



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 21, 2016 – 11:08 PM EDT

PDB ID : 4V8X  
Title : Structure of Thermus thermophilus ribosome  
Authors : Feng, S.; Chen, Y.; Kamada, K.; Wang, H.; Tang, K.; Wang, M.; Gao, Y.G.  
Deposited on : 2013-07-19  
Resolution : 3.35 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027790

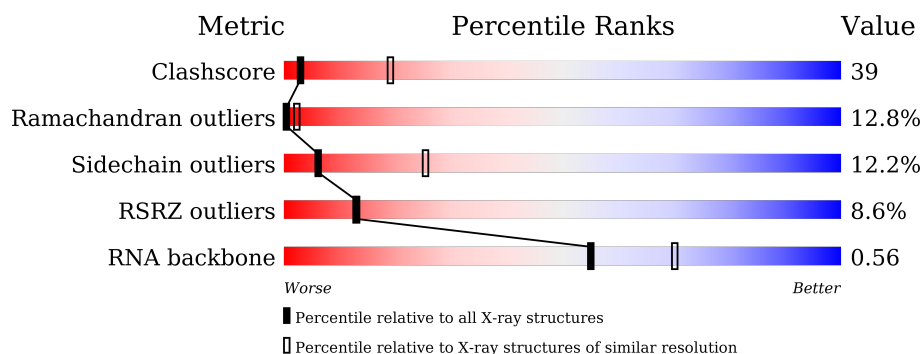
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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.





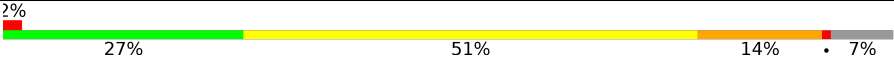
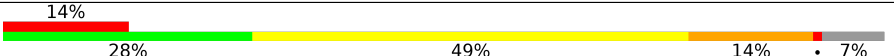
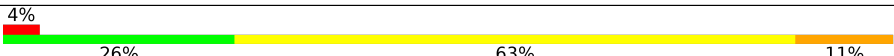
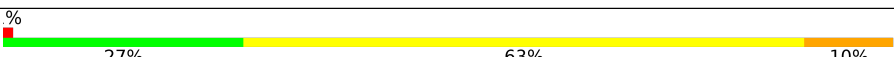
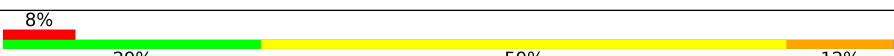
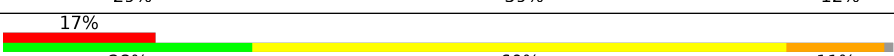
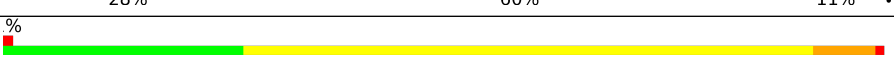
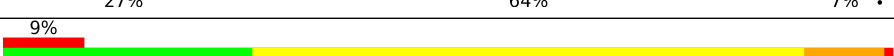
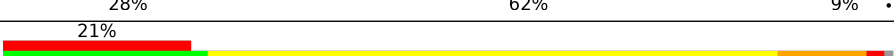
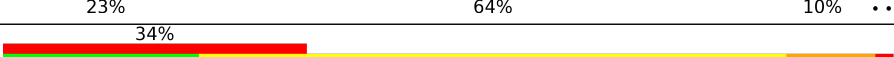

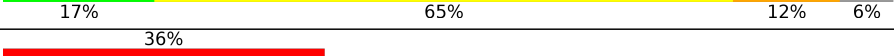
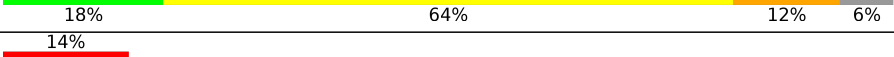
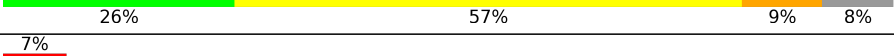
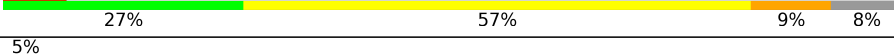

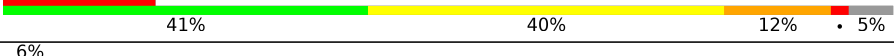
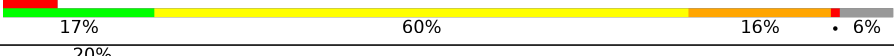
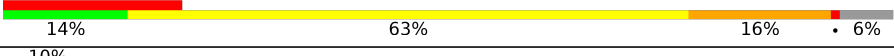
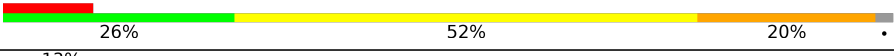
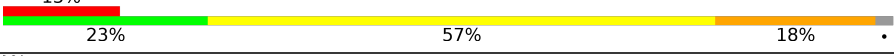


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)
RNA backbone	2183	1016 (3.92-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1504	<div> <div>2%</div> <div>29%</div> <div>60%</div> <div>11%</div> <div>.</div> </div>
1	CA	1504	<div> <div>3%</div> <div>27%</div> <div>62%</div> <div>10%</div> <div>.</div> </div>
2	AB	256	<div> <div>11%</div> <div>20%</div> <div>61%</div> <div>11%</div> <div>8%</div> </div>
2	CB	256	<div> <div>11%</div> <div>18%</div> <div>63%</div> <div>10%</div> <div>.</div> <div>8%</div> </div>
3	AC	239	<div> <div>5%</div> <div>21%</div> <div>52%</div> <div>13%</div> <div>.</div> <div>13%</div> </div>
3	CC	239	<div> <div>16%</div> <div>21%</div> <div>51%</div> <div>13%</div> <div>.</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	

