4%)	28	62
7	CG	126/127 (99%)	120 (95%)	6 (5%)	23	57
8	AH	119/119 (100%)	108 (91%)	11 (9%)	8	33
8	CH	119/119 (100%)	108 (91%)	11 (9%)	8	33
9	AI	98/99 (99%)	90 (92%)	8 (8%)	10	37
9	CI	98/99 (99%)	90 (92%)	8 (8%)	10	37
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	11	38
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	11	38
11	AK	90/99 (91%)	81 (90%)	9 (10%)	7	29
11	CK	90/99 (91%)	81 (90%)	9 (10%)	7	29
12	AL	104/111 (94%)	92 (88%)	12 (12%)	5	24
12	CL	104/111 (94%)	91 (88%)	13 (12%)	4	20
13	AM	93/101 (92%)	87 (94%)	6 (6%)	15	47
13	CM	93/101 (92%)	88 (95%)	5 (5%)	20	53
14	AN	49/50 (98%)	46 (94%)	3 (6%)	17	49
14	CN	49/50 (98%)	46 (94%)	3 (6%)	17	49
15	AO	79/80 (99%)	70 (89%)	9 (11%)	5	24
15	CO	79/80 (99%)	71 (90%)	8 (10%)	7	29
16	AP	72/74 (97%)	59 (82%)	13 (18%)	2	9
16	CP	72/74 (97%)	59 (82%)	13 (18%)	2	9
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	8	31
18	AR	61/77 (79%)	56 (92%)	5 (8%)	10	37
18	CR	61/77 (79%)	55 (90%)	6 (10%)	7	30
19	AS	69/80 (86%)	63 (91%)	6 (9%)	9	35
19	CS	69/80 (86%)	63 (91%)	6 (9%)	9	35
20	AT	76/82 (93%)	65 (86%)	11 (14%)	3	15
20	CT	76/82 (93%)	65 (86%)	11 (14%)	3	15
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
22	B0	61/67 (91%)	53 (87%)	8 (13%)	4	19
22	D0	61/67 (91%)	51 (84%)	10 (16%)	2	12
23	B1	73/83 (88%)	52 (71%)	21 (29%)	0	2
23	D1	73/83 (88%)	53 (73%)	20 (27%)	0	2
24	B2	46/67 (69%)	25 (54%)	21 (46%)	0	0
24	D2	46/67 (69%)	25 (54%)	21 (46%)	0	0
25	B3	51/52 (98%)	44 (86%)	7 (14%)	3	17
25	D3	51/52 (98%)	44 (86%)	7 (14%)	3	17
27	B5	51/52 (98%)	38 (74%)	13 (26%)	0	3
27	D5	51/52 (98%)	38 (74%)	13 (26%)	0	3
28	B6	43/52 (83%)	23 (54%)	20 (46%)	0	0
28	D6	43/52 (83%)	24 (56%)	19 (44%)	0	0
29	B7	41/42 (98%)	33 (80%)	8 (20%)	1	8
29	D7	41/42 (98%)	33 (80%)	8 (20%)	1	8
30	B8	53/55 (96%)	40 (76%)	13 (24%)	1	4
30	D8	53/55 (96%)	41 (77%)	12 (23%)	1	5
33	BD	213/218 (98%)	167 (78%)	46 (22%)	1	6
33	DD	213/218 (98%)	167 (78%)	46 (22%)	1	6
34	BE	165/166 (99%)	126 (76%)	39 (24%)	1	4
34	DE	165/166 (99%)	125 (76%)	40 (24%)	1	4
35	BF	165/166 (99%)	126 (76%)	39 (24%)	1	4
35	DF	165/166 (99%)	124 (75%)	41 (25%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BG	155/156 (99%)	135 (87%)	20 (13%)	4	19
36	DG	155/156 (99%)	136 (88%)	19 (12%)	4	21
37	BH	132/148 (89%)	102 (77%)	30 (23%)	1	5
37	DH	132/148 (89%)	102 (77%)	30 (23%)	1	5
38	BI	122/124 (98%)	101 (83%)	21 (17%)	2	11
38	DI	122/124 (98%)	103 (84%)	19 (16%)	2	13
39	BN	117/119 (98%)	78 (67%)	39 (33%)	0	1
39	DN	117/119 (98%)	78 (67%)	39 (33%)	0	1
40	BO	100/100 (100%)	81 (81%)	19 (19%)	1	8
40	DO	100/100 (100%)	81 (81%)	19 (19%)	1	8
41	BP	112/116 (97%)	73 (65%)	39 (35%)	0	1
41	DP	112/116 (97%)	72 (64%)	40 (36%)	0	1
42	BQ	106/111 (96%)	78 (74%)	28 (26%)	0	3
42	DQ	106/111 (96%)	77 (73%)	29 (27%)	0	2
43	BR	100/101 (99%)	70 (70%)	30 (30%)	0	1
43	DR	100/101 (99%)	73 (73%)	27 (27%)	0	2
44	BS	77/88 (88%)	52 (68%)	25 (32%)	0	1
44	DS	77/88 (88%)	51 (66%)	26 (34%)	0	1
45	BT	116/127 (91%)	79 (68%)	37 (32%)	0	1
45	DT	116/127 (91%)	83 (72%)	33 (28%)	0	2
46	BU	92/94 (98%)	72 (78%)	20 (22%)	1	6
46	DU	92/94 (98%)	71 (77%)	21 (23%)	1	5
47	BV	82/82 (100%)	51 (62%)	31 (38%)	0	1
47	DV	82/82 (100%)	49 (60%)	33 (40%)	0	1
48	BW	91/92 (99%)	72 (79%)	19 (21%)	1	7
48	DW	91/92 (99%)	67 (74%)	24 (26%)	0	3
49	BX	74/78 (95%)	52 (70%)	22 (30%)	0	2
49	DX	74/78 (95%)	51 (69%)	23 (31%)	0	1
50	BY	84/91 (92%)	60 (71%)	24 (29%)	0	2
50	DY	84/91 (92%)	57 (68%)	27 (32%)	0	1
51	BZ	155/179 (87%)	129 (83%)	26 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	DZ	155/179 (87%)	129 (83%)	26 (17%)	2 11
All	All	9322/9874 (94%)	7560 (81%)	1762 (19%)	1 9

5 of 1762 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CD	94	LEU
25	D3	47	VAL
51	DZ	124	ILE
45	DT	82	LEU
5	CE	73	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 314 such sidechains are listed below:

Mol	Chain	Res	Type
30	D8	35	GLN
44	DS	34	HIS
33	DD	186	HIS
37	DH	158	HIS
48	DW	34	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	283 (18%)	29 (1%)
1	CA	1503/1522 (98%)	280 (18%)	29 (1%)
31	BA	2723/2787 (97%)	734 (26%)	73 (2%)
31	DA	2723/2787 (97%)	736 (27%)	70 (2%)
32	BB	118/122 (96%)	36 (30%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	1 (0%)
All	All	8688/8862 (98%)	2104 (24%)	203 (2%)

5 of 2104 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C

5 of 203 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	484	G
31	DA	474	G
31	DA	2796	U
1	CA	687	A
1	CA	1498	U

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 838 ligands modelled in this entry, 836 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	ERY	DA	3330	-	53,53,53	1.26	6 (11%)	82,82,82	0.99	4 (4%)
55	ERY	BA	3364	-	53,53,53	1.26	5 (9%)	82,82,82	0.99	4 (4%)

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	ERY	DA	3330	-	-	4/72/107/107	0/3/3/3
55	ERY	BA	3364	-	-	4/72/107/107	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BA	3364	ERY	C6-C5	3.39	1.61	1.55
55	DA	3330	ERY	C6-C5	3.37	1.61	1.55
55	BA	3364	ERY	C7-C6	2.59	1.58	1.54
55	DA	3330	ERY	C7-C6	2.57	1.58	1.54
55	DA	3330	ERY	O2-C13	2.30	1.50	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	3330	ERY	C3-C2-C1	-2.59	104.69	109.93
55	BA	3364	ERY	C3-C2-C1	-2.59	104.70	109.93
55	DA	3330	ERY	C25-C24-C23	-2.48	106.45	110.02
55	BA	3364	ERY	C25-C24-C23	-2.47	106.46	110.02
55	BA	3364	ERY	O5-C16-C17	2.13	106.95	103.86

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	BA	3364	ERY	O9-C22-O7-C5
55	DA	3330	ERY	O9-C22-O7-C5
55	BA	3364	ERY	O7-C5-C6-C7
55	DA	3330	ERY	O7-C5-C6-C7
55	BA	3364	ERY	C23-C22-O7-C5

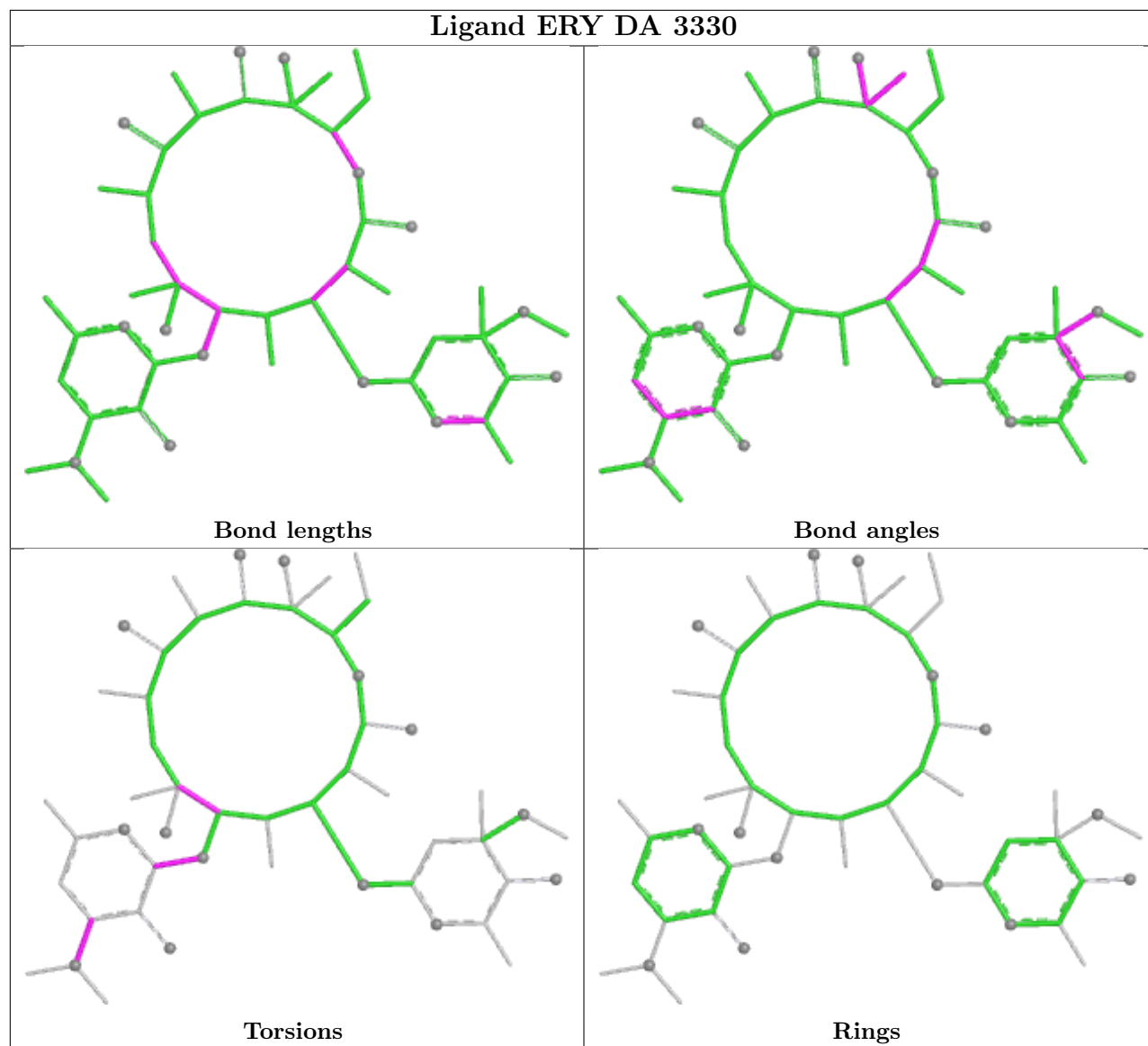
There are no ring outliers.

