



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 11:13 PM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

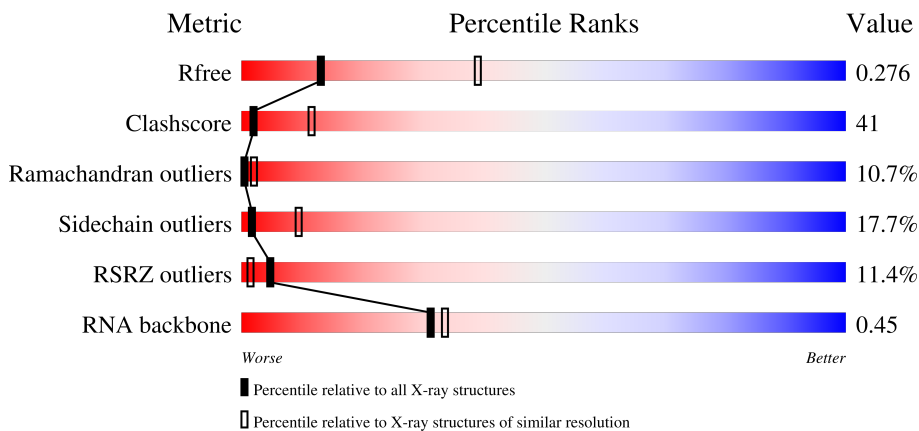
1 Overall quality at a glance i

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>19%</p> </div> <div style="text-align: center;"> <p>22%</p> </div> <div style="text-align: center;"> <p>61%</p> </div> <div style="text-align: center;"> <p>15%</p> </div> </div>
1	CA	1522	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>16%</p> </div> <div style="text-align: center;"> <p>22%</p> </div> <div style="text-align: center;"> <p>60%</p> </div> <div style="text-align: center;"> <p>16%</p> </div> </div>
2	AB	256	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>14%</p> </div> <div style="text-align: center;"> <p>25%</p> </div> <div style="text-align: center;"> <p>53%</p> </div> <div style="text-align: center;"> <p>11%</p> </div> <div style="text-align: center;"> <p>8%</p> </div> </div>
2	CB	256	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>20%</p> </div> <div style="text-align: center;"> <p>27%</p> </div> <div style="text-align: center;"> <p>50%</p> </div> <div style="text-align: center;"> <p>12%</p> </div> <div style="text-align: center;"> <p>8%</p> </div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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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	




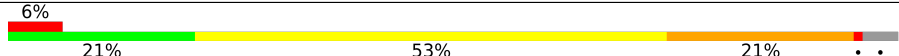
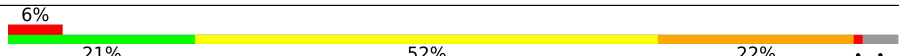
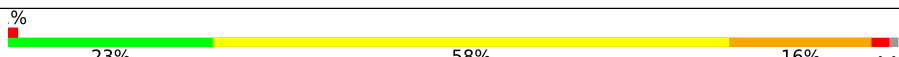
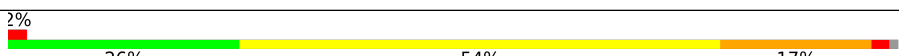
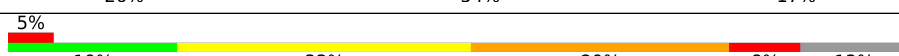

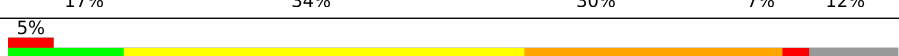
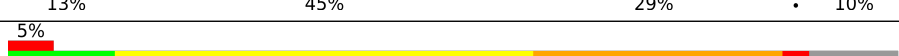
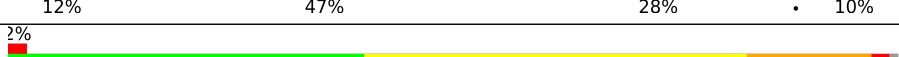

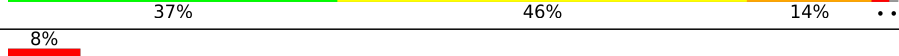

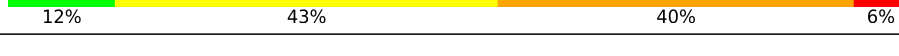
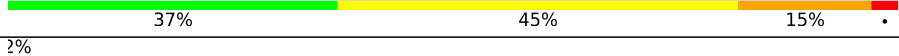

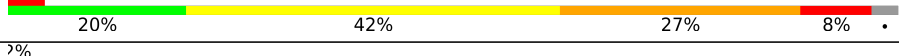


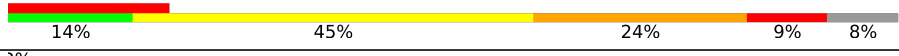
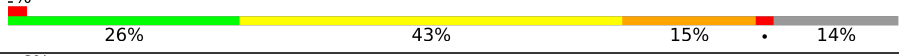
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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	AA	1637	-	-	-	X
52	MG	AA	1643	-	-	-	X
52	MG	AA	1644	-	-	-	X
52	MG	AA	1654	-	-	-	X
52	MG	BA	3007	-	-	-	X
52	MG	BA	3072	-	-	-	X
52	MG	BA	3074	-	-	-	X
52	MG	BA	3088	-	-	-	X
52	MG	BA	3128	-	-	-	X
52	MG	BA	3131	-	-	-	X
52	MG	BA	3150	-	-	-	X
52	MG	BA	3159	-	-	-	X
52	MG	BA	3167	-	-	-	X
52	MG	BA	3171	-	-	-	X
52	MG	BA	3175	-	-	-	X
52	MG	BA	3176	-	-	-	X
52	MG	BA	3180	-	-	-	X
52	MG	BA	3247	-	-	-	X
52	MG	BA	3313	-	-	-	X
52	MG	BA	3330	-	-	-	X
52	MG	BA	3337	-	-	-	X
52	MG	BA	3349	-	-	-	X
52	MG	BA	3355	-	-	-	X
52	MG	BA	3358	-	-	-	X
52	MG	CA	1626	-	-	-	X
52	MG	CA	1627	-	-	-	X
52	MG	CA	1630	-	-	-	X
52	MG	CA	1638	-	-	-	X
52	MG	DA	3025	-	-	-	X
52	MG	DA	3074	-	-	-	X
52	MG	DA	3075	-	-	-	X
52	MG	DA	3106	-	-	-	X
52	MG	DA	3149	-	-	-	X
52	MG	DA	3153	-	-	-	X
52	MG	DA	3166	-	-	-	X
52	MG	DA	3180	-	-	-	X
52	MG	DA	3187	-	-	-	X
52	MG	DA	3195	-	-	-	X
52	MG	DA	3208	-	-	-	X
52	MG	DA	3232	-	-	-	X
52	MG	DA	3236	-	-	-	X
52	MG	DA	3243	-	-	-	X
52	MG	DA	3252	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3267	-	-	-	X
52	MG	DA	3271	-	-	-	X
52	MG	DA	3274	-	-	-	X
52	MG	DA	3280	-	-	-	X
52	MG	DA	3281	-	-	-	X
52	MG	DA	3283	-	-	-	X
52	MG	DA	3289	-	-	-	X
52	MG	DA	3290	-	-	-	X
52	MG	DA	3295	-	-	-	X
52	MG	DA	3297	-	-	-	X
52	MG	DA	3305	-	-	-	X
52	MG	DA	3310	-	-	-	X
52	MG	DA	3325	-	-	-	X
52	MG	DA	3328	-	-	-	X
52	MG	DU	201	-	-	-	X
53	ZN	CD	301	-	-	X	-

2 Entry composition

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
10	AJ	99	Total 795	C 499	N 157	O 138	S 1	0	0	1
10	CJ	99	Total 795	C 499	N 157	O 138	S 1	0	0	1

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AL	125	Total 971	C 611	N 196	O 163	S 1	0	0	1
12	CL	125	Total 971	C 611	N 196	O 163	S 1	0	0	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
			Total	C	N	O	S			
13	AM	115	Total 921	C 569	N 190	O 160	S 2	0	0	0
13	CM	115	Total 921	C 569	N 190	O 160	S 2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
51	DZ	177	1404	897	253	252	2	0	0	1

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

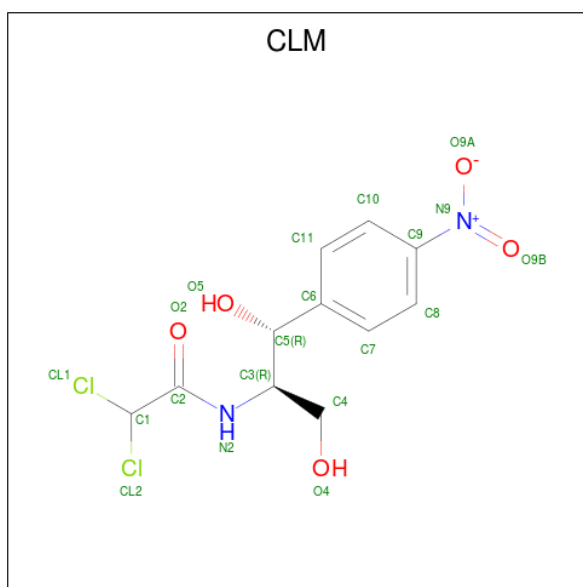
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: K) (formula: K).

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

- Molecule 55 is CHLORAMPHENICOL (three-letter code: CLM) (formula: C₁₁H₁₂Cl₂N₂O₅).

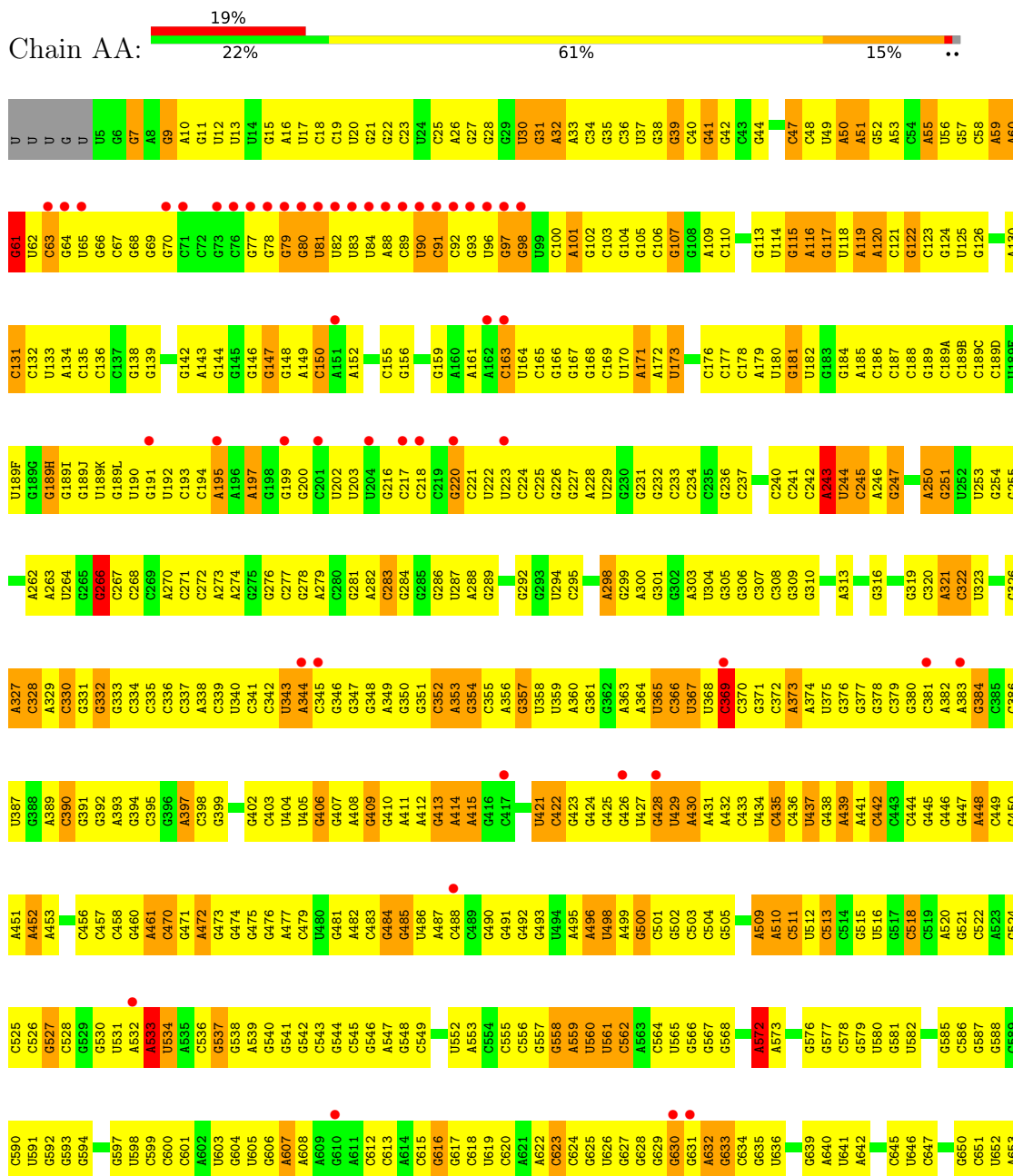


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
55	BA	1	20	11	2	2	5	0	0
55	DA	1	20	11	2	2	5	0	0

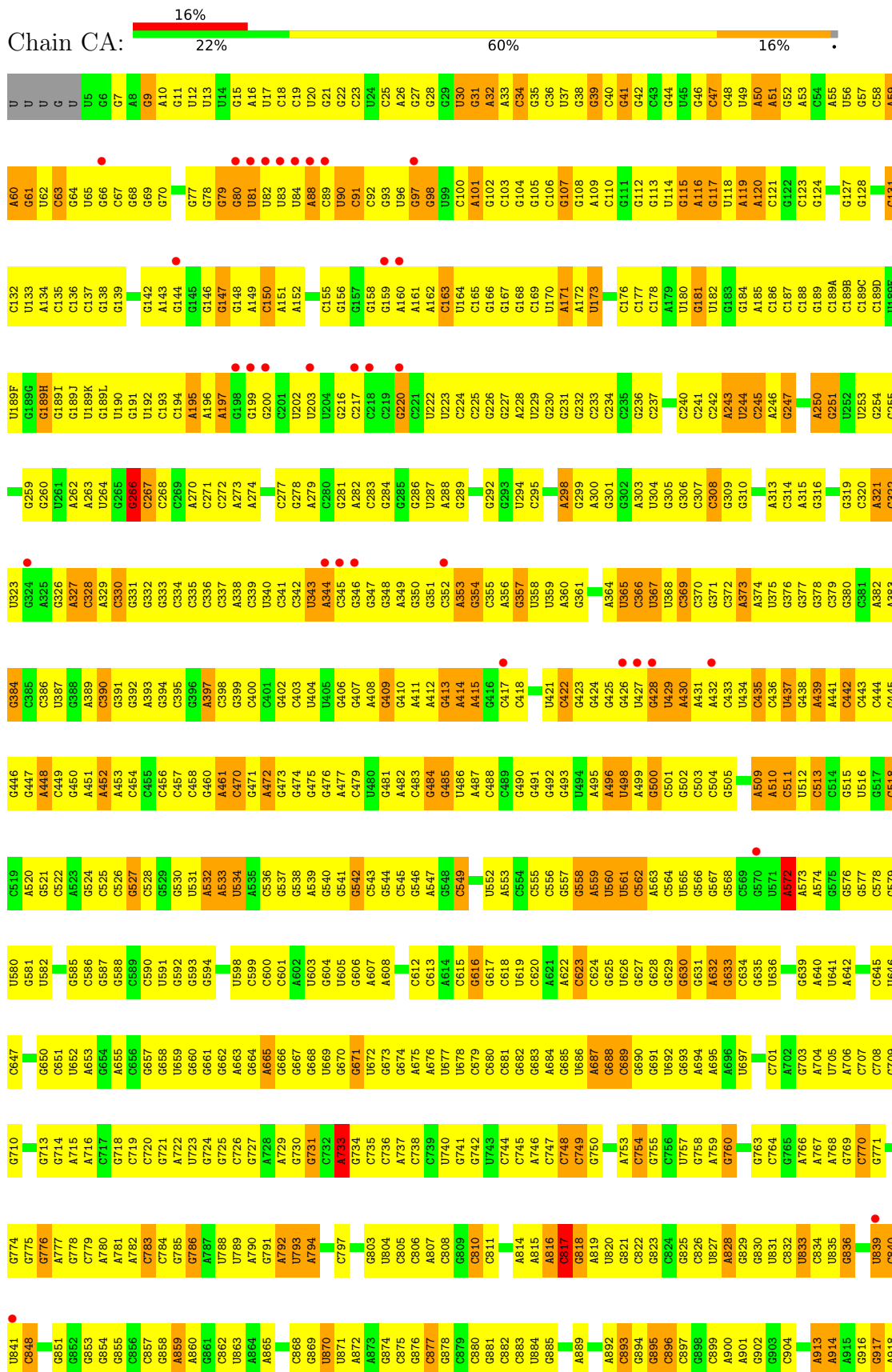
3 Residue-property plots

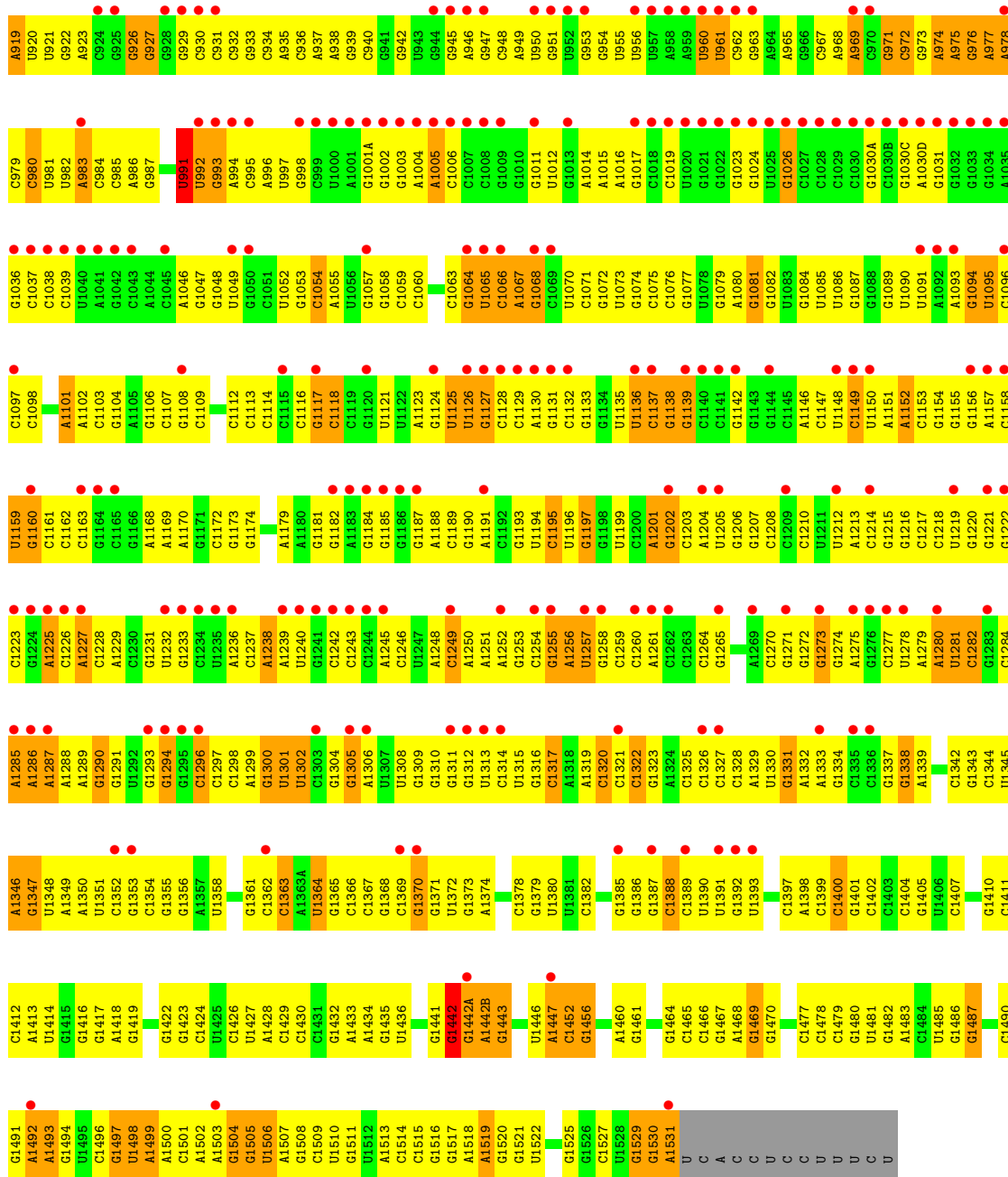
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

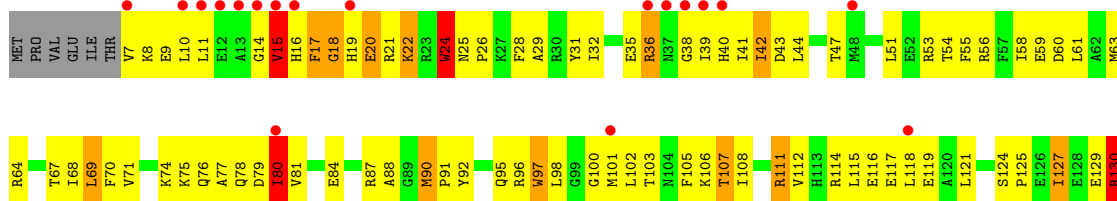


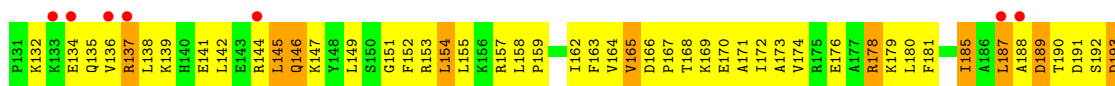
• Molecule 1: 16S rRNA



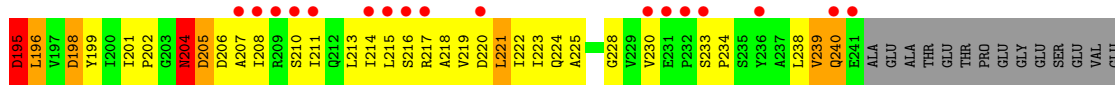
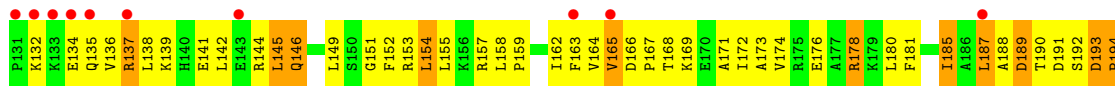
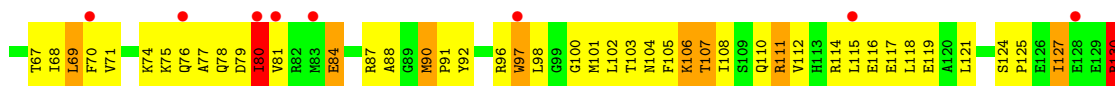
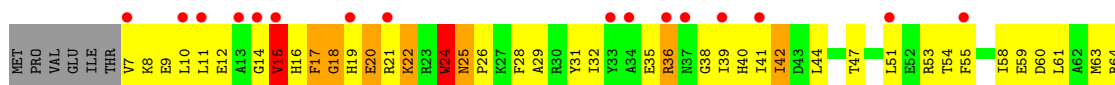


• Molecule 2: 30S ribosomal protein S2



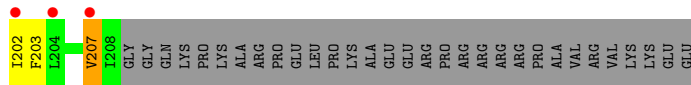
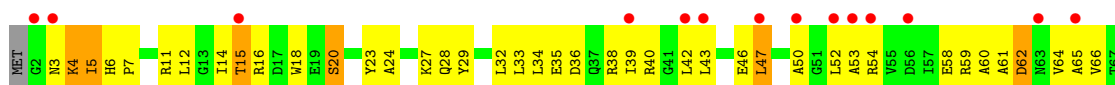


• Molecule 2: 30S ribosomal protein S2



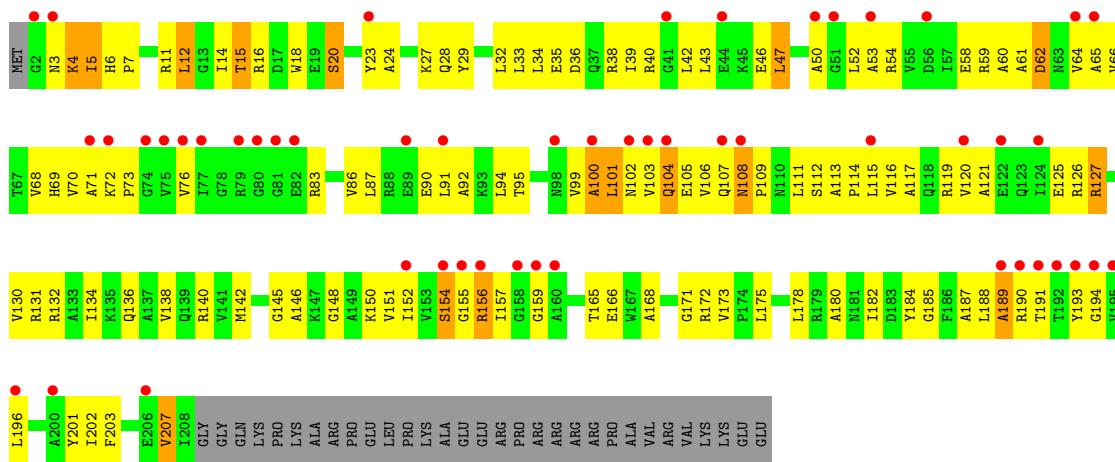
ALA

• Molecule 3: 30S ribosomal protein S3

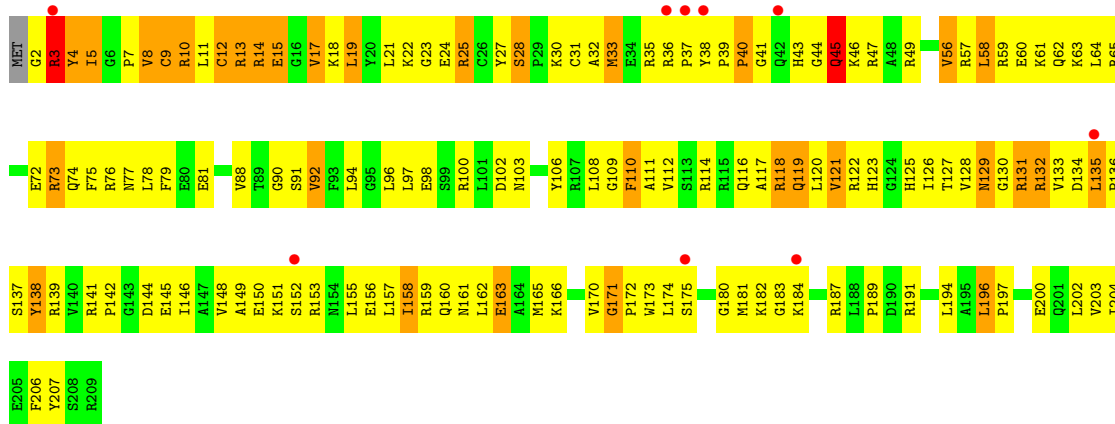


• Molecule 3: 30S ribosomal protein S3

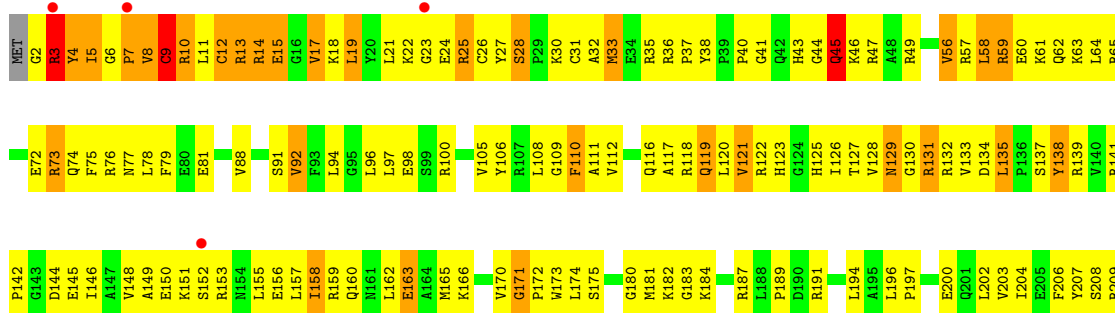




• Molecule 4: 30S ribosomal protein S4

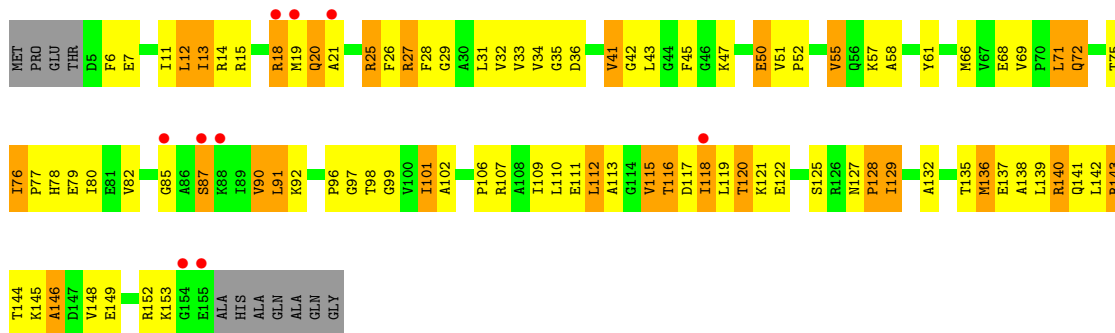


• Molecule 4: 30S ribosomal protein S4

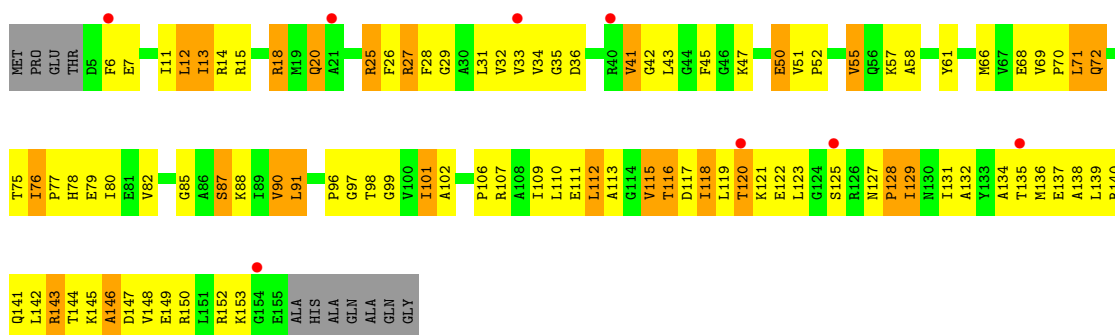


• Molecule 5: 30S ribosomal protein S5

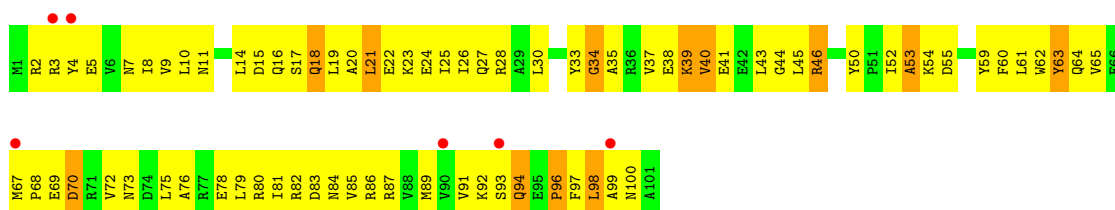




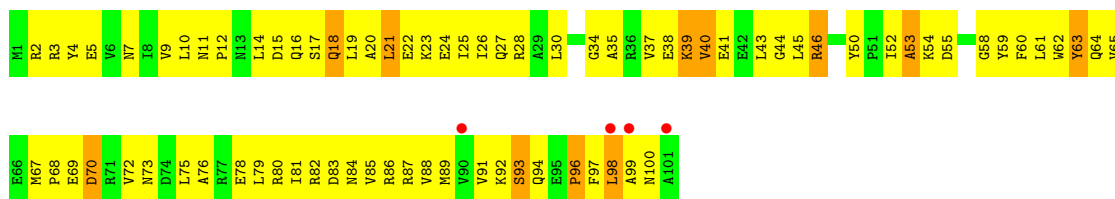
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