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Mol	Chain	Length	Quality of chain
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
23	AW	77	
23	CV	77	
23	CW	77	
24	AX	25	
25	AY	84	
25	AZ	84	
25	CY	84	
25	CZ	84	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	
28	B2	72	

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Mol	Chain	Length	Quality of chain
28	D2	72	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%</div><div>25%</div><div>56%</div><div>14%</div><div>• •</div></div>
29	B3	60	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>13%</div><div>53%</div><div>40%</div><div>5%</div><div>•</div></div>
29	D3	60	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div>53%</div><div>40%</div><div>5%</div><div>•</div></div>
30	B4	71	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>8%</div><div>7%</div><div>46%</div><div>23%</div><div>6%</div><div>18%</div></div>
30	D4	71	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%</div><div>8%</div><div>46%</div><div>21%</div><div>6%</div><div>18%</div></div>
31	B5	60	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%</div><div>35%</div><div>45%</div><div>10%</div><div>•</div><div>7%</div></div>
31	D5	60	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%</div><div>40%</div><div>40%</div><div>10%</div><div>•</div><div>7%</div></div>
32	B6	54	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>35%</div><div>13%</div><div>39%</div><div>33%</div><div>7%</div><div>7%</div></div>
32	D6	54	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>26%</div><div>13%</div><div>37%</div><div>33%</div><div>9%</div><div>7%</div></div>
33	B7	49	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div>55%</div><div>39%</div><div>•</div><div>•</div></div>
33	D7	49	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%</div><div>53%</div><div>43%</div><div>•</div><div>•</div></div>
34	B8	65	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%</div><div>22%</div><div>51%</div><div>17%</div><div>9%</div><div>•</div></div>
34	D8	65	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%</div><div>18%</div><div>54%</div><div>18%</div><div>8%</div><div>•</div></div>
35	B9	37	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>41%</div><div>35%</div><div>57%</div><div>8%</div></div>
35	D9	37	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>51%</div><div>38%</div><div>54%</div><div>8%</div></div>
36	BA	2848	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%</div><div>36%</div><div>51%</div><div>12%</div><div>•</div></div>
36	DA	2848	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%</div><div>36%</div><div>51%</div><div>12%</div><div>•</div></div>
37	BB	119	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div>22%</div><div>58%</div><div>19%</div><div>•</div></div>
37	DB	119	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%</div><div>20%</div><div>61%</div><div>18%</div><div>•</div></div>
38	BC	229	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>41%</div><div>17%</div><div>32%</div><div>•</div><div>48%</div></div>
38	DC	229	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>40%</div><div>17%</div><div>32%</div><div>•</div><div>48%</div></div>
39	BD	276	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>1%</div><div>36%</div><div>48%</div><div>13%</div><div>• •</div></div>
39	DD	276	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>1%</div><div>35%</div><div>48%</div><div>14%</div><div>• •</div></div>
40	BE	206	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%</div><div>31%</div><div>50%</div><div>18%</div><div>•</div></div>
40	DE	206	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div>34%</div><div>47%</div><div>17%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BI	148	
44	DI	148	
45	BJ	130	
45	DJ	130	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	
52	DT	146	
53	BU	118	

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Mol	Chain	Length	Quality of chain
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	
59	CX	10	