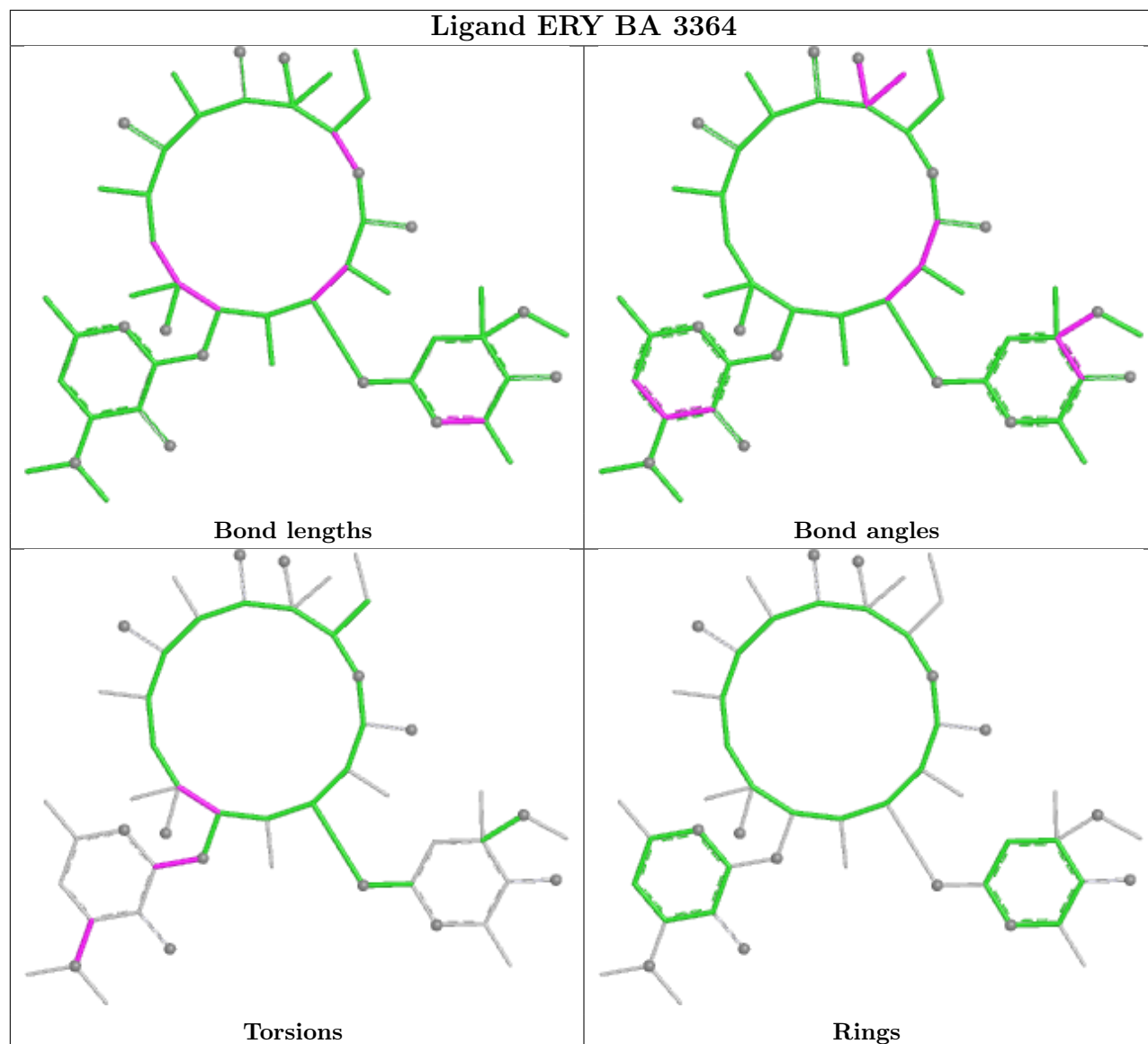
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	DA	3330	ERY	2	0
55	BA	3364	ERY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
36	DG	1
36	BG	1

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Mol	Chain	Number of breaks
28	B6	1
28	D6	1
9	AI	1
9	CI	1

The worst 5 of 12 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	5.58
1	AM	69:GLU	C	70:LEU	N	5.57
1	DG	112:PRO	C	113:ARG	N	4.82
1	BG	112:PRO	C	113:ARG	N	4.80
1	CM	97:PRO	C	98:VAL	N	4.38

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%)	1.47	387 (25%) 1 1	46, 116, 201, 202	0
1	CA	1504/1522 (98%)	1.41	353 (23%) 2 1	50, 115, 201, 203	0
2	AB	235/256 (91%)	1.86	75 (31%) 1 1	99, 157, 195, 200	0
2	CB	235/256 (91%)	1.77	85 (36%) 1 1	99, 162, 195, 201	0
3	AC	207/239 (86%)	1.75	58 (28%) 1 1	108, 163, 190, 198	0
3	CC	207/239 (86%)	1.90	75 (36%) 1 1	110, 168, 192, 198	0
4	AD	208/209 (99%)	1.88	84 (40%) 0 1	65, 126, 175, 189	0
4	CD	208/209 (99%)	2.08	89 (42%) 0 1	66, 124, 173, 191	0
5	AE	151/160 (94%)	1.39	35 (23%) 2 1	65, 111, 162, 199	0
5	CE	151/160 (94%)	1.64	48 (31%) 1 1	72, 115, 172, 198	0
6	AF	101/101 (100%)	1.47	24 (23%) 2 1	82, 123, 173, 192	0
6	CF	101/101 (100%)	1.90	37 (36%) 1 1	84, 130, 177, 196	0
7	AG	155/156 (99%)	2.04	69 (44%) 0 1	126, 177, 196, 201	0
7	CG	155/156 (99%)	1.83	53 (34%) 1 1	122, 177, 196, 200	0
8	AH	138/138 (100%)	1.67	41 (29%) 1 1	78, 113, 157, 171	0
8	CH	138/138 (100%)	1.69	42 (30%) 1 1	79, 115, 162, 171	0
9	AI	127/128 (99%)	2.54	72 (56%) 0 0	132, 189, 200, 201	0
9	CI	127/128 (99%)	2.60	78 (61%) 0 0	131, 190, 200, 202	0
10	AJ	99/105 (94%)	2.25	51 (51%) 0 0	119, 178, 199, 200	0
10	CJ	99/105 (94%)	2.45	59 (59%) 0 0	116, 182, 200, 201	0
11	AK	119/129 (92%)	1.82	48 (40%) 0 1	63, 113, 163, 199	0
11	CK	119/129 (92%)	1.80	41 (34%) 1 1	64, 116, 165, 199	0
12	AL	125/135 (92%)	1.78	45 (36%) 1 1	59, 98, 164, 201	0
12	CL	125/135 (92%)	1.94	47 (37%) 1 1	58, 99, 167, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	2.42	62 (53%)	0	0	157, 191, 200, 201	0
13	CM	115/126 (91%)	2.13	53 (46%)	0	0	152, 189, 199, 201	0
14	AN	60/61 (98%)	2.36	34 (56%)	0	0	112, 172, 197, 199	0
14	CN	60/61 (98%)	2.62	35 (58%)	0	0	112, 171, 197, 199	0
15	AO	88/89 (98%)	1.46	27 (30%)	1	1	70, 105, 160, 169	0
15	CO	88/89 (98%)	1.23	20 (22%)	2	1	71, 107, 162, 171	0
16	AP	84/88 (95%)	2.08	42 (50%)	0	0	82, 109, 170, 187	0
16	CP	84/88 (95%)	2.29	47 (55%)	0	0	80, 107, 165, 183	0
17	AQ	100/105 (95%)	1.71	35 (35%)	1	1	71, 104, 154, 185	0
17	CQ	100/105 (95%)	1.76	33 (33%)	1	1	74, 103, 154, 190	0
18	AR	70/88 (79%)	1.73	21 (30%)	1	1	80, 116, 173, 182	0
18	CR	70/88 (79%)	1.39	14 (20%)	3	2	83, 124, 175, 185	0
19	AS	79/93 (84%)	2.12	36 (45%)	0	0	127, 192, 200, 200	0
19	CS	79/93 (84%)	2.13	37 (46%)	0	0	131, 190, 200, 201	0
20	AT	99/106 (93%)	2.10	44 (44%)	0	1	75, 115, 162, 186	0
20	CT	99/106 (93%)	1.78	35 (35%)	1	1	74, 115, 160, 189	0
21	AU	25/27 (92%)	4.40	23 (92%)	0	0	144, 182, 197, 199	0
21	CU	25/27 (92%)	4.27	21 (84%)	0	0	139, 173, 194, 197	0
22	B0	85/85 (100%)	1.46	27 (31%)	1	1	39, 60, 177, 193	0
22	D0	85/85 (100%)	1.21	14 (16%)	4	3	44, 65, 177, 193	0
23	B1	89/98 (90%)	1.91	33 (37%)	1	1	39, 64, 143, 170	0
23	D1	89/98 (90%)	1.86	36 (40%)	0	1	41, 66, 144, 183	0
24	B2	51/72 (70%)	3.20	35 (68%)	0	0	47, 85, 185, 196	0
24	D2	51/72 (70%)	2.36	21 (41%)	0	1	53, 92, 191, 198	0
25	B3	60/60 (100%)	1.21	10 (16%)	4	3	36, 59, 135, 186	0
25	D3	60/60 (100%)	0.88	9 (15%)	5	3	42, 66, 141, 182	0
26	B4	32/71 (45%)	2.34	19 (59%)	0	0	133, 155, 186, 193	0
26	D4	32/71 (45%)	2.15	16 (50%)	0	0	143, 169, 187, 197	0
27	B5	58/60 (96%)	1.17	12 (20%)	2	2	20, 47, 177, 199	0
27	D5	58/60 (96%)	0.99	13 (22%)	2	1	23, 50, 176, 199	0
28	B6	45/54 (83%)	2.45	24 (53%)	0	0	41, 74, 129, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	1.89	19 (42%) 0 1	44, 77, 143, 178	0
29	B7	49/49 (100%)	0.68	7 (14%) 6 3	26, 33, 119, 175	0
29	D7	49/49 (100%)	0.56	7 (14%) 6 3	26, 35, 126, 174	0
30	B8	64/65 (98%)	2.01	23 (35%) 1 1	33, 54, 148, 179	0
30	D8	64/65 (98%)	1.65	19 (29%) 1 1	36, 58, 148, 180	0
31	BA	2725/2787 (97%)	0.23	224 (8%) 17 9	25, 47, 144, 203	0
31	DA	2725/2787 (97%)	0.25	180 (6%) 24 12	25, 52, 155, 202	0
32	BB	119/122 (97%)	1.95	46 (38%) 1 1	44, 92, 137, 191	0
32	DB	119/122 (97%)	1.97	45 (37%) 1 1	51, 101, 165, 190	0
33	BD	272/276 (98%)	0.53	22 (8%) 18 9	25, 49, 105, 183	0
33	DD	272/276 (98%)	0.57	25 (9%) 14 8	23, 53, 109, 172	0
34	BE	205/206 (99%)	0.84	39 (19%) 3 2	26, 54, 140, 193	0
34	DE	205/206 (99%)	0.85	29 (14%) 6 4	30, 58, 146, 193	0
35	BF	208/210 (99%)	0.92	31 (14%) 5 3	21, 65, 175, 198	0
35	DF	208/210 (99%)	0.79	25 (12%) 9 5	27, 68, 175, 199	0
36	BG	181/182 (99%)	2.44	91 (50%) 0 0	95, 145, 191, 201	0
36	DG	181/182 (99%)	2.44	93 (51%) 0 0	104, 162, 195, 202	0
37	BH	160/180 (88%)	2.80	100 (62%) 0 0	62, 103, 161, 193	0
37	DH	160/180 (88%)	1.75	56 (35%) 1 1	68, 117, 171, 193	0
38	BI	146/148 (98%)	2.19	67 (45%) 0 0	56, 144, 191, 200	0
38	DI	146/148 (98%)	2.89	88 (60%) 0 0	52, 164, 194, 201	0
39	BN	139/140 (99%)	1.56	43 (30%) 1 1	35, 63, 136, 190	0
39	DN	139/140 (99%)	1.06	24 (17%) 4 3	41, 69, 144, 191	0
40	BO	122/122 (100%)	0.52	5 (4%) 41 23	34, 57, 109, 141	0
40	DO	122/122 (100%)	0.49	9 (7%) 20 10	37, 59, 116, 146	0
41	BP	146/150 (97%)	2.07	64 (43%) 0 1	23, 83, 151, 201	0
41	DP	146/150 (97%)	1.67	47 (32%) 1 1	25, 88, 155, 201	0
42	BQ	136/141 (96%)	2.10	41 (30%) 1 1	38, 68, 149, 195	0
42	DQ	136/141 (96%)	1.63	37 (27%) 1 1	43, 74, 146, 195	0
43	BR	117/118 (99%)	0.50	14 (11%) 9 5	29, 45, 120, 144	0
43	DR	117/118 (99%)	0.56	14 (11%) 9 5	31, 51, 125, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	2.36	54 (54%)	0	0	49, 98, 144, 184	0
44	DS	99/112 (88%)	2.27	42 (42%)	0	1	59, 105, 160, 188	0
45	BT	132/146 (90%)	1.63	45 (34%)	1	1	43, 76, 154, 194	0
45	DT	132/146 (90%)	1.36	35 (26%)	1	1	47, 79, 162, 197	0
46	BU	117/118 (99%)	1.21	27 (23%)	2	1	29, 51, 121, 190	0
46	DU	117/118 (99%)	1.14	28 (23%)	2	1	35, 58, 130, 192	0
47	BV	101/101 (100%)	2.94	70 (69%)	0	0	32, 98, 188, 199	0
47	DV	101/101 (100%)	1.83	35 (34%)	1	1	39, 105, 189, 199	0
48	BW	113/113 (100%)	0.40	13 (11%)	9	6	27, 39, 106, 171	0