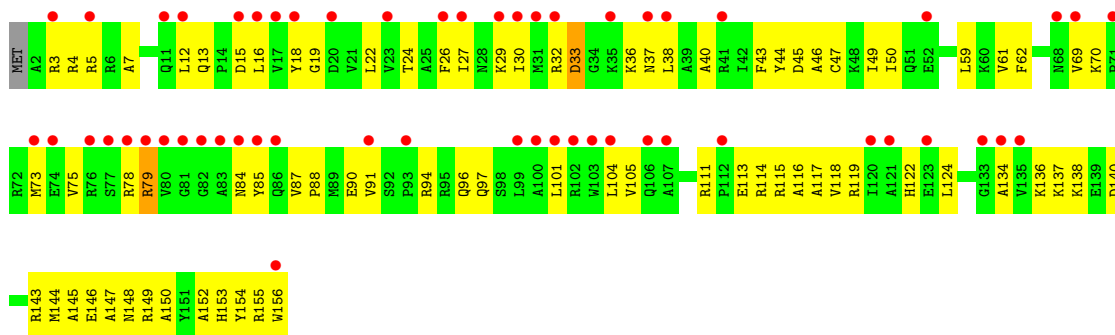


• Molecule 6: 30S ribosomal protein S6

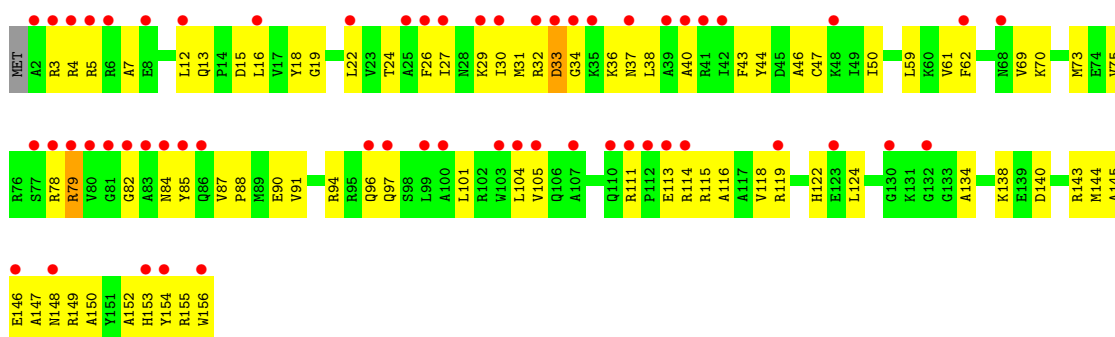
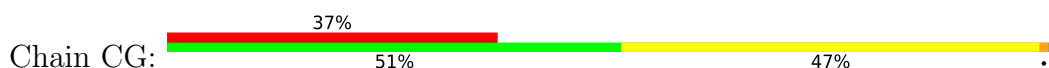


• Molecule 7: 30S ribosomal protein S7

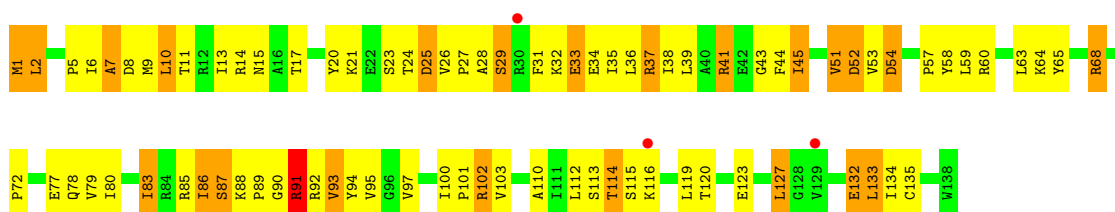




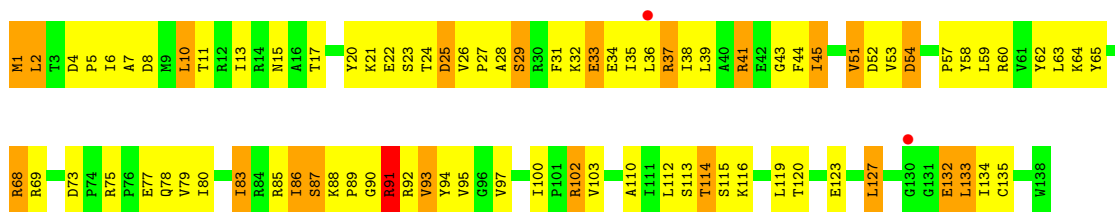
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

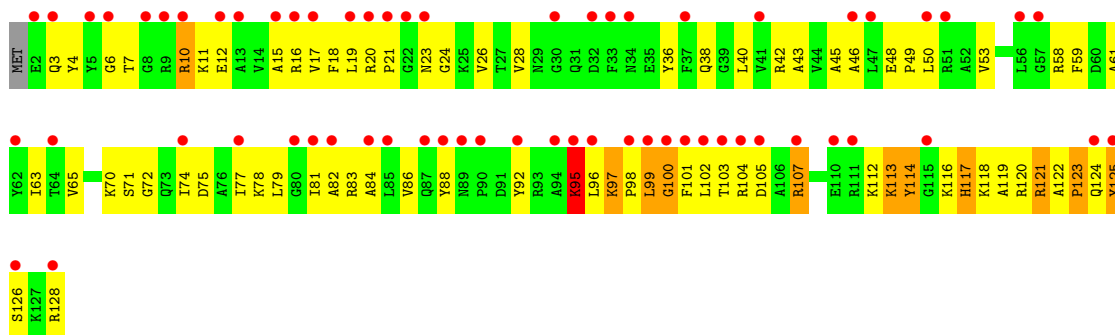


• Molecule 8: 30S ribosomal protein S8

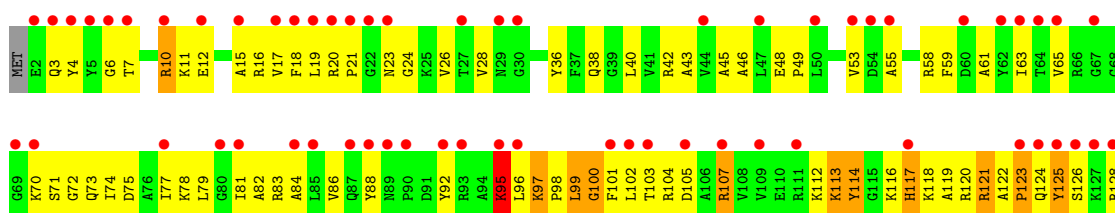


• Molecule 9: 30S ribosomal protein S9

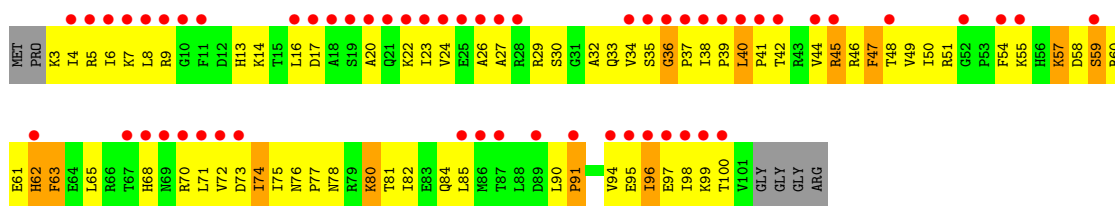




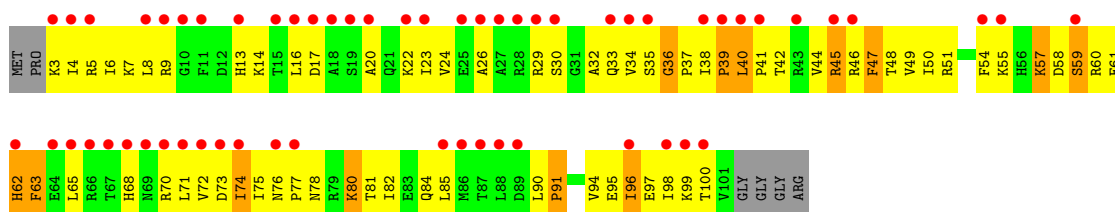
• Molecule 9: 30S ribosomal protein S9



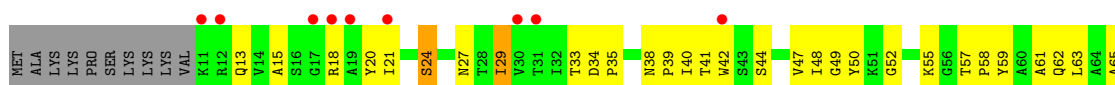
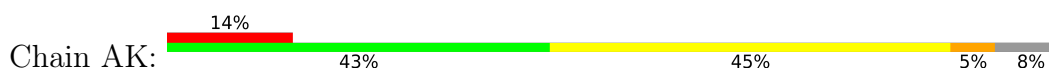
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10

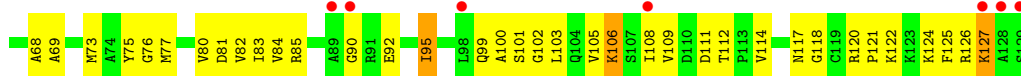
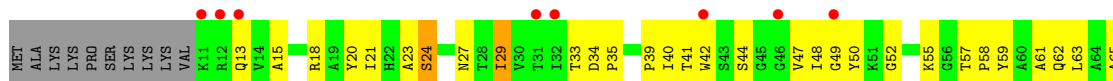


• Molecule 11: 30S ribosomal protein S11

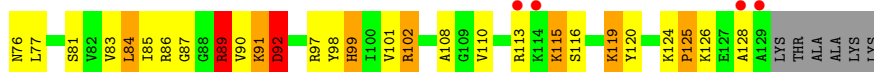
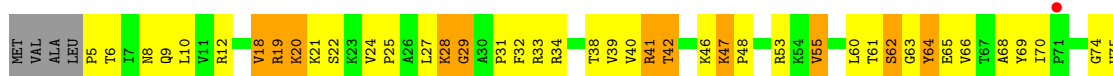




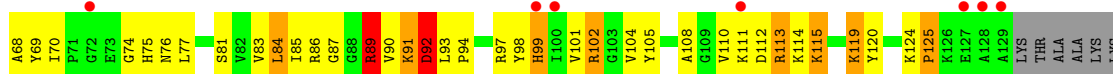
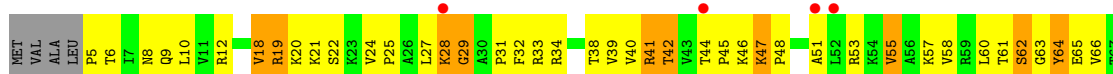
• Molecule 11: 30S ribosomal protein S11



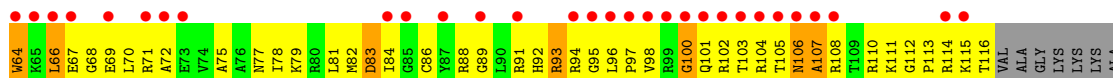
• Molecule 12: 30S ribosomal protein S12



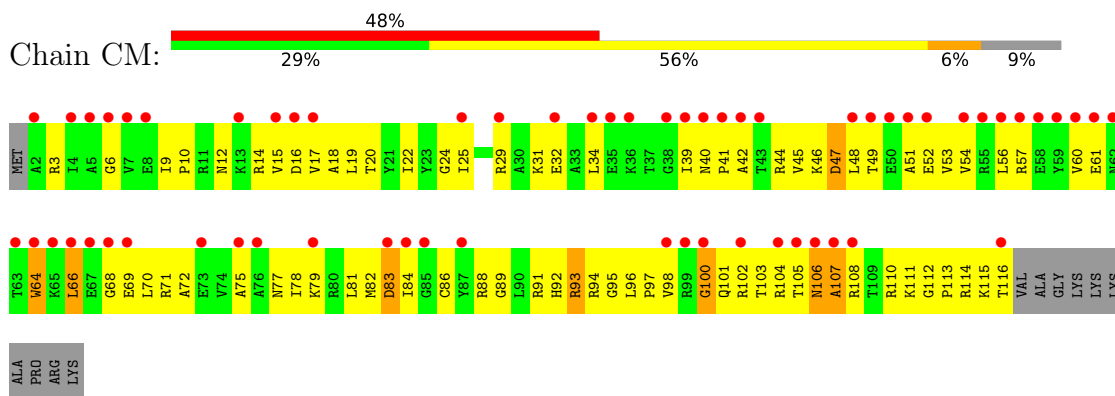
• Molecule 12: 30S ribosomal protein S12



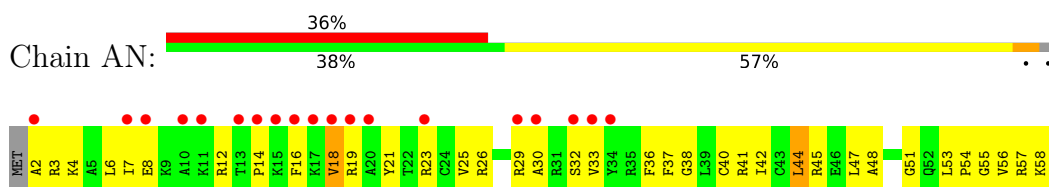
• Molecule 13: 30S ribosomal protein S13



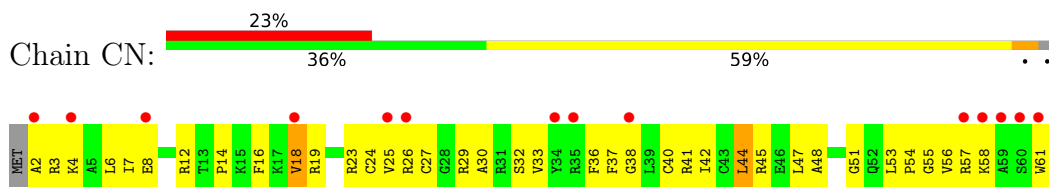
- Molecule 13: 30S ribosomal protein S13



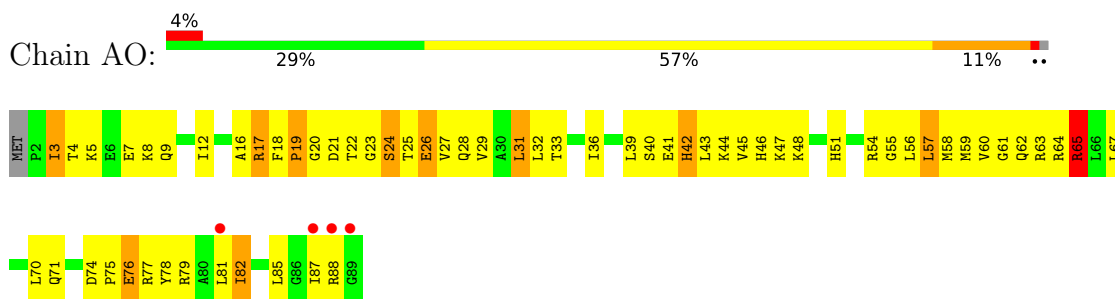
- Molecule 14: 30S ribosomal protein S14



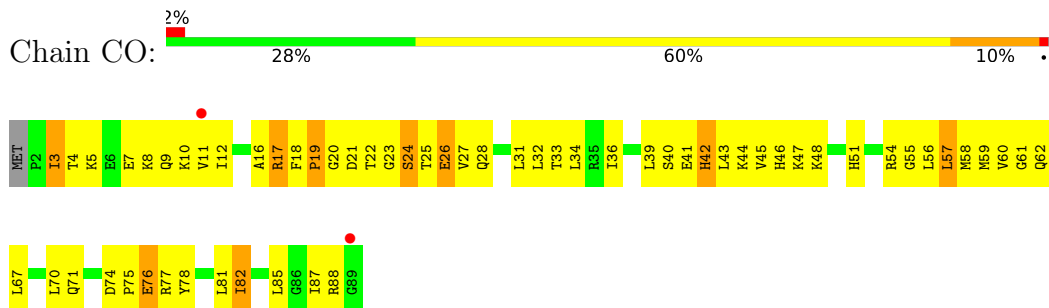
- Molecule 14: 30S ribosomal protein S14



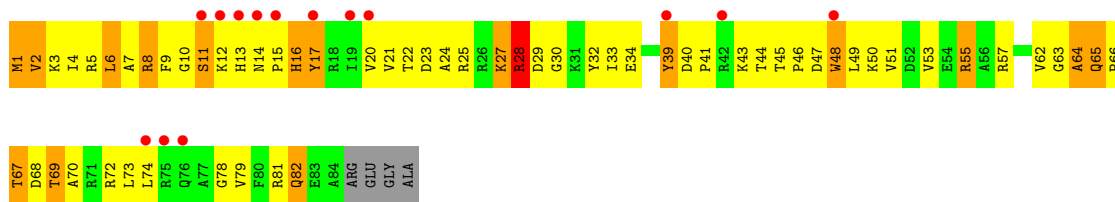
- Molecule 15: 30S ribosomal protein S15



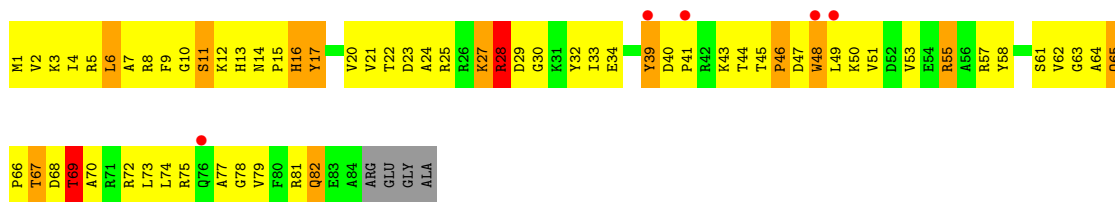
- Molecule 15: 30S ribosomal protein S15



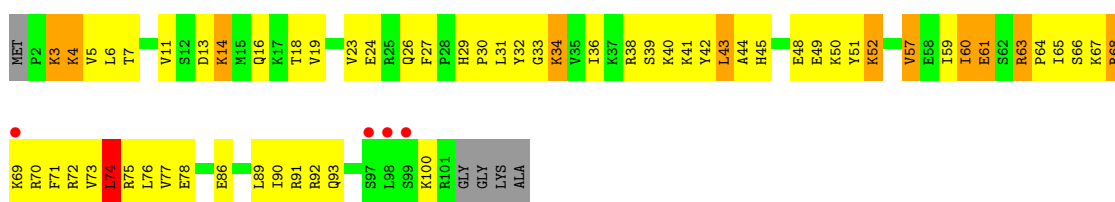
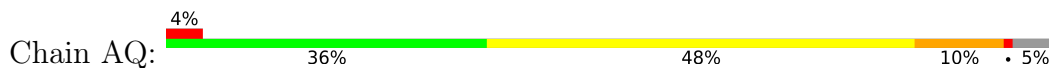
- Molecule 16: 30S ribosomal protein S16



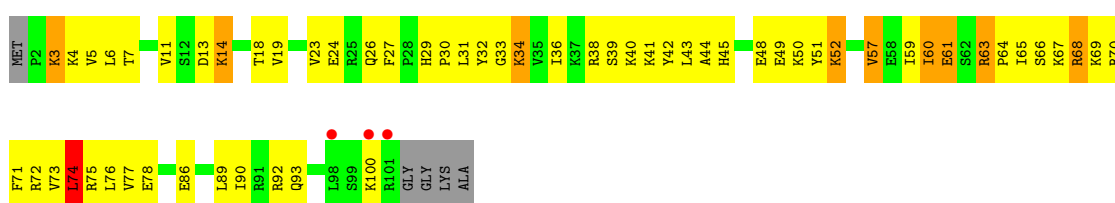
• Molecule 16: 30S ribosomal protein S16



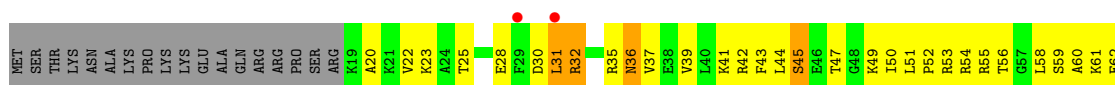
• Molecule 17: 30S ribosomal protein S17

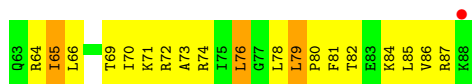


• Molecule 17: 30S ribosomal protein S17

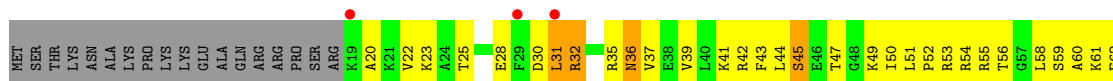


• Molecule 18: 30S ribosomal protein S18

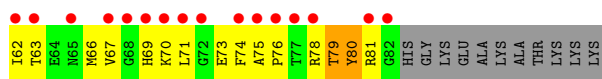
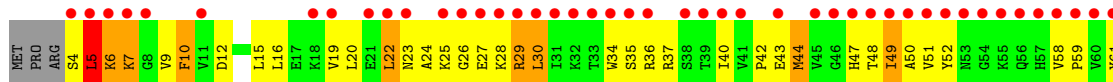




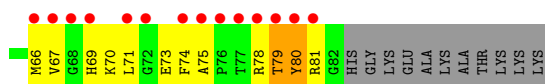
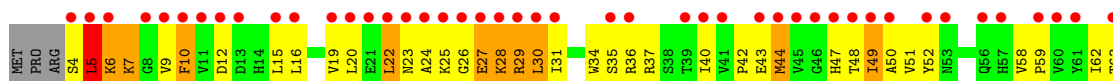
- Molecule 18: 30S ribosomal protein S18



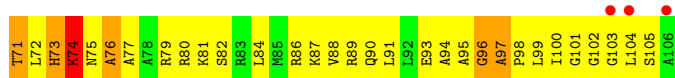
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

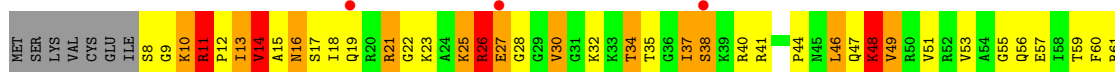
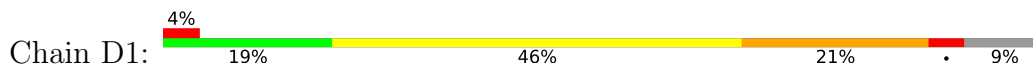


- Molecule 20: 30S ribosomal protein S20





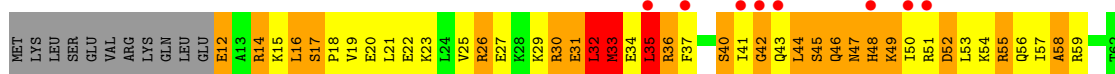
• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



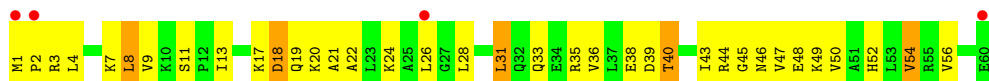
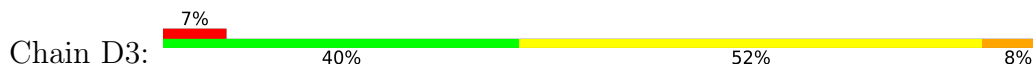
• Molecule 24: 50S ribosomal protein L29



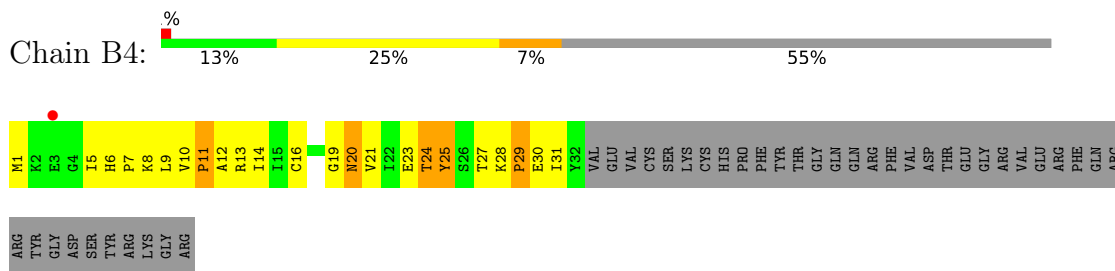
• Molecule 25: 50S ribosomal protein L30



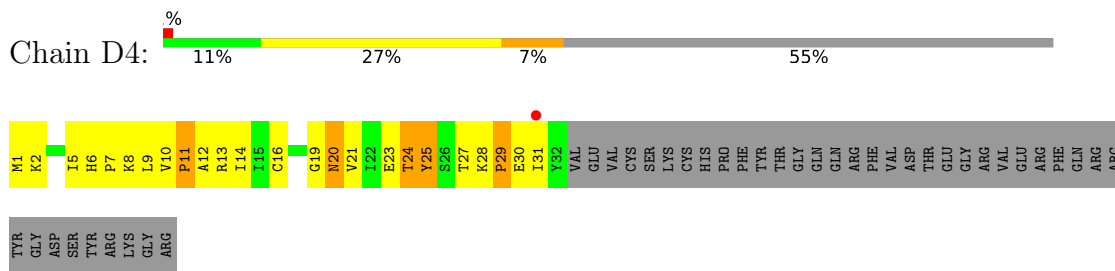
• Molecule 25: 50S ribosomal protein L30



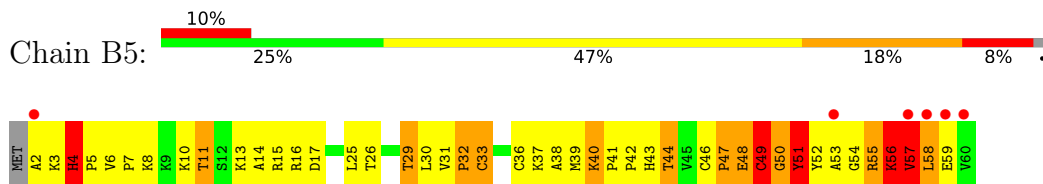
- Molecule 26: 50S ribosomal protein L31



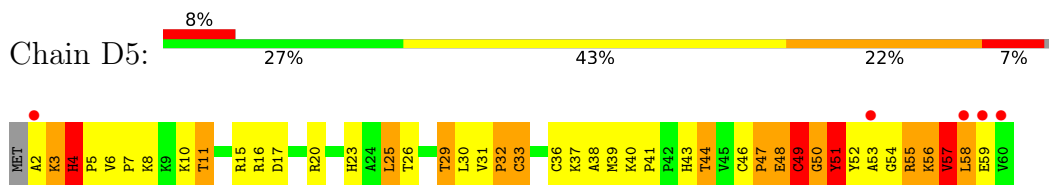
- Molecule 26: 50S ribosomal protein L31