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
24	OMU	AX	19	-	-	X	-
24	A2M	AX	20	-	-	X	-
24	A2M	AX	21	-	-	X	-
59	OMU	CX	19	-	-	X	-
59	A2M	CX	20	-	-	X	-
59	A2M	CX	21	-	-	X	-
60	MG	AA	1603	-	-	-	X
60	MG	AA	1605	-	-	-	X
60	MG	AA	1608	-	-	-	X
60	MG	AA	1616	-	-	-	X
60	MG	AA	1617	-	-	-	X
60	MG	AA	1620	-	-	-	X
60	MG	AA	1622	-	-	-	X
60	MG	AA	1623	-	-	-	X
60	MG	AA	1628	-	-	-	X
60	MG	AA	1629	-	-	-	X
60	MG	AA	1635	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	1651	-	-	-	X
60	MG	AA	1652	-	-	-	X
60	MG	AA	1658	-	-	-	X
60	MG	AA	1662	-	-	-	X
60	MG	AA	1671	-	-	-	X
60	MG	AA	1676	-	-	-	X
60	MG	AA	1680	-	-	-	X
60	MG	AA	1686	-	-	-	X
60	MG	AA	1702	-	-	-	X
60	MG	B1	102	-	-	-	X
60	MG	BA	2903	-	-	-	X
60	MG	BA	2904	-	-	-	X
60	MG	BA	2907	-	-	-	X
60	MG	BA	2909	-	-	-	X
60	MG	BA	2912	-	-	-	X
60	MG	BA	2915	-	-	-	X
60	MG	BA	2916	-	-	-	X
60	MG	BA	2918	-	-	-	X
60	MG	BA	2919	-	-	-	X
60	MG	BA	2921	-	-	-	X
60	MG	BA	2922	-	-	-	X
60	MG	BA	2928	-	-	-	X
60	MG	BA	2930	-	-	-	X
60	MG	BA	2933	-	-	-	X
60	MG	BA	2934	-	-	-	X
60	MG	BA	2936	-	-	-	X
60	MG	BA	2937	-	-	-	X
60	MG	BA	2939	-	-	-	X
60	MG	BA	2940	-	-	-	X
60	MG	BA	2942	-	-	-	X
60	MG	BA	2943	-	-	-	X
60	MG	BA	2944	-	-	-	X
60	MG	BA	2945	-	-	-	X
60	MG	BA	2946	-	-	-	X
60	MG	BA	2949	-	-	-	X
60	MG	BA	2954	-	-	-	X
60	MG	BA	2955	-	-	-	X
60	MG	BA	2960	-	-	-	X
60	MG	BA	2966	-	-	-	X
60	MG	BA	2967	-	-	-	X
60	MG	BA	2968	-	-	-	X
60	MG	BA	2969	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	2972	-	-	-	X
60	MG	BA	2973	-	-	-	X
60	MG	BA	2974	-	-	-	X
60	MG	BA	2987	-	-	-	X
60	MG	BA	2990	-	-	-	X
60	MG	BA	2992	-	-	-	X
60	MG	BA	2993	-	-	-	X
60	MG	BA	2994	-	-	-	X
60	MG	BA	2995	-	-	-	X
60	MG	BA	2996	-	-	-	X
60	MG	BA	3003	-	-	-	X
60	MG	BA	3006	-	-	-	X
60	MG	BA	3014	-	-	-	X
60	MG	BA	3015	-	-	-	X
60	MG	BA	3016	-	-	-	X
60	MG	BA	3025	-	-	-	X
60	MG	BA	3027	-	-	-	X
60	MG	BA	3030	-	-	-	X
60	MG	BA	3038	-	-	-	X
60	MG	BA	3039	-	-	-	X
60	MG	BA	3045	-	-	-	X
60	MG	BA	3047	-	-	-	X
60	MG	BA	3057	-	-	-	X
60	MG	BA	3059	-	-	-	X
60	MG	BA	3064	-	-	-	X
60	MG	BA	3071	-	-	-	X
60	MG	BA	3077	-	-	-	X
60	MG	BA	3078	-	-	-	X
60	MG	BA	3079	-	-	-	X
60	MG	BA	3082	-	-	-	X
60	MG	BA	3088	-	-	-	X
60	MG	BA	3098	-	-	-	X
60	MG	BA	3100	-	-	-	X
60	MG	BA	3102	-	-	-	X
60	MG	BA	3104	-	-	-	X
60	MG	BA	3107	-	-	-	X
60	MG	BA	3110	-	-	-	X
60	MG	BA	3122	-	-	-	X
60	MG	BA	3133	-	-	-	X
60	MG	BA	3135	-	-	-	X
60	MG	BA	3136	-	-	-	X
60	MG	BF	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	1612	-	-	-	X
60	MG	CA	1613	-	-	-	X
60	MG	CA	1614	-	-	-	X
60	MG	CA	1622	-	-	-	X
60	MG	CA	1626	-	-	-	X
60	MG	CA	1628	-	-	-	X
60	MG	CA	1647	-	-	-	X
60	MG	CA	1655	-	-	-	X
60	MG	CA	1656	-	-	-	X
60	MG	CA	1657	-	-	-	X
60	MG	CA	1663	-	-	-	X
60	MG	CA	1678	-	-	-	X
60	MG	CA	1681	-	-	-	X
60	MG	CA	1687	-	-	-	X
60	MG	CA	1701	-	-	-	X
60	MG	CV	101	-	-	-	X
60	MG	D1	101	-	-	-	X
60	MG	DA	2903	-	-	-	X
60	MG	DA	2904	-	-	-	X
60	MG	DA	2907	-	-	-	X
60	MG	DA	2909	-	-	-	X
60	MG	DA	2910	-	-	-	X
60	MG	DA	2911	-	-	-	X
60	MG	DA	2914	-	-	-	X
60	MG	DA	2915	-	-	-	X
60	MG	DA	2917	-	-	-	X
60	MG	DA	2918	-	-	-	X
60	MG	DA	2921	-	-	-	X
60	MG	DA	2927	-	-	-	X
60	MG	DA	2929	-	-	-	X
60	MG	DA	2932	-	-	-	X
60	MG	DA	2933	-	-	-	X
60	MG	DA	2935	-	-	-	X
60	MG	DA	2937	-	-	-	X
60	MG	DA	2938	-	-	-	X
60	MG	DA	2940	-	-	-	X
60	MG	DA	2941	-	-	-	X
60	MG	DA	2942	-	-	-	X
60	MG	DA	2943	-	-	-	X
60	MG	DA	2946	-	-	-	X
60	MG	DA	2950	-	-	-	X
60	MG	DA	2957	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	2958	-	-	-	X
60	MG	DA	2965	-	-	-	X
60	MG	DA	2967	-	-	-	X
60	MG	DA	2968	-	-	-	X
60	MG	DA	2971	-	-	-	X
60	MG	DA	2972	-	-	-	X
60	MG	DA	2973	-	-	-	X
60	MG	DA	2974	-	-	-	X
60	MG	DA	2978	-	-	-	X
60	MG	DA	2979	-	-	-	X
60	MG	DA	2994	-	-	-	X
60	MG	DA	2995	-	-	-	X
60	MG	DA	2996	-	-	-	X
60	MG	DA	2998	-	-	-	X
60	MG	DA	2999	-	-	-	X
60	MG	DA	3005	-	-	-	X
60	MG	DA	3006	-	-	-	X
60	MG	DA	3008	-	-	-	X
60	MG	DA	3022	-	-	-	X
60	MG	DA	3025	-	-	-	X
60	MG	DA	3029	-	-	-	X
60	MG	DA	3035	-	-	-	X
60	MG	DA	3037	-	-	-	X
60	MG	DA	3038	-	-	-	X
60	MG	DA	3040	-	-	-	X
60	MG	DA	3042	-	-	-	X
60	MG	DA	3044	-	-	-	X
60	MG	DA	3052	-	-	-	X
60	MG	DA	3062	-	-	-	X
60	MG	DA	3065	-	-	-	X
60	MG	DA	3067	-	-	-	X
60	MG	DA	3074	-	-	-	X
60	MG	DA	3075	-	-	-	X
60	MG	DA	3076	-	-	-	X
60	MG	DA	3077	-	-	-	X
60	MG	DA	3083	-	-	-	X
60	MG	DA	3092	-	-	-	X
60	MG	DA	3094	-	-	-	X
60	MG	DA	3096	-	-	-	X
60	MG	DA	3103	-	-	-	X
60	MG	DA	3105	-	-	-	X
60	MG	DA	3108	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3109	-	-	-	X
60	MG	DA	3111	-	-	-	X
60	MG	DR	201	-	-	-	X
61	ZN	AD	301	-	-	X	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298206 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 RNA (1504-MER).