48	DW	113/113 (100%)	0.40	11 (9%)	13	7	28, 43, 109, 180	0
49	BX	93/96 (96%)	1.67	32 (34%)	1	1	37, 63, 144, 187	0
49	DX	93/96 (96%)	1.50	27 (29%)	1	1	40, 66, 144, 186	0
50	BY	101/110 (91%)	3.11	64 (63%)	0	0	44, 92, 194, 201	0
50	DY	101/110 (91%)	2.43	57 (56%)	0	0	53, 99, 192, 201	0
51	BZ	177/206 (85%)	1.92	70 (39%)	1	1	58, 103, 152, 180	0
51	DZ	177/206 (85%)	1.48	44 (24%)	2	1	63, 110, 156, 188	0
All	All	20062/20918 (95%)	1.26	5072 (25%)	1	1	20, 90, 194, 203	0

The worst 5 of 5072 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AG	5	ARG	24.6
42	BQ	140	ALA	21.9
17	CQ	101	ARG	17.7
42	BQ	141	GLN	16.8
42	BQ	91	GLU	14.8

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	AA	1644	1/1	0.51	0.30	87,87,87,87	0
52	MG	DA	3131	1/1	0.59	0.28	82,82,82,82	0
52	MG	BA	3254	1/1	0.73	0.22	55,55,55,55	0
52	MG	AA	1648	1/1	0.74	0.21	82,82,82,82	0
52	MG	BA	3361	1/1	0.76	0.17	60,60,60,60	0
52	MG	D3	101	1/1	0.76	0.39	52,52,52,52	0
52	MG	BA	3151	1/1	0.76	0.27	54,54,54,54	0
52	MG	AA	1642	1/1	0.77	0.36	73,73,73,73	0
52	MG	DA	3324	1/1	0.77	0.38	69,69,69,69	0
52	MG	DA	3162	1/1	0.78	0.24	51,51,51,51	0
52	MG	BA	3154	1/1	0.78	0.37	79,79,79,79	0
52	MG	CA	1630	1/1	0.79	0.36	73,73,73,73	0
52	MG	AA	1645	1/1	0.79	0.26	75,75,75,75	0
52	MG	BA	3165	1/1	0.79	0.15	44,44,44,44	0
52	MG	AA	1649	1/1	0.79	0.36	62,62,62,62	0
52	MG	DA	3309	1/1	0.79	0.27	62,62,62,62	0
52	MG	AA	1646	1/1	0.79	0.15	51,51,51,51	0
52	MG	BA	3304	1/1	0.80	0.25	55,55,55,55	0
52	MG	BA	3243	1/1	0.80	0.19	57,57,57,57	0
52	MG	CA	1608	1/1	0.80	0.33	74,74,74,74	0
52	MG	DA	3209	1/1	0.80	0.41	58,58,58,58	0
52	MG	DA	3247	1/1	0.80	0.34	76,76,76,76	0
52	MG	AA	1640	1/1	0.80	0.14	67,67,67,67	0
52	MG	CA	1649	1/1	0.80	0.15	63,63,63,63	0
52	MG	CA	1618	1/1	0.81	0.27	65,65,65,65	0
52	MG	BA	3311	1/1	0.81	0.27	62,62,62,62	0
52	MG	DA	3225	1/1	0.81	0.15	51,51,51,51	0
52	MG	BA	3174	1/1	0.81	0.17	40,40,40,40	0
52	MG	DA	3271	1/1	0.81	0.24	61,61,61,61	0
52	MG	DA	3277	1/1	0.81	0.29	76,76,76,76	0
52	MG	AA	1606	1/1	0.81	0.25	89,89,89,89	0
52	MG	CA	1612	1/1	0.81	0.20	68,68,68,68	0
52	MG	AA	1616	1/1	0.82	0.33	76,76,76,76	0
52	MG	DA	3176	1/1	0.82	0.26	44,44,44,44	0
52	MG	BA	3357	1/1	0.82	0.27	71,71,71,71	0
52	MG	BA	3358	1/1	0.82	0.41	80,80,80,80	0
52	MG	BA	3288	1/1	0.82	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3248	1/1	0.82	0.27	46,46,46,46	0
52	MG	DA	3005	1/1	0.82	0.13	63,63,63,63	0
52	MG	DA	3072	1/1	0.82	0.45	58,58,58,58	0
52	MG	DA	3316	1/1	0.82	0.20	60,60,60,60	0
52	MG	CA	1610	1/1	0.82	0.14	90,90,90,90	0
52	MG	DA	3276	1/1	0.83	0.20	65,65,65,65	0
52	MG	DA	3220	1/1	0.83	0.24	40,40,40,40	0
52	MG	CA	1637	1/1	0.83	0.19	61,61,61,61	0
52	MG	AA	1647	1/1	0.83	0.32	62,62,62,62	0
52	MG	BA	3175	1/1	0.83	0.16	62,62,62,62	0
52	MG	BA	3347	1/1	0.84	0.25	43,43,43,43	0
52	MG	CA	1625	1/1	0.84	0.15	54,54,54,54	0
52	MG	DA	3185	1/1	0.84	0.40	53,53,53,53	0
52	MG	DA	3189	1/1	0.84	0.23	42,42,42,42	0
52	MG	BA	3155	1/1	0.84	0.21	55,55,55,55	0
52	MG	CA	1634	1/1	0.84	0.23	63,63,63,63	0
52	MG	CA	1635	1/1	0.84	0.18	77,77,77,77	0
52	MG	DA	3246	1/1	0.84	0.24	67,67,67,67	0
52	MG	BA	3162	1/1	0.84	0.24	60,60,60,60	0
52	MG	DA	3248	1/1	0.84	0.18	82,82,82,82	0
52	MG	BA	3112	1/1	0.84	0.20	38,38,38,38	0
52	MG	AA	1638	1/1	0.84	0.20	67,67,67,67	0
52	MG	AA	1651	1/1	0.84	0.37	57,57,57,57	0
52	MG	CA	1611	1/1	0.84	0.27	65,65,65,65	0
52	MG	BA	3217	1/1	0.84	0.14	38,38,38,38	0
52	MG	DA	3144	1/1	0.84	0.18	48,48,48,48	0
52	MG	BA	3166	1/1	0.85	0.18	47,47,47,47	0
52	MG	BA	3238	1/1	0.85	0.16	40,40,40,40	0
52	MG	DA	3191	1/1	0.85	0.20	45,45,45,45	0
52	MG	CA	1639	1/1	0.85	0.31	70,70,70,70	0
52	MG	BA	3305	1/1	0.85	0.24	43,43,43,43	0
52	MG	BA	3003	1/1	0.85	0.21	52,52,52,52	0
52	MG	BA	3330	1/1	0.85	0.15	72,72,72,72	0
52	MG	BA	3074	1/1	0.85	0.37	60,60,60,60	0
52	MG	DA	3079	1/1	0.85	0.21	41,41,41,41	0
52	MG	DA	3081	1/1	0.85	0.31	48,48,48,48	0
52	MG	DA	3123	1/1	0.85	0.10	57,57,57,57	0
52	MG	CA	1624	1/1	0.85	0.16	55,55,55,55	0
52	MG	BA	3206	1/1	0.85	0.38	57,57,57,57	0
52	MG	BA	3263	1/1	0.85	0.11	26,26,26,26	0
52	MG	BA	3360	1/1	0.85	0.17	64,64,64,64	0
52	MG	CA	1648	1/1	0.86	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	CA	1613	1/1	0.86	0.34	68,68,68,68	0
52	MG	BA	3120	1/1	0.86	0.17	45,45,45,45	0
52	MG	BA	3245	1/1	0.86	0.16	56,56,56,56	0
52	MG	DA	3200	1/1	0.86	0.24	46,46,46,46	0
52	MG	BA	3333	1/1	0.86	0.13	51,51,51,51	0
52	MG	DA	3074	1/1	0.86	0.26	55,55,55,55	0
52	MG	DA	3223	1/1	0.86	0.09	41,41,41,41	0
52	MG	CA	1604	1/1	0.86	0.24	88,88,88,88	0
52	MG	DA	3233	1/1	0.86	0.34	52,52,52,52	0
52	MG	BA	3336	1/1	0.86	0.26	69,69,69,69	0
52	MG	DA	3092	1/1	0.86	0.37	40,40,40,40	0
52	MG	BA	3344	1/1	0.86	0.27	60,60,60,60	0
52	MG	DA	3258	1/1	0.86	0.17	52,52,52,52	0
52	MG	DA	3130	1/1	0.86	0.35	59,59,59,59	0
52	MG	BA	3110	1/1	0.86	0.35	36,36,36,36	0
52	MG	CA	1638	1/1	0.86	0.21	61,61,61,61	0
52	MG	DA	3158	1/1	0.86	0.09	53,53,53,53	0
52	MG	DA	3313	1/1	0.86	0.22	66,66,66,66	0
52	MG	AA	1613	1/1	0.86	0.22	76,76,76,76	0
52	MG	DA	3164	1/1	0.86	0.20	49,49,49,49	0
52	MG	DA	3325	1/1	0.86	0.27	67,67,67,67	0
52	MG	DA	3222	1/1	0.87	0.16	44,44,44,44	0
52	MG	AA	1607	1/1	0.87	0.27	58,58,58,58	0
52	MG	AA	1614	1/1	0.87	0.28	49,49,49,49	0
52	MG	AA	1608	1/1	0.87	0.31	80,80,80,80	0
52	MG	DA	3239	1/1	0.87	0.13	29,29,29,29	0
52	MG	BA	3204	1/1	0.87	0.26	43,43,43,43	0
52	MG	AA	1622	1/1	0.87	0.31	63,63,63,63	0
52	MG	BA	3208	1/1	0.87	0.15	41,41,41,41	0
52	MG	BA	3315	1/1	0.87	0.37	52,52,52,52	0
52	MG	BA	3327	1/1	0.87	0.17	48,48,48,48	0
52	MG	AA	1653	1/1	0.87	0.12	61,61,61,61	0
52	MG	AA	1654	1/1	0.87	0.26	69,69,69,69	0
52	MG	DA	3297	1/1	0.87	0.09	21,21,21,21	0
52	MG	DA	3300	1/1	0.87	0.33	64,64,64,64	0
52	MG	DA	3301	1/1	0.87	0.30	54,54,54,54	0
52	MG	DA	3306	1/1	0.87	0.13	69,69,69,69	0
52	MG	DA	3068	1/1	0.87	0.24	56,56,56,56	0
52	MG	AA	1611	1/1	0.87	0.12	82,82,82,82	0
52	MG	BA	3031	1/1	0.87	0.25	50,50,50,50	0
52	MG	BA	3054	1/1	0.87	0.14	47,47,47,47	0
52	MG	CA	1627	1/1	0.87	0.36	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3328	1/1	0.87	0.35	81,81,81,81	0
54	K	DA	3329	1/1	0.87	0.12	55,55,55,55	0
52	MG	DA	3190	1/1	0.88	0.27	43,43,43,43	0
52	MG	AA	1650	1/1	0.88	0.23	60,60,60,60	0
52	MG	BA	3240	1/1	0.88	0.13	42,42,42,42	0
52	MG	BA	3183	1/1	0.88	0.09	54,54,54,54	0