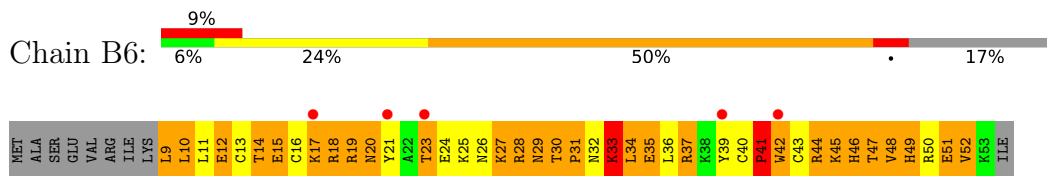
- Molecule 27: 50S ribosomal protein L32



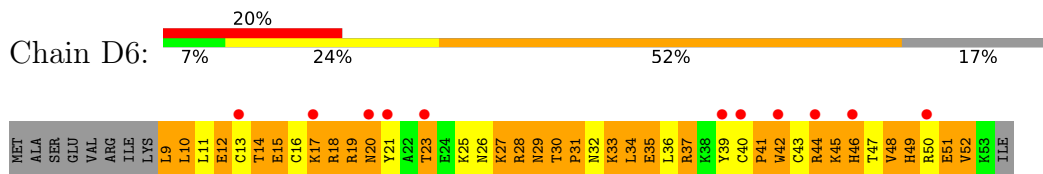
- Molecule 27: 50S ribosomal protein L32



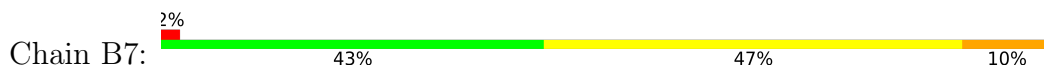
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



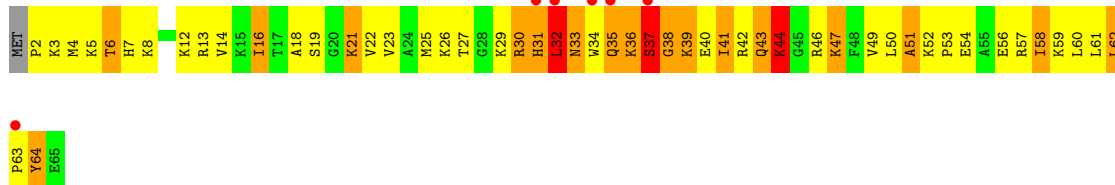
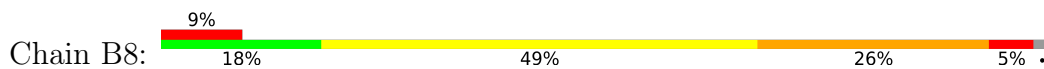
- Molecule 29: 50S ribosomal protein L34



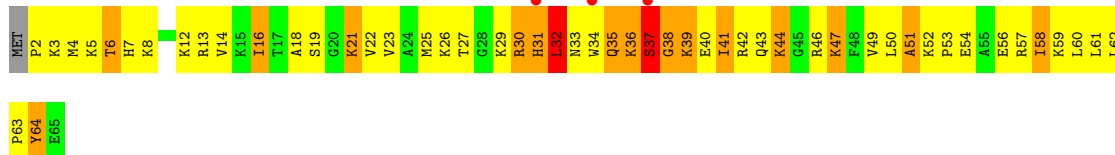
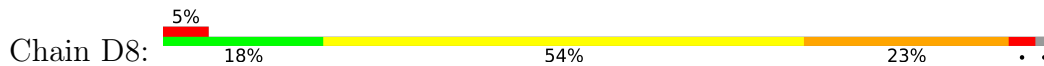
• Molecule 29: 50S ribosomal protein L34



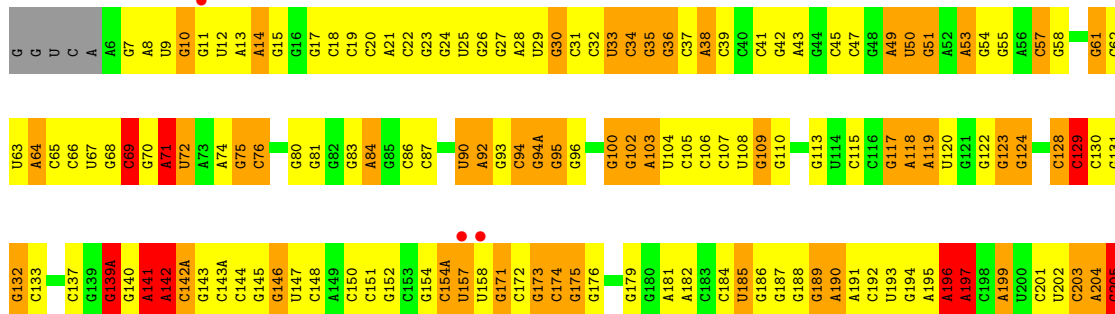
• Molecule 30: 50S ribosomal protein L35

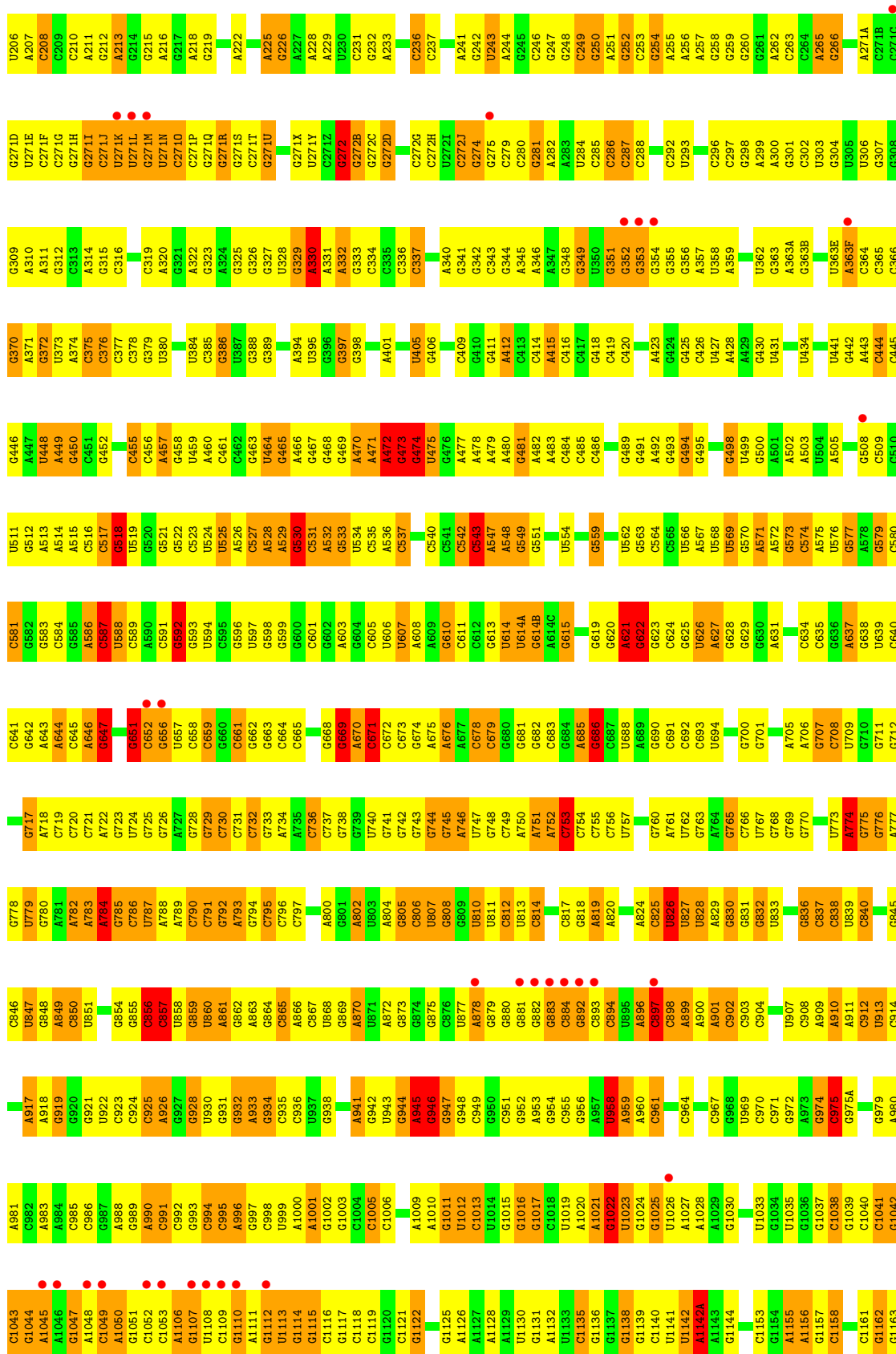


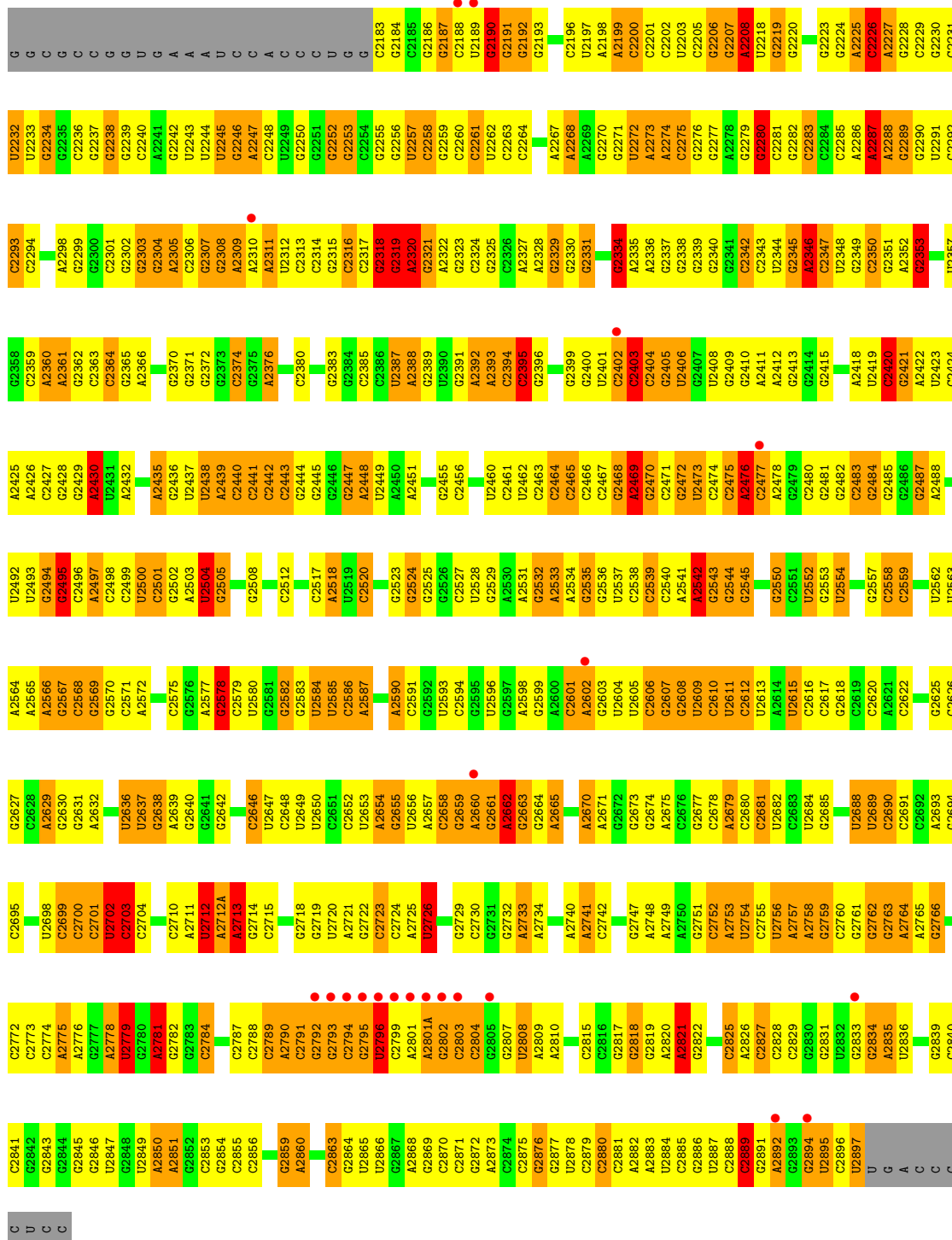
• Molecule 30: 50S ribosomal protein L35



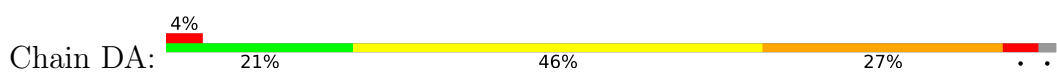
• Molecule 31: 23S ribosomal RNA

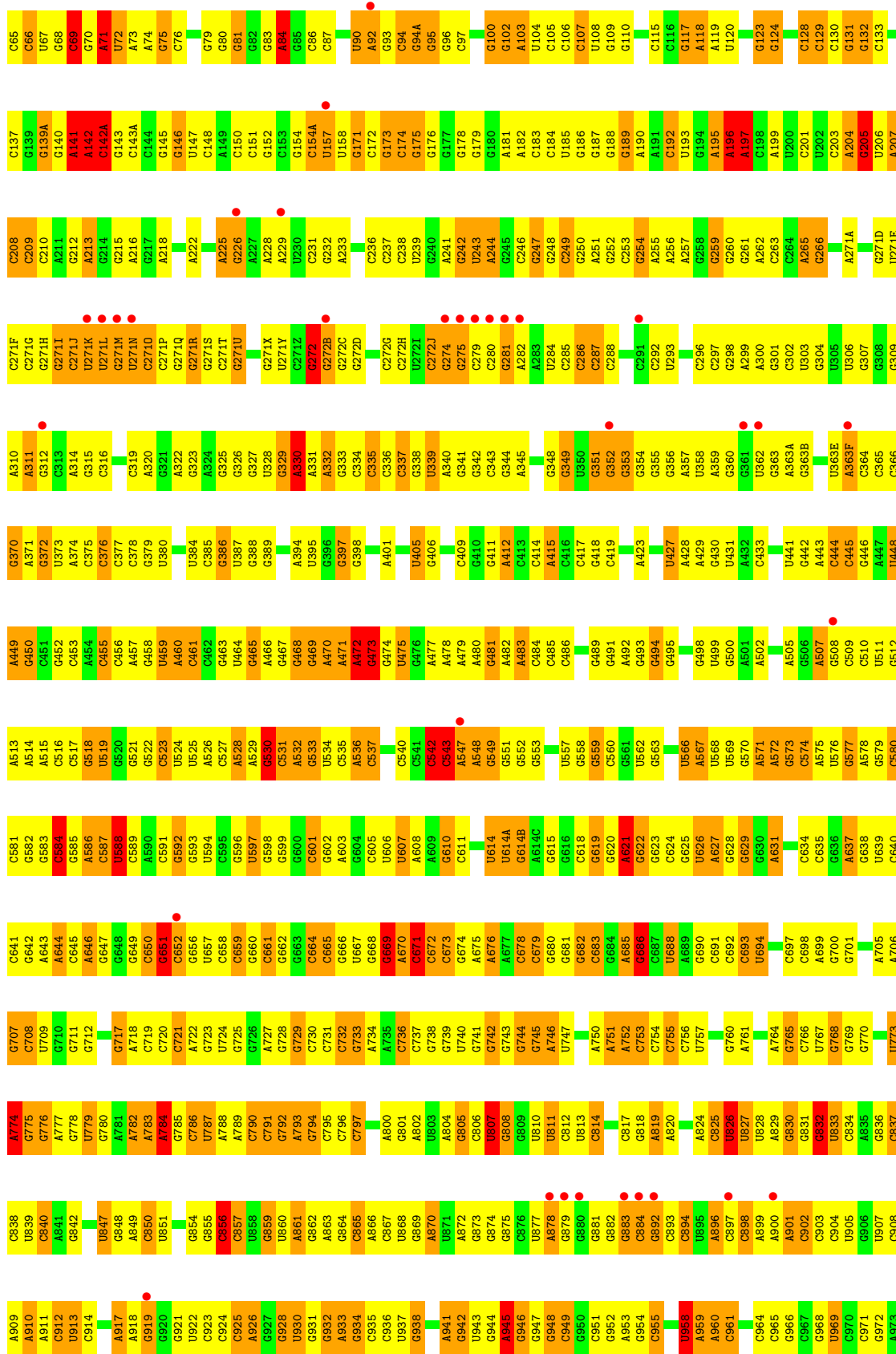






• Molecule 31: 23S ribosomal RNA

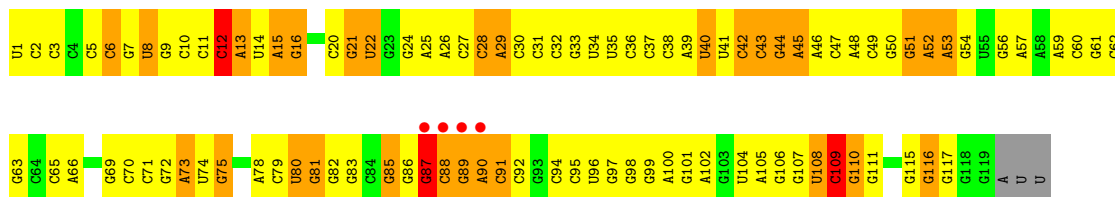
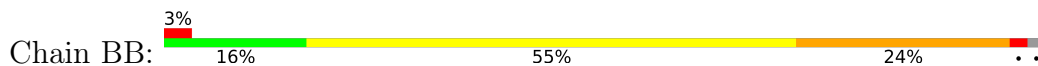




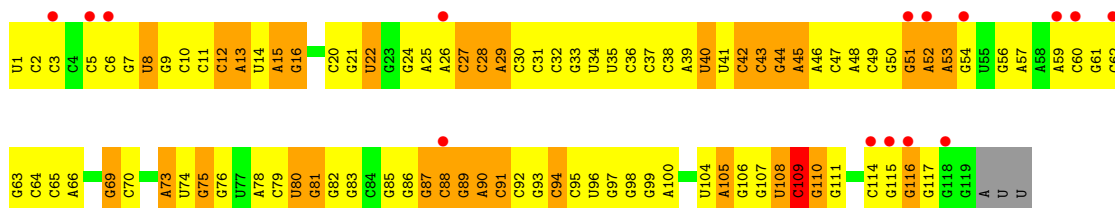
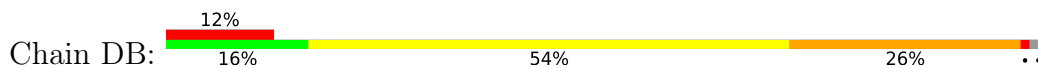
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U2870	U2739	A2665	A2600	G2536	A2600	G2536	G2472	G2407	G2341	G2279	U2218	A2057	U1993
U2871	A2740	U2666	G2601	U2537	U2601	U2537	U2473	U2408	G2342	G2280	G2219	A2058	C1994
U2872	A2741	A2667	C2538	C2538	C2538	C2538	C2474	G2409	C2343	C2281	G2220	G2063	G1997
U2873	C2742	A2670	C2539	C2539	C2539	C2539	C2475	G2410	U2344	G2282	G2221	A2060	G1998
U2874	G2743	G2672	U2604	U2540	U2604	U2540	A2476	A2411	G2345	C2283	G2223	G2064	C1999
U2875	G2744	G2673	U2605	A2541	U2605	A2541	C2477	A2412	A2346	C2284	G2224	C2065	G2000
U2876	G2745	C2674	C2606	A2542	C2606	A2542	A2478	G2413	A2347	C2285	A2225	A2062	A2001
U2877	G2746	C2675	G2607	G2543	G2607	G2543	G2479	G2414	U2348	A2286	G2226	G2063	G2002
U2878	G2747	C2676	G2608	G2544	G2608	G2544	C2480	G2415	G2349	A2287	A2227	C2065	A2005
U2879	A2748	A2679	U2609	G2545	U2609	G2545	G2481	C2416	C2350	A2288	G2228	C2066	C2006
U2880	A2749	C2680	C2610	U2546	C2610	U2546	G2482	C2417	G2351	G2289	C2229	G2067	C2007
U2881	U2750	C2681	U2611	U2547	U2611	U2547	C2483	A2418	C2352	G2290	G2230	U2068	C2008
U2882	C2751	U2682	U2612	G2550	U2612	G2550	G2484	U2419	G2353	U2291	U2232	G2070	G2009
U2883	G2752	G2685	U2613	C2551	U2613	C2551	G2485	C2420	G2354	C2292	U2233	A2071	G2010
U2884	A2753	G2686	A2614	U2552	A2614	U2552	G2486	G2421	G2355	C2293	G2234	G2072	U2011
U2885	U2754	U2687	C2616	G2553	C2616	G2553	A2487	A2422	U2357	C2294	G2235	C2073	G2012
U2886	C2755	U2688	C2617	U2554	C2617	U2554	A2488	U2423	G2358	G2298	G2236	C2074	A2013
U2887	U2756	U2689	G2618	G2555	G2618	G2555	G2489	C2424	C2359	A2298	C2237	U2074	A2014
U2888	A2757	U2690	C2619	G2556	C2619	G2556	U2492	A2425	A2360	G2299	G2237	U2075	A2015
U2889	U2758	C2691	C2620	U2557	C2620	U2557	U2493	A2426	A2361	G2300	G2238	A2076	G2016
U2890	G2759	C2692	A2621	C2558	A2621	C2558	G2494	C2427	G2362	C2301	G2239	A2077	U2016
U2891	C2760	C2693	A2622	C2559	A2622	C2559	G2495	G2428	C2363	G2302	C2240	C2078	U2017
U2892	G2761	A2694	C2622	C2560	C2622	C2560	C2496	G2429	G2364	G2303	A2241	U2079	G2018
U2893	G2762	G2695	G2623	A2561	G2623	A2561	A2497	A2430	G2365	G2304	G2242	G2080	A2019
U2894	G2763	C2696	C2624	U2562	C2624	U2562	C2498	U2431	A2366	A2305	U2243	C2081	A2020
U2895	A2764	U2698	G2625	U2563	G2625	U2563	C2499	A2432	G2370	G2306	U2244	A2082	A2021
U2896	G2765	C2699	A2626	A2564	A2626	A2564	U2500	A2433	G2371	G2307	U2245	G2083	U2022
U2897	G2766	C2700	G2626	A2565	G2626	A2565	C2501	A2434	G2371	G2308	G2246	C2084	G2023
U2898	C2772	C2701	G2627	A2566	G2627	A2566	G2502	A2435	G2374	A2309	A2247	C2085	G2024
U2899	C2773	U2702	A2627	C2567	A2627	C2567	A2503	G2375	C2374	A2310	C2248	U2086	C2025
U2900	C2774	C2703	G2628	C2568	A2628	C2568	U2504	U2438	G2376	U2312	U2249	G2087	C2026
U2901	A2775	C2704	C2629	C2569	C2629	C2569	G2505	A2439	A2376	U2313	U2250	G2088	C2027
U2902	C2776	C2705	U2630	G2570	U2630	G2570	U2506	C2440	A2377	C2313	G2251	U2089	U2028
U2903	G2777	C2706	G2631	C2571	U2631	C2571	C2507	C2441	A2378	C2314	G2252	G2090	G2029
U2904	U2778	C2707	G2632	A2572	U2632	A2572	G2508	C2442	G2379	C2315	G2253	U2091	A2030
U2905	A2779	U2708	A2633	U2573	U2633	U2573	G2509	C2443	C2380	C2316	G2254	U2092	A2031
U2906	U2780	U2709	G2634	C2574	U2634	C2574	U2511	G2444	C2381	C2317	G2255	G2093	G2032
U2907	A2781	A2712	A2713	G2575	U2635	G2575	U2512	G2445	G2382	C2318	G2256	G2094	A2033
U2908	U2782	A2713	A2714	A2577	U2636	A2577	G2513	G2446	G2384	G2319	C2185	C2095	

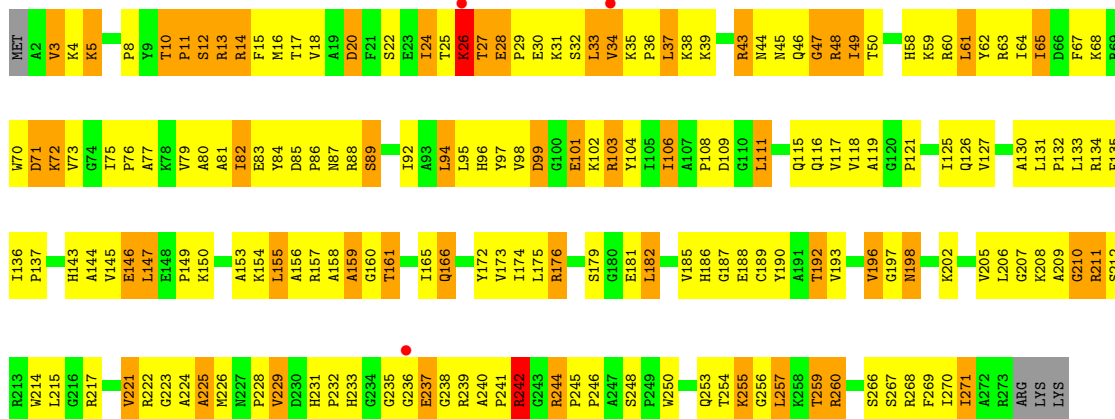
• Molecule 32: 5S ribosomal RNA



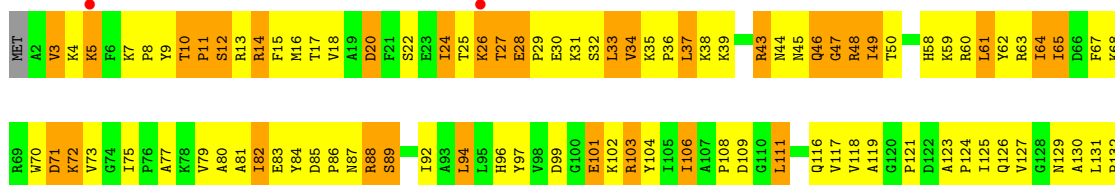
• Molecule 32: 5S ribosomal RNA

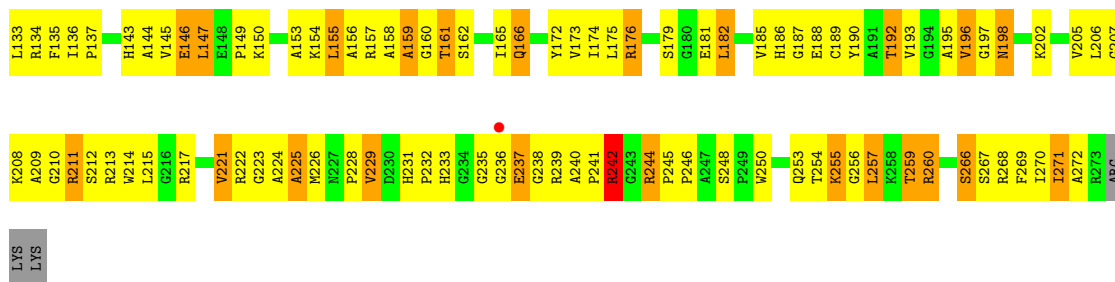


• Molecule 33: 50S ribosomal protein L2

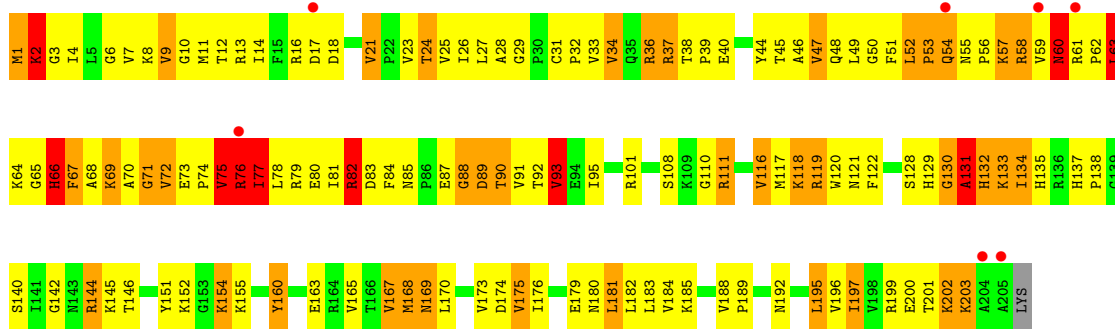
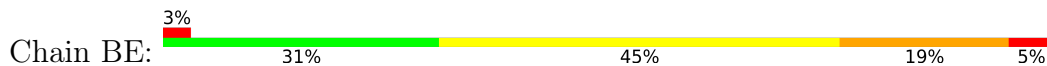