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

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			
13	CM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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			
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 RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 23 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 24 is a RNA chain called 5'-R(\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*AP\*GP\*GP\*UP\*AP\*AP\*AP \*AP\*AP\*UP\*G U2M A2M A2MP\*AP\*AP\*AP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			239	111	49	69	10			

- Molecule 25 is a protein called TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	84	Total	C	N	O	S	0	0	0
			722	464	126	130	2			
25	AZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
25	CY	84	Total	C	N	O	S	0	0	0
			722	464	126	130	2			
25	CZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
26	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
27	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
28	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
30	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			
33	D7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called RNA (2848-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			
36	DA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			

- Molecule 37 is a RNA chain called RNA (119-MER).

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
38	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
43	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BJ	130	Total	C	N	O		0	0	0
			651	390	130	131				
45	DJ	130	Total	C	N	O		0	0	0
			651	390	130	131				

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	7			
49	DQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	7			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			
52	DT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1
58	DZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1

- Molecule 59 is a RNA chain called BACTERIAL TOXIN YOEB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	10	Total 217	C 101	N 44	O 63	P 9	0	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	236	Total 236	Mg 236	0	0
60	CA	103	Total 103	Mg 103	0	0
60	DF	1	Total 1	Mg 1	0	0
60	CV	2	Total 2	Mg 2	0	0
60	B1	2	Total 2	Mg 2	0	0
60	BP	1	Total 1	Mg 1	0	0
60	AX	1	Total 1	Mg 1	0	0
60	DR	1	Total 1	Mg 1	0	0
60	B5	2	Total 2	Mg 2	0	0
60	BB	2	Total 2	Mg 2	0	0
60	BF	1	Total 1	Mg 1	0	0
60	AV	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	AA	103	Total 103	Mg 103	0	0
60	CG	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DX	1	Total 1	Mg 1	0	0
60	DA	242	Total 242	Mg 242	0	0
60	AL	1	Total 1	Mg 1	0	0
60	D1	1	Total 1	Mg 1	0	0
60	D5	1	Total 1	Mg 1	0	0
60	B0	1	Total 1	Mg 1	0	0
60	CL	1	Total 1	Mg 1	0	0
60	DB	1	Total 1	Mg 1	0	0

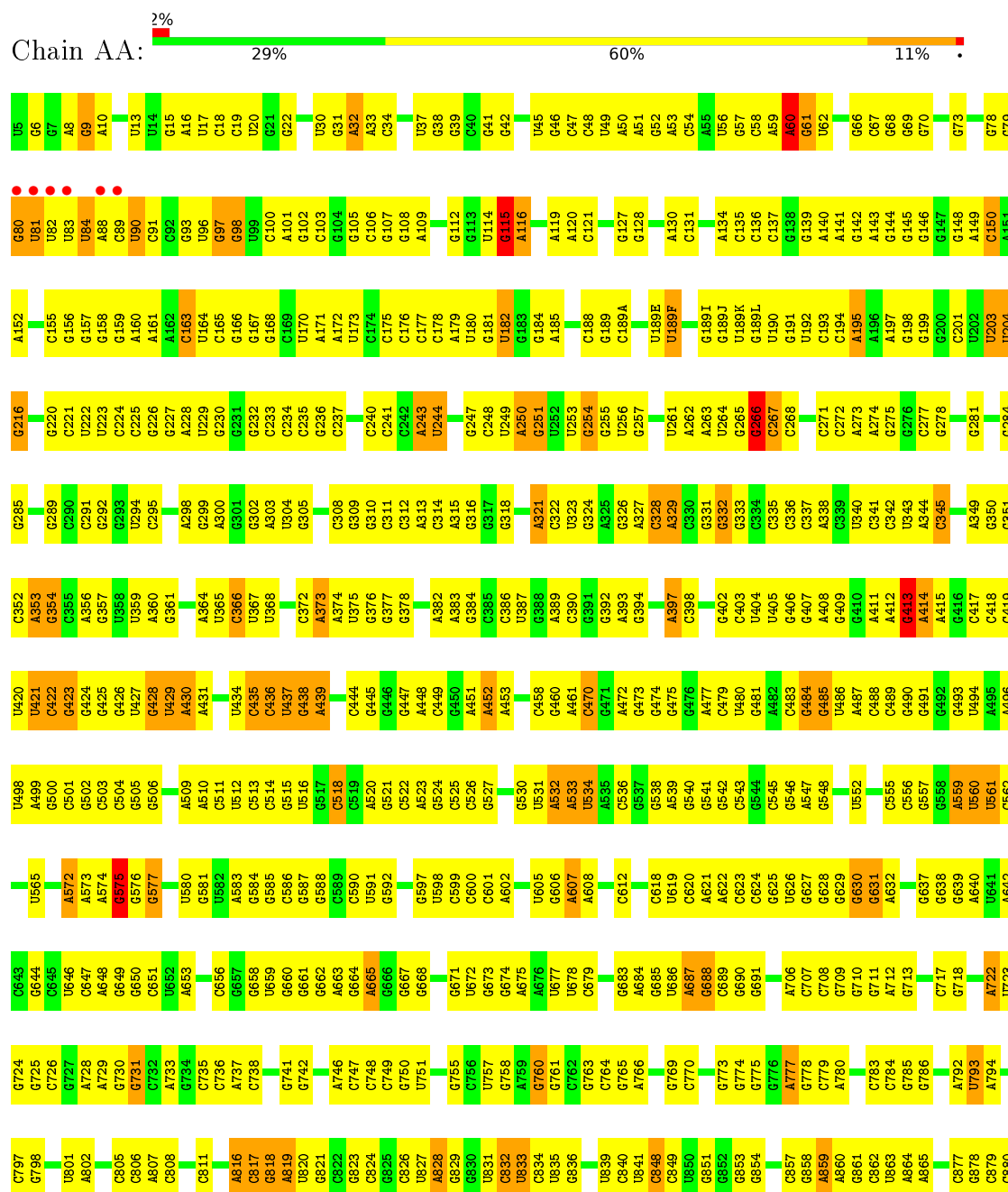
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