52	MG	DA	3018	1/1	0.88	0.10	23,23,23,23	0
52	MG	BA	3187	1/1	0.88	0.20	48,48,48,48	0
52	MG	BA	3196	1/1	0.88	0.16	30,30,30,30	0
52	MG	BA	3201	1/1	0.88	0.41	51,51,51,51	0
52	MG	AA	1635	1/1	0.88	0.15	69,69,69,69	0
52	MG	BA	3345	1/1	0.88	0.25	48,48,48,48	0
52	MG	DA	3083	1/1	0.88	0.29	38,38,38,38	0
52	MG	DA	3091	1/1	0.88	0.24	31,31,31,31	0
52	MG	BA	3278	1/1	0.88	0.12	39,39,39,39	0
52	MG	DA	3120	1/1	0.88	0.36	55,55,55,55	0
52	MG	CA	1628	1/1	0.88	0.17	73,73,73,73	0
52	MG	DA	3128	1/1	0.88	0.16	47,47,47,47	0
52	MG	CA	1629	1/1	0.88	0.11	67,67,67,67	0
52	MG	DA	3280	1/1	0.88	0.31	64,64,64,64	0
52	MG	DA	3293	1/1	0.88	0.25	62,62,62,62	0
52	MG	DA	3294	1/1	0.88	0.30	65,65,65,65	0
52	MG	DA	3295	1/1	0.88	0.09	46,46,46,46	0
52	MG	BA	3350	1/1	0.88	0.07	65,65,65,65	0
52	MG	DA	3134	1/1	0.88	0.12	67,67,67,67	0
52	MG	BA	3107	1/1	0.88	0.15	28,28,28,28	0
52	MG	DA	3146	1/1	0.88	0.28	52,52,52,52	0
52	MG	BA	3152	1/1	0.88	0.17	55,55,55,55	0
52	MG	AA	1604	1/1	0.88	0.22	73,73,73,73	0
52	MG	BA	3306	1/1	0.88	0.23	52,52,52,52	0
52	MG	DA	3172	1/1	0.88	0.25	56,56,56,56	0
52	MG	BA	3310	1/1	0.88	0.30	59,59,59,59	0
52	MG	DA	3326	1/1	0.88	0.19	52,52,52,52	0
52	MG	DA	3327	1/1	0.88	0.31	60,60,60,60	0
52	MG	CA	1643	1/1	0.88	0.33	57,57,57,57	0
52	MG	DB	201	1/1	0.88	0.39	58,58,58,58	0
52	MG	DR	201	1/1	0.88	0.11	37,37,37,37	0
52	MG	CA	1607	1/1	0.88	0.40	58,58,58,58	0
52	MG	DA	3034	1/1	0.89	0.28	51,51,51,51	0
52	MG	DA	3136	1/1	0.89	0.13	33,33,33,33	0
52	MG	DA	3041	1/1	0.89	0.24	31,31,31,31	0
52	MG	CA	1606	1/1	0.89	0.25	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	3252	1/1	0.89	0.32	54,54,54,54	0
52	MG	DA	3256	1/1	0.89	0.24	82,82,82,82	0
52	MG	DA	3150	1/1	0.89	0.39	72,72,72,72	0
52	MG	DA	3267	1/1	0.89	0.28	49,49,49,49	0
52	MG	DA	3270	1/1	0.89	0.13	44,44,44,44	0
52	MG	DA	3069	1/1	0.89	0.23	65,65,65,65	0
52	MG	DA	3272	1/1	0.89	0.18	42,42,42,42	0
52	MG	BA	3295	1/1	0.89	0.26	34,34,34,34	0
52	MG	DA	3163	1/1	0.89	0.24	59,59,59,59	0
52	MG	DA	3278	1/1	0.89	0.32	74,74,74,74	0
52	MG	BA	3242	1/1	0.89	0.21	44,44,44,44	0
52	MG	DA	3289	1/1	0.89	0.29	65,65,65,65	0
52	MG	DA	3170	1/1	0.89	0.12	61,61,61,61	0
52	MG	BA	3090	1/1	0.89	0.17	18,18,18,18	0
52	MG	BA	3170	1/1	0.89	0.23	31,31,31,31	0
52	MG	AA	1617	1/1	0.89	0.14	57,57,57,57	0
52	MG	DA	3084	1/1	0.89	0.25	38,38,38,38	0
52	MG	DA	3090	1/1	0.89	0.20	34,34,34,34	0
52	MG	BA	3352	1/1	0.89	0.33	62,62,62,62	0
52	MG	DA	3308	1/1	0.89	0.17	36,36,36,36	0
52	MG	AA	1637	1/1	0.89	0.23	53,53,53,53	0
52	MG	DA	3204	1/1	0.89	0.25	53,53,53,53	0
52	MG	DA	3117	1/1	0.89	0.18	45,45,45,45	0
52	MG	DA	3219	1/1	0.89	0.20	57,57,57,57	0
52	MG	AA	1609	1/1	0.89	0.28	50,50,50,50	0
52	MG	AA	1639	1/1	0.89	0.24	49,49,49,49	0
52	MG	CA	1626	1/1	0.89	0.25	65,65,65,65	0
52	MG	BA	3285	1/1	0.89	0.21	59,59,59,59	0
52	MG	DA	3226	1/1	0.89	0.15	40,40,40,40	0
52	MG	DA	3231	1/1	0.89	0.34	58,58,58,58	0
52	MG	BA	3121	1/1	0.89	0.23	38,38,38,38	0
52	MG	DA	3037	1/1	0.90	0.28	35,35,35,35	0
52	MG	CA	1619	1/1	0.90	0.28	47,47,47,47	0
52	MG	BA	3185	1/1	0.90	0.14	46,46,46,46	0
52	MG	DA	3262	1/1	0.90	0.23	57,57,57,57	0
52	MG	DA	3264	1/1	0.90	0.31	58,58,58,58	0
52	MG	DA	3266	1/1	0.90	0.20	74,74,74,74	0
52	MG	BA	3356	1/1	0.90	0.28	60,60,60,60	0
52	MG	AA	1629	1/1	0.90	0.09	41,41,41,41	0
52	MG	BA	3159	1/1	0.90	0.22	43,43,43,43	0
52	MG	BA	3115	1/1	0.90	0.07	49,49,49,49	0
52	MG	AA	1631	1/1	0.90	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BP	203	1/1	0.90	0.29	55,55,55,55	0
52	MG	CA	1632	1/1	0.90	0.18	63,63,63,63	0
52	MG	CA	1601	1/1	0.90	0.19	72,72,72,72	0
52	MG	CA	1603	1/1	0.90	0.25	44,44,44,44	0
52	MG	BA	3100	1/1	0.90	0.21	28,28,28,28	0
52	MG	DA	3207	1/1	0.90	0.16	56,56,56,56	0
52	MG	BA	3142	1/1	0.90	0.23	33,33,33,33	0
52	MG	DA	3214	1/1	0.90	0.28	48,48,48,48	0
52	MG	DA	3298	1/1	0.90	0.14	46,46,46,46	0
52	MG	DA	3218	1/1	0.90	0.18	41,41,41,41	0
52	MG	BA	3101	1/1	0.90	0.23	43,43,43,43	0
52	MG	DA	3305	1/1	0.90	0.41	83,83,83,83	0
52	MG	BA	3226	1/1	0.90	0.14	14,14,14,14	0
52	MG	BA	3340	1/1	0.90	0.23	45,45,45,45	0
52	MG	BA	3291	1/1	0.90	0.14	38,38,38,38	0
52	MG	BA	3293	1/1	0.90	0.17	36,36,36,36	0
52	MG	BA	3037	1/1	0.90	0.22	22,22,22,22	0
52	MG	DA	3320	1/1	0.90	0.40	68,68,68,68	0
52	MG	DA	3321	1/1	0.90	0.06	34,34,34,34	0
52	MG	DA	3229	1/1	0.90	0.26	52,52,52,52	0
52	MG	DA	3014	1/1	0.90	0.29	56,56,56,56	0
52	MG	DA	3139	1/1	0.90	0.19	44,44,44,44	0
52	MG	DA	3236	1/1	0.90	0.19	43,43,43,43	0
52	MG	CA	1616	1/1	0.90	0.33	67,67,67,67	0
52	MG	DA	3033	1/1	0.90	0.14	43,43,43,43	0
52	MG	AA	1605	1/1	0.90	0.27	69,69,69,69	0
54	K	BA	3363	1/1	0.90	0.11	43,43,43,43	0
52	MG	DA	3156	1/1	0.90	0.12	39,39,39,39	0
52	MG	DA	3138	1/1	0.91	0.31	47,47,47,47	0
52	MG	BA	3319	1/1	0.91	0.11	64,64,64,64	0
52	MG	DA	3141	1/1	0.91	0.43	70,70,70,70	0
52	MG	DA	3021	1/1	0.91	0.14	48,48,48,48	0
52	MG	DA	3254	1/1	0.91	0.17	68,68,68,68	0
52	MG	DA	3022	1/1	0.91	0.19	39,39,39,39	0
52	MG	DA	3023	1/1	0.91	0.27	38,38,38,38	0
52	MG	DA	3260	1/1	0.91	0.15	65,65,65,65	0
52	MG	DA	3153	1/1	0.91	0.24	54,54,54,54	0
52	MG	BA	3237	1/1	0.91	0.22	40,40,40,40	0
52	MG	BA	3362	1/1	0.91	0.27	70,70,70,70	0
52	MG	BA	3001	1/1	0.91	0.26	46,46,46,46	0
52	MG	AA	1620	1/1	0.91	0.36	51,51,51,51	0
52	MG	DA	3043	1/1	0.91	0.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3058	1/1	0.91	0.20	48,48,48,48	0
52	MG	DA	3063	1/1	0.91	0.28	44,44,44,44	0
52	MG	BA	3292	1/1	0.91	0.29	56,56,56,56	0
52	MG	DA	3181	1/1	0.91	0.33	44,44,44,44	0
52	MG	DA	3184	1/1	0.91	0.21	57,57,57,57	0
52	MG	DA	3282	1/1	0.91	0.08	48,48,48,48	0
52	MG	DA	3283	1/1	0.91	0.36	67,67,67,67	0
52	MG	DA	3285	1/1	0.91	0.06	49,49,49,49	0
52	MG	BA	3337	1/1	0.91	0.22	47,47,47,47	0
52	MG	DA	3290	1/1	0.91	0.08	46,46,46,46	0
52	MG	DA	3292	1/1	0.91	0.17	54,54,54,54	0
52	MG	BA	3021	1/1	0.91	0.11	22,22,22,22	0
52	MG	DA	3073	1/1	0.91	0.21	31,31,31,31	0
52	MG	BA	3202	1/1	0.91	0.15	54,54,54,54	0
52	MG	DA	3193	1/1	0.91	0.11	46,46,46,46	0
52	MG	DA	3195	1/1	0.91	0.24	42,42,42,42	0
52	MG	AA	1630	1/1	0.91	0.25	51,51,51,51	0
52	MG	AA	1612	1/1	0.91	0.33	70,70,70,70	0
52	MG	DA	3304	1/1	0.91	0.17	65,65,65,65	0
52	MG	AA	1634	1/1	0.91	0.36	55,55,55,55	0
52	MG	BA	3113	1/1	0.91	0.27	33,33,33,33	0
52	MG	DA	3088	1/1	0.91	0.14	32,32,32,32	0
52	MG	CA	1642	1/1	0.91	0.22	55,55,55,55	0