• Molecule 33: 50S ribosomal protein L2

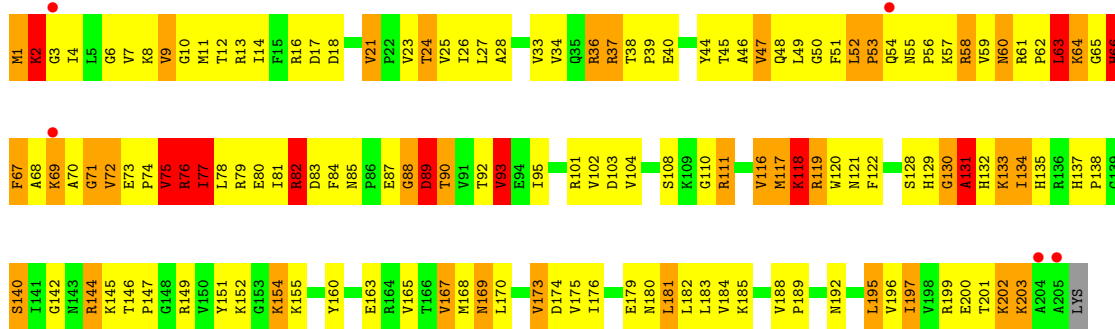




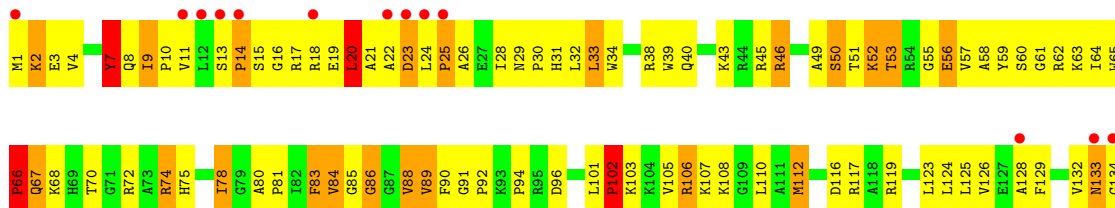
• Molecule 34: 50S ribosomal protein L3

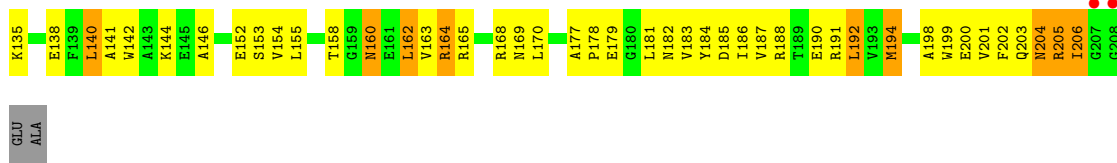


• Molecule 34: 50S ribosomal protein L3

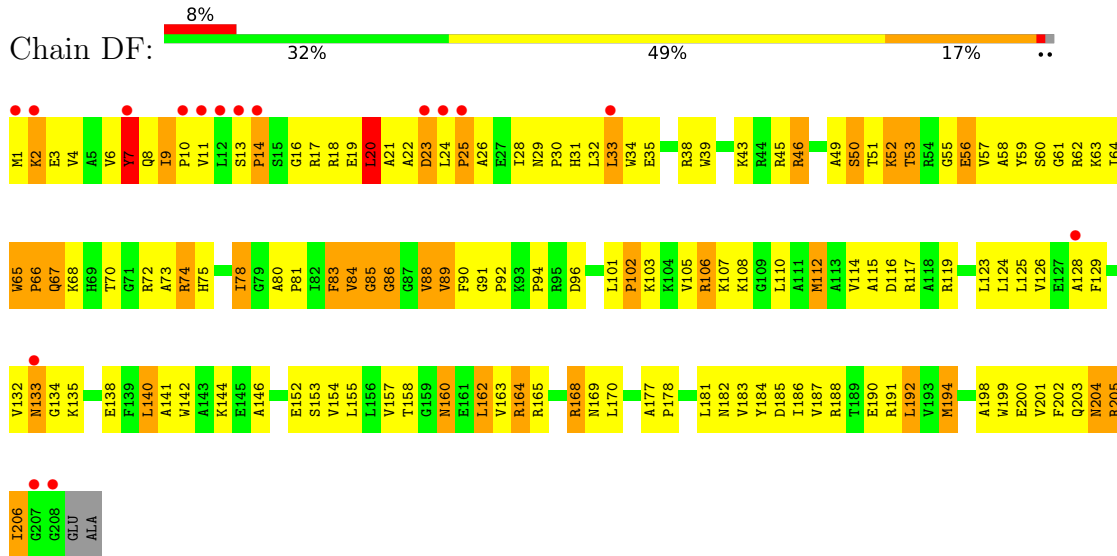


• Molecule 35: 50S ribosomal protein L4

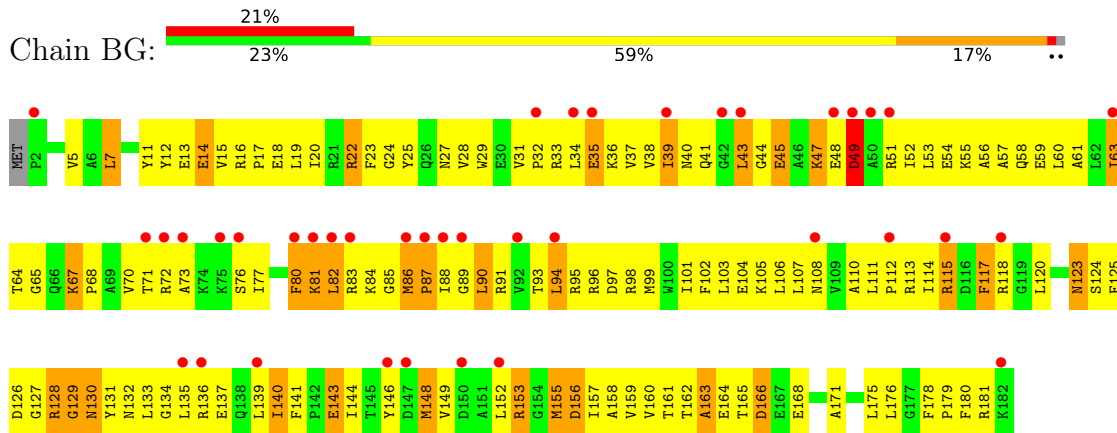




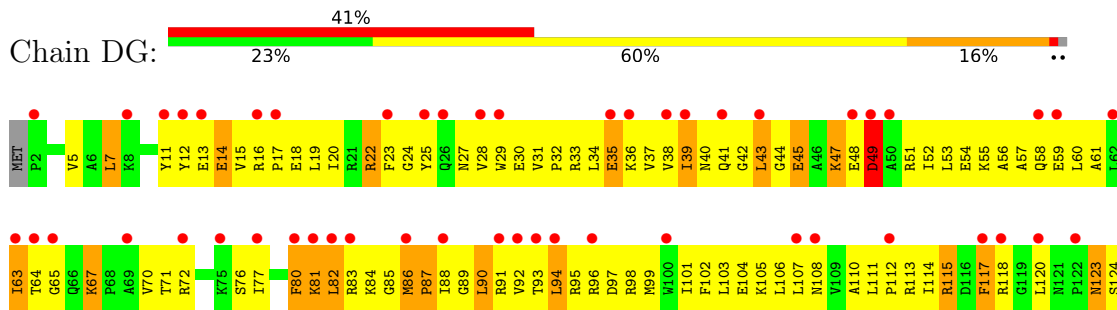
• Molecule 35: 50S ribosomal protein L4

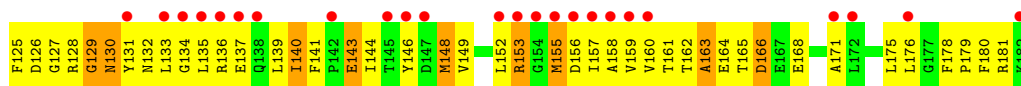


• Molecule 36: 50S ribosomal protein L5

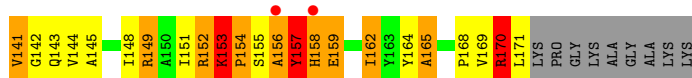
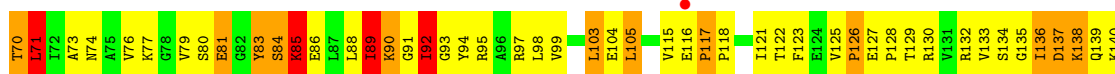
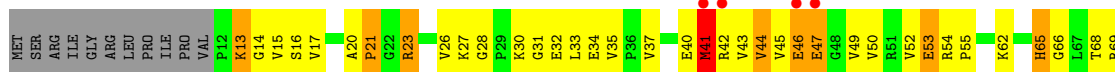


• Molecule 36: 50S ribosomal protein L5

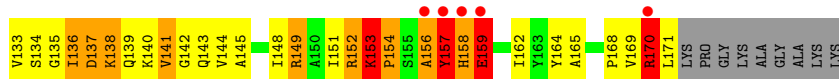
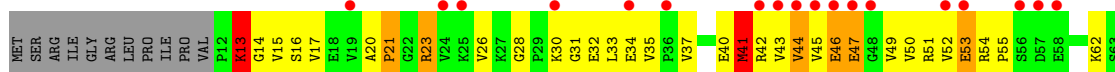




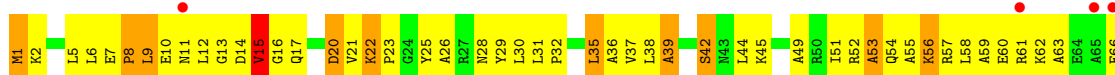
• Molecule 37: 50S ribosomal protein L6



• Molecule 37: 50S ribosomal protein L6

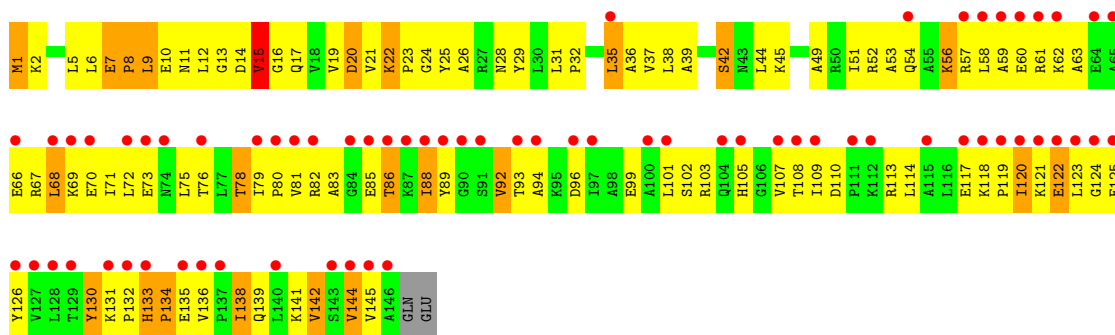


• Molecule 38: 50S ribosomal protein L9

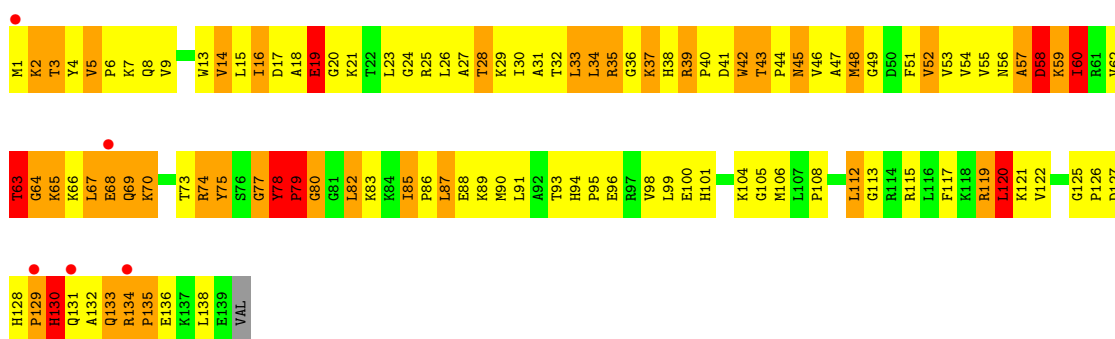
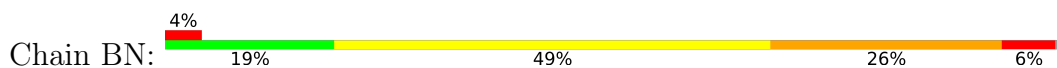


• Molecule 38: 50S ribosomal protein L9

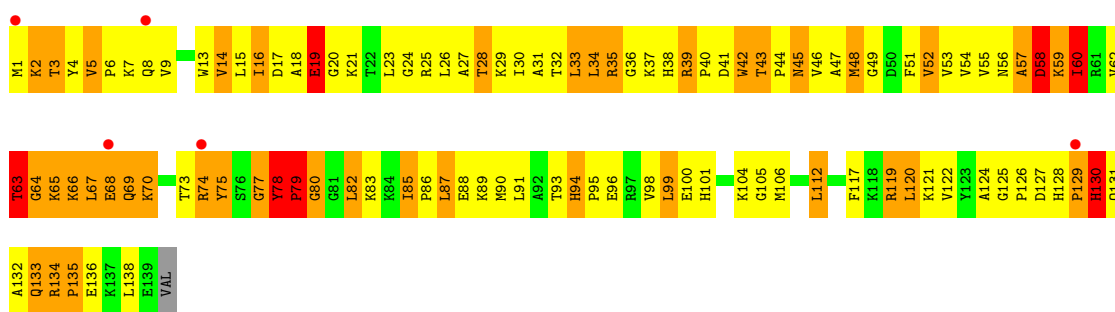
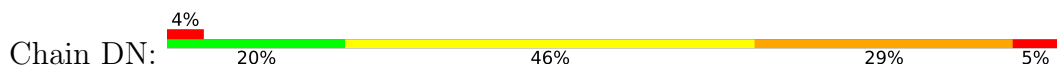




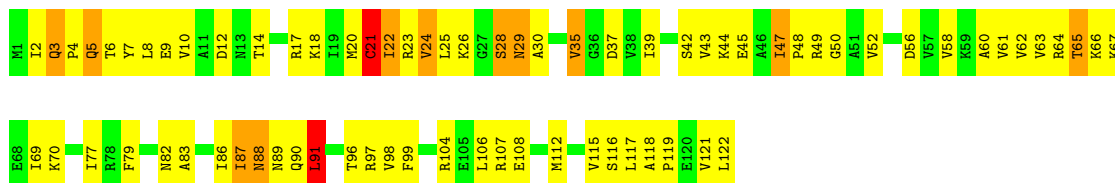
• Molecule 39: 50S ribosomal protein L13



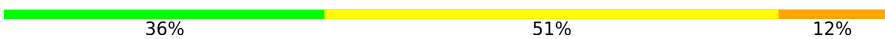
• Molecule 39: 50S ribosomal protein L13

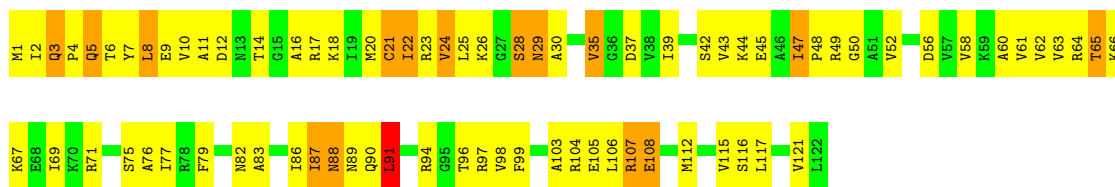


• Molecule 40: 50S ribosomal protein L14




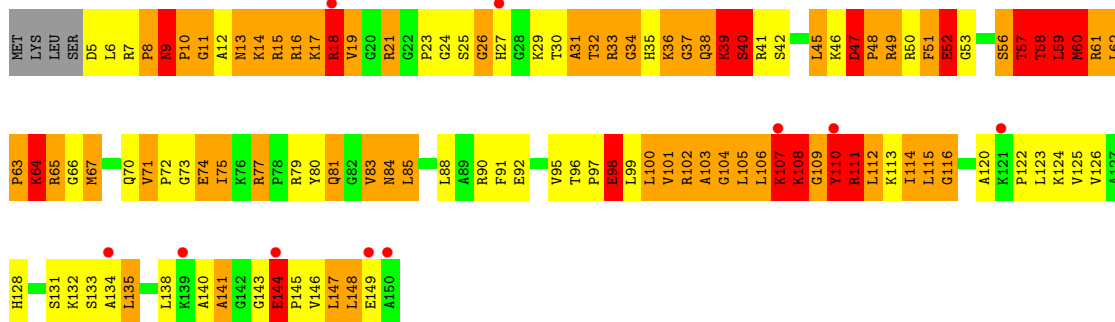
• Molecule 40: 50S ribosomal protein L14

Chain DO:  36% 51% 12%




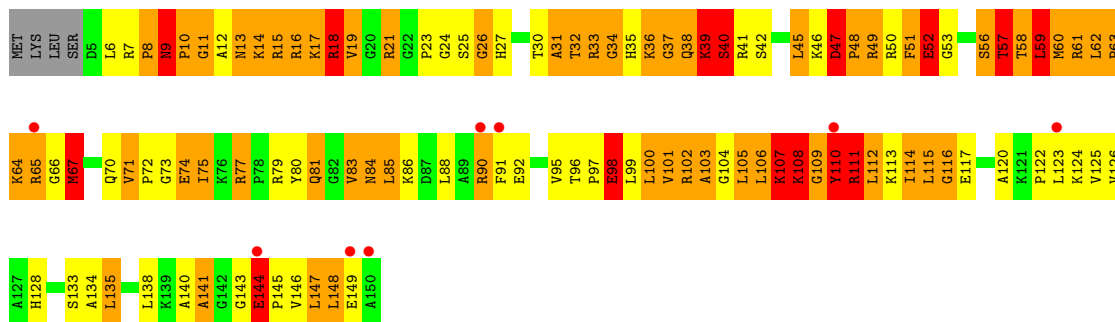
• Molecule 41: 50S ribosomal protein L15

Chain BP:  7% 19% 32% 35% 11%



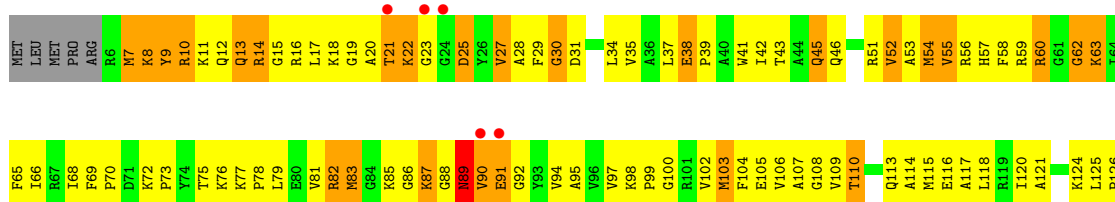
• Molecule 41: 50S ribosomal protein L15

Chain DP:  5% 21% 31% 36% 10%



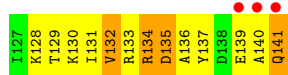
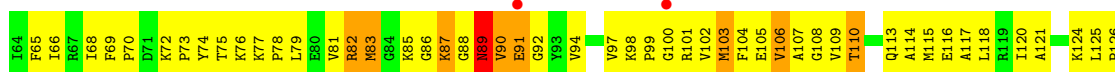
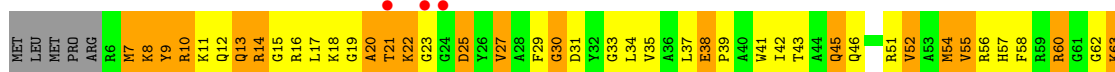
• Molecule 42: 50S ribosomal protein L16

Chain BQ:  6% 21% 53% 21%





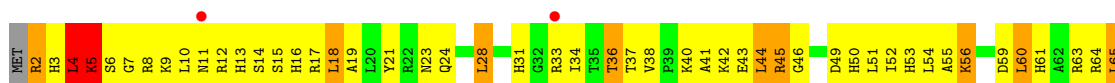
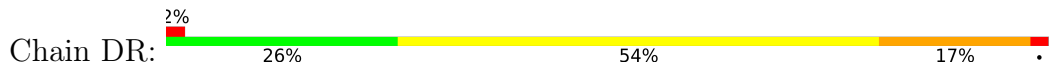
- Molecule 42: 50S ribosomal protein L16



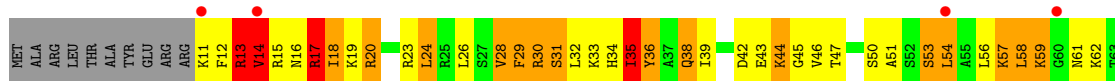
- Molecule 43: 50S ribosomal protein L17



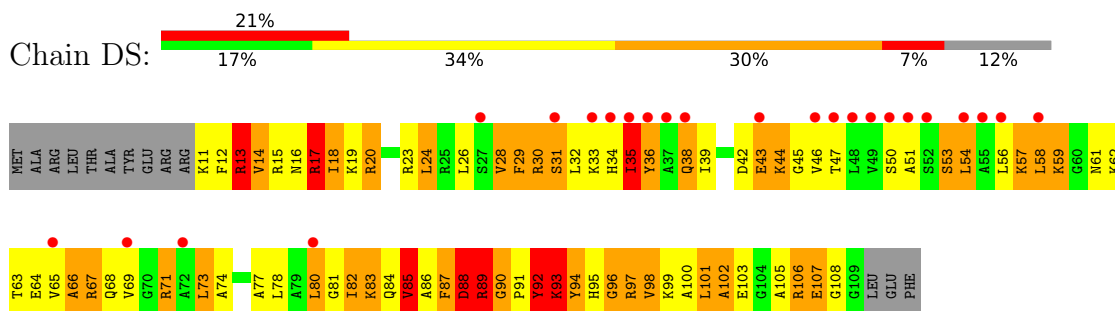
- Molecule 43: 50S ribosomal protein L17



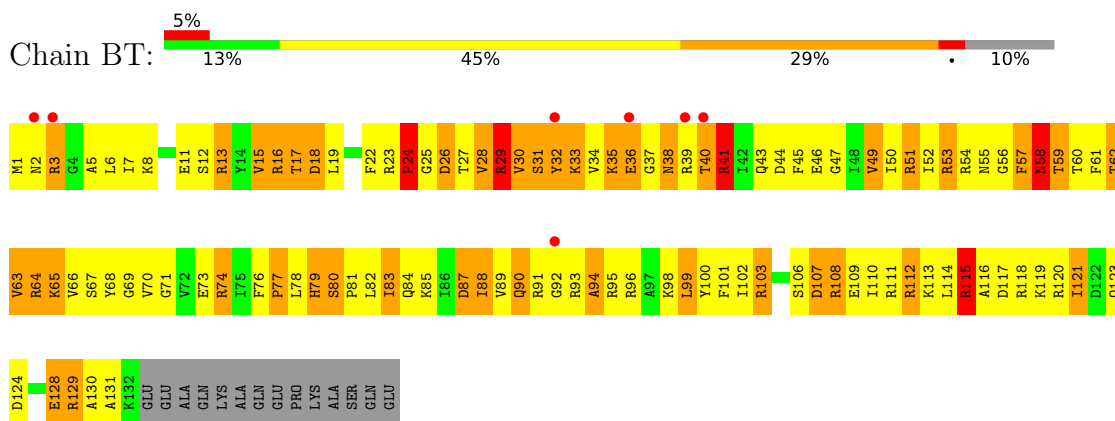
- Molecule 44: 50S ribosomal protein L18



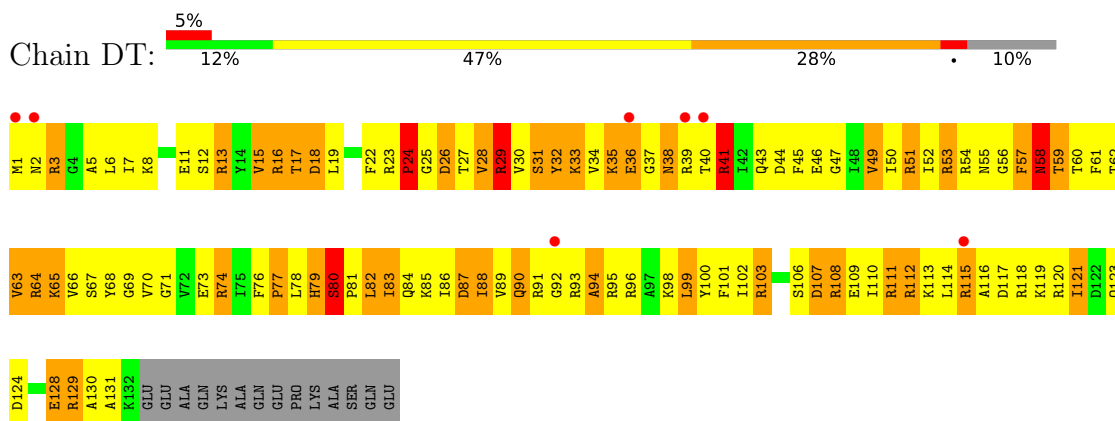
- Molecule 44: 50S ribosomal protein L18



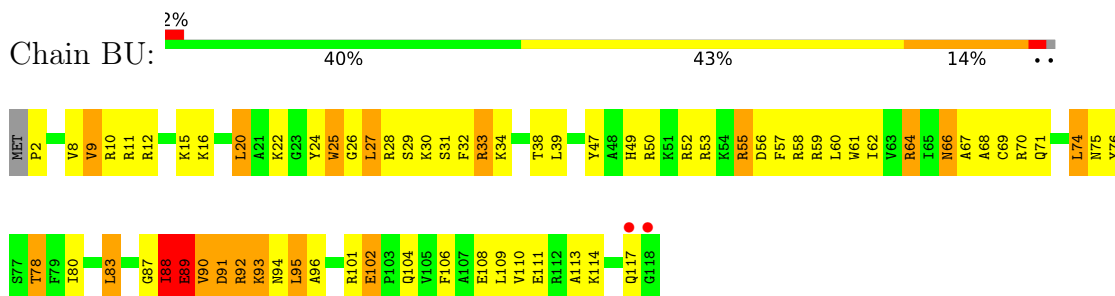
- Molecule 45: 50S ribosomal protein L19



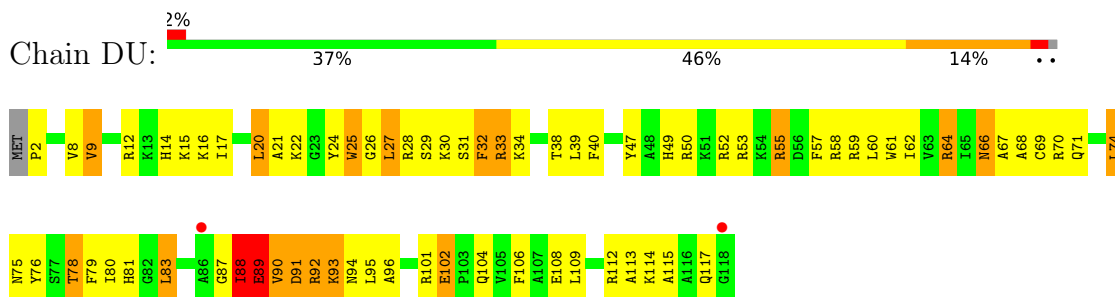
- Molecule 45: 50S ribosomal protein L19



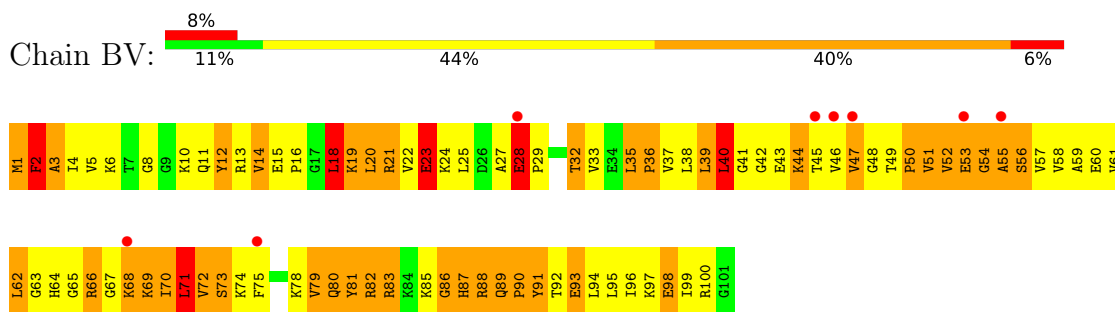
- Molecule 46: 50S ribosomal protein L20



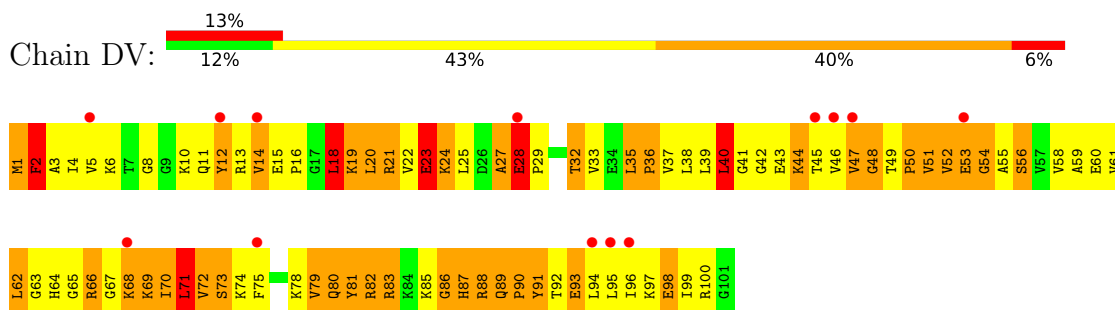
- Molecule 46: 50S ribosomal protein L20



• Molecule 47: 50S ribosomal protein L21



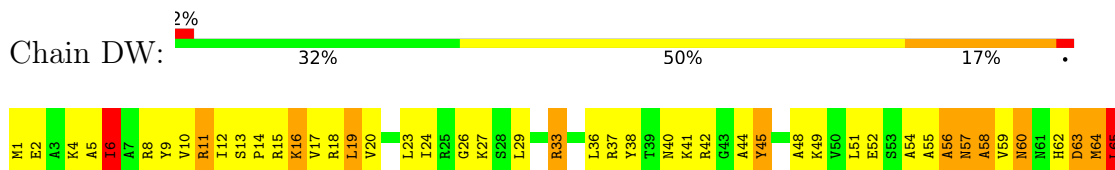
• Molecule 47: 50S ribosomal protein L21