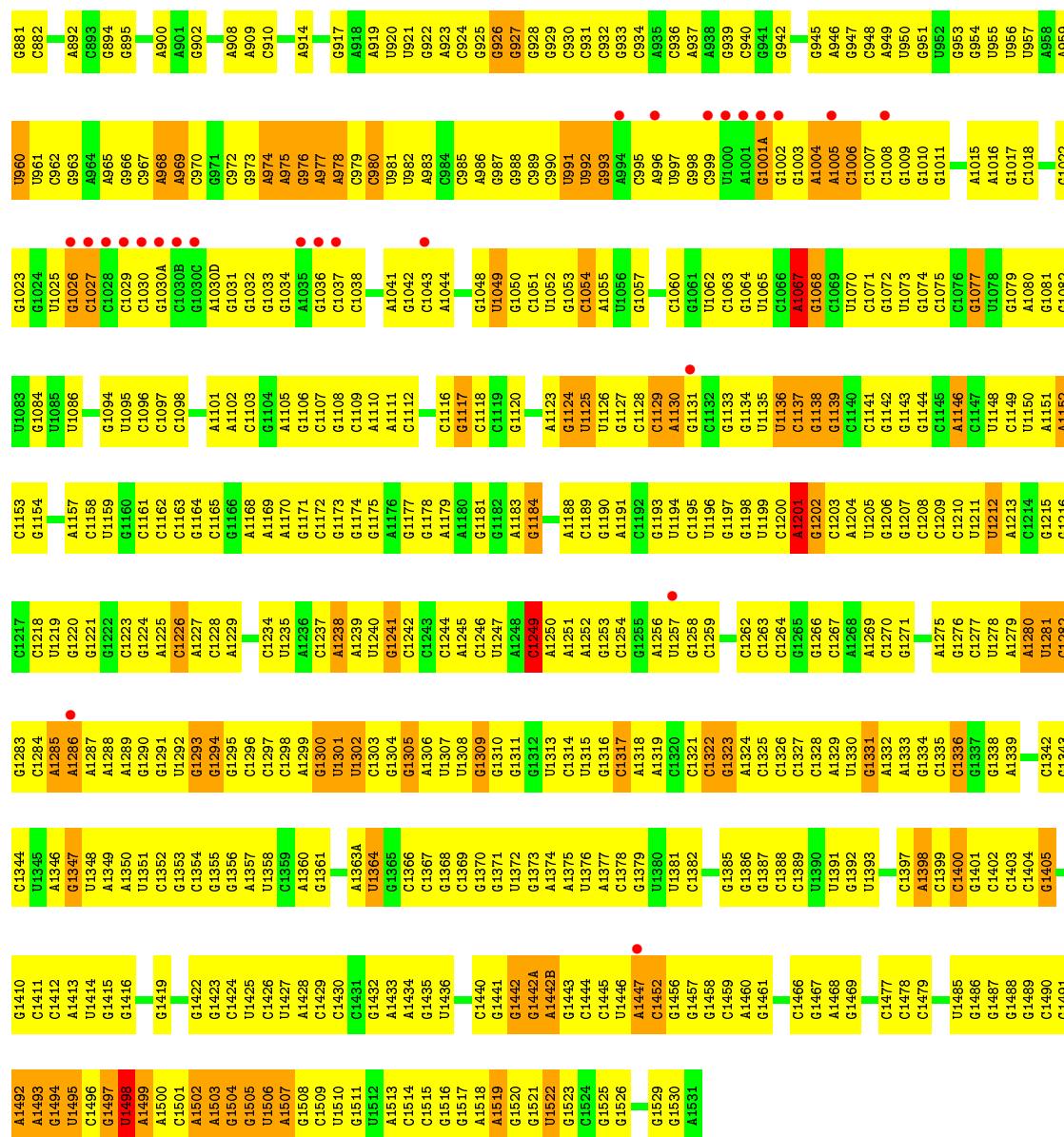
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CN	1	Total 1	Zn 1	0	0
61	AD	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0
61	AN	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