52	MG	AA	1624	1/1	0.91	0.34	58,58,58,58	0
52	MG	CA	1644	1/1	0.91	0.25	62,62,62,62	0
52	MG	CA	1645	1/1	0.91	0.26	64,64,64,64	0
52	MG	DA	3119	1/1	0.91	0.18	50,50,50,50	0
52	MG	CA	1646	1/1	0.91	0.29	59,59,59,59	0
52	MG	CA	1647	1/1	0.91	0.16	66,66,66,66	0
52	MG	CA	1615	1/1	0.91	0.23	69,69,69,69	0
52	MG	BA	3312	1/1	0.91	0.11	40,40,40,40	0
52	MG	BA	3282	1/1	0.91	0.28	55,55,55,55	0
52	MG	BA	3359	1/1	0.91	0.20	52,52,52,52	0
52	MG	DB	202	1/1	0.91	0.23	51,51,51,51	0
52	MG	DF	301	1/1	0.91	0.21	57,57,57,57	0
52	MG	CA	1621	1/1	0.91	0.28	54,54,54,54	0
52	MG	DA	3240	1/1	0.91	0.20	42,42,42,42	0
52	MG	DA	3244	1/1	0.91	0.18	32,32,32,32	0
52	MG	DA	3108	1/1	0.92	0.21	30,30,30,30	0
52	MG	DA	3235	1/1	0.92	0.15	40,40,40,40	0
52	MG	BA	3064	1/1	0.92	0.23	52,52,52,52	0
52	MG	DA	3237	1/1	0.92	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3238	1/1	0.92	0.23	59,59,59,59	0
52	MG	BA	3173	1/1	0.92	0.19	31,31,31,31	0
52	MG	BB	207	1/1	0.92	0.15	62,62,62,62	0
52	MG	DA	3242	1/1	0.92	0.20	53,53,53,53	0
52	MG	DA	3121	1/1	0.92	0.26	44,44,44,44	0
52	MG	DA	3122	1/1	0.92	0.12	48,48,48,48	0
52	MG	BP	202	1/1	0.92	0.05	0,0,0,0	0
52	MG	AA	1628	1/1	0.92	0.34	70,70,70,70	0
52	MG	BA	3309	1/1	0.92	0.09	55,55,55,55	0
52	MG	DA	3253	1/1	0.92	0.12	58,58,58,58	0
52	MG	BA	3140	1/1	0.92	0.05	46,46,46,46	0
52	MG	BA	3176	1/1	0.92	0.11	45,45,45,45	0
52	MG	BA	3004	1/1	0.92	0.32	28,28,28,28	0
52	MG	DA	3137	1/1	0.92	0.24	31,31,31,31	0
52	MG	DA	3261	1/1	0.92	0.22	63,63,63,63	0
52	MG	D5	101	1/1	0.92	0.23	35,35,35,35	0
52	MG	BA	3313	1/1	0.92	0.17	38,38,38,38	0
52	MG	DA	3140	1/1	0.92	0.20	52,52,52,52	0
52	MG	DA	3010	1/1	0.92	0.28	51,51,51,51	0
52	MG	BA	3314	1/1	0.92	0.18	49,49,49,49	0
52	MG	BA	3244	1/1	0.92	0.21	60,60,60,60	0
52	MG	BA	3316	1/1	0.92	0.12	31,31,31,31	0
52	MG	BA	3010	1/1	0.92	0.29	33,33,33,33	0
52	MG	AA	1652	1/1	0.92	0.17	66,66,66,66	0
52	MG	DA	3027	1/1	0.92	0.35	34,34,34,34	0
52	MG	DA	3279	1/1	0.92	0.16	59,59,59,59	0
52	MG	DA	3161	1/1	0.92	0.32	57,57,57,57	0
52	MG	DA	3031	1/1	0.92	0.13	62,62,62,62	0
52	MG	BA	3249	1/1	0.92	0.25	63,63,63,63	0
52	MG	BA	3332	1/1	0.92	0.21	40,40,40,40	0
52	MG	CA	1617	1/1	0.92	0.31	54,54,54,54	0
52	MG	DA	3038	1/1	0.92	0.25	26,26,26,26	0
52	MG	DA	3291	1/1	0.92	0.23	62,62,62,62	0
52	MG	BA	3190	1/1	0.92	0.24	23,23,23,23	0
52	MG	DA	3177	1/1	0.92	0.14	34,34,34,34	0
52	MG	DA	3179	1/1	0.92	0.34	39,39,39,39	0
52	MG	BA	3257	1/1	0.92	0.06	23,23,23,23	0
52	MG	DA	3183	1/1	0.92	0.28	56,56,56,56	0
52	MG	DA	3051	1/1	0.92	0.26	36,36,36,36	0
52	MG	DA	3056	1/1	0.92	0.10	14,14,14,14	0
52	MG	BA	3105	1/1	0.92	0.25	34,34,34,34	0
52	MG	BA	3338	1/1	0.92	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3268	1/1	0.92	0.10	39,39,39,39	0
52	MG	BA	3200	1/1	0.92	0.32	36,36,36,36	0
52	MG	BA	3281	1/1	0.92	0.33	61,61,61,61	0
52	MG	BA	3022	1/1	0.92	0.15	37,37,37,37	0
52	MG	BA	3349	1/1	0.92	0.07	33,33,33,33	0
52	MG	DA	3315	1/1	0.92	0.16	48,48,48,48	0
52	MG	AA	1633	1/1	0.92	0.06	39,39,39,39	0
52	MG	DA	3208	1/1	0.92	0.18	57,57,57,57	0
52	MG	BA	3203	1/1	0.92	0.28	46,46,46,46	0
52	MG	BA	3032	1/1	0.92	0.26	28,28,28,28	0
52	MG	BA	3163	1/1	0.92	0.22	31,31,31,31	0
52	MG	CA	1636	1/1	0.92	0.47	76,76,76,76	0
52	MG	DA	3089	1/1	0.92	0.17	29,29,29,29	0
52	MG	DA	3221	1/1	0.92	0.26	40,40,40,40	0
52	MG	AA	1603	1/1	0.92	0.15	45,45,45,45	0
52	MG	AA	1627	1/1	0.92	0.15	51,51,51,51	0
52	MG	BA	3300	1/1	0.92	0.20	48,48,48,48	0
52	MG	DP	201	1/1	0.92	0.06	27,27,27,27	0
52	MG	DA	3093	1/1	0.92	0.27	48,48,48,48	0
52	MG	DX	101	1/1	0.92	0.15	63,63,63,63	0
52	MG	DA	3105	1/1	0.92	0.09	43,43,43,43	0
52	MG	DA	3107	1/1	0.92	0.23	30,30,30,30	0
52	MG	BA	3083	1/1	0.93	0.29	35,35,35,35	0
52	MG	DA	3196	1/1	0.93	0.25	45,45,45,45	0
52	MG	BA	3234	1/1	0.93	0.19	53,53,53,53	0
52	MG	DA	3057	1/1	0.93	0.23	35,35,35,35	0
52	MG	BA	3235	1/1	0.93	0.17	34,34,34,34	0
52	MG	BA	3117	1/1	0.93	0.13	42,42,42,42	0
52	MG	DA	3064	1/1	0.93	0.19	47,47,47,47	0
52	MG	DA	3213	1/1	0.93	0.24	30,30,30,30	0
52	MG	BA	3086	1/1	0.93	0.20	24,24,24,24	0
52	MG	BA	3036	1/1	0.93	0.25	19,19,19,19	0
52	MG	CA	1620	1/1	0.93	0.26	58,58,58,58	0
52	MG	BA	3122	1/1	0.93	0.20	35,35,35,35	0
52	MG	BA	3123	1/1	0.93	0.31	39,39,39,39	0
52	MG	DA	3077	1/1	0.93	0.16	33,33,33,33	0
52	MG	BA	3137	1/1	0.93	0.18	10,10,10,10	0
52	MG	DA	3080	1/1	0.93	0.39	46,46,46,46	0
52	MG	BA	3320	1/1	0.93	0.24	50,50,50,50	0
52	MG	DA	3227	1/1	0.93	0.30	42,42,42,42	0
52	MG	DA	3082	1/1	0.93	0.18	47,47,47,47	0
52	MG	BA	3321	1/1	0.93	0.09	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	BA	3093	1/1	0.93	0.23	37,37,37,37	0
52	MG	DA	3234	1/1	0.93	0.16	46,46,46,46	0
52	MG	DA	3085	1/1	0.93	0.10	22,22,22,22	0
52	MG	BA	3328	1/1	0.93	0.26	56,56,56,56	0
52	MG	BA	3246	1/1	0.93	0.15	46,46,46,46	0
52	MG	BA	3097	1/1	0.93	0.22	54,54,54,54	0
52	MG	BA	3186	1/1	0.93	0.17	38,38,38,38	0
52	MG	BA	3144	1/1	0.93	0.31	37,37,37,37	0
52	MG	BA	3188	1/1	0.93	0.21	57,57,57,57	0
52	MG	DA	3094	1/1	0.93	0.24	34,34,34,34	0
52	MG	DA	3097	1/1	0.93	0.16	33,33,33,33	0
52	MG	DA	3098	1/1	0.93	0.22	28,28,28,28	0
52	MG	DA	3100	1/1	0.93	0.21	37,37,37,37	0
52	MG	BA	3262	1/1	0.93	0.17	25,25,25,25	0
52	MG	BA	3146	1/1	0.93	0.21	37,37,37,37	0
52	MG	BA	3265	1/1	0.93	0.15	41,41,41,41	0
52	MG	DA	3109	1/1	0.93	0.15	42,42,42,42	0
52	MG	DA	3110	1/1	0.93	0.11	45,45,45,45	0
52	MG	DA	3259	1/1	0.93	0.11	49,49,49,49	0
52	MG	DA	3113	1/1	0.93	0.31	52,52,52,52	0
52	MG	DA	3115	1/1	0.93	0.29	44,44,44,44	0
52	MG	DA	3116	1/1	0.93	0.09	62,62,62,62	0
52	MG	CA	1640	1/1	0.93	0.19	42,42,42,42	0
52	MG	BA	3266	1/1	0.93	0.17	48,48,48,48	0
52	MG	BA	3191	1/1	0.93	0.17	21,21,21,21	0
52	MG	BA	3269	1/1	0.93	0.11	43,43,43,43	0
52	MG	BA	3270	1/1	0.93	0.22	66,66,66,66	0
52	MG	BA	3271	1/1	0.93	0.29	38,38,38,38	0
52	MG	DA	3127	1/1	0.93	0.18	38,38,38,38	0
52	MG	BA	3274	1/1	0.93	0.22	36,36,36,36	0
52	MG	BA	3275	1/1	0.93	0.23	40,40,40,40	0
52	MG	BA	3195	1/1	0.93	0.24	31,31,31,31	0
52	MG	CA	1650	1/1	0.93	0.23	58,58,58,58	0
52	MG	DA	3281	1/1	0.93	0.19	51,51,51,51	0
52	MG	D0	101	1/1	0.93	0.08	46,46,46,46	0
52	MG	AA	1619	1/1	0.93	0.21	49,49,49,49	0
52	MG	BA	3197	1/1	0.93	0.26	47,47,47,47	0
52	MG	D7	101	1/1	0.93	0.10	38,38,38,38	0
52	MG	DA	3001	1/1	0.93	0.13	56,56,56,56	0
52	MG	DA	3004	1/1	0.93	0.24	29,29,29,29	0