• Molecule 48: 50S ribosomal protein L22

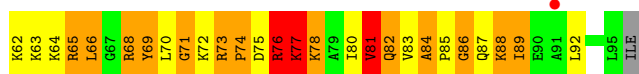
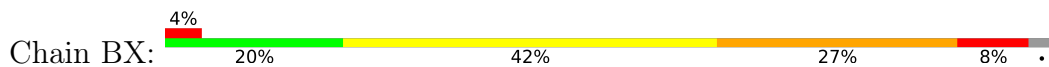


• Molecule 48: 50S ribosomal protein L22

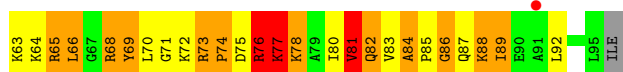
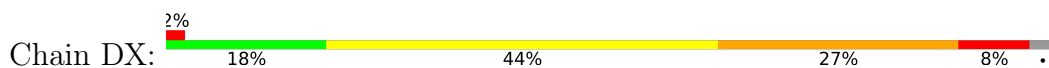




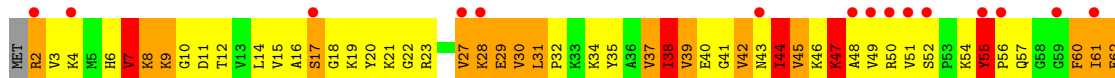
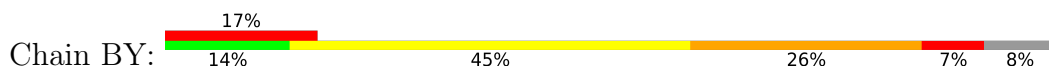
• Molecule 49: 50S ribosomal protein L23



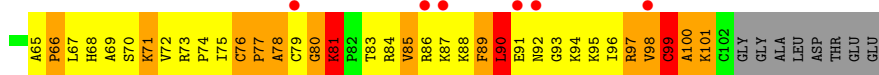
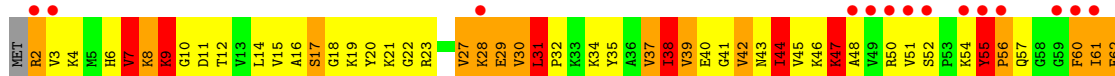
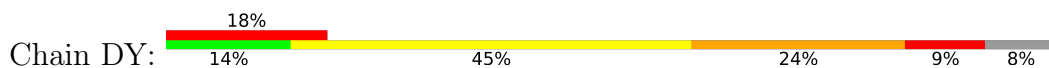
• Molecule 49: 50S ribosomal protein L23



• Molecule 50: 50S ribosomal protein L24

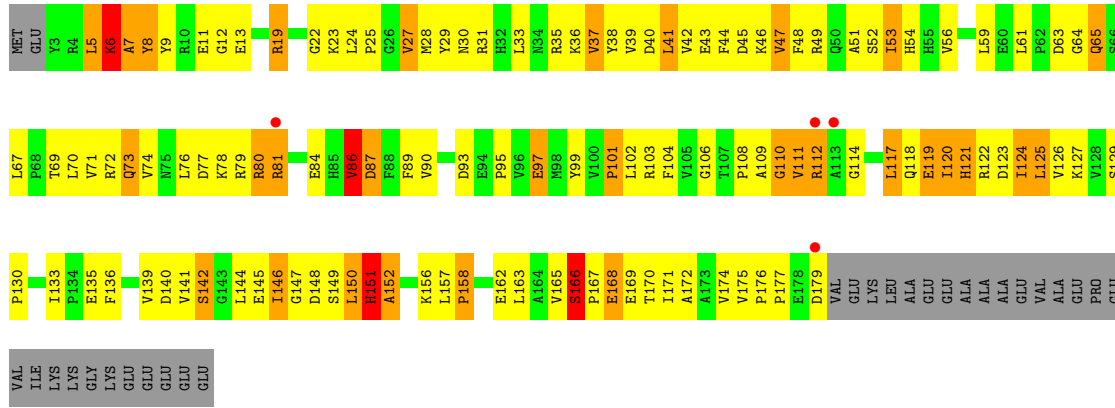


• Molecule 50: 50S ribosomal protein L24

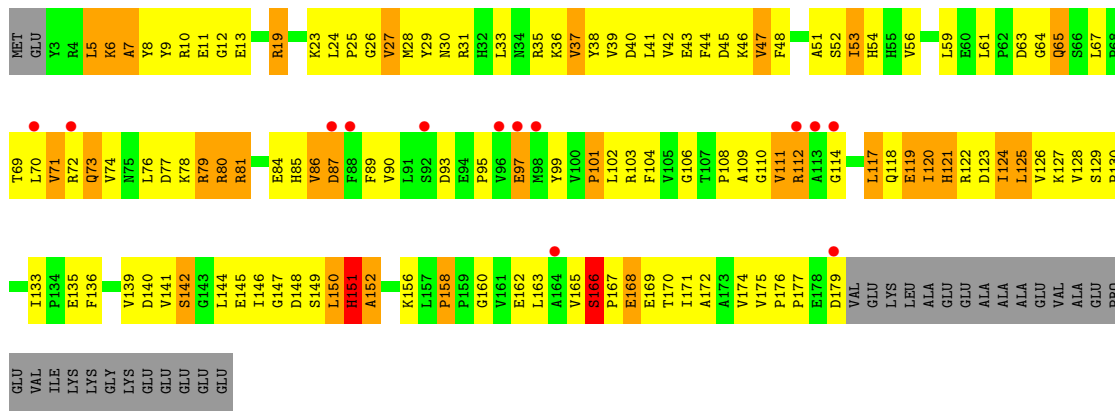


• Molecule 51: 50S ribosomal protein L25





• Molecule 51: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.18Å 448.40Å 621.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.00 49.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.57-3.00) 98.6 (49.57-3.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.01Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.244 , 0.281 0.242 , 0.276	Depositor DCC
R_{free} test set	57089 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 86.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	277987	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CLM, ZN, K, MG

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	0.54	0/36190	0.92	37/56486 (0.1%)
1	CA	0.53	0/36190	0.93	55/56486 (0.1%)
2	AB	0.29	0/1936	0.51	0/2611
2	CB	0.29	0/1936	0.50	0/2611
3	AC	0.27	0/1637	0.44	0/2207
3	CC	0.26	0/1637	0.44	0/2207
4	AD	0.36	0/1733	0.54	0/2318
4	CD	0.38	1/1733 (0.1%)	0.55	0/2318
5	AE	0.38	0/1163	0.58	0/1566
5	CE	0.37	0/1163	0.59	0/1566
6	AF	0.38	0/856	0.58	0/1154
6	CF	0.36	0/856	0.58	0/1154
7	AG	0.25	0/1276	0.44	0/1709
7	CG	0.25	0/1276	0.44	0/1709
8	AH	0.34	0/1136	0.56	0/1527
8	CH	0.34	0/1136	0.55	0/1527
9	AI	0.25	0/1028	0.44	0/1375
9	CI	0.25	0/1028	0.44	0/1375
10	AJ	0.27	0/808	0.48	0/1087
10	CJ	0.26	0/808	0.49	0/1087
11	AK	0.33	0/900	0.55	0/1213
11	CK	0.35	0/900	0.54	0/1213
12	AL	0.42	0/987	0.65	0/1322
12	CL	0.42	0/987	0.65	0/1322
13	AM	0.26	0/928	0.47	0/1238
13	CM	0.26	0/928	0.46	0/1238
14	AN	0.26	0/501	0.42	0/664
14	CN	0.26	0/501	0.42	0/664
15	AO	0.36	0/745	0.59	0/992
15	CO	0.35	0/745	0.58	0/992
16	AP	0.34	0/717	0.59	0/965
16	CP	0.35	0/717	0.60	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.36	0/837	0.58	0/1119
17	CQ	0.37	0/837	0.59	0/1119
18	AR	0.35	0/579	0.58	0/768
18	CR	0.36	0/579	0.57	0/768
19	AS	0.26	0/643	0.43	0/867
19	CS	0.26	0/643	0.44	0/867
20	AT	0.36	0/765	0.57	0/1007
20	CT	0.35	0/765	0.56	0/1007
21	AU	0.26	0/213	0.43	0/279
21	CU	0.26	0/213	0.43	0/279
22	B0	0.53	0/658	0.70	0/878
22	D0	0.49	0/658	0.70	0/878
23	B1	0.78	0/700	0.99	2/931 (0.2%)
23	D1	0.67	0/700	0.95	1/931 (0.1%)
24	B2	0.66	0/423	0.94	0/560
24	D2	0.55	0/423	0.89	0/560
25	B3	0.61	0/473	0.69	0/636
25	D3	0.49	0/473	0.67	0/636
26	B4	0.30	0/156	0.68	0/215
26	D4	0.30	0/156	0.65	0/215
27	B5	0.84	1/473 (0.2%)	1.02	2/639 (0.3%)
27	D5	0.77	0/473	0.97	1/639 (0.2%)
28	B6	0.89	0/387	1.07	0/517
28	D6	0.71	0/387	1.01	0/517
29	B7	0.64	0/427	0.79	0/563
29	D7	0.67	0/427	0.76	0/563
30	B8	0.72	0/516	1.09	2/681 (0.3%)
30	D8	0.64	0/516	1.04	0/681
31	BA	1.06	84/65745 (0.1%)	1.42	971/102639 (0.9%)
31	DA	0.85	35/65745 (0.1%)	1.41	1008/102639 (1.0%)
32	BB	0.83	0/2853	1.18	23/4451 (0.5%)
32	DB	0.66	0/2853	1.13	19/4451 (0.4%)
33	BD	0.63	0/2155	0.85	2/2907 (0.1%)
33	DD	0.59	0/2155	0.83	1/2907 (0.0%)
34	BE	0.63	0/1597	0.82	0/2155
34	DE	0.56	0/1597	0.81	0/2155
35	BF	0.60	0/1659	0.76	0/2246
35	DF	0.52	1/1659 (0.1%)	0.74	0/2246
36	BG	0.34	0/1498	0.55	0/2013
36	DG	0.30	0/1498	0.54	0/2013
37	BH	0.60	0/1246	0.74	0/1684
37	DH	0.44	0/1246	0.69	0/1684
38	BI	0.38	0/1147	0.61	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.40	0/1147	0.61	0/1553
39	BN	0.71	0/1132	0.93	2/1527 (0.1%)
39	DN	0.59	0/1132	0.87	1/1527 (0.1%)
40	BO	0.59	1/943 (0.1%)	0.73	0/1269
40	DO	0.52	0/943	0.73	1/1269 (0.1%)
41	BP	0.69	0/1131	1.03	8/1504 (0.5%)
41	DP	0.60	0/1131	0.98	6/1504 (0.4%)
42	BQ	0.70	0/1100	0.85	1/1470 (0.1%)
42	DQ	0.60	0/1100	0.83	0/1470
43	BR	0.63	0/974	0.82	1/1302 (0.1%)
43	DR	0.56	0/974	0.80	1/1302 (0.1%)
44	BS	0.50	0/779	0.77	0/1038
44	DS	0.43	0/779	0.73	0/1038
45	BT	0.59	0/1114	0.85	2/1488 (0.1%)
45	DT	0.52	0/1114	0.83	1/1488 (0.1%)
46	BU	0.69	0/975	0.76	0/1297
46	DU	0.56	0/975	0.72	0/1297
47	BV	0.72	0/789	0.95	1/1054 (0.1%)
47	DV	0.58	0/789	0.89	1/1054 (0.1%)
48	BW	0.68	0/907	0.84	2/1216 (0.2%)
48	DW	0.58	0/907	0.81	2/1216 (0.2%)
49	BX	0.70	0/740	0.96	2/995 (0.2%)
49	DX	0.63	0/740	0.94	2/995 (0.2%)
50	BY	0.70	1/789 (0.1%)	0.91	0/1053
50	DY	0.60	0/789	0.87	1/1053 (0.1%)
51	BZ	0.47	0/1436	0.67	2/1951 (0.1%)
51	DZ	0.41	0/1436	0.66	1/1951 (0.1%)
All	All	0.75	124/301000 (0.0%)	1.13	2162/449812 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	B1	0	1
23	D1	0	1
24	B2	0	1
24	D2	0	1
27	B5	0	1
27	D5	0	1
28	B6	0	1

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

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	669	G	C4'-C3'	-11.30	1.40	1.53
31	DA	669	G	C4'-C3'	-10.33	1.41	1.53
31	BA	1300	U	C4'-C3'	-9.89	1.42	1.53
31	BA	1332	G	N9-C4	-9.70	1.30	1.38
31	DA	783	A	N9-C4	-9.28	1.32	1.37

The worst 5 of 2162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BA	1332	G	N3-C4-C5	18.18	137.69	128.60
31	DA	1779	U	C5-C6-N1	-17.02	114.19	122.70
31	BA	1779	U	C5-C6-N1	-16.17	114.61	122.70
31	BA	1332	G	N3-C4-N9	-15.97	116.42	126.00
31	BA	1332	G	C2-N3-C4	-15.30	104.25	111.90

5 of 38 chirality outliers are listed below:

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

5 of 55 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1597	0
1	CA	32329	0	16318	1553	0
2	AB	1901	0	1951	215	0
2	CB	1901	0	1951	207	0
3	AC	1613	0	1677	116	0
3	CC	1613	0	1677	116	0
4	AD	1703	0	1765	190	0
4	CD	1703	0	1764	192	0
5	AE	1147	0	1207	101	0
5	CE	1147	0	1207	100	0
6	AF	843	0	857	96	0
6	CF	843	0	857	98	0
7	AG	1257	0	1296	75	0
7	CG	1257	0	1296	75	0
8	AH	1116	0	1177	101	0
8	CH	1116	0	1177	99	0
9	AI	1011	0	1042	101	0
9	CI	1011	0	1042	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	105	0
10	CJ	795	0	840	102	0
11	AK	885	0	904	63	0
11	CK	885	0	904	68	0
12	AL	971	0	1057	100	0
12	CL	971	0	1057	103	0
13	AM	921	0	976	88	0
13	CM	921	0	976	91	0
14	AN	492	0	530	47	0
14	CN	492	0	529	46	0
15	AO	734	0	771	76	0
15	CO	734	0	771	78	0
16	AP	701	0	720	91	0
16	CP	701	0	720	97	0
17	AQ	824	0	891	66	0
17	CQ	824	0	891	55	0
18	AR	574	0	644	76	0
18	CR	574	0	644	78	0
19	AS	630	0	652	51	0
19	CS	630	0	652	52	0
20	AT	763	0	861	82	0
20	CT	763	0	861	73	0
21	AU	209	0	221	9	0
21	CU	209	0	221	9	0
22	B0	650	0	654	55	0
22	D0	650	0	654	57	0
23	B1	693	0	764	146	0
23	D1	693	0	764	143	0
24	B2	421	0	461	119	0
24	D2	421	0	461	123	0
25	B3	468	0	523	32	0
25	D3	468	0	523	41	0
26	B4	157	0	69	20	0
26	D4	157	0	69	21	0
27	B5	459	0	480	94	0
27	D5	459	0	480	86	0
28	B6	381	0	390	102	0
28	D6	381	0	390	97	0
29	B7	419	0	467	37	0
29	D7	419	0	467	39	0
30	B8	508	0	576	158	0
30	D8	508	0	576	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29590	2607	0
31	DA	58698	0	29591	2784	0
32	BB	2551	0	1295	145	0
32	DB	2551	0	1295	156	0
33	BD	2105	0	2182	325	0
33	DD	2105	0	2182	333	0
34	BE	1564	0	1629	240	0
34	DE	1564	0	1629	249	0
35	BF	1624	0	1677	182	0
35	DF	1624	0	1677	185	0
36	BG	1474	0	1534	190	0
36	DG	1474	0	1534	187	0
37	BH	1223	0	1282	162	0
37	DH	1223	0	1282	157	0
38	BI	1132	0	1218	120	0
38	DI	1132	0	1218	125	0
39	BN	1105	0	1180	218	0
39	DN	1105	0	1180	229	0
40	BO	933	0	996	77	0
40	DO	933	0	996	86	0
41	BP	1114	0	1187	302	0
41	DP	1114	0	1187	289	0
42	BQ	1080	0	1127	165	0
42	DQ	1080	0	1127	176	0
43	BR	960	0	1021	135	0
43	DR	960	0	1021	132	0
44	BS	771	0	832	149	0
44	DS	771	0	832	139	0
45	BT	1100	0	1164	210	0
45	DT	1100	0	1164	201	0
46	BU	958	0	1015	145	0
46	DU	958	0	1015	151	0
47	BV	779	0	851	224	0
47	DV	779	0	851	225	0
48	BW	896	0	953	76	0
48	DW	896	0	953	84	0
49	BX	726	0	778	168	0
49	DX	726	0	778	164	0
50	BY	776	0	870	177	0
50	DY	776	0	870	178	0
51	BZ	1404	0	1432	153	0
51	DZ	1404	0	1432	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	56	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	BA	368	0	0	0	0
52	BB	7	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	2	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	2	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	53	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	DA	332	0	0	0	0
52	DB	4	0	0	0	0
52	DD	1	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	2	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	20	0	10	0	0
55	DA	20	0	10	0	0
All	All	277987	0	189127	18994	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 41.

The worst 5 of 18994 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B5:46:CYS:SG	27:B5:47:PRO:HD2	1.78	1.22
31:BA:1899:G:H22	31:BA:1902:C:N4	1.41	1.18
30:B8:32:LEU:CB	30:B8:35:GLN:H	1.57	1.17
32:DB:20:C:H2'	32:DB:21:G:H5''	1.25	1.17
41:BP:141:ALA:HB3	25:D3:1:MET:SD	1.86	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	155 (66%)	61 (26%)	17 (7%)	1	5
2	CB	233/256 (91%)	155 (66%)	60 (26%)	18 (8%)	1	5
3	AC	205/239 (86%)	148 (72%)	46 (22%)	11 (5%)	2	11
3	CC	205/239 (86%)	148 (72%)	45 (22%)	12 (6%)	1	9
4	AD	206/209 (99%)	129 (63%)	57 (28%)	20 (10%)	0	2
4	CD	206/209 (99%)	131 (64%)	55 (27%)	20 (10%)	0	2
5	AE	149/162 (92%)	103 (69%)	36 (24%)	10 (7%)	1	6
5	CE	149/162 (92%)	104 (70%)	36 (24%)	9 (6%)	1	9
6	AF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	12
6	CF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	12
7	AG	153/156 (98%)	123 (80%)	28 (18%)	2 (1%)	12	45
7	CG	153/156 (98%)	124 (81%)	27 (18%)	2 (1%)	12	45
8	AH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	0	3
8	CH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	3
9	AI	123/128 (96%)	89 (72%)	26 (21%)	8 (6%)	1	7
9	CI	123/128 (96%)	91 (74%)	24 (20%)	8 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	78 (80%)	15 (16%)	4 (4%)	3	16
10	CJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	2	12
11	AK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	9	39
11	CK	117/129 (91%)	90 (77%)	25 (21%)	2 (2%)	9	39
12	AL	123/135 (91%)	85 (69%)	25 (20%)	13 (11%)	0	2
12	CL	123/135 (91%)	82 (67%)	27 (22%)	14 (11%)	0	2
13	AM	107/126 (85%)	80 (75%)	21 (20%)	6 (6%)	2	10
13	CM	107/126 (85%)	81 (76%)	19 (18%)	7 (6%)	1	7
14	AN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	39
14	CN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	39
15	AO	86/89 (97%)	65 (76%)	14 (16%)	7 (8%)	1	4
15	CO	86/89 (97%)	64 (74%)	16 (19%)	6 (7%)	1	6
16	AP	82/88 (93%)	51 (62%)	18 (22%)	13 (16%)	0	1
16	CP	82/88 (93%)	52 (63%)	18 (22%)	12 (15%)	0	1
17	AQ	98/105 (93%)	79 (81%)	11 (11%)	8 (8%)	1	4
17	CQ	98/105 (93%)	78 (80%)	13 (13%)	7 (7%)	1	5
18	AR	68/88 (77%)	49 (72%)	14 (21%)	5 (7%)	1	5
18	CR	68/88 (77%)	46 (68%)	16 (24%)	6 (9%)	1	3
19	AS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	3
19	CS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	3
20	AT	97/106 (92%)	70 (72%)	18 (19%)	9 (9%)	0	3
20	CT	97/106 (92%)	68 (70%)	20 (21%)	9 (9%)	0	3
21	AU	23/27 (85%)	17 (74%)	5 (22%)	1 (4%)	2	15
21	CU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	3
22	B0	83/85 (98%)	69 (83%)	10 (12%)	4 (5%)	2	13
22	D0	83/85 (98%)	68 (82%)	11 (13%)	4 (5%)	2	13
23	B1	87/98 (89%)	47 (54%)	24 (28%)	16 (18%)	0	0
23	D1	87/98 (89%)	46 (53%)	24 (28%)	17 (20%)	0	0
24	B2	49/72 (68%)	23 (47%)	14 (29%)	12 (24%)	0	0
24	D2	49/72 (68%)	22 (45%)	15 (31%)	12 (24%)	0	0
25	B3	58/60 (97%)	50 (86%)	8 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D3	58/60 (97%)	48 (83%)	10 (17%)	0	100	100
26	B4	30/71 (42%)	4 (13%)	14 (47%)	12 (40%)	0	0
26	D4	30/71 (42%)	3 (10%)	15 (50%)	12 (40%)	0	0
27	B5	57/60 (95%)	43 (75%)	4 (7%)	10 (18%)	0	0
27	D5	57/60 (95%)	42 (74%)	6 (10%)	9 (16%)	0	1
28	B6	41/54 (76%)	21 (51%)	6 (15%)	14 (34%)	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%)	42 (89%)	5 (11%)	0	100	100
30	B8	62/65 (95%)	41 (66%)	12 (19%)	9 (14%)	0	1
30	D8	62/65 (95%)	42 (68%)	12 (19%)	8 (13%)	0	1
33	BD	270/276 (98%)	211 (78%)	44 (16%)	15 (6%)	2	10
33	DD	270/276 (98%)	208 (77%)	46 (17%)	16 (6%)	1	9
34	BE	203/206 (98%)	147 (72%)	31 (15%)	25 (12%)	0	1
34	DE	203/206 (98%)	144 (71%)	37 (18%)	22 (11%)	0	2
35	BF	206/210 (98%)	158 (77%)	34 (16%)	14 (7%)	1	6
35	DF	206/210 (98%)	154 (75%)	36 (18%)	16 (8%)	1	4
36	BG	177/182 (97%)	125 (71%)	35 (20%)	17 (10%)	0	3
36	DG	177/182 (97%)	126 (71%)	34 (19%)	17 (10%)	0	3
37	BH	158/180 (88%)	102 (65%)	31 (20%)	25 (16%)	0	1
37	DH	158/180 (88%)	101 (64%)	31 (20%)	26 (16%)	0	0
38	BI	144/148 (97%)	98 (68%)	30 (21%)	16 (11%)	0	2
38	DI	144/148 (97%)	99 (69%)	33 (23%)	12 (8%)	1	4
39	BN	137/140 (98%)	89 (65%)	28 (20%)	20 (15%)	0	1
39	DN	137/140 (98%)	92 (67%)	25 (18%)	20 (15%)	0	1
40	BO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	39
40	DO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	5	28
41	BP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
41	DP	144/150 (96%)	70 (49%)	33 (23%)	41 (28%)	0	0
42	BQ	134/141 (95%)	97 (72%)	21 (16%)	16 (12%)	0	1
42	DQ	134/141 (95%)	92 (69%)	25 (19%)	17 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BR	115/118 (98%)	86 (75%)	22 (19%)	7 (6%)	1	8
43	DR	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	1	8
44	BS	97/112 (87%)	45 (46%)	22 (23%)	30 (31%)	0	0
44	DS	97/112 (87%)	44 (45%)	22 (23%)	31 (32%)	0	0
45	BT	130/146 (89%)	91 (70%)	21 (16%)	18 (14%)	0	1
45	DT	130/146 (89%)	91 (70%)	21 (16%)	18 (14%)	0	1
46	BU	115/118 (98%)	89 (77%)	18 (16%)	8 (7%)	1	6
46	DU	115/118 (98%)	86 (75%)	21 (18%)	8 (7%)	1	6
47	BV	97/101 (96%)	54 (56%)	18 (19%)	25 (26%)	0	0
47	DV	97/101 (96%)	53 (55%)	19 (20%)	25 (26%)	0	0
48	BW	111/113 (98%)	85 (77%)	17 (15%)	9 (8%)	1	4
48	DW	111/113 (98%)	83 (75%)	19 (17%)	9 (8%)	1	4
49	BX	91/96 (95%)	47 (52%)	23 (25%)	21 (23%)	0	0
49	DX	91/96 (95%)	48 (53%)	23 (25%)	20 (22%)	0	0
50	BY	99/110 (90%)	47 (48%)	22 (22%)	30 (30%)	0	0
50	DY	99/110 (90%)	44 (44%)	25 (25%)	30 (30%)	0	0
51	BZ	175/206 (85%)	123 (70%)	32 (18%)	20 (11%)	0	2
51	DZ	175/206 (85%)	121 (69%)	36 (21%)	18 (10%)	0	2
All	All	11148/12060 (92%)	7786 (70%)	2170 (20%)	1192 (11%)	0	2

5 of 1192 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	20	GLU
2	AB	106	LYS
2	AB	165	VAL
2	AB	195	ASP

5.3.2 Protein sidechains [i](#)

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%)	170 (84%)	32 (16%)	2	12
2	CB	202/220 (92%)	168 (83%)	34 (17%)	2	11
3	AC	160/188 (85%)	153 (96%)	7 (4%)	28	65
3	CC	160/188 (85%)	153 (96%)	7 (4%)	28	65
4	AD	180/181 (99%)	156 (87%)	24 (13%)	4	17
4	CD	180/181 (99%)	156 (87%)	24 (13%)	4	17
5	AE	115/123 (94%)	95 (83%)	20 (17%)	2	10
5	CE	115/123 (94%)	95 (83%)	20 (17%)	2	10
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	21
6	CF	90/90 (100%)	78 (87%)	12 (13%)	4	17
7	AG	126/127 (99%)	122 (97%)	4 (3%)	39	74
7	CG	126/127 (99%)	122 (97%)	4 (3%)	39	74
8	AH	119/119 (100%)	106 (89%)	13 (11%)	6	25
8	CH	119/119 (100%)	106 (89%)	13 (11%)	6	25
9	AI	98/99 (99%)	90 (92%)	8 (8%)	11	39
9	CI	98/99 (99%)	90 (92%)	8 (8%)	11	39
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
11	AK	90/99 (91%)	82 (91%)	8 (9%)	9	35
11	CK	90/99 (91%)	83 (92%)	7 (8%)	12	42
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%)	17	50
13	CM	93/101 (92%)	87 (94%)	6 (6%)	17	50
14	AN	49/50 (98%)	45 (92%)	4 (8%)	11	39
14	CN	49/50 (98%)	45 (92%)	4 (8%)	11	39
15	AO	79/80 (99%)	68 (86%)	11 (14%)	3	16
15	CO	79/80 (99%)	68 (86%)	11 (14%)	3	16
16	AP	72/74 (97%)	58 (81%)	14 (19%)	1	7
16	CP	72/74 (97%)	59 (82%)	13 (18%)	1	9
17	AQ	94/97 (97%)	82 (87%)	12 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	4	19
18	AR	61/77 (79%)	55 (90%)	6 (10%)	8	30
18	CR	61/77 (79%)	55 (90%)	6 (10%)	8	30
19	AS	69/80 (86%)	62 (90%)	7 (10%)	7	29
19	CS	69/80 (86%)	62 (90%)	7 (10%)	7	29
20	AT	76/82 (93%)	68 (90%)	8 (10%)	7	27
20	CT	76/82 (93%)	68 (90%)	8 (10%)	7	27
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	18
22	D0	61/67 (91%)	53 (87%)	8 (13%)	4	18
23	B1	73/83 (88%)	53 (73%)	20 (27%)	0	2
23	D1	73/83 (88%)	55 (75%)	18 (25%)	0	3
24	B2	46/67 (69%)	33 (72%)	13 (28%)	0	2
24	D2	46/67 (69%)	33 (72%)	13 (28%)	0	2
25	B3	51/52 (98%)	45 (88%)	6 (12%)	5	22
25	D3	51/52 (98%)	44 (86%)	7 (14%)	3	17
27	B5	51/52 (98%)	40 (78%)	11 (22%)	1	5
27	D5	51/52 (98%)	38 (74%)	13 (26%)	0	3
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	0
28	D6	43/52 (83%)	28 (65%)	15 (35%)	0	1
29	B7	41/42 (98%)	33 (80%)	8 (20%)	1	7
29	D7	41/42 (98%)	32 (78%)	9 (22%)	1	4
30	B8	53/55 (96%)	40 (76%)	13 (24%)	0	3
30	D8	53/55 (96%)	41 (77%)	12 (23%)	1	4
33	BD	213/218 (98%)	166 (78%)	47 (22%)	1	4
33	DD	213/218 (98%)	165 (78%)	48 (22%)	1	4
34	BE	165/166 (99%)	122 (74%)	43 (26%)	0	2
34	DE	165/166 (99%)	122 (74%)	43 (26%)	0	2
35	BF	165/166 (99%)	134 (81%)	31 (19%)	1	8
35	DF	165/166 (99%)	137 (83%)	28 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	BG	155/156 (99%)	134 (86%)	21 (14%)	4 17
36	DG	155/156 (99%)	134 (86%)	21 (14%)	4 17
37	BH	132/148 (89%)	105 (80%)	27 (20%)	1 6
37	DH	132/148 (89%)	105 (80%)	27 (20%)	1 6
38	BI	122/124 (98%)	104 (85%)	18 (15%)	3 14
38	DI	122/124 (98%)	104 (85%)	18 (15%)	3 14
39	BN	117/119 (98%)	79 (68%)	38 (32%)	0 1
39	DN	117/119 (98%)	79 (68%)	38 (32%)	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%)	72 (64%)	40 (36%)	0 1
41	DP	112/116 (97%)	72 (64%)	40 (36%)	0 1
42	BQ	106/111 (96%)	86 (81%)	20 (19%)	1 8
42	DQ	106/111 (96%)	85 (80%)	21 (20%)	1 7
43	BR	100/101 (99%)	81 (81%)	19 (19%)	1 8
43	DR	100/101 (99%)	80 (80%)	20 (20%)	1 7
44	BS	77/88 (88%)	53 (69%)	24 (31%)	0 1
44	DS	77/88 (88%)	54 (70%)	23 (30%)	0 1
45	BT	116/127 (91%)	81 (70%)	35 (30%)	0 1
45	DT	116/127 (91%)	81 (70%)	35 (30%)	0 1
46	BU	92/94 (98%)	79 (86%)	13 (14%)	3 16
46	DU	92/94 (98%)	79 (86%)	13 (14%)	3 16
47	BV	82/82 (100%)	53 (65%)	29 (35%)	0 1
47	DV	82/82 (100%)	53 (65%)	29 (35%)	0 1
48	BW	91/92 (99%)	70 (77%)	21 (23%)	1 4
48	DW	91/92 (99%)	71 (78%)	20 (22%)	1 4
49	BX	74/78 (95%)	54 (73%)	20 (27%)	0 2
49	DX	74/78 (95%)	53 (72%)	21 (28%)	0 2
50	BY	84/91 (92%)	60 (71%)	24 (29%)	0 2
50	DY	84/91 (92%)	61 (73%)	23 (27%)	0 2
51	BZ	155/179 (87%)	130 (84%)	25 (16%)	2 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	DZ	155/179 (87%)	130 (84%)	25 (16%)	2 12
All	All	9322/9876 (94%)	7670 (82%)	1652 (18%)	2 9

5 of 1652 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	CG	156	TRP
33	DD	27	THR
49	DX	65	ARG
10	CJ	62	HIS
7	CG	79	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 277 such sidechains are listed below:

Mol	Chain	Res	Type
39	DN	56	ASN
40	DO	82	ASN
46	DU	72	HIS
41	BP	13	ASN
39	BN	130	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	280 (18%)	31 (2%)
1	CA	1503/1522 (98%)	283 (18%)	31 (2%)
31	BA	2723/2787 (97%)	712 (26%)	70 (2%)
31	DA	2723/2787 (97%)	706 (25%)	69 (2%)
32	BB	118/122 (96%)	34 (28%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	1 (0%)
All	All	8688/8862 (98%)	2050 (23%)	203 (2%)

5 of 2050 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	41	G

5 of 203 RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	CLM	DA	3334	54	19,20,20	1.22	1 (5%)	23,27,27	0.90	0
55	CLM	BA	3370	54	19,20,20	1.22	1 (5%)	23,27,27	0.90	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3334	CLM	C9-N9	-4.29	1.34	1.45
55	BA	3370	CLM	C9-N9	-4.26	1.34	1.45

There are no bond angle outliers.