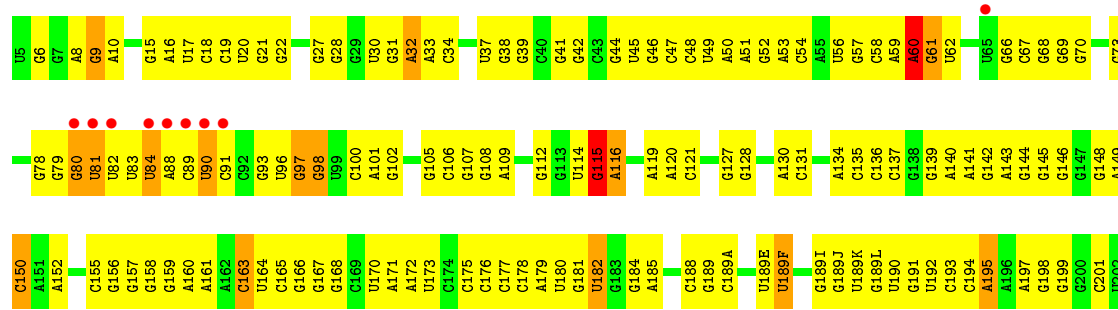
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: RNA (1504-MER)

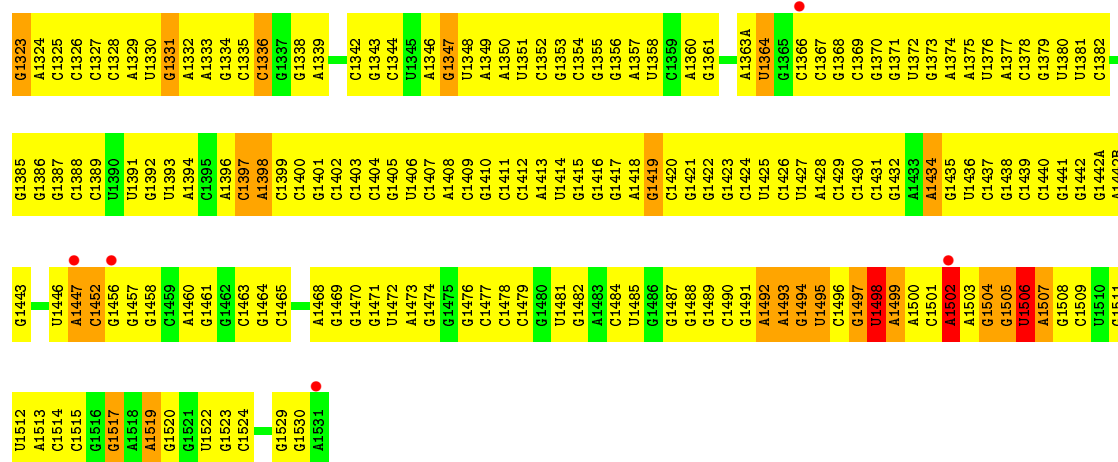




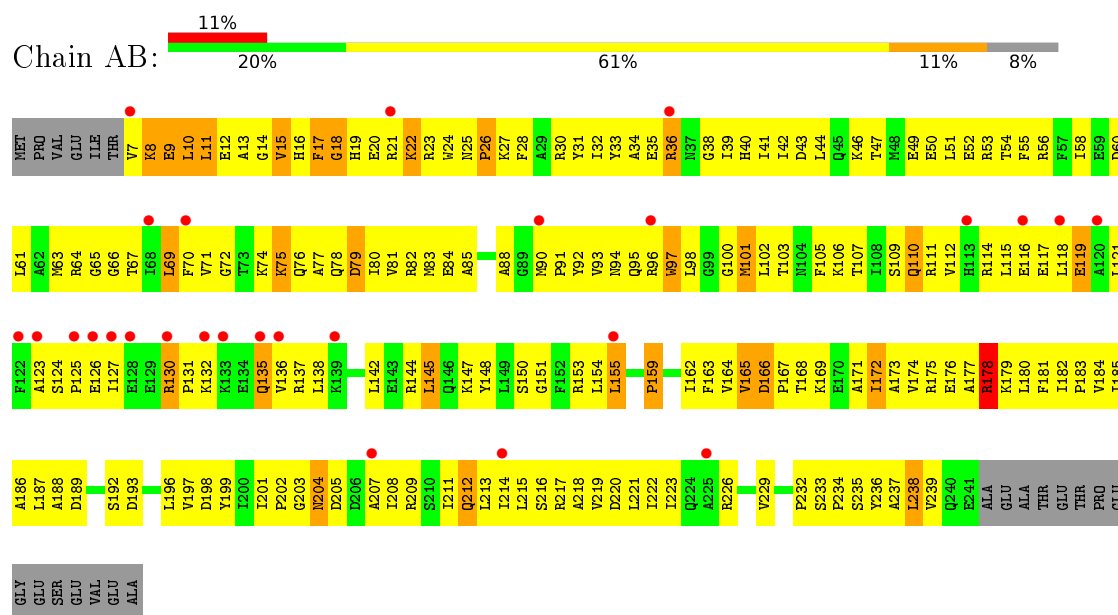
● Molecule 1: RNA (1504-MER)