52	MG	DA	3142	1/1	0.93	0.26	37,37,37,37	0
52	MG	AA	1621	1/1	0.93	0.36	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3145	1/1	0.93	0.24	59,59,59,59	0
52	MG	BA	3056	1/1	0.93	0.08	24,24,24,24	0
52	MG	BB	205	1/1	0.93	0.12	64,64,64,64	0
52	MG	DA	3151	1/1	0.93	0.27	47,47,47,47	0
52	MG	DA	3152	1/1	0.93	0.13	30,30,30,30	0
52	MG	DA	3015	1/1	0.93	0.20	39,39,39,39	0
52	MG	DA	3303	1/1	0.93	0.06	47,47,47,47	0
52	MG	DA	3154	1/1	0.93	0.09	49,49,49,49	0
52	MG	B1	101	1/1	0.93	0.19	35,35,35,35	0
52	MG	DA	3157	1/1	0.93	0.44	52,52,52,52	0
52	MG	DA	3020	1/1	0.93	0.28	35,35,35,35	0
52	MG	DA	3159	1/1	0.93	0.20	48,48,48,48	0
52	MG	DA	3310	1/1	0.93	0.30	56,56,56,56	0
52	MG	DA	3311	1/1	0.93	0.14	45,45,45,45	0
52	MG	BA	3156	1/1	0.93	0.26	26,26,26,26	0
52	MG	BA	3158	1/1	0.93	0.18	30,30,30,30	0
52	MG	BA	3294	1/1	0.93	0.07	38,38,38,38	0
52	MG	DA	3318	1/1	0.93	0.05	45,45,45,45	0
52	MG	DA	3026	1/1	0.93	0.08	66,66,66,66	0
52	MG	BA	3205	1/1	0.93	0.25	43,43,43,43	0
52	MG	DA	3323	1/1	0.93	0.14	57,57,57,57	0
52	MG	BA	3297	1/1	0.93	0.20	37,37,37,37	0
52	MG	DA	3173	1/1	0.93	0.16	41,41,41,41	0
52	MG	BA	3067	1/1	0.93	0.22	28,28,28,28	0
52	MG	BA	3301	1/1	0.93	0.21	41,41,41,41	0
52	MG	BA	3071	1/1	0.93	0.23	33,33,33,33	0
52	MG	B5	102	1/1	0.93	0.10	56,56,56,56	0
52	MG	DA	3040	1/1	0.93	0.40	50,50,50,50	0
52	MG	BA	3220	1/1	0.93	0.27	46,46,46,46	0
52	MG	DA	3042	1/1	0.93	0.26	37,37,37,37	0
52	MG	BA	3307	1/1	0.93	0.24	44,44,44,44	0
52	MG	DA	3045	1/1	0.93	0.23	29,29,29,29	0
52	MG	DA	3046	1/1	0.93	0.23	48,48,48,48	0
52	MG	DA	3050	1/1	0.93	0.15	39,39,39,39	0
52	MG	BA	3108	1/1	0.94	0.17	42,42,42,42	0
52	MG	DA	3217	1/1	0.94	0.17	23,23,23,23	0
52	MG	BA	3060	1/1	0.94	0.24	27,27,27,27	0
52	MG	CA	1631	1/1	0.94	0.20	73,73,73,73	0
52	MG	BA	3063	1/1	0.94	0.21	36,36,36,36	0
52	MG	AA	1626	1/1	0.94	0.20	46,46,46,46	0
52	MG	BA	3322	1/1	0.94	0.23	50,50,50,50	0
52	MG	BA	3323	1/1	0.94	0.20	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	3114	1/1	0.94	0.20	37,37,37,37	0
52	MG	DA	3095	1/1	0.94	0.10	39,39,39,39	0
52	MG	BA	3023	1/1	0.94	0.27	35,35,35,35	0
52	MG	DA	3228	1/1	0.94	0.14	52,52,52,52	0
52	MG	BA	3329	1/1	0.94	0.17	32,32,32,32	0
52	MG	BA	3068	1/1	0.94	0.25	35,35,35,35	0
52	MG	DA	3104	1/1	0.94	0.28	36,36,36,36	0
52	MG	BA	3177	1/1	0.94	0.23	38,38,38,38	0
52	MG	BA	3118	1/1	0.94	0.31	40,40,40,40	0
52	MG	BA	3335	1/1	0.94	0.06	44,44,44,44	0
52	MG	BA	3006	1/1	0.94	0.29	30,30,30,30	0
52	MG	BA	3258	1/1	0.94	0.19	30,30,30,30	0
52	MG	DA	3111	1/1	0.94	0.27	31,31,31,31	0
52	MG	BA	3259	1/1	0.94	0.16	23,23,23,23	0
52	MG	BA	3261	1/1	0.94	0.06	27,27,27,27	0
52	MG	BA	3342	1/1	0.94	0.18	38,38,38,38	0
52	MG	BA	3072	1/1	0.94	0.33	39,39,39,39	0
52	MG	BA	3009	1/1	0.94	0.25	27,27,27,27	0
52	MG	BA	3075	1/1	0.94	0.27	44,44,44,44	0
52	MG	BA	3127	1/1	0.94	0.21	39,39,39,39	0
52	MG	BA	3267	1/1	0.94	0.23	37,37,37,37	0
52	MG	BA	3131	1/1	0.94	0.20	21,21,21,21	0
52	MG	DA	3126	1/1	0.94	0.18	42,42,42,42	0
52	MG	BA	3355	1/1	0.94	0.14	64,64,64,64	0
52	MG	BA	3135	1/1	0.94	0.27	28,28,28,28	0
52	MG	DA	3007	1/1	0.94	0.11	53,53,53,53	0
52	MG	BA	3077	1/1	0.94	0.16	21,21,21,21	0
52	MG	DA	3132	1/1	0.94	0.26	25,25,25,25	0
52	MG	DA	3263	1/1	0.94	0.11	45,45,45,45	0
52	MG	DA	3013	1/1	0.94	0.21	18,18,18,18	0
52	MG	DA	3265	1/1	0.94	0.23	47,47,47,47	0
52	MG	BA	3139	1/1	0.94	0.29	60,60,60,60	0
52	MG	BA	3081	1/1	0.94	0.23	23,23,23,23	0
52	MG	AA	1615	1/1	0.94	0.26	49,49,49,49	0
52	MG	BA	3013	1/1	0.94	0.19	24,24,24,24	0
52	MG	BA	3279	1/1	0.94	0.23	37,37,37,37	0
52	MG	BB	202	1/1	0.94	0.21	26,26,26,26	0
52	MG	BA	3039	1/1	0.94	0.21	32,32,32,32	0
52	MG	BA	3150	1/1	0.94	0.17	40,40,40,40	0
52	MG	BF	301	1/1	0.94	0.10	51,51,51,51	0
52	MG	DA	3028	1/1	0.94	0.32	36,36,36,36	0
52	MG	DA	3147	1/1	0.94	0.24	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BP	201	1/1	0.94	0.21	39,39,39,39	0
52	MG	BA	3091	1/1	0.94	0.15	20,20,20,20	0
52	MG	BA	3287	1/1	0.94	0.15	44,44,44,44	0
52	MG	BR	201	1/1	0.94	0.12	24,24,24,24	0
52	MG	BX	101	1/1	0.94	0.07	38,38,38,38	0
52	MG	DA	3155	1/1	0.94	0.19	30,30,30,30	0
52	MG	BA	3047	1/1	0.94	0.28	28,28,28,28	0
52	MG	CA	1602	1/1	0.94	0.26	55,55,55,55	0
52	MG	BA	3290	1/1	0.94	0.19	46,46,46,46	0
52	MG	BA	3207	1/1	0.94	0.18	27,27,27,27	0
52	MG	DA	3296	1/1	0.94	0.24	55,55,55,55	0
52	MG	CA	1605	1/1	0.94	0.20	84,84,84,84	0
52	MG	BA	3096	1/1	0.94	0.23	19,19,19,19	0
52	MG	DA	3299	1/1	0.94	0.36	57,57,57,57	0
52	MG	BA	3209	1/1	0.94	0.27	31,31,31,31	0
52	MG	BA	3210	1/1	0.94	0.20	33,33,33,33	0
52	MG	DA	3302	1/1	0.94	0.19	64,64,64,64	0
52	MG	DA	3168	1/1	0.94	0.16	35,35,35,35	0
52	MG	DA	3169	1/1	0.94	0.06	35,35,35,35	0
52	MG	DA	3055	1/1	0.94	0.18	30,30,30,30	0
52	MG	BA	3214	1/1	0.94	0.05	12,12,12,12	0
52	MG	BA	3215	1/1	0.94	0.27	41,41,41,41	0
52	MG	BA	3049	1/1	0.94	0.30	33,33,33,33	0
52	MG	BA	3218	1/1	0.94	0.22	27,27,27,27	0
52	MG	DA	3178	1/1	0.94	0.06	58,58,58,58	0
52	MG	DA	3312	1/1	0.94	0.12	55,55,55,55	0
52	MG	CA	1614	1/1	0.94	0.13	71,71,71,71	0
52	MG	DA	3314	1/1	0.94	0.13	58,58,58,58	0
52	MG	DA	3066	1/1	0.94	0.24	40,40,40,40	0
52	MG	BA	3302	1/1	0.94	0.18	46,46,46,46	0
52	MG	BA	3050	1/1	0.94	0.19	27,27,27,27	0
52	MG	DA	3319	1/1	0.94	0.10	40,40,40,40	0
52	MG	DA	3070	1/1	0.94	0.17	28,28,28,28	0
52	MG	DA	3071	1/1	0.94	0.28	35,35,35,35	0
52	MG	BA	3225	1/1	0.94	0.04	20,20,20,20	0
52	MG	BA	3052	1/1	0.94	0.19	24,24,24,24	0
52	MG	BA	3231	1/1	0.94	0.18	35,35,35,35	0
52	MG	DA	3194	1/1	0.94	0.25	47,47,47,47	0
52	MG	BA	3233	1/1	0.94	0.09	21,21,21,21	0
52	MG	DA	3078	1/1	0.94	0.19	37,37,37,37	0
52	MG	BA	3102	1/1	0.94	0.17	23,23,23,23	0
52	MG	DA	3201	1/1	0.94	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3160	1/1	0.94	0.40	62,62,62,62	0
52	MG	BA	3236	1/1	0.94	0.16	25,25,25,25	0
52	MG	DQ	201	1/1	0.94	0.06	46,46,46,46	0
52	MG	BA	3014	1/1	0.94	0.26	29,29,29,29	0
52	MG	B5	101	1/1	0.94	0.19	40,40,40,40	0
52	MG	DA	3210	1/1	0.94	0.18	43,43,43,43	0
52	MG	BA	3239	1/1	0.94	0.16	50,50,50,50	0
55	ERY	BA	3364	51/51	0.94	0.31	94,94,94,94	0
55	ERY	DA	3330	51/51	0.94	0.24	94,94,94,94	0
52	MG	DA	3149	1/1	0.95	0.13	29,29,29,29	0
52	MG	BA	3061	1/1	0.95	0.21	27,27,27,27	0
52	MG	BA	3130	1/1	0.95	0.28	55,55,55,55	0
52	MG	BQ	201	1/1	0.95	0.04	19,19,19,19	0