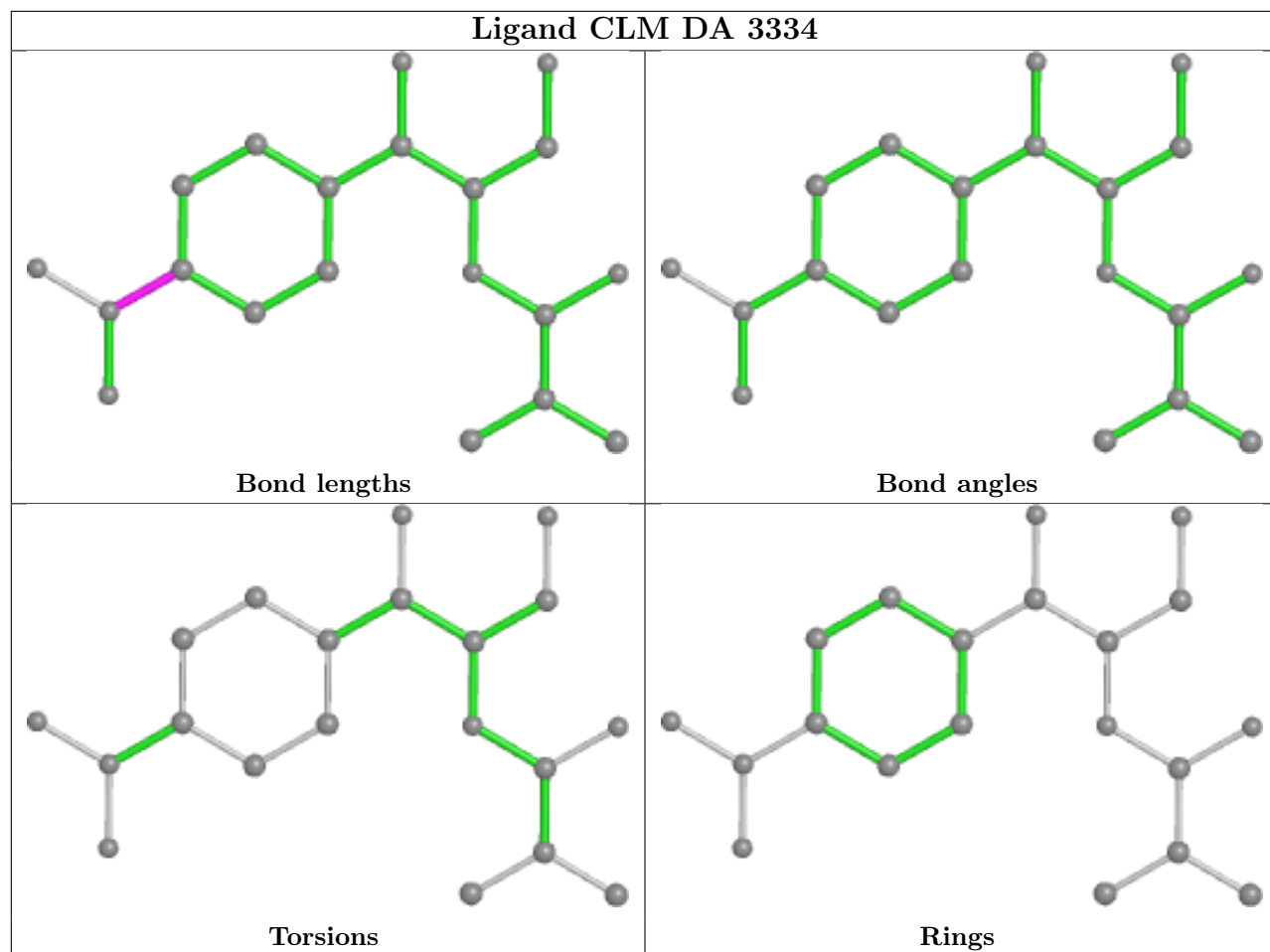
There are no chirality outliers.

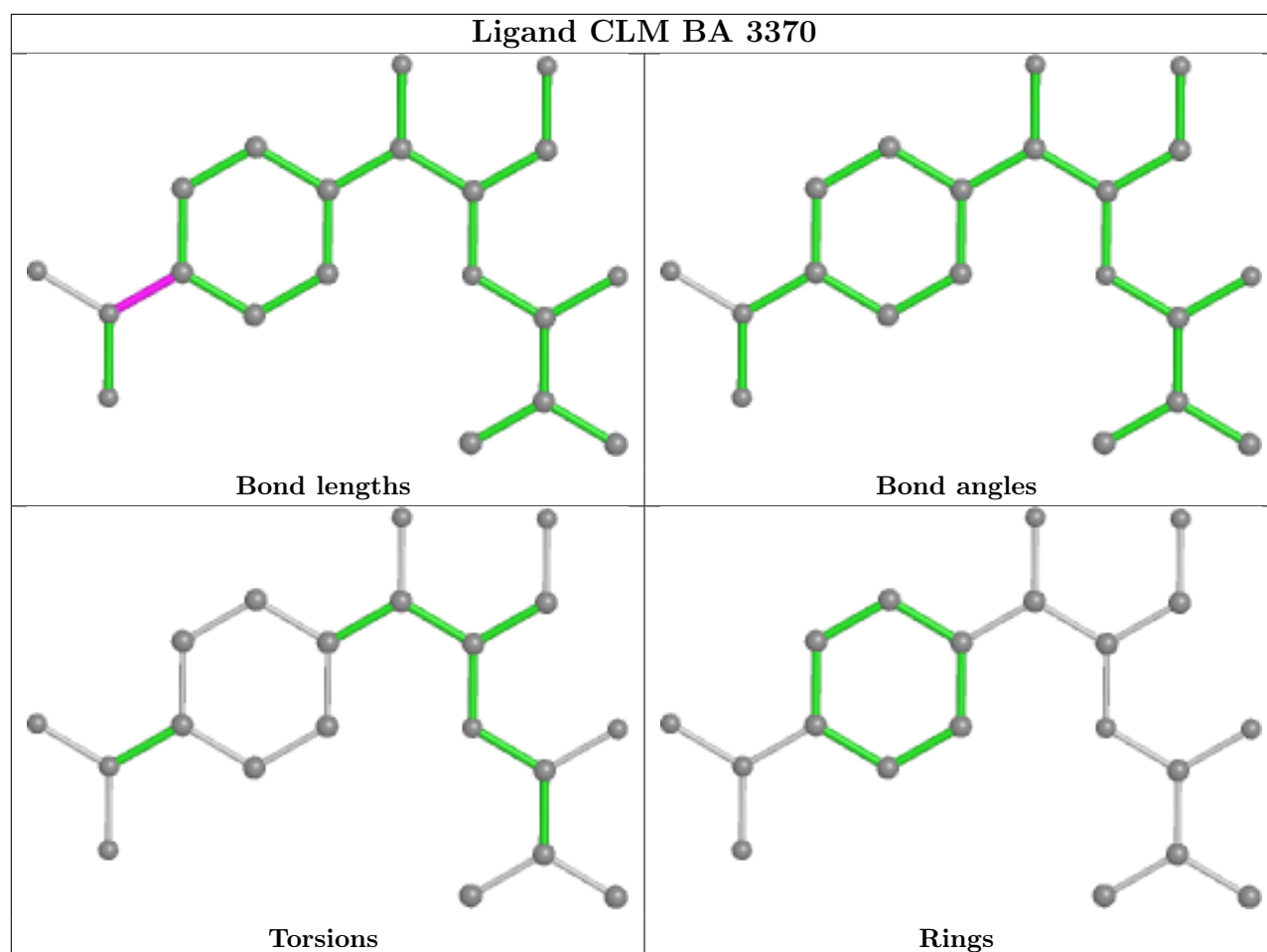
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

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Mol	Chain	Number of breaks
47	DV	1

The worst 5 of 14 chain breaks are listed below:

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

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	1.11	291 (19%) 1 0	42, 106, 199, 201	0
1	CA	1504/1522 (98%)	0.93	239 (15%) 1 1	46, 105, 198, 201	0
2	AB	235/256 (91%)	0.71	35 (14%) 2 1	83, 146, 188, 195	0
2	CB	235/256 (91%)	0.90	51 (21%) 0 0	84, 149, 187, 196	0
3	AC	207/239 (86%)	1.13	52 (25%) 0 0	97, 158, 187, 194	0
3	CC	207/239 (86%)	1.19	51 (24%) 0 0	98, 160, 187, 194	0
4	AD	208/209 (99%)	0.35	9 (4%) 35 13	72, 112, 165, 186	0
4	CD	208/209 (99%)	0.19	4 (1%) 66 37	70, 111, 164, 185	0
5	AE	151/162 (93%)	0.43	9 (5%) 21 7	59, 97, 151, 194	0
5	CE	151/162 (93%)	0.45	8 (5%) 26 10	64, 98, 153, 194	0
6	AF	101/101 (100%)	0.21	6 (5%) 22 7	66, 111, 160, 183	0
6	CF	101/101 (100%)	0.17	4 (3%) 38 15	67, 113, 160, 188	0
7	AG	155/156 (99%)	1.77	55 (35%) 0 0	124, 172, 192, 197	0
7	CG	155/156 (99%)	1.93	58 (37%) 0 0	125, 172, 192, 198	0
8	AH	138/138 (100%)	0.06	3 (2%) 62 33	67, 102, 147, 162	0
8	CH	138/138 (100%)	0.13	2 (1%) 75 49	66, 102, 147, 163	0
9	AI	127/128 (99%)	2.47	62 (48%) 0 0	125, 179, 196, 199	0
9	CI	127/128 (99%)	2.38	60 (47%) 0 0	126, 180, 197, 199	0
10	AJ	99/105 (94%)	3.03	57 (57%) 0 0	122, 175, 196, 198	0
10	CJ	99/105 (94%)	2.81	58 (58%) 0 0	121, 176, 197, 199	0
11	AK	119/129 (92%)	0.67	18 (15%) 2 1	63, 105, 164, 188	0
11	CK	119/129 (92%)	0.79	15 (12%) 3 1	65, 104, 168, 191	0
12	AL	125/135 (92%)	0.33	5 (4%) 38 15	57, 89, 154, 198	0
12	CL	125/135 (92%)	0.57	11 (8%) 10 3	55, 89, 158, 198	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	2.67	65 (56%) 0 0	136, 190, 198, 200	0
13	CM	115/126 (91%)	2.58	61 (53%) 0 0	136, 188, 197, 199	0
14	AN	60/61 (98%)	1.68	22 (36%) 0 0	113, 167, 193, 196	0
14	CN	60/61 (98%)	1.31	14 (23%) 0 0	112, 168, 191, 196	0
15	AO	88/89 (98%)	0.11	4 (4%) 33 12	59, 91, 149, 155	0
15	CO	88/89 (98%)	0.12	2 (2%) 60 31	63, 92, 150, 157	0
16	AP	84/88 (95%)	0.94	14 (16%) 1 0	77, 101, 161, 188	0
16	CP	84/88 (95%)	0.49	5 (5%) 21 7	78, 100, 154, 186	0
17	AQ	100/105 (95%)	0.17	4 (4%) 38 15	62, 93, 138, 158	0
17	CQ	100/105 (95%)	0.14	3 (3%) 50 22	59, 92, 140, 157	0
18	AR	70/88 (79%)	0.36	3 (4%) 35 13	73, 98, 167, 197	0
18	CR	70/88 (79%)	0.93	7 (10%) 7 2	74, 100, 167, 196	0
19	AS	79/93 (84%)	4.19	61 (77%) 0 0	142, 191, 198, 199	0
19	CS	79/93 (84%)	3.55	59 (74%) 0 0	142, 190, 198, 199	0
20	AT	99/106 (93%)	0.18	4 (4%) 38 15	73, 110, 157, 186	0
20	CT	99/106 (93%)	0.39	9 (9%) 9 3	74, 108, 156, 189	0
21	AU	25/27 (92%)	4.40	19 (76%) 0 0	138, 175, 193, 196	0
21	CU	25/27 (92%)	3.38	17 (68%) 0 0	135, 172, 193, 195	0
22	B0	85/85 (100%)	0.69	8 (9%) 8 3	34, 59, 182, 197	0
22	D0	85/85 (100%)	0.62	12 (14%) 2 1	40, 64, 178, 197	0
23	B1	89/98 (90%)	0.36	2 (2%) 62 33	37, 64, 140, 187	0
23	D1	89/98 (90%)	0.17	4 (4%) 33 12	40, 66, 142, 191	0
24	B2	51/72 (70%)	0.87	8 (15%) 2 1	49, 87, 184, 193	0
24	D2	51/72 (70%)	0.52	8 (15%) 2 1	50, 91, 183, 195	0
25	B3	60/60 (100%)	0.05	1 (1%) 70 41	36, 56, 132, 180	0
25	D3	60/60 (100%)	0.40	4 (6%) 17 5	42, 61, 138, 178	0
26	B4	32/71 (45%)	0.00	1 (3%) 49 21	109, 156, 186, 191	0
26	D4	32/71 (45%)	0.21	1 (3%) 49 21	112, 161, 188, 195	0
27	B5	59/60 (98%)	0.68	6 (10%) 6 2	25, 47, 180, 195	0
27	D5	59/60 (98%)	0.35	5 (8%) 10 3	28, 50, 184, 195	0
28	B6	45/54 (83%)	0.77	5 (11%) 5 1	36, 70, 133, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	0.89	11 (24%) 0 0	42, 74, 138, 184	0
29	B7	49/49 (100%)	0.29	1 (2%) 65 36	26, 33, 117, 170	0
29	D7	49/49 (100%)	0.33	1 (2%) 65 36	27, 37, 118, 170	0
30	B8	64/65 (98%)	0.45	6 (9%) 8 3	34, 57, 138, 181	0
30	D8	64/65 (98%)	0.18	3 (4%) 31 11	38, 59, 139, 183	0
31	BA	2725/2787 (97%)	0.40	76 (2%) 53 25	26, 46, 145, 201	0
31	DA	2725/2787 (97%)	0.21	103 (3%) 40 16	27, 51, 148, 201	0
32	BB	119/122 (97%)	0.55	4 (3%) 45 19	39, 91, 140, 185	0
32	DB	119/122 (97%)	0.78	15 (12%) 3 1	48, 95, 154, 190	0
33	BD	272/276 (98%)	-0.10	3 (1%) 80 56	27, 47, 100, 177	0
33	DD	272/276 (98%)	-0.15	3 (1%) 80 56	29, 50, 104, 181	0
34	BE	205/206 (99%)	0.16	7 (3%) 45 19	25, 52, 145, 189	0
34	DE	205/206 (99%)	-0.03	5 (2%) 59 30	29, 56, 142, 189	0
35	BF	208/210 (99%)	0.45	15 (7%) 15 4	24, 58, 180, 197	0
35	DF	208/210 (99%)	0.38	16 (7%) 13 4	27, 63, 178, 197	0
36	BG	181/182 (99%)	1.17	39 (21%) 0 0	87, 145, 189, 199	0
36	DG	181/182 (99%)	1.94	74 (40%) 0 0	91, 153, 193, 199	0
37	BH	160/180 (88%)	0.38	7 (4%) 34 13	62, 102, 150, 193	0
37	DH	160/180 (88%)	1.08	37 (23%) 0 0	70, 110, 157, 195	0
38	BI	146/148 (98%)	0.50	14 (9%) 8 2	52, 143, 185, 195	0
38	DI	146/148 (98%)	3.26	68 (46%) 0 0	56, 156, 188, 198	0
39	BN	139/140 (99%)	0.20	5 (3%) 42 17	32, 60, 140, 187	0
39	DN	139/140 (99%)	-0.07	5 (3%) 42 17	38, 65, 142, 188	0
40	BO	122/122 (100%)	-0.20	0 100 100	32, 52, 105, 141	0
40	DO	122/122 (100%)	-0.45	0 100 100	35, 55, 111, 146	0
41	BP	146/150 (97%)	0.78	10 (6%) 17 5	22, 79, 148, 199	0
41	DP	146/150 (97%)	0.46	8 (5%) 25 9	27, 81, 150, 198	0
42	BQ	136/141 (96%)	0.52	9 (6%) 18 5	39, 64, 150, 189	0
42	DQ	136/141 (96%)	0.38	8 (5%) 22 7	43, 69, 149, 190	0
43	BR	117/118 (99%)	-0.02	1 (0%) 84 63	28, 44, 113, 143	0
43	DR	117/118 (99%)	-0.17	2 (1%) 70 41	30, 49, 115, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	0.44	6 (6%) 21 7	53, 98, 141, 178	0
44	DS	99/112 (88%)	1.12	24 (24%) 0 0	63, 103, 146, 180	0
45	BT	132/146 (90%)	0.31	7 (5%) 26 10	42, 73, 157, 191	0
45	DT	132/146 (90%)	0.14	7 (5%) 26 10	46, 77, 159, 194	0
46	BU	117/118 (99%)	0.24	2 (1%) 70 41	23, 50, 114, 190	0
46	DU	117/118 (99%)	0.12	2 (1%) 70 41	32, 56, 119, 193	0
47	BV	101/101 (100%)	0.80	8 (7%) 12 4	32, 91, 171, 194	0
47	DV	101/101 (100%)	0.76	13 (12%) 3 1	35, 97, 169, 195	0
48	BW	113/113 (100%)	-0.20	0 100 100	28, 40, 101, 168	0
48	DW	113/113 (100%)	-0.33	2 (1%) 68 40	31, 43, 106, 175	0
49	BX	93/96 (96%)	0.34	4 (4%) 35 13	36, 65, 142, 184	0
49	DX	93/96 (96%)	0.01	2 (2%) 62 33	42, 69, 147, 185	0
50	BY	101/110 (91%)	1.12	19 (18%) 1 0	39, 91, 191, 199	0
50	DY	101/110 (91%)	0.93	20 (19%) 1 0	40, 96, 191, 198	0
51	BZ	177/206 (85%)	0.22	4 (2%) 60 31	56, 100, 150, 175	0
51	DZ	177/206 (85%)	0.49	13 (7%) 15 4	63, 103, 153, 179	0
All	All	20064/20922 (95%)	0.64	2290 (11%) 5 1	22, 84, 190, 201	0

The worst 5 of 2290 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BF	208	GLY	23.7
42	BQ	140	ALA	18.8
38	DI	100	ALA	18.7
42	DQ	140	ALA	17.0
1	AA	88	A	16.4

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 monosaccharides in this entry.