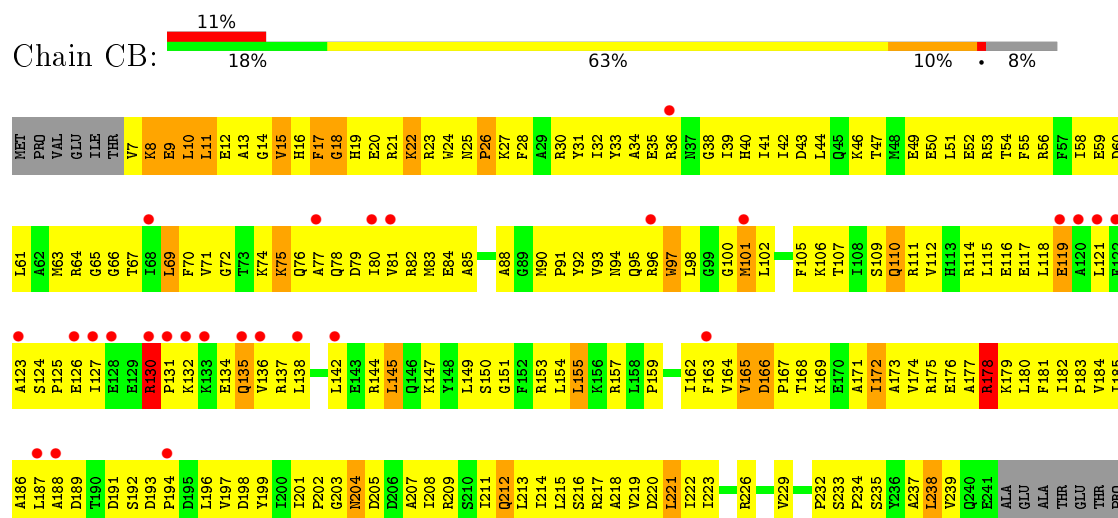




• Molecule 2: 30S RIBOSOMAL PROTEIN S2



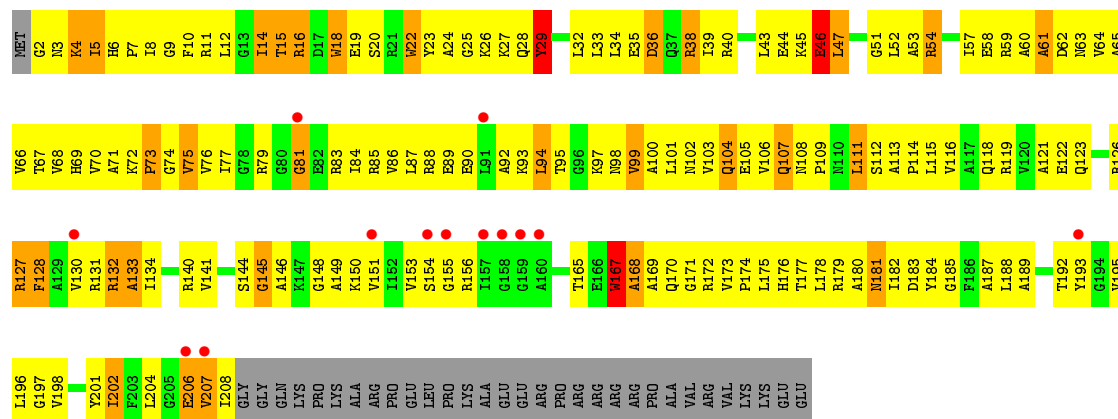
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



GLU  
GLY  
GLU  
SER  
GLU  
VAL  
GLU  
ALA

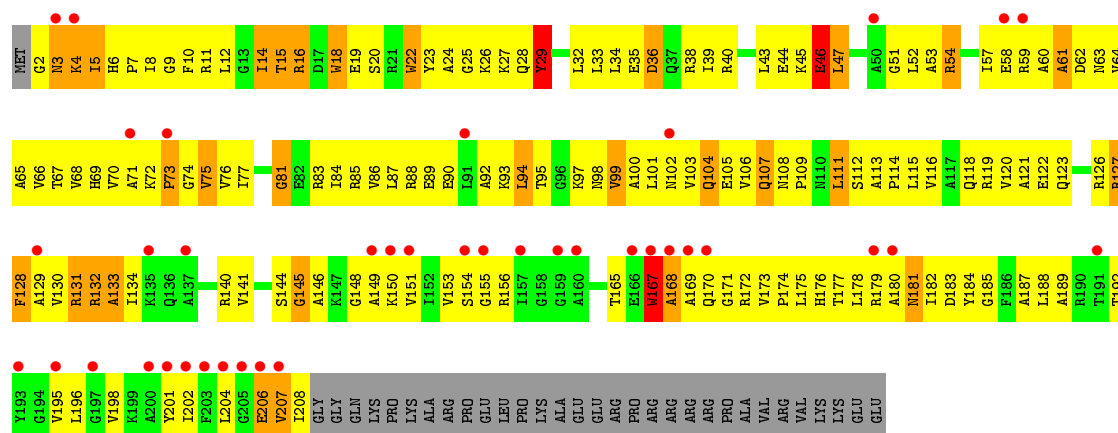
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC: 5% 21% 52% 13% 13%



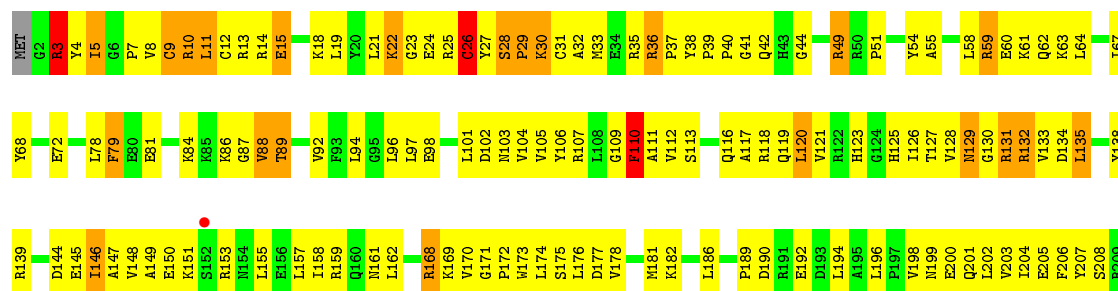
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: 16% 21% 51% 13% 13%