52	MG	DA	3249	1/1	0.95	0.26	51,51,51,51	0
52	MG	DA	3250	1/1	0.95	0.14	41,41,41,41	0
52	MG	DA	3251	1/1	0.95	0.17	57,57,57,57	0
52	MG	BA	3317	1/1	0.95	0.10	45,45,45,45	0
52	MG	BA	3094	1/1	0.95	0.34	31,31,31,31	0
52	MG	DA	3076	1/1	0.95	0.19	29,29,29,29	0
52	MG	DA	3255	1/1	0.95	0.12	50,50,50,50	0
52	MG	BA	3134	1/1	0.95	0.21	36,36,36,36	0
52	MG	BA	3230	1/1	0.95	0.06	21,21,21,21	0
52	MG	BA	3062	1/1	0.95	0.06	19,19,19,19	0
52	MG	AA	1618	1/1	0.95	0.08	59,59,59,59	0
52	MG	DA	3160	1/1	0.95	0.19	33,33,33,33	0
52	MG	BA	3326	1/1	0.95	0.27	37,37,37,37	0
52	MG	BA	3098	1/1	0.95	0.22	39,39,39,39	0
52	MG	AA	1625	1/1	0.95	0.25	41,41,41,41	0
52	MG	BA	3141	1/1	0.95	0.32	32,32,32,32	0
52	MG	DA	3008	1/1	0.95	0.19	36,36,36,36	0
52	MG	DA	3087	1/1	0.95	0.19	34,34,34,34	0
52	MG	DA	3268	1/1	0.95	0.21	52,52,52,52	0
52	MG	BA	3283	1/1	0.95	0.19	33,33,33,33	0
52	MG	BA	3331	1/1	0.95	0.21	49,49,49,49	0
52	MG	BA	3066	1/1	0.95	0.23	29,29,29,29	0
52	MG	DA	3175	1/1	0.95	0.14	44,44,44,44	0
52	MG	BA	3286	1/1	0.95	0.14	30,30,30,30	0
52	MG	DA	3017	1/1	0.95	0.20	34,34,34,34	0
52	MG	BA	3015	1/1	0.95	0.16	33,33,33,33	0
52	MG	BA	3104	1/1	0.95	0.24	31,31,31,31	0
52	MG	DA	3180	1/1	0.95	0.25	45,45,45,45	0
52	MG	BA	3193	1/1	0.95	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	3182	1/1	0.95	0.07	39,39,39,39	0
52	MG	DA	3284	1/1	0.95	0.36	51,51,51,51	0
52	MG	DA	3096	1/1	0.95	0.18	45,45,45,45	0
52	MG	DA	3286	1/1	0.95	0.16	47,47,47,47	0
52	MG	BA	3148	1/1	0.95	0.19	26,26,26,26	0
52	MG	BA	3041	1/1	0.95	0.18	24,24,24,24	0
52	MG	DA	3187	1/1	0.95	0.15	54,54,54,54	0
52	MG	BA	3341	1/1	0.95	0.19	70,70,70,70	0
52	MG	DA	3102	1/1	0.95	0.32	36,36,36,36	0
52	MG	BA	3043	1/1	0.95	0.14	31,31,31,31	0
52	MG	BA	3343	1/1	0.95	0.23	44,44,44,44	0
52	MG	DA	3029	1/1	0.95	0.24	45,45,45,45	0
52	MG	DA	3030	1/1	0.95	0.17	32,32,32,32	0
52	MG	CA	1623	1/1	0.95	0.25	62,62,62,62	0
52	MG	DA	3197	1/1	0.95	0.23	46,46,46,46	0
52	MG	DA	3198	1/1	0.95	0.14	38,38,38,38	0
52	MG	DA	3199	1/1	0.95	0.07	37,37,37,37	0
52	MG	BA	3046	1/1	0.95	0.16	28,28,28,28	0
52	MG	AA	1636	1/1	0.95	0.20	44,44,44,44	0
52	MG	DA	3035	1/1	0.95	0.19	32,32,32,32	0
52	MG	DA	3205	1/1	0.95	0.38	62,62,62,62	0
52	MG	AA	1643	1/1	0.95	0.25	59,59,59,59	0
52	MG	BA	3348	1/1	0.95	0.18	38,38,38,38	0
52	MG	BA	3298	1/1	0.95	0.27	59,59,59,59	0
52	MG	DA	3118	1/1	0.95	0.21	35,35,35,35	0
52	MG	BA	3008	1/1	0.95	0.22	24,24,24,24	0
52	MG	BA	3253	1/1	0.95	0.29	42,42,42,42	0
52	MG	BA	3078	1/1	0.95	0.25	30,30,30,30	0
52	MG	DA	3044	1/1	0.95	0.21	32,32,32,32	0
52	MG	BA	3303	1/1	0.95	0.22	65,65,65,65	0
52	MG	CA	1633	1/1	0.95	0.19	48,48,48,48	0
52	MG	DA	3047	1/1	0.95	0.22	36,36,36,36	0
52	MG	DA	3048	1/1	0.95	0.22	35,35,35,35	0
52	MG	DA	3129	1/1	0.95	0.13	54,54,54,54	0
52	MG	DA	3224	1/1	0.95	0.10	54,54,54,54	0
52	MG	BA	3256	1/1	0.95	0.07	39,39,39,39	0
52	MG	BA	3027	1/1	0.95	0.23	19,19,19,19	0
52	MG	DA	3052	1/1	0.95	0.18	40,40,40,40	0
52	MG	DA	3054	1/1	0.95	0.20	43,43,43,43	0
52	MG	BA	3029	1/1	0.95	0.11	16,16,16,16	0
52	MG	DA	3230	1/1	0.95	0.13	57,57,57,57	0
52	MG	BA	3085	1/1	0.95	0.09	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3308	1/1	0.95	0.12	41,41,41,41	0
52	MG	AA	1632	1/1	0.95	0.34	68,68,68,68	0
52	MG	DA	3059	1/1	0.95	0.20	26,26,26,26	0
52	MG	BA	3164	1/1	0.95	0.14	30,30,30,30	0
52	MG	BA	3088	1/1	0.95	0.22	34,34,34,34	0
52	MG	BA	3059	1/1	0.95	0.14	26,26,26,26	0
53	ZN	AD	301	1/1	0.95	0.23	120,120,120,120	0
52	MG	DA	3067	1/1	0.95	0.21	49,49,49,49	0
52	MG	BA	3167	1/1	0.95	0.24	31,31,31,31	0
52	MG	AA	1623	1/1	0.95	0.20	37,37,37,37	0
52	MG	DA	3243	1/1	0.95	0.07	41,41,41,41	0
52	MG	BA	3069	1/1	0.96	0.21	45,45,45,45	0
52	MG	BA	3070	1/1	0.96	0.16	9,9,9,9	0
52	MG	B0	101	1/1	0.96	0.15	37,37,37,37	0
52	MG	BA	3095	1/1	0.96	0.21	33,33,33,33	0
52	MG	DA	3009	1/1	0.96	0.29	49,49,49,49	0
52	MG	BA	3040	1/1	0.96	0.26	37,37,37,37	0
52	MG	DA	3166	1/1	0.96	0.29	54,54,54,54	0
52	MG	BA	3318	1/1	0.96	0.22	40,40,40,40	0
52	MG	BA	3264	1/1	0.96	0.14	48,48,48,48	0
52	MG	BA	3073	1/1	0.96	0.20	20,20,20,20	0
52	MG	DA	3171	1/1	0.96	0.16	39,39,39,39	0
52	MG	DA	3016	1/1	0.96	0.21	31,31,31,31	0
52	MG	BA	3124	1/1	0.96	0.16	10,10,10,10	0
52	MG	DA	3174	1/1	0.96	0.17	67,67,67,67	0
52	MG	BA	3126	1/1	0.96	0.14	33,33,33,33	0
52	MG	DA	3019	1/1	0.96	0.23	21,21,21,21	0
52	MG	BA	3058	1/1	0.96	0.16	35,35,35,35	0
52	MG	CA	1609	1/1	0.96	0.07	34,34,34,34	0
52	MG	BA	3324	1/1	0.96	0.20	40,40,40,40	0
52	MG	BA	3325	1/1	0.96	0.31	58,58,58,58	0
52	MG	DA	3025	1/1	0.96	0.18	44,44,44,44	0
52	MG	BA	3128	1/1	0.96	0.17	39,39,39,39	0
52	MG	DA	3273	1/1	0.96	0.25	52,52,52,52	0
52	MG	DA	3099	1/1	0.96	0.28	42,42,42,42	0
52	MG	BA	3024	1/1	0.96	0.17	28,28,28,28	0
52	MG	BA	3076	1/1	0.96	0.14	21,21,21,21	0
52	MG	DA	3186	1/1	0.96	0.36	45,45,45,45	0
52	MG	BA	3272	1/1	0.96	0.12	28,28,28,28	0
52	MG	BA	3216	1/1	0.96	0.16	26,26,26,26	0
52	MG	BA	3168	1/1	0.96	0.14	28,28,28,28	0
52	MG	DA	3032	1/1	0.96	0.23	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3192	1/1	0.96	0.08	29,29,29,29	0
52	MG	BA	3133	1/1	0.96	0.18	37,37,37,37	0
52	MG	BA	3172	1/1	0.96	0.23	52,52,52,52	0
52	MG	BA	3334	1/1	0.96	0.12	24,24,24,24	0
52	MG	DA	3112	1/1	0.96	0.10	30,30,30,30	0
52	MG	DA	3036	1/1	0.96	0.25	29,29,29,29	0
52	MG	DA	3114	1/1	0.96	0.20	47,47,47,47	0
52	MG	BA	3223	1/1	0.96	0.17	41,41,41,41	0
52	MG	CA	1622	1/1	0.96	0.26	51,51,51,51	0
52	MG	BA	3026	1/1	0.96	0.11	48,48,48,48	0
52	MG	BA	3103	1/1	0.96	0.17	24,24,24,24	0
52	MG	BA	3227	1/1	0.96	0.35	37,37,37,37	0
52	MG	DA	3206	1/1	0.96	0.19	38,38,38,38	0
52	MG	BA	3229	1/1	0.96	0.37	45,45,45,45	0
52	MG	BA	3034	1/1	0.96	0.22	61,61,61,61	0
52	MG	BA	3035	1/1	0.96	0.13	26,26,26,26	0
52	MG	BA	3289	1/1	0.96	0.20	37,37,37,37	0
52	MG	DA	3211	1/1	0.96	0.15	35,35,35,35	0
52	MG	DA	3212	1/1	0.96	0.22	38,38,38,38	0
52	MG	DA	3124	1/1	0.96	0.13	42,42,42,42	0
52	MG	DA	3125	1/1	0.96	0.06	45,45,45,45	0
52	MG	DA	3216	1/1	0.96	0.20	31,31,31,31	0
52	MG	BA	3106	1/1	0.96	0.19	18,18,18,18	0
52	MG	BA	3180	1/1	0.96	0.16	48,48,48,48	0
52	MG	DA	3049	1/1	0.96	0.22	42,42,42,42	0
52	MG	BA	3346	1/1	0.96	0.18	60,60,60,60	0
52	MG	BA	3181	1/1	0.96	0.19	35,35,35,35	0
52	MG	BA	3182	1/1	0.96	0.14	43,43,43,43	0
52	MG	BA	3082	1/1	0.96	0.21	33,33,33,33	0
52	MG	BA	3048	1/1	0.96	0.26	23,23,23,23	0