6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
52	MG	DA	3309	1/1	0.36	0.17	66,66,66,66	0
52	MG	DA	3232	1/1	0.48	0.87	63,63,63,63	0
52	MG	BA	3362	1/1	0.48	0.38	50,50,50,50	0
52	MG	AA	1643	1/1	0.49	1.02	66,66,66,66	0
52	MG	DA	3297	1/1	0.56	0.51	55,55,55,55	0
52	MG	DA	3124	1/1	0.56	0.29	49,49,49,49	0
52	MG	DA	3310	1/1	0.59	0.45	56,56,56,56	0
52	MG	BA	3349	1/1	0.62	0.78	65,65,65,65	0
52	MG	DA	3133	1/1	0.62	0.12	55,55,55,55	0
52	MG	BA	3128	1/1	0.62	0.91	45,45,45,45	0
52	MG	AA	1654	1/1	0.63	0.83	64,64,64,64	0
52	MG	BA	3167	1/1	0.65	0.54	51,51,51,51	0
52	MG	BA	3175	1/1	0.65	0.64	43,43,43,43	0
52	MG	BA	3072	1/1	0.66	0.56	41,41,41,41	0
52	MG	BF	301	1/1	0.66	0.40	43,43,43,43	0
52	MG	BA	3098	1/1	0.66	0.34	59,59,59,59	0
52	MG	AA	1635	1/1	0.66	0.14	53,53,53,53	0
52	MG	DA	3236	1/1	0.67	0.57	71,71,71,71	0
52	MG	DA	3305	1/1	0.67	0.99	46,46,46,46	0
52	MG	DA	3074	1/1	0.69	0.59	54,54,54,54	0
52	MG	BA	3150	1/1	0.69	0.43	40,40,40,40	0
52	MG	BA	3088	1/1	0.69	0.40	33,33,33,33	0
52	MG	AA	1604	1/1	0.70	0.32	62,62,62,62	0
52	MG	DA	3167	1/1	0.70	0.26	63,63,63,63	0
52	MG	BA	3151	1/1	0.71	0.39	47,47,47,47	0
52	MG	DA	3280	1/1	0.71	0.42	70,70,70,70	0
52	MG	BA	3346	1/1	0.71	0.12	63,63,63,63	0
52	MG	CA	1626	1/1	0.72	0.48	68,68,68,68	0
52	MG	DA	3303	1/1	0.72	0.28	43,43,43,43	0
52	MG	BA	3271	1/1	0.72	0.16	53,53,53,53	0
52	MG	BA	3313	1/1	0.72	0.66	56,56,56,56	0
52	MG	BA	3007	1/1	0.72	0.70	40,40,40,40	0
52	MG	DA	3290	1/1	0.73	0.55	55,55,55,55	0
52	MG	DA	3295	1/1	0.73	0.65	73,73,73,73	0
52	MG	BA	3171	1/1	0.73	0.77	35,35,35,35	0
52	MG	BA	3292	1/1	0.73	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3243	1/1	0.73	0.52	56,56,56,56	0
52	MG	DA	3252	1/1	0.73	0.47	57,57,57,57	0
52	MG	AA	1649	1/1	0.73	0.26	76,76,76,76	0
52	MG	CA	1608	1/1	0.74	0.33	68,68,68,68	0
52	MG	BA	3363	1/1	0.74	0.20	54,54,54,54	0
52	MG	DA	3166	1/1	0.74	0.62	64,64,64,64	0
52	MG	BA	3154	1/1	0.74	0.37	77,77,77,77	0
52	MG	DA	3328	1/1	0.74	0.52	61,61,61,61	0
52	MG	BA	3203	1/1	0.75	0.13	47,47,47,47	0
52	MG	BA	3307	1/1	0.75	0.36	38,38,38,38	0
52	MG	BA	3247	1/1	0.75	0.56	35,35,35,35	0
52	MG	BA	3131	1/1	0.75	0.52	45,45,45,45	0
52	MG	BA	3180	1/1	0.76	0.64	46,46,46,46	0
52	MG	BA	3336	1/1	0.76	0.34	49,49,49,49	0
52	MG	BA	3141	1/1	0.76	0.18	47,47,47,47	0
52	MG	DA	3331	1/1	0.76	0.15	67,67,67,67	0
52	MG	DA	3153	1/1	0.77	0.77	73,73,73,73	0
52	MG	DA	3281	1/1	0.77	0.81	63,63,63,63	0
52	MG	BA	3159	1/1	0.77	0.70	52,52,52,52	0
52	MG	AA	1637	1/1	0.77	0.69	51,51,51,51	0
52	MG	DA	3184	1/1	0.77	0.29	32,32,32,32	0
52	MG	DA	3187	1/1	0.77	0.57	44,44,44,44	0
52	MG	DA	3195	1/1	0.77	0.48	36,36,36,36	0
52	MG	BA	3355	1/1	0.77	0.85	51,51,51,51	0
52	MG	BA	3361	1/1	0.77	0.33	52,52,52,52	0
52	MG	AA	1611	1/1	0.77	0.17	72,72,72,72	0
52	MG	AA	1644	1/1	0.77	0.41	68,68,68,68	0
52	MG	DA	3283	1/1	0.78	0.65	52,52,52,52	0
52	MG	DA	3289	1/1	0.78	0.45	53,53,53,53	0
52	MG	CA	1630	1/1	0.78	0.62	66,66,66,66	0
52	MG	BA	3113	1/1	0.78	0.21	26,26,26,26	0
52	MG	BA	3181	1/1	0.78	0.15	32,32,32,32	0
52	MG	DA	3249	1/1	0.78	0.23	48,48,48,48	0
52	MG	BA	3291	1/1	0.78	0.21	54,54,54,54	0
52	MG	DA	3264	1/1	0.78	0.26	58,58,58,58	0
52	MG	DA	3274	1/1	0.78	0.42	71,71,71,71	0
52	MG	DA	3322	1/1	0.78	0.39	45,45,45,45	0
52	MG	BA	3176	1/1	0.78	0.42	58,58,58,58	0
52	MG	DA	3201	1/1	0.78	0.23	43,43,43,43	0
52	MG	DA	3180	1/1	0.79	0.50	38,38,38,38	0
52	MG	CA	1638	1/1	0.79	1.28	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3025	1/1	0.79	0.44	46,46,46,46	0
52	MG	BA	3246	1/1	0.79	0.37	40,40,40,40	0
52	MG	DA	3106	1/1	0.79	0.91	53,53,53,53	0
52	MG	DA	3208	1/1	0.79	0.57	34,34,34,34	0
52	MG	BA	3330	1/1	0.79	0.55	48,48,48,48	0
52	MG	BA	3351	1/1	0.79	0.30	48,48,48,48	0
52	MG	DA	3149	1/1	0.79	0.58	54,54,54,54	0
52	MG	BA	3074	1/1	0.79	0.50	48,48,48,48	0
52	MG	DA	3159	1/1	0.79	0.24	40,40,40,40	0
52	MG	BA	3358	1/1	0.79	0.50	59,59,59,59	0
52	MG	DA	3325	1/1	0.79	0.56	46,46,46,46	0
52	MG	DA	3271	1/1	0.79	0.56	56,56,56,56	0
52	MG	BA	3337	1/1	0.79	0.47	32,32,32,32	0
52	MG	DU	201	1/1	0.79	0.47	60,60,60,60	0
52	MG	BA	3289	1/1	0.80	0.27	44,44,44,44	0
52	MG	CA	1627	1/1	0.80	0.75	81,81,81,81	0
52	MG	DA	3298	1/1	0.80	0.64	59,59,59,59	0
52	MG	AA	1656	1/1	0.80	0.17	62,62,62,62	0
52	MG	DA	3304	1/1	0.80	0.79	63,63,63,63	0
52	MG	DA	3267	1/1	0.80	0.45	46,46,46,46	0
52	MG	BA	3215	1/1	0.80	0.20	10,10,10,10	0
52	MG	BA	3259	1/1	0.80	0.41	40,40,40,40	0
52	MG	DA	3221	1/1	0.80	0.68	43,43,43,43	0
52	MG	DA	3225	1/1	0.80	0.20	37,37,37,37	0
52	MG	BA	3237	1/1	0.80	0.50	42,42,42,42	0
52	MG	DA	3075	1/1	0.80	0.45	38,38,38,38	0
52	MG	BA	3282	1/1	0.80	0.59	46,46,46,46	0
52	MG	BA	3116	1/1	0.81	0.11	41,41,41,41	0
52	MG	BA	3234	1/1	0.81	0.19	16,16,16,16	0
52	MG	CA	1625	1/1	0.81	0.56	59,59,59,59	0
52	MG	DA	3245	1/1	0.81	0.19	65,65,65,65	0
52	MG	DA	3123	1/1	0.81	0.22	38,38,38,38	0
52	MG	CA	1642	1/1	0.81	1.23	71,71,71,71	0
52	MG	DA	3293	1/1	0.81	0.74	54,54,54,54	0
52	MG	DA	3173	1/1	0.81	0.77	57,57,57,57	0
52	MG	DA	3329	1/1	0.81	0.34	51,51,51,51	0
52	MG	DA	3222	1/1	0.81	0.52	41,41,41,41	0
52	MG	BA	3127	1/1	0.81	0.50	44,44,44,44	0
52	MG	AA	1612	1/1	0.82	0.59	56,56,56,56	0
52	MG	DA	3090	1/1	0.82	0.34	33,33,33,33	0
52	MG	DA	3287	1/1	0.82	1.20	61,61,61,61	0
52	MG	AA	1638	1/1	0.82	0.52	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	CA	1611	1/1	0.82	0.84	76,76,76,76	0
52	MG	BA	3009	1/1	0.82	0.55	38,38,38,38	0
52	MG	BA	3093	1/1	0.82	1.00	50,50,50,50	0
52	MG	BA	3198	1/1	0.82	0.89	62,62,62,62	0
52	MG	BA	3323	1/1	0.82	0.63	42,42,42,42	0
52	MG	BA	3360	1/1	0.82	0.51	48,48,48,48	0
52	MG	BA	3326	1/1	0.82	0.43	40,40,40,40	0
52	MG	CA	1649	1/1	0.82	0.36	55,55,55,55	0
52	MG	DA	3170	1/1	0.82	0.15	42,42,42,42	0
52	MG	DA	3263	1/1	0.82	0.29	65,65,65,65	0
52	MG	DA	3009	1/1	0.82	0.43	47,47,47,47	0
52	MG	DA	3265	1/1	0.82	0.14	38,38,38,38	0
52	MG	DA	3175	1/1	0.82	0.48	51,51,51,51	0
52	MG	BA	3094	1/1	0.82	0.57	30,30,30,30	0
52	MG	DA	3054	1/1	0.82	0.28	55,55,55,55	0
52	MG	BA	3062	1/1	0.82	0.17	30,30,30,30	0
55	CLM	DA	3334	20/20	0.82	0.50	90,90,90,90	0
52	MG	BA	3056	1/1	0.83	0.16	20,20,20,20	0
52	MG	BA	3305	1/1	0.83	0.27	54,54,54,54	0
52	MG	DA	3137	1/1	0.83	0.17	69,69,69,69	0
52	MG	BA	3350	1/1	0.83	0.38	54,54,54,54	0
52	MG	AA	1624	1/1	0.83	0.49	59,59,59,59	0
52	MG	AA	1629	1/1	0.83	0.34	49,49,49,49	0
52	MG	BA	3318	1/1	0.83	0.38	34,34,34,34	0
52	MG	BA	3320	1/1	0.83	1.17	52,52,52,52	0
52	MG	BA	3274	1/1	0.83	0.46	33,33,33,33	0
52	MG	BA	3278	1/1	0.83	0.16	31,31,31,31	0
52	MG	AA	1613	1/1	0.83	0.29	62,62,62,62	0
52	MG	BB	203	1/1	0.83	0.11	55,55,55,55	0
52	MG	DA	3312	1/1	0.83	0.59	45,45,45,45	0
52	MG	BA	3238	1/1	0.83	0.77	43,43,43,43	0
52	MG	DA	3085	1/1	0.83	0.17	19,19,19,19	0
52	MG	DA	3327	1/1	0.83	0.14	41,41,41,41	0
52	MG	AA	1620	1/1	0.83	0.61	52,52,52,52	0
52	MG	DA	3278	1/1	0.83	0.52	54,54,54,54	0
52	MG	CA	1610	1/1	0.83	0.27	66,66,66,66	0
52	MG	DA	3206	1/1	0.83	0.64	45,45,45,45	0
52	MG	BA	3338	1/1	0.83	0.38	50,50,50,50	0
52	MG	DA	3234	1/1	0.84	0.72	60,60,60,60	0
52	MG	DA	3072	1/1	0.84	0.89	71,71,71,71	0
52	MG	BA	3139	1/1	0.84	0.68	30,30,30,30	0
52	MG	BA	3359	1/1	0.84	0.58	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3276	1/1	0.84	0.36	35,35,35,35	0
52	MG	AA	1630	1/1	0.84	0.53	49,49,49,49	0
52	MG	DA	3257	1/1	0.84	0.36	46,46,46,46	0
52	MG	DA	3259	1/1	0.84	0.51	79,79,79,79	0
52	MG	DA	3101	1/1	0.84	0.33	34,34,34,34	0
52	MG	BA	3345	1/1	0.84	0.25	43,43,43,43	0
52	MG	BA	3207	1/1	0.84	0.72	32,32,32,32	0
52	MG	AA	1632	1/1	0.84	0.65	51,51,51,51	0
52	MG	DA	3270	1/1	0.84	0.43	55,55,55,55	0
52	MG	DA	3127	1/1	0.84	0.21	33,33,33,33	0
52	MG	BA	3221	1/1	0.84	0.25	31,31,31,31	0
52	MG	BP	201	1/1	0.84	0.56	35,35,35,35	0
52	MG	BA	3075	1/1	0.84	0.47	38,38,38,38	0
52	MG	DA	3029	1/1	0.84	0.23	43,43,43,43	0
52	MG	DB	201	1/1	0.84	0.46	57,57,57,57	0
52	MG	DB	204	1/1	0.84	0.47	37,37,37,37	0
52	MG	BA	3300	1/1	0.84	0.41	45,45,45,45	0
52	MG	DX	101	1/1	0.84	0.25	45,45,45,45	0
54	K	DA	3333	1/1	0.84	0.30	62,62,62,62	0
52	MG	DA	3165	1/1	0.84	0.28	38,38,38,38	0
52	MG	BA	3229	1/1	0.85	0.36	26,26,26,26	0
52	MG	DA	3047	1/1	0.85	0.55	33,33,33,33	0
52	MG	BA	3248	1/1	0.85	0.35	33,33,33,33	0
52	MG	DA	3210	1/1	0.85	0.23	46,46,46,46	0
52	MG	DA	3214	1/1	0.85	0.43	39,39,39,39	0
52	MG	BA	3249	1/1	0.85	0.33	54,54,54,54	0
52	MG	BA	3255	1/1	0.85	0.44	54,54,54,54	0
52	MG	BA	3118	1/1	0.85	0.20	38,38,38,38	0
52	MG	CA	1628	1/1	0.85	0.63	50,50,50,50	0
52	MG	BA	3365	1/1	0.85	0.36	43,43,43,43	0
52	MG	CA	1631	1/1	0.85	0.08	71,71,71,71	0
52	MG	DA	3239	1/1	0.85	0.78	41,41,41,41	0
52	MG	BA	3209	1/1	0.85	0.39	36,36,36,36	0
52	MG	DA	3177	1/1	0.85	0.41	37,37,37,37	0
52	MG	DD	301	1/1	0.85	0.44	32,32,32,32	0
52	MG	DF	301	1/1	0.85	0.41	53,53,53,53	0
52	MG	DQ	201	1/1	0.85	0.36	42,42,42,42	0
52	MG	BA	3199	1/1	0.85	0.40	42,42,42,42	0
52	MG	BA	3356	1/1	0.85	0.08	60,60,60,60	0
52	MG	CA	1606	1/1	0.85	0.86	52,52,52,52	0
52	MG	AA	1651	1/1	0.85	0.32	45,45,45,45	0
52	MG	DA	3156	1/1	0.86	0.35	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BR	202	1/1	0.86	0.68	31,31,31,31	0
52	MG	DA	3164	1/1	0.86	0.56	41,41,41,41	0
52	MG	DA	3302	1/1	0.86	0.24	39,39,39,39	0
52	MG	AA	1648	1/1	0.86	1.32	80,80,80,80	0
52	MG	BA	3003	1/1	0.86	0.80	44,44,44,44	0
52	MG	BA	3115	1/1	0.86	0.44	34,34,34,34	0
52	MG	BA	3279	1/1	0.86	0.36	39,39,39,39	0
52	MG	CA	1614	1/1	0.86	0.63	57,57,57,57	0
52	MG	BA	3314	1/1	0.86	0.50	41,41,41,41	0
52	MG	BA	3240	1/1	0.86	0.38	50,50,50,50	0
52	MG	BA	3347	1/1	0.86	0.43	47,47,47,47	0
52	MG	BA	3258	1/1	0.86	0.24	21,21,21,21	0
52	MG	DA	3105	1/1	0.86	0.20	39,39,39,39	0
52	MG	BA	3366	1/1	0.86	0.14	52,52,52,52	0
52	MG	BA	3367	1/1	0.86	0.10	47,47,47,47	0
52	MG	CA	1637	1/1	0.86	0.35	65,65,65,65	0
52	MG	DA	3126	1/1	0.86	0.16	36,36,36,36	0
52	MG	BA	3368	1/1	0.86	0.07	60,60,60,60	0
52	MG	DA	3132	1/1	0.86	0.77	53,53,53,53	0
52	MG	DA	3216	1/1	0.86	0.56	45,45,45,45	0
52	MG	BA	3243	1/1	0.86	0.20	30,30,30,30	0
52	MG	BA	3325	1/1	0.86	0.63	53,53,53,53	0
52	MG	D5	102	1/1	0.86	0.51	58,58,58,58	0
52	MG	AA	1646	1/1	0.86	0.12	48,48,48,48	0
52	MG	BA	3331	1/1	0.87	0.53	37,37,37,37	0
52	MG	BA	3352	1/1	0.87	0.27	51,51,51,51	0
52	MG	BA	3244	1/1	0.87	0.36	50,50,50,50	0
52	MG	DA	3136	1/1	0.87	0.36	48,48,48,48	0
52	MG	BA	3317	1/1	0.87	0.36	53,53,53,53	0
52	MG	DA	3055	1/1	0.87	0.52	34,34,34,34	0
52	MG	BA	3111	1/1	0.87	0.55	41,41,41,41	0
52	MG	BA	3341	1/1	0.87	0.65	66,66,66,66	0
52	MG	BQ	202	1/1	0.87	0.35	37,37,37,37	0
52	MG	CA	1635	1/1	0.87	0.79	73,73,73,73	0
52	MG	BA	3299	1/1	0.87	0.38	37,37,37,37	0
52	MG	CA	1604	1/1	0.87	0.32	67,67,67,67	0
52	MG	BA	3225	1/1	0.87	0.60	32,32,32,32	0
52	MG	DA	3233	1/1	0.87	0.56	51,51,51,51	0
52	MG	DA	3285	1/1	0.87	0.20	33,33,33,33	0
52	MG	BA	3049	1/1	0.87	0.56	23,23,23,23	0
52	MG	DA	3115	1/1	0.87	0.27	47,47,47,47	0
52	MG	CA	1652	1/1	0.87	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3176	1/1	0.87	0.20	66,66,66,66	0
52	MG	BA	3286	1/1	0.87	0.51	44,44,44,44	0
52	MG	BA	3160	1/1	0.87	0.58	41,41,41,41	0
52	MG	DA	3250	1/1	0.87	0.35	56,56,56,56	0
52	MG	BA	3124	1/1	0.88	0.43	39,39,39,39	0
52	MG	DA	3103	1/1	0.88	0.56	33,33,33,33	0
52	MG	BA	3315	1/1	0.88	0.23	43,43,43,43	0
52	MG	BA	3250	1/1	0.88	0.70	48,48,48,48	0
52	MG	DA	3110	1/1	0.88	0.22	50,50,50,50	0
52	MG	BA	3288	1/1	0.88	0.52	46,46,46,46	0
52	MG	DA	3116	1/1	0.88	0.28	45,45,45,45	0
52	MG	DA	3118	1/1	0.88	0.33	43,43,43,43	0
52	MG	BB	205	1/1	0.88	0.16	59,59,59,59	0
52	MG	BA	3319	1/1	0.88	0.48	46,46,46,46	0
52	MG	DA	3299	1/1	0.88	0.18	41,41,41,41	0
52	MG	CA	1645	1/1	0.88	0.35	45,45,45,45	0
52	MG	BA	3205	1/1	0.88	0.50	34,34,34,34	0
52	MG	BA	3155	1/1	0.88	0.32	39,39,39,39	0
52	MG	BA	3089	1/1	0.88	0.39	15,15,15,15	0
52	MG	DA	3306	1/1	0.88	0.44	54,54,54,54	0
52	MG	DA	3135	1/1	0.88	0.68	39,39,39,39	0
52	MG	DA	3006	1/1	0.88	0.58	38,38,38,38	0
52	MG	DA	3007	1/1	0.88	0.49	48,48,48,48	0
52	MG	BA	3296	1/1	0.88	0.07	36,36,36,36	0
52	MG	DA	3014	1/1	0.88	0.40	71,71,71,71	0
52	MG	DA	3326	1/1	0.88	0.22	49,49,49,49	0
52	MG	DA	3016	1/1	0.88	0.59	29,29,29,29	0
52	MG	DA	3021	1/1	0.88	0.35	38,38,38,38	0
52	MG	BA	3148	1/1	0.88	0.48	23,23,23,23	0
52	MG	BA	3112	1/1	0.88	0.25	14,14,14,14	0
52	MG	DA	3332	1/1	0.88	0.15	69,69,69,69	0
52	MG	BA	3332	1/1	0.88	0.41	35,35,35,35	0
52	MG	DB	202	1/1	0.88	0.41	60,60,60,60	0
52	MG	BA	3335	1/1	0.88	0.42	57,57,57,57	0
52	MG	AA	1652	1/1	0.88	0.73	44,44,44,44	0
52	MG	CA	1622	1/1	0.88	0.45	46,46,46,46	0
52	MG	BA	3200	1/1	0.88	0.33	12,12,12,12	0
52	MG	BA	3232	1/1	0.88	0.31	27,27,27,27	0
52	MG	BA	3364	1/1	0.88	0.35	64,64,64,64	0
52	MG	DA	3086	1/1	0.88	0.20	34,34,34,34	0
52	MG	BA	3340	1/1	0.88	0.23	39,39,39,39	0
52	MG	CA	1633	1/1	0.89	0.87	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3354	1/1	0.89	0.39	40,40,40,40	0
52	MG	DA	3301	1/1	0.89	0.20	15,15,15,15	0
52	MG	BA	3322	1/1	0.89	0.50	41,41,41,41	0
52	MG	AA	1622	1/1	0.89	0.47	40,40,40,40	0
52	MG	CA	1613	1/1	0.89	0.35	58,58,58,58	0
52	MG	DA	3260	1/1	0.89	0.48	34,34,34,34	0
52	MG	DA	3262	1/1	0.89	0.71	60,60,60,60	0
52	MG	DA	3211	1/1	0.89	0.90	50,50,50,50	0
52	MG	BA	3097	1/1	0.89	0.41	32,32,32,32	0
52	MG	DA	3215	1/1	0.89	0.28	27,27,27,27	0
52	MG	BA	3269	1/1	0.89	0.44	34,34,34,34	0
52	MG	DA	3220	1/1	0.89	0.21	40,40,40,40	0
52	MG	DA	3061	1/1	0.89	0.42	34,34,34,34	0
52	MG	DA	3272	1/1	0.89	0.47	47,47,47,47	0
52	MG	DA	3065	1/1	0.89	0.19	30,30,30,30	0
52	MG	DA	3276	1/1	0.89	0.85	44,44,44,44	0
52	MG	DA	3277	1/1	0.89	0.17	38,38,38,38	0
52	MG	DA	3223	1/1	0.89	0.62	37,37,37,37	0
52	MG	BA	3161	1/1	0.89	0.27	32,32,32,32	0
52	MG	BA	3196	1/1	0.89	0.40	26,26,26,26	0
52	MG	DA	3001	1/1	0.89	0.43	45,45,45,45	0
52	MG	BA	3025	1/1	0.89	0.27	29,29,29,29	0
52	MG	DA	3235	1/1	0.89	0.28	48,48,48,48	0
52	MG	BA	3277	1/1	0.89	0.34	10,10,10,10	0
52	MG	BA	3026	1/1	0.89	0.39	45,45,45,45	0
52	MG	DA	3242	1/1	0.89	0.33	35,35,35,35	0
52	MG	AA	1650	1/1	0.89	0.56	49,49,49,49	0
52	MG	DA	3193	1/1	0.89	0.74	40,40,40,40	0
52	MG	BA	3321	1/1	0.90	0.31	33,33,33,33	0
52	MG	BA	3184	1/1	0.90	0.52	40,40,40,40	0
52	MG	DA	3107	1/1	0.90	0.44	15,15,15,15	0
52	MG	BB	201	1/1	0.90	0.54	35,35,35,35	0
52	MG	BA	3188	1/1	0.90	0.51	36,36,36,36	0
52	MG	CA	1621	1/1	0.90	0.43	50,50,50,50	0
52	MG	CA	1648	1/1	0.90	0.90	53,53,53,53	0
52	MG	DA	3266	1/1	0.90	0.61	45,45,45,45	0
52	MG	BA	3309	1/1	0.90	0.58	49,49,49,49	0
52	MG	CA	1650	1/1	0.90	0.31	45,45,45,45	0
52	MG	BA	3204	1/1	0.90	0.26	36,36,36,36	0
52	MG	DA	3313	1/1	0.90	0.67	48,48,48,48	0
52	MG	DA	3316	1/1	0.90	0.21	62,62,62,62	0
52	MG	DA	3227	1/1	0.90	0.24	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
52	MG	CA	1653	1/1	0.90	0.19	47,47,47,47	0
52	MG	BA	3228	1/1	0.90	0.42	27,27,27,27	0
52	MG	BA	3177	1/1	0.90	0.87	67,67,67,67	0
52	MG	AA	1641	1/1	0.90	0.22	64,64,64,64	0
52	MG	DA	3188	1/1	0.90	0.62	43,43,43,43	0
52	MG	AA	1631	1/1	0.90	0.62	52,52,52,52	0
52	MG	DA	3282	1/1	0.90	0.23	61,61,61,61	0
52	MG	DA	3008	1/1	0.90	0.40	33,33,33,33	0
52	MG	DA	3198	1/1	0.90	0.31	37,37,37,37	0
52	MG	DB	203	1/1	0.90	0.14	73,73,73,73	0
52	MG	BA	3283	1/1	0.90	0.36	50,50,50,50	0
52	MG	DA	3288	1/1	0.90	0.22	42,42,42,42	0
52	MG	DA	3246	1/1	0.90	0.10	43,43,43,43	0
52	MG	BA	3304	1/1	0.90	0.53	49,49,49,49	0
52	MG	DA	3207	1/1	0.90	0.46	54,54,54,54	0
52	MG	DA	3251	1/1	0.90	0.19	72,72,72,72	0
52	MG	DA	3296	1/1	0.90	0.31	45,45,45,45	0
55	CLM	BA	3370	20/20	0.90	0.46	90,90,90,90	0
52	MG	DA	3154	1/1	0.90	0.53	51,51,51,51	0
52	MG	DA	3069	1/1	0.91	0.29	63,63,63,63	0
52	MG	BA	3117	1/1	0.91	0.31	50,50,50,50	0
52	MG	BA	3324	1/1	0.91	0.45	53,53,53,53	0
52	MG	DA	3191	1/1	0.91	0.44	38,38,38,38	0
52	MG	BA	3085	1/1	0.91	0.17	9,9,9,9	0
52	MG	AA	1618	1/1	0.91	0.19	53,53,53,53	0
52	MG	BA	3013	1/1	0.91	0.41	7,7,7,7	0
52	MG	CA	1636	1/1	0.91	0.26	77,77,77,77	0
52	MG	DA	3096	1/1	0.91	0.47	61,61,61,61	0
52	MG	BA	3235	1/1	0.91	0.56	38,38,38,38	0
52	MG	AA	1609	1/1	0.91	0.45	52,52,52,52	0
52	MG	CA	1639	1/1	0.91	0.56	50,50,50,50	0
52	MG	BA	3333	1/1	0.91	0.48	50,50,50,50	0
52	MG	CA	1643	1/1	0.91	0.29	42,42,42,42	0
52	MG	DA	3292	1/1	0.91	0.32	52,52,52,52	0
52	MG	DA	3109	1/1	0.91	0.34	48,48,48,48	0
52	MG	AA	1621	1/1	0.91	0.49	37,37,37,37	0
52	MG	BA	3046	1/1	0.91	0.37	24,24,24,24	0
52	MG	AA	1653	1/1	0.91	0.33	46,46,46,46	0
52	MG	BA	3146	1/1	0.91	0.40	33,33,33,33	0
52	MG	CA	1651	1/1	0.91	0.69	51,51,51,51	0
52	MG	BA	3103	1/1	0.91	0.36	27,27,27,27	0
52	MG	DA	3125	1/1	0.91	0.16	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3231	1/1	0.91	0.55	54,54,54,54	0
52	MG	BA	3108	1/1	0.91	0.18	31,31,31,31	0
52	MG	BA	3109	1/1	0.91	0.82	40,40,40,40	0
52	MG	CA	1601	1/1	0.91	0.20	61,61,61,61	0
52	MG	DA	3003	1/1	0.91	0.71	39,39,39,39	0
52	MG	CA	1602	1/1	0.91	0.58	40,40,40,40	0
52	MG	BA	3201	1/1	0.91	0.63	31,31,31,31	0
52	MG	DA	3241	1/1	0.91	0.12	54,54,54,54	0
52	MG	DA	3315	1/1	0.91	0.17	43,43,43,43	0
52	MG	BA	3202	1/1	0.91	0.61	35,35,35,35	0
52	MG	BA	3110	1/1	0.91	0.52	27,27,27,27	0
52	MG	DA	3323	1/1	0.91	0.67	62,62,62,62	0
52	MG	DA	3150	1/1	0.91	0.51	32,32,32,32	0
52	MG	AA	1605	1/1	0.91	0.39	71,71,71,71	0
52	MG	AA	1634	1/1	0.91	0.64	51,51,51,51	0
52	MG	BA	3260	1/1	0.91	0.30	13,13,13,13	0
52	MG	AA	1615	1/1	0.91	0.21	35,35,35,35	0
52	MG	DA	3160	1/1	0.91	0.59	51,51,51,51	0
52	MG	CA	1618	1/1	0.91	0.46	58,58,58,58	0
52	MG	DA	3032	1/1	0.91	0.37	31,31,31,31	0
52	MG	BA	3004	1/1	0.91	0.35	14,14,14,14	0
52	MG	DA	3052	1/1	0.91	0.51	36,36,36,36	0
52	MG	DA	3169	1/1	0.91	0.55	45,45,45,45	0
52	MG	BA	3272	1/1	0.91	0.44	36,36,36,36	0
52	MG	BA	3166	1/1	0.91	0.19	27,27,27,27	0
52	MG	DA	3058	1/1	0.91	0.34	42,42,42,42	0
52	MG	AA	1628	1/1	0.91	0.70	70,70,70,70	0
52	MG	DA	3268	1/1	0.91	0.94	63,63,63,63	0
54	K	BA	3369	1/1	0.91	0.16	41,41,41,41	0
52	MG	DA	3269	1/1	0.91	0.20	61,61,61,61	0
52	MG	BA	3169	1/1	0.91	0.34	33,33,33,33	0
52	MG	DA	3067	1/1	0.91	0.29	35,35,35,35	0
52	MG	BA	3206	1/1	0.92	0.56	29,29,29,29	0
52	MG	DA	3200	1/1	0.92	0.19	37,37,37,37	0
52	MG	BA	3241	1/1	0.92	0.18	44,44,44,44	0
52	MG	DA	3202	1/1	0.92	0.54	46,46,46,46	0
52	MG	CA	1605	1/1	0.92	0.29	68,68,68,68	0
52	MG	BA	3134	1/1	0.92	0.27	36,36,36,36	0
52	MG	DA	3284	1/1	0.92	0.72	49,49,49,49	0
52	MG	CA	1607	1/1	0.92	0.46	46,46,46,46	0
52	MG	B1	101	1/1	0.92	0.32	25,25,25,25	0
52	MG	BA	3245	1/1	0.92	0.52	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3287	1/1	0.92	0.34	27,27,27,27	0
52	MG	CA	1612	1/1	0.92	0.34	48,48,48,48	0
52	MG	DA	3121	1/1	0.92	0.28	49,49,49,49	0
52	MG	BA	3357	1/1	0.92	0.41	44,44,44,44	0
52	MG	BA	3162	1/1	0.92	0.30	45,45,45,45	0
52	MG	AA	1645	1/1	0.92	0.59	61,61,61,61	0
52	MG	BA	3033	1/1	0.92	0.30	18,18,18,18	0
52	MG	BA	3327	1/1	0.92	0.30	48,48,48,48	0
52	MG	DA	3226	1/1	0.92	0.65	55,55,55,55	0
52	MG	DA	3131	1/1	0.92	0.28	55,55,55,55	0
52	MG	DA	3026	1/1	0.92	0.43	55,55,55,55	0
52	MG	BA	3226	1/1	0.92	0.20	14,14,14,14	0
52	MG	DA	3030	1/1	0.92	0.26	37,37,37,37	0