52	MG	BA	3351	1/1	0.96	0.15	39,39,39,39	0
52	MG	BA	3143	1/1	0.96	0.24	28,28,28,28	0
52	MG	BA	3109	1/1	0.96	0.24	31,31,31,31	0
52	MG	BA	3299	1/1	0.96	0.21	38,38,38,38	0
52	MG	DA	3061	1/1	0.96	0.17	36,36,36,36	0
52	MG	DA	3062	1/1	0.96	0.06	24,24,24,24	0
52	MG	BA	3145	1/1	0.96	0.16	33,33,33,33	0
52	MG	BA	3189	1/1	0.96	0.27	36,36,36,36	0
52	MG	AA	1610	1/1	0.96	0.10	41,41,41,41	0
52	MG	BA	3147	1/1	0.96	0.22	37,37,37,37	0
52	MG	BA	3028	1/1	0.96	0.29	22,22,22,22	0
52	MG	BA	3194	1/1	0.96	0.24	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DB	203	1/1	0.96	0.27	46,46,46,46	0
52	MG	BA	3087	1/1	0.96	0.20	18,18,18,18	0
52	MG	BA	3250	1/1	0.96	0.16	37,37,37,37	0
52	MG	BB	206	1/1	0.96	0.29	50,50,50,50	0
52	MG	DA	3241	1/1	0.96	0.09	36,36,36,36	0
52	MG	DU	201	1/1	0.96	0.10	60,60,60,60	0
52	MG	BA	3252	1/1	0.96	0.18	30,30,30,30	0
52	MG	BA	3051	1/1	0.96	0.22	17,17,17,17	0
53	ZN	CD	301	1/1	0.96	0.20	116,116,116,116	0
52	MG	DA	3075	1/1	0.96	0.18	36,36,36,36	0
52	MG	BA	3038	1/1	0.96	0.20	14,14,14,14	0
52	MG	BA	3198	1/1	0.96	0.16	36,36,36,36	0
52	MG	BA	3153	1/1	0.96	0.25	47,47,47,47	0
52	MG	DA	3274	1/1	0.97	0.13	36,36,36,36	0
52	MG	BA	3136	1/1	0.97	0.18	28,28,28,28	0
52	MG	DA	3039	1/1	0.97	0.20	53,53,53,53	0
52	MG	BA	3260	1/1	0.97	0.17	37,37,37,37	0
52	MG	BA	3042	1/1	0.97	0.20	14,14,14,14	0
52	MG	BA	3012	1/1	0.97	0.18	23,23,23,23	0
52	MG	BA	3228	1/1	0.97	0.17	21,21,21,21	0
52	MG	BA	3339	1/1	0.97	0.08	53,53,53,53	0
52	MG	BA	3045	1/1	0.97	0.15	21,21,21,21	0
52	MG	BA	3199	1/1	0.97	0.19	20,20,20,20	0
52	MG	BA	3157	1/1	0.97	0.15	22,22,22,22	0
52	MG	DA	3101	1/1	0.97	0.05	28,28,28,28	0
52	MG	DA	3287	1/1	0.97	0.06	40,40,40,40	0
52	MG	DA	3288	1/1	0.97	0.26	51,51,51,51	0
52	MG	BA	3232	1/1	0.97	0.07	4,4,4,4	0
52	MG	DA	3103	1/1	0.97	0.26	32,32,32,32	0
52	MG	BA	3178	1/1	0.97	0.23	30,30,30,30	0
52	MG	BA	3179	1/1	0.97	0.29	41,41,41,41	0
52	MG	DA	3106	1/1	0.97	0.26	63,63,63,63	0
52	MG	DA	3165	1/1	0.97	0.27	35,35,35,35	0
52	MG	BA	3055	1/1	0.97	0.16	16,16,16,16	0
52	MG	DA	3167	1/1	0.97	0.07	44,44,44,44	0
52	MG	DA	3002	1/1	0.97	0.28	29,29,29,29	0
52	MG	BA	3099	1/1	0.97	0.13	21,21,21,21	0
52	MG	DA	3232	1/1	0.97	0.16	50,50,50,50	0
52	MG	AA	1601	1/1	0.97	0.14	59,59,59,59	0
52	MG	DA	3006	1/1	0.97	0.31	30,30,30,30	0
52	MG	BA	3273	1/1	0.97	0.26	42,42,42,42	0
52	MG	BA	3161	1/1	0.97	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3184	1/1	0.97	0.22	44,44,44,44	0
52	MG	DA	3060	1/1	0.97	0.21	38,38,38,38	0
52	MG	BA	3277	1/1	0.97	0.14	41,41,41,41	0
52	MG	DA	3307	1/1	0.97	0.14	41,41,41,41	0
52	MG	DA	3011	1/1	0.97	0.29	30,30,30,30	0
52	MG	DA	3012	1/1	0.97	0.16	25,25,25,25	0
52	MG	BA	3353	1/1	0.97	0.08	26,26,26,26	0
52	MG	BA	3089	1/1	0.97	0.10	12,12,12,12	0
52	MG	AA	1641	1/1	0.97	0.15	57,57,57,57	0
52	MG	DA	3245	1/1	0.97	0.07	38,38,38,38	0
52	MG	BA	3280	1/1	0.97	0.14	33,33,33,33	0
52	MG	BA	3011	1/1	0.97	0.23	19,19,19,19	0
52	MG	BA	3211	1/1	0.97	0.15	34,34,34,34	0
52	MG	DA	3317	1/1	0.97	0.11	42,42,42,42	0
52	MG	BA	3212	1/1	0.97	0.19	26,26,26,26	0
52	MG	BA	3116	1/1	0.97	0.26	55,55,55,55	0
52	MG	BA	3247	1/1	0.97	0.20	31,31,31,31	0
52	MG	BB	201	1/1	0.97	0.25	35,35,35,35	0
52	MG	DA	3322	1/1	0.97	0.24	48,48,48,48	0
52	MG	BA	3132	1/1	0.97	0.10	18,18,18,18	0
52	MG	DA	3024	1/1	0.97	0.13	35,35,35,35	0
52	MG	BB	204	1/1	0.97	0.22	43,43,43,43	0
52	MG	BA	3149	1/1	0.97	0.20	19,19,19,19	0
52	MG	DA	3257	1/1	0.97	0.22	38,38,38,38	0
52	MG	DA	3133	1/1	0.97	0.36	42,42,42,42	0
52	MG	BA	3016	1/1	0.97	0.18	21,21,21,21	0
52	MG	BA	3251	1/1	0.97	0.03	40,40,40,40	0
52	MG	BD	301	1/1	0.97	0.15	25,25,25,25	0
52	MG	BA	3192	1/1	0.97	0.05	37,37,37,37	0
52	MG	BA	3018	1/1	0.97	0.15	20,20,20,20	0
52	MG	BA	3221	1/1	0.97	0.20	29,29,29,29	0
52	MG	BA	3222	1/1	0.97	0.23	32,32,32,32	0
52	MG	DA	3202	1/1	0.97	0.24	64,64,64,64	0
52	MG	DA	3086	1/1	0.97	0.12	25,25,25,25	0
52	MG	BA	3119	1/1	0.97	0.23	32,32,32,32	0
53	ZN	AN	101	1/1	0.97	0.04	157,157,157,157	0
52	MG	DA	3269	1/1	0.97	0.26	39,39,39,39	0
52	MG	BQ	202	1/1	0.97	0.16	38,38,38,38	0
52	MG	CA	1641	1/1	0.97	0.25	52,52,52,52	0
52	MG	BA	3224	1/1	0.97	0.19	30,30,30,30	0
52	MG	DA	3148	1/1	0.97	0.19	41,41,41,41	0
52	MG	BA	3020	1/1	0.98	0.09	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3284	1/1	0.98	0.07	25,25,25,25	0
52	MG	BE	301	1/1	0.98	0.17	25,25,25,25	0
52	MG	BA	3213	1/1	0.98	0.10	20,20,20,20	0
52	MG	BA	3129	1/1	0.98	0.03	35,35,35,35	0
52	MG	DA	3143	1/1	0.98	0.16	32,32,32,32	0
52	MG	BA	3169	1/1	0.98	0.27	38,38,38,38	0
52	MG	DA	3065	1/1	0.98	0.15	39,39,39,39	0
52	MG	BA	3025	1/1	0.98	0.08	29,29,29,29	0
52	MG	BA	3171	1/1	0.98	0.28	32,32,32,32	0
52	MG	BA	3005	1/1	0.98	0.13	24,24,24,24	0
52	MG	BA	3354	1/1	0.98	0.12	34,34,34,34	0
52	MG	BU	201	1/1	0.98	0.18	31,31,31,31	0
52	MG	BA	3084	1/1	0.98	0.17	21,21,21,21	0
52	MG	BA	3057	1/1	0.98	0.10	24,24,24,24	0
52	MG	BA	3255	1/1	0.98	0.05	24,24,24,24	0
52	MG	BA	3044	1/1	0.98	0.18	14,14,14,14	0
52	MG	DE	301	1/1	0.98	0.08	23,23,23,23	0
52	MG	BA	3002	1/1	0.98	0.26	28,28,28,28	0
52	MG	BA	3296	1/1	0.98	0.09	43,43,43,43	0
52	MG	BA	3276	1/1	0.98	0.09	17,17,17,17	0
52	MG	DA	3275	1/1	0.98	0.29	60,60,60,60	0
52	MG	BA	3019	1/1	0.98	0.23	19,19,19,19	0
52	MG	BA	3241	1/1	0.98	0.12	26,26,26,26	0
52	MG	DA	3188	1/1	0.98	0.27	44,44,44,44	0
52	MG	DA	3003	1/1	0.98	0.25	41,41,41,41	0
52	MG	BA	3053	1/1	0.98	0.23	27,27,27,27	0
53	ZN	CN	101	1/1	0.98	0.06	139,139,139,139	0
52	MG	BA	3138	1/1	0.98	0.31	34,34,34,34	0
52	MG	DA	3135	1/1	0.98	0.31	29,29,29,29	0
52	MG	BA	3079	1/1	0.98	0.09	17,17,17,17	0
52	MG	BA	3080	1/1	0.98	0.24	17,17,17,17	0
52	MG	AA	1602	1/1	0.99	0.30	41,41,41,41	0
52	MG	BA	3033	1/1	0.99	0.06	27,27,27,27	0
52	MG	BB	203	1/1	0.99	0.04	41,41,41,41	0
52	MG	DA	3053	1/1	0.99	0.14	27,27,27,27	0
52	MG	BA	3125	1/1	0.99	0.08	18,18,18,18	0
52	MG	BA	3017	1/1	0.99	0.26	32,32,32,32	0
52	MG	BA	3065	1/1	0.99	0.16	26,26,26,26	0
52	MG	BA	3111	1/1	0.99	0.04	17,17,17,17	0
52	MG	DA	3215	1/1	0.99	0.04	37,37,37,37	0
52	MG	BA	3219	1/1	0.99	0.23	25,25,25,25	0
52	MG	DA	3203	1/1	0.99	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3030	1/1	0.99	0.11	15,15,15,15	0
52	MG	BA	3007	1/1	0.99	0.22	28,28,28,28	0
52	MG	BA	3092	1/1	0.99	0.12	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.