52	MG	BA	3227	1/1	0.92	0.61	22,22,22,22	0
52	MG	DA	3035	1/1	0.92	0.45	31,31,31,31	0
52	MG	DA	3143	1/1	0.92	0.43	40,40,40,40	0
52	MG	BA	3298	1/1	0.92	0.36	41,41,41,41	0
52	MG	DA	3049	1/1	0.92	0.55	42,42,42,42	0
52	MG	DA	3051	1/1	0.92	0.51	29,29,29,29	0
52	MG	BA	3083	1/1	0.92	0.55	34,34,34,34	0
52	MG	BA	3170	1/1	0.92	0.65	36,36,36,36	0
52	MG	DA	3318	1/1	0.92	0.36	43,43,43,43	0
52	MG	DA	3319	1/1	0.92	0.63	55,55,55,55	0
52	MG	DA	3157	1/1	0.92	0.24	48,48,48,48	0
52	MG	DA	3248	1/1	0.92	0.33	33,33,33,33	0
52	MG	BA	3230	1/1	0.92	0.76	37,37,37,37	0
52	MG	BA	3061	1/1	0.92	0.38	35,35,35,35	0
52	MG	CA	1634	1/1	0.92	0.16	47,47,47,47	0
52	MG	DA	3063	1/1	0.92	0.39	38,38,38,38	0
52	MG	BA	3041	1/1	0.92	0.44	24,24,24,24	0
52	MG	DA	3330	1/1	0.92	0.28	53,53,53,53	0
52	MG	BA	3063	1/1	0.92	0.54	45,45,45,45	0
52	MG	BB	204	1/1	0.92	0.43	41,41,41,41	0
52	MG	DA	3070	1/1	0.92	0.32	35,35,35,35	0
52	MG	BA	3312	1/1	0.92	0.20	41,41,41,41	0
52	MG	BE	301	1/1	0.92	0.49	16,16,16,16	0
52	MG	BA	3344	1/1	0.92	0.09	56,56,56,56	0
52	MG	BA	3236	1/1	0.92	0.26	31,31,31,31	0
52	MG	BA	3090	1/1	0.92	0.42	14,14,14,14	0
52	MG	DA	3089	1/1	0.92	0.61	31,31,31,31	0
52	MG	DA	3185	1/1	0.92	0.47	49,49,49,49	0
52	MG	BA	3069	1/1	0.92	0.31	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
53	ZN	AN	101	1/1	0.92	0.15	144,144,144,144	0
52	MG	DA	3094	1/1	0.92	0.69	38,38,38,38	0
52	MG	DA	3095	1/1	0.92	0.41	47,47,47,47	0
52	MG	BX	101	1/1	0.92	0.26	21,21,21,21	0
52	MG	BA	3239	1/1	0.92	0.17	32,32,32,32	0
52	MG	DA	3113	1/1	0.93	0.09	59,59,59,59	0
52	MG	DA	3048	1/1	0.93	0.48	30,30,30,30	0
52	MG	BA	3193	1/1	0.93	0.55	46,46,46,46	0
52	MG	DA	3179	1/1	0.93	0.33	29,29,29,29	0
52	MG	DA	3244	1/1	0.93	0.62	36,36,36,36	0
52	MG	AA	1636	1/1	0.93	0.52	47,47,47,47	0
52	MG	DA	3182	1/1	0.93	0.55	41,41,41,41	0
52	MG	DA	3183	1/1	0.93	0.45	35,35,35,35	0
52	MG	DA	3120	1/1	0.93	0.29	36,36,36,36	0
52	MG	BA	3001	1/1	0.93	0.38	36,36,36,36	0
52	MG	AA	1608	1/1	0.93	0.45	70,70,70,70	0
52	MG	BA	3039	1/1	0.93	0.72	37,37,37,37	0
52	MG	DA	3308	1/1	0.93	0.15	43,43,43,43	0
52	MG	DA	3254	1/1	0.93	0.19	46,46,46,46	0
52	MG	DA	3256	1/1	0.93	0.30	46,46,46,46	0
52	MG	AA	1626	1/1	0.93	0.44	46,46,46,46	0
52	MG	CA	1620	1/1	0.93	0.34	45,45,45,45	0
52	MG	DA	3314	1/1	0.93	0.23	40,40,40,40	0
52	MG	AA	1639	1/1	0.93	0.35	48,48,48,48	0
52	MG	DA	3128	1/1	0.93	0.23	29,29,29,29	0
52	MG	D1	101	1/1	0.93	0.34	47,47,47,47	0
52	MG	D5	101	1/1	0.93	0.47	30,30,30,30	0
52	MG	BA	3080	1/1	0.93	0.68	14,14,14,14	0
52	MG	CA	1624	1/1	0.93	0.40	50,50,50,50	0
52	MG	BA	3256	1/1	0.93	0.12	24,24,24,24	0
52	MG	BA	3152	1/1	0.93	0.12	49,49,49,49	0
52	MG	BA	3122	1/1	0.93	0.51	37,37,37,37	0
52	MG	DA	3145	1/1	0.93	0.55	40,40,40,40	0
52	MG	DA	3212	1/1	0.93	0.21	33,33,33,33	0
52	MG	DA	3148	1/1	0.93	0.29	51,51,51,51	0
52	MG	BA	3104	1/1	0.93	0.19	22,22,22,22	0
52	MG	BA	3263	1/1	0.93	0.17	29,29,29,29	0
52	MG	DA	3088	1/1	0.93	0.48	40,40,40,40	0
52	MG	BA	3265	1/1	0.93	0.31	43,43,43,43	0
52	MG	AA	1603	1/1	0.93	0.38	43,43,43,43	0
52	MG	BA	3329	1/1	0.93	0.33	49,49,49,49	0
52	MG	AA	1642	1/1	0.93	0.34	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3018	1/1	0.93	0.29	27,27,27,27	0
52	MG	DA	3027	1/1	0.93	0.60	36,36,36,36	0
52	MG	DR	201	1/1	0.93	0.45	34,34,34,34	0
52	MG	BA	3306	1/1	0.93	0.56	35,35,35,35	0
52	MG	DA	3286	1/1	0.93	0.43	43,43,43,43	0
52	MG	BA	3218	1/1	0.93	0.33	30,30,30,30	0
52	MG	BA	3308	1/1	0.93	0.37	45,45,45,45	0
52	MG	CA	1641	1/1	0.93	0.40	45,45,45,45	0
52	MG	DA	3040	1/1	0.93	0.95	58,58,58,58	0
52	MG	BA	3189	1/1	0.93	0.19	46,46,46,46	0
52	MG	BA	3029	1/1	0.94	0.32	25,25,25,25	0
52	MG	AA	1607	1/1	0.94	0.72	47,47,47,47	0
52	MG	BA	3099	1/1	0.94	0.30	34,34,34,34	0
52	MG	DA	3279	1/1	0.94	0.59	44,44,44,44	0
52	MG	DA	3005	1/1	0.94	0.19	49,49,49,49	0
52	MG	DA	3114	1/1	0.94	0.22	46,46,46,46	0
52	MG	BA	3281	1/1	0.94	0.21	41,41,41,41	0
52	MG	BA	3132	1/1	0.94	0.27	15,15,15,15	0
52	MG	DA	3117	1/1	0.94	0.12	54,54,54,54	0
52	MG	BA	3101	1/1	0.94	0.35	24,24,24,24	0
52	MG	BA	3284	1/1	0.94	0.28	39,39,39,39	0
52	MG	BA	3137	1/1	0.94	0.32	34,34,34,34	0
52	MG	BA	3339	1/1	0.94	0.34	31,31,31,31	0
52	MG	CA	1609	1/1	0.94	0.34	41,41,41,41	0
52	MG	BA	3186	1/1	0.94	0.50	38,38,38,38	0
52	MG	BA	3102	1/1	0.94	0.44	38,38,38,38	0
52	MG	DA	3218	1/1	0.94	0.31	24,24,24,24	0
52	MG	DA	3294	1/1	0.94	0.18	46,46,46,46	0
52	MG	DA	3219	1/1	0.94	0.37	25,25,25,25	0
52	MG	BA	3342	1/1	0.94	1.39	69,69,69,69	0
52	MG	BA	3038	1/1	0.94	0.48	17,17,17,17	0
52	MG	BA	3143	1/1	0.94	0.63	29,29,29,29	0
52	MG	CA	1617	1/1	0.94	0.53	48,48,48,48	0
52	MG	DA	3300	1/1	0.94	0.47	54,54,54,54	0
52	MG	BA	3195	1/1	0.94	0.42	49,49,49,49	0
52	MG	BA	3145	1/1	0.94	0.52	33,33,33,33	0
52	MG	DA	3042	1/1	0.94	0.25	29,29,29,29	0
52	MG	DA	3230	1/1	0.94	0.15	25,25,25,25	0
52	MG	BA	3197	1/1	0.94	0.18	27,27,27,27	0
52	MG	DA	3140	1/1	0.94	0.47	42,42,42,42	0
52	MG	BA	3071	1/1	0.94	0.44	22,22,22,22	0
52	MG	DA	3144	1/1	0.94	0.60	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3105	1/1	0.94	0.54	19,19,19,19	0
52	MG	BA	3106	1/1	0.94	0.57	37,37,37,37	0
52	MG	AA	1619	1/1	0.94	0.37	44,44,44,44	0
52	MG	BA	3040	1/1	0.94	0.65	37,37,37,37	0
52	MG	BA	3153	1/1	0.94	0.41	34,34,34,34	0
52	MG	DA	3056	1/1	0.94	0.30	24,24,24,24	0
52	MG	B5	102	1/1	0.94	0.59	44,44,44,44	0
52	MG	BA	3252	1/1	0.94	0.22	50,50,50,50	0
52	MG	BA	3311	1/1	0.94	0.20	38,38,38,38	0
52	MG	BA	3254	1/1	0.94	0.70	34,34,34,34	0
52	MG	BA	3042	1/1	0.94	0.31	7,7,7,7	0
52	MG	BA	3016	1/1	0.94	0.34	11,11,11,11	0
52	MG	BA	3048	1/1	0.94	0.55	22,22,22,22	0
52	MG	AA	1647	1/1	0.94	0.47	46,46,46,46	0
52	MG	DA	3168	1/1	0.94	0.55	32,32,32,32	0
52	MG	AA	1616	1/1	0.94	0.08	57,57,57,57	0
52	MG	BA	3057	1/1	0.94	0.29	37,37,37,37	0
52	MG	DA	3258	1/1	0.94	0.24	38,38,38,38	0
52	MG	BA	3219	1/1	0.94	0.59	24,24,24,24	0
52	MG	DA	3174	1/1	0.94	0.34	54,54,54,54	0
52	MG	BA	3266	1/1	0.94	0.44	37,37,37,37	0
52	MG	BA	3267	1/1	0.94	0.19	41,41,41,41	0
52	MG	CA	1646	1/1	0.94	0.79	58,58,58,58	0
52	MG	BA	3091	1/1	0.94	0.25	14,14,14,14	0
52	MG	BA	3270	1/1	0.94	0.55	26,26,26,26	0
52	MG	BA	3224	1/1	0.94	0.31	27,27,27,27	0
52	MG	BA	3119	1/1	0.94	0.40	34,34,34,34	0
52	MG	DA	3098	1/1	0.94	0.47	34,34,34,34	0
52	MG	BA	3059	1/1	0.94	0.34	25,25,25,25	0
52	MG	BA	3328	1/1	0.94	0.29	27,27,27,27	0
52	MG	BP	202	1/1	0.94	0.28	0,0,0,0	0
52	MG	AA	1640	1/1	0.94	0.47	60,60,60,60	0
52	MG	DA	3275	1/1	0.94	0.60	51,51,51,51	0
52	MG	BA	3054	1/1	0.95	0.29	48,48,48,48	0
52	MG	BA	3147	1/1	0.95	0.57	28,28,28,28	0
52	MG	BA	3027	1/1	0.95	0.49	25,25,25,25	0
52	MG	BA	3008	1/1	0.95	0.45	27,27,27,27	0
52	MG	BA	3280	1/1	0.95	0.40	41,41,41,41	0
52	MG	B5	101	1/1	0.95	0.39	28,28,28,28	0
52	MG	BA	3060	1/1	0.95	0.36	31,31,31,31	0
52	MG	BB	207	1/1	0.95	0.20	58,58,58,58	0
52	MG	DA	3080	1/1	0.95	0.82	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3083	1/1	0.95	0.45	37,37,37,37	0
52	MG	BA	3036	1/1	0.95	0.45	8,8,8,8	0
52	MG	DA	3273	1/1	0.95	0.28	39,39,39,39	0
52	MG	AA	1617	1/1	0.95	0.52	57,57,57,57	0
52	MG	BA	3285	1/1	0.95	0.42	35,35,35,35	0
52	MG	BA	3120	1/1	0.95	0.42	25,25,25,25	0
52	MG	BA	3157	1/1	0.95	0.44	13,13,13,13	0
52	MG	BA	3334	1/1	0.95	0.40	39,39,39,39	0
52	MG	BA	3158	1/1	0.95	0.35	9,9,9,9	0
52	MG	AA	1625	1/1	0.95	0.58	40,40,40,40	0
52	MG	BA	3064	1/1	0.95	0.48	41,41,41,41	0
52	MG	DA	3099	1/1	0.95	0.63	34,34,34,34	0
52	MG	AA	1655	1/1	0.95	0.21	45,45,45,45	0
52	MG	DA	3192	1/1	0.95	0.65	36,36,36,36	0
52	MG	BA	3293	1/1	0.95	0.36	47,47,47,47	0
52	MG	DA	3002	1/1	0.95	0.48	22,22,22,22	0
52	MG	DA	3197	1/1	0.95	0.47	46,46,46,46	0
52	MG	BA	3070	1/1	0.95	0.35	24,24,24,24	0
52	MG	DA	3199	1/1	0.95	0.57	43,43,43,43	0
52	MG	BA	3163	1/1	0.95	0.51	53,53,53,53	0
52	MG	DA	3291	1/1	0.95	0.20	36,36,36,36	0
52	MG	BA	3165	1/1	0.95	0.30	26,26,26,26	0
52	MG	BA	3130	1/1	0.95	0.13	36,36,36,36	0
52	MG	DA	3204	1/1	0.95	0.30	42,42,42,42	0
52	MG	DA	3112	1/1	0.95	0.44	28,28,28,28	0
52	MG	BA	3301	1/1	0.95	0.66	36,36,36,36	0
52	MG	BA	3303	1/1	0.95	0.23	37,37,37,37	0
52	MG	DA	3013	1/1	0.95	0.46	10,10,10,10	0
52	MG	BA	3021	1/1	0.95	0.44	19,19,19,19	0
52	MG	BA	3348	1/1	0.95	0.26	34,34,34,34	0
52	MG	DA	3213	1/1	0.95	0.42	26,26,26,26	0
52	MG	DA	3018	1/1	0.95	0.33	29,29,29,29	0
52	MG	DA	3119	1/1	0.95	0.40	36,36,36,36	0
52	MG	DA	3019	1/1	0.95	0.63	25,25,25,25	0
52	MG	BA	3217	1/1	0.95	0.35	34,34,34,34	0
52	MG	DA	3122	1/1	0.95	0.67	40,40,40,40	0
52	MG	DA	3022	1/1	0.95	0.29	38,38,38,38	0
52	MG	DA	3023	1/1	0.95	0.48	27,27,27,27	0
52	MG	CA	1615	1/1	0.95	0.39	64,64,64,64	0
52	MG	DA	3311	1/1	0.95	0.28	29,29,29,29	0
52	MG	BA	3022	1/1	0.95	0.36	37,37,37,37	0
52	MG	DA	3224	1/1	0.95	0.61	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
52	MG	BA	3044	1/1	0.95	0.28	9,9,9,9	0
52	MG	CA	1619	1/1	0.95	0.53	40,40,40,40	0
52	MG	DA	3129	1/1	0.95	0.32	36,36,36,36	0
52	MG	DA	3228	1/1	0.95	0.23	38,38,38,38	0
52	MG	BA	3220	1/1	0.95	0.69	22,22,22,22	0
52	MG	BA	3023	1/1	0.95	0.39	13,13,13,13	0
52	MG	BA	3223	1/1	0.95	0.43	25,25,25,25	0
52	MG	DA	3324	1/1	0.95	0.17	38,38,38,38	0
52	MG	DA	3038	1/1	0.95	0.57	25,25,25,25	0
52	MG	BA	3264	1/1	0.95	0.25	11,11,11,11	0
52	MG	BA	3076	1/1	0.95	0.24	21,21,21,21	0
52	MG	DA	3139	1/1	0.95	0.83	43,43,43,43	0
52	MG	DA	3237	1/1	0.95	0.26	57,57,57,57	0
52	MG	BA	3140	1/1	0.95	0.54	44,44,44,44	0
52	MG	AA	1610	1/1	0.95	0.21	33,33,33,33	0
52	MG	BA	3316	1/1	0.95	0.36	41,41,41,41	0
52	MG	DA	3050	1/1	0.95	0.34	33,33,33,33	0
52	MG	DA	3146	1/1	0.95	0.34	37,37,37,37	0
52	MG	DA	3147	1/1	0.95	0.26	43,43,43,43	0
52	MG	CA	1629	1/1	0.95	0.16	57,57,57,57	0
52	MG	AA	1627	1/1	0.95	0.20	60,60,60,60	0
52	MG	DE	301	1/1	0.95	0.43	31,31,31,31	0
52	MG	BA	3144	1/1	0.95	0.60	29,29,29,29	0
52	MG	DP	201	1/1	0.95	0.18	19,19,19,19	0
52	MG	DA	3152	1/1	0.95	0.40	36,36,36,36	0
52	MG	CA	1632	1/1	0.95	0.35	56,56,56,56	0
52	MG	BA	3182	1/1	0.95	0.49	37,37,37,37	0
52	MG	DA	3057	1/1	0.95	0.32	32,32,32,32	0
52	MG	BA	3052	1/1	0.95	0.53	23,23,23,23	0
52	MG	DA	3060	1/1	0.95	0.31	46,46,46,46	0
52	MG	BA	3231	1/1	0.95	0.11	26,26,26,26	0
52	MG	DA	3161	1/1	0.95	0.15	44,44,44,44	0
52	MG	DA	3163	1/1	0.95	0.66	30,30,30,30	0
52	MG	BA	3257	1/1	0.96	0.22	35,35,35,35	0
52	MG	DA	3155	1/1	0.96	0.13	41,41,41,41	0
52	MG	BA	3295	1/1	0.96	0.23	35,35,35,35	0
52	MG	DA	3017	1/1	0.96	0.45	37,37,37,37	0
52	MG	BA	3058	1/1	0.96	0.29	30,30,30,30	0
52	MG	DA	3229	1/1	0.96	0.55	36,36,36,36	0
52	MG	BA	3297	1/1	0.96	0.34	31,31,31,31	0
52	MG	DA	3097	1/1	0.96	0.37	30,30,30,30	0
52	MG	BB	202	1/1	0.96	0.34	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	AA	1614	1/1	0.96	0.34	47,47,47,47	0
52	MG	BA	3164	1/1	0.96	0.33	33,33,33,33	0
52	MG	DA	3024	1/1	0.96	0.40	47,47,47,47	0
52	MG	BA	3030	1/1	0.96	0.26	17,17,17,17	0
52	MG	BA	3031	1/1	0.96	0.22	39,39,39,39	0
52	MG	BD	301	1/1	0.96	0.43	25,25,25,25	0
52	MG	DA	3240	1/1	0.96	0.18	40,40,40,40	0
52	MG	DA	3108	1/1	0.96	0.47	39,39,39,39	0
52	MG	DA	3028	1/1	0.96	0.33	34,34,34,34	0
52	MG	BA	3082	1/1	0.96	0.33	6,6,6,6	0
52	MG	BA	3006	1/1	0.96	0.62	33,33,33,33	0
52	MG	BA	3233	1/1	0.96	0.29	20,20,20,20	0
52	MG	BA	3268	1/1	0.96	0.52	38,38,38,38	0
52	MG	BA	3034	1/1	0.96	0.23	45,45,45,45	0
52	MG	BA	3343	1/1	0.96	0.55	40,40,40,40	0
52	MG	DA	3041	1/1	0.96	0.34	29,29,29,29	0
52	MG	CA	1640	1/1	0.96	0.12	53,53,53,53	0
52	MG	BA	3035	1/1	0.96	0.33	18,18,18,18	0
52	MG	BA	3172	1/1	0.96	0.53	18,18,18,18	0
52	MG	BA	3173	1/1	0.96	0.29	50,50,50,50	0
52	MG	BA	3065	1/1	0.96	0.29	28,28,28,28	0
52	MG	DA	3190	1/1	0.96	0.40	43,43,43,43	0
52	MG	DA	3320	1/1	0.96	0.42	31,31,31,31	0
52	MG	BA	3129	1/1	0.96	0.19	33,33,33,33	0
52	MG	BA	3066	1/1	0.96	0.44	34,34,34,34	0
52	MG	DA	3261	1/1	0.96	0.06	51,51,51,51	0
52	MG	BA	3014	1/1	0.96	0.54	30,30,30,30	0
52	MG	BA	3211	1/1	0.96	0.29	30,30,30,30	0
52	MG	BA	3212	1/1	0.96	0.33	30,30,30,30	0
52	MG	BA	3002	1/1	0.96	0.54	23,23,23,23	0
52	MG	AA	1601	1/1	0.96	0.22	50,50,50,50	0
52	MG	BA	3136	1/1	0.96	0.50	22,22,22,22	0
52	MG	BA	3185	1/1	0.96	0.27	45,45,45,45	0
52	MG	BA	3095	1/1	0.96	0.44	38,38,38,38	0
52	MG	BA	3114	1/1	0.96	0.49	21,21,21,21	0
52	MG	CA	1616	1/1	0.96	0.50	45,45,45,45	0
52	MG	DA	3068	1/1	0.96	0.44	57,57,57,57	0
52	MG	DA	3138	1/1	0.96	0.38	31,31,31,31	0
52	MG	BA	3222	1/1	0.96	0.58	20,20,20,20	0
52	MG	DA	3004	1/1	0.96	0.25	19,19,19,19	0
52	MG	DA	3141	1/1	0.96	0.54	35,35,35,35	0
52	MG	DA	3071	1/1	0.96	0.54	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
52	MG	BA	3253	1/1	0.96	0.30	17,17,17,17	0
52	MG	BA	3020	1/1	0.96	0.35	8,8,8,8	0
52	MG	BA	3290	1/1	0.96	0.28	40,40,40,40	0
52	MG	DA	3077	1/1	0.96	0.27	38,38,38,38	0
52	MG	BA	3190	1/1	0.96	0.55	36,36,36,36	0
53	ZN	CD	301	1/1	0.96	0.28	107,107,107,107	0
52	MG	BA	3192	1/1	0.96	0.35	17,17,17,17	0
52	MG	DA	3010	1/1	0.96	0.36	35,35,35,35	0
52	MG	DA	3011	1/1	0.96	0.51	27,27,27,27	0
52	MG	CA	1623	1/1	0.96	0.12	50,50,50,50	0
52	MG	DA	3130	1/1	0.97	0.20	53,53,53,53	0
52	MG	BA	3068	1/1	0.97	0.60	35,35,35,35	0
52	MG	BA	3086	1/1	0.97	0.35	27,27,27,27	0
52	MG	DA	3062	1/1	0.97	0.16	24,24,24,24	0
52	MG	DA	3134	1/1	0.97	0.54	28,28,28,28	0
52	MG	BA	3123	1/1	0.97	0.38	40,40,40,40	0
52	MG	BA	3174	1/1	0.97	0.48	29,29,29,29	0
52	MG	BA	3087	1/1	0.97	0.20	10,10,10,10	0
52	MG	BA	3242	1/1	0.97	0.40	33,33,33,33	0
52	MG	BA	3208	1/1	0.97	0.32	17,17,17,17	0
52	MG	BA	3125	1/1	0.97	0.53	18,18,18,18	0
52	MG	BA	3210	1/1	0.97	0.51	29,29,29,29	0
52	MG	DA	3217	1/1	0.97	0.13	36,36,36,36	0
52	MG	BA	3126	1/1	0.97	0.21	29,29,29,29	0
52	MG	BA	3178	1/1	0.97	0.28	32,32,32,32	0
52	MG	BA	3214	1/1	0.97	0.20	23,23,23,23	0
52	MG	DA	3076	1/1	0.97	0.24	23,23,23,23	0
52	MG	BA	3179	1/1	0.97	0.46	25,25,25,25	0
52	MG	DA	3015	1/1	0.97	0.39	52,52,52,52	0
52	MG	DA	3081	1/1	0.97	0.56	24,24,24,24	0
52	MG	DA	3082	1/1	0.97	0.48	44,44,44,44	0
52	MG	DA	3151	1/1	0.97	0.44	40,40,40,40	0
52	MG	BA	3216	1/1	0.97	0.53	35,35,35,35	0
52	MG	BA	3251	1/1	0.97	0.17	40,40,40,40	0
52	MG	BA	3047	1/1	0.97	0.56	22,22,22,22	0
52	MG	DA	3087	1/1	0.97	0.12	24,24,24,24	0
52	MG	BA	3107	1/1	0.97	0.25	7,7,7,7	0
52	MG	BA	3011	1/1	0.97	0.47	17,17,17,17	0
52	MG	BA	3294	1/1	0.97	0.56	40,40,40,40	0
52	MG	DA	3307	1/1	0.97	0.32	42,42,42,42	0
52	MG	DA	3092	1/1	0.97	0.70	47,47,47,47	0
52	MG	BB	206	1/1	0.97	0.74	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3162	1/1	0.97	0.53	50,50,50,50	0
52	MG	BA	3012	1/1	0.97	0.47	38,38,38,38	0
52	MG	BA	3156	1/1	0.97	0.49	12,12,12,12	0
52	MG	BA	3050	1/1	0.97	0.31	21,21,21,21	0
52	MG	BA	3187	1/1	0.97	0.61	33,33,33,33	0
52	MG	BA	3073	1/1	0.97	0.28	7,7,7,7	0
52	MG	BA	3019	1/1	0.97	0.58	13,13,13,13	0
52	MG	BA	3261	1/1	0.97	0.26	27,27,27,27	0
52	MG	BR	201	1/1	0.97	0.39	7,7,7,7	0
52	MG	DA	3172	1/1	0.97	0.32	48,48,48,48	0
52	MG	DA	3033	1/1	0.97	0.29	31,31,31,31	0
52	MG	BA	3262	1/1	0.97	0.15	30,30,30,30	0
52	MG	DA	3036	1/1	0.97	0.46	12,12,12,12	0
52	MG	BU	201	1/1	0.97	0.36	25,25,25,25	0
52	MG	DA	3039	1/1	0.97	0.53	48,48,48,48	0
52	MG	DA	3178	1/1	0.97	0.41	30,30,30,30	0
52	MG	DA	3255	1/1	0.97	0.45	49,49,49,49	0
52	MG	BA	3135	1/1	0.97	0.24	30,30,30,30	0
52	MG	CA	1644	1/1	0.97	0.25	43,43,43,43	0
52	MG	DA	3181	1/1	0.97	0.67	29,29,29,29	0
52	MG	BA	3053	1/1	0.97	0.44	6,6,6,6	0
52	MG	DA	3043	1/1	0.97	0.25	49,49,49,49	0
52	MG	DA	3044	1/1	0.97	0.36	35,35,35,35	0
52	MG	DA	3045	1/1	0.97	0.40	30,30,30,30	0
52	MG	DA	3186	1/1	0.97	0.25	42,42,42,42	0
52	MG	BA	3096	1/1	0.97	0.43	16,16,16,16	0
52	MG	CA	1647	1/1	0.97	0.28	49,49,49,49	0
52	MG	BA	3138	1/1	0.97	0.38	4,4,4,4	0
52	MG	AA	1606	1/1	0.97	0.60	86,86,86,86	0
52	MG	BA	3077	1/1	0.97	0.28	20,20,20,20	0
52	MG	BA	3010	1/1	0.97	0.40	37,37,37,37	0
52	MG	DA	3194	1/1	0.97	0.35	22,22,22,22	0
52	MG	BA	3142	1/1	0.97	0.41	26,26,26,26	0
52	MG	DA	3196	1/1	0.97	0.48	33,33,33,33	0
52	MG	BA	3168	1/1	0.97	0.45	21,21,21,21	0
52	MG	BA	3015	1/1	0.97	0.36	29,29,29,29	0
52	MG	BA	3353	1/1	0.97	0.12	31,31,31,31	0
52	MG	BA	3067	1/1	0.97	0.57	28,28,28,28	0
52	MG	DA	3059	1/1	0.97	0.41	24,24,24,24	0
52	MG	DA	3253	1/1	0.98	0.59	32,32,32,32	0
52	MG	DA	3205	1/1	0.98	0.70	39,39,39,39	0
52	MG	BA	3191	1/1	0.98	0.42	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3079	1/1	0.98	0.22	36,36,36,36	0
52	MG	CA	1603	1/1	0.98	0.42	32,32,32,32	0
52	MG	DA	3209	1/1	0.98	0.40	51,51,51,51	0
52	MG	DA	3046	1/1	0.98	0.51	34,34,34,34	0
52	MG	BA	3028	1/1	0.98	0.48	24,24,24,24	0
52	MG	BA	3078	1/1	0.98	0.45	22,22,22,22	0
52	MG	DA	3084	1/1	0.98	0.45	31,31,31,31	0
52	MG	DA	3020	1/1	0.98	0.60	33,33,33,33	0
52	MG	BA	3092	1/1	0.98	0.50	19,19,19,19	0
52	MG	BA	3213	1/1	0.98	0.47	17,17,17,17	0
52	MG	BA	3079	1/1	0.98	0.24	36,36,36,36	0
52	MG	DA	3053	1/1	0.98	0.46	21,21,21,21	0
52	MG	BA	3149	1/1	0.98	0.19	8,8,8,8	0
52	MG	DA	3317	1/1	0.98	0.06	48,48,48,48	0
52	MG	DA	3091	1/1	0.98	0.43	11,11,11,11	0
52	MG	BA	3310	1/1	0.98	0.52	31,31,31,31	0
52	MG	DA	3093	1/1	0.98	0.48	44,44,44,44	0
52	MG	BA	3051	1/1	0.98	0.50	19,19,19,19	0
52	MG	BA	3121	1/1	0.98	0.27	34,34,34,34	0
52	MG	AA	1623	1/1	0.98	0.46	31,31,31,31	0
52	MG	BA	3183	1/1	0.98	0.39	43,43,43,43	0
52	MG	BA	3275	1/1	0.98	0.46	29,29,29,29	0
52	MG	DA	3031	1/1	0.98	0.17	51,51,51,51	0
52	MG	DA	3100	1/1	0.98	0.48	35,35,35,35	0
52	MG	AA	1602	1/1	0.98	0.56	32,32,32,32	0
52	MG	DA	3142	1/1	0.98	0.57	32,32,32,32	0
52	MG	DA	3102	1/1	0.98	0.55	24,24,24,24	0
52	MG	BA	3037	1/1	0.98	0.50	1,1,1,1	0
52	MG	DA	3104	1/1	0.98	0.43	41,41,41,41	0
52	MG	DA	3189	1/1	0.98	0.14	42,42,42,42	0
52	MG	DA	3034	1/1	0.98	0.37	38,38,38,38	0
52	MG	DA	3066	1/1	0.98	0.42	29,29,29,29	0
52	MG	DA	3238	1/1	0.98	0.30	36,36,36,36	0
52	MG	BQ	201	1/1	0.98	0.22	18,18,18,18	0
52	MG	BA	3055	1/1	0.98	0.41	19,19,19,19	0
52	MG	DA	3037	1/1	0.98	0.76	33,33,33,33	0
52	MG	AA	1633	1/1	0.98	0.10	42,42,42,42	0
52	MG	DA	3111	1/1	0.98	0.63	39,39,39,39	0
52	MG	BA	3100	1/1	0.98	0.39	23,23,23,23	0
52	MG	DA	3012	1/1	0.98	0.48	26,26,26,26	0
52	MG	DA	3073	1/1	0.98	0.30	27,27,27,27	0
52	MG	BA	3032	1/1	0.98	0.34	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	ZN	CN	101	1/1	0.98	0.16	136,136,136,136	0
52	MG	BA	3005	1/1	0.98	0.36	26,26,26,26	0
52	MG	DA	3158	1/1	0.98	0.31	33,33,33,33	0
52	MG	DA	3203	1/1	0.98	0.32	38,38,38,38	0
52	MG	BA	3302	1/1	0.98	0.72	31,31,31,31	0
52	MG	BA	3017	1/1	0.99	0.46	27,27,27,27	0
52	MG	DA	3064	1/1	0.99	0.51	44,44,44,44	0
52	MG	DA	3247	1/1	0.99	0.15	37,37,37,37	0
52	MG	BA	3081	1/1	0.99	0.43	7,7,7,7	0
52	MG	BA	3273	1/1	0.99	0.20	3,3,3,3	0
52	MG	BA	3045	1/1	0.99	0.41	14,14,14,14	0
52	MG	DA	3078	1/1	0.99	0.50	31,31,31,31	0
53	ZN	AD	301	1/1	0.99	0.28	109,109,109,109	0
52	MG	BA	3194	1/1	0.99	0.50	30,30,30,30	0
52	MG	BA	3024	1/1	0.99	0.33	20,20,20,20	0
52	MG	BA	3084	1/1	0.99	0.37	5,5,5,5	0
52	MG	BA	3133	1/1	0.99	0.31	25,25,25,25	0
52	MG	DA	3321	1/1	0.99	0.07	41,41,41,41	0
52	MG	DA	3171	1/1	0.99	0.35	26,26,26,26	0
52	MG	BA	3043	1/1	0.99	0.18	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.