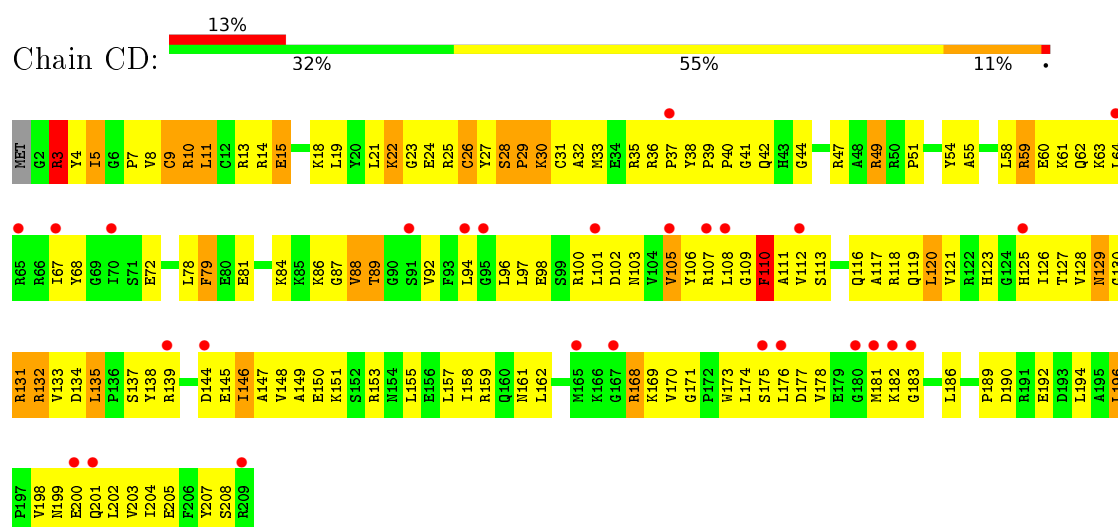


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

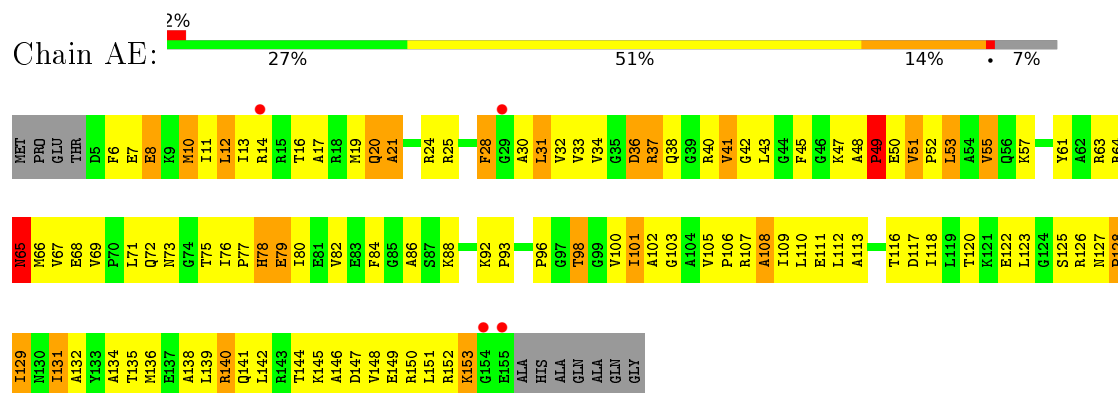
Chain AD: 33% 55% 11%



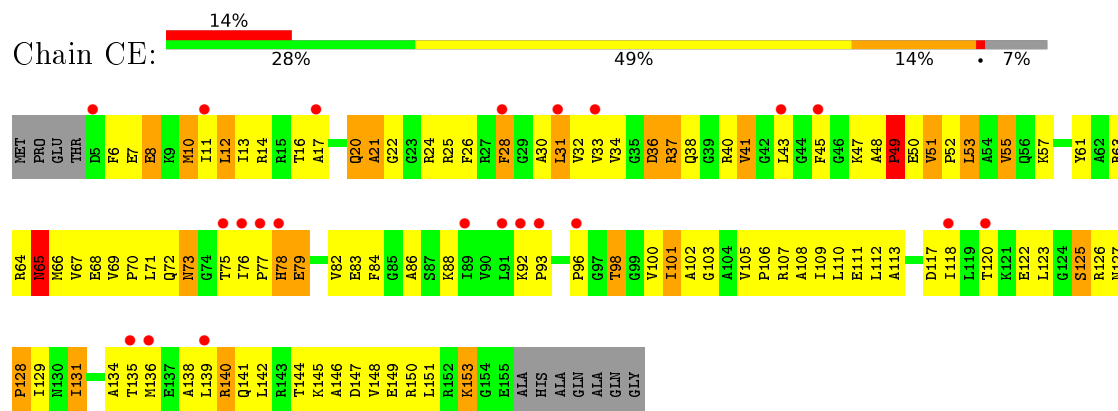
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



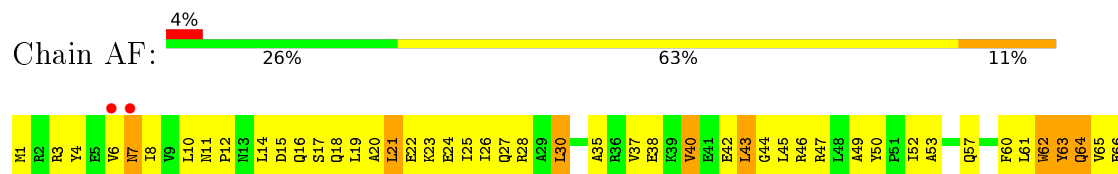
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

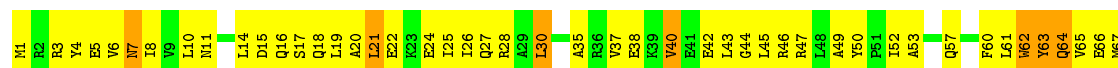


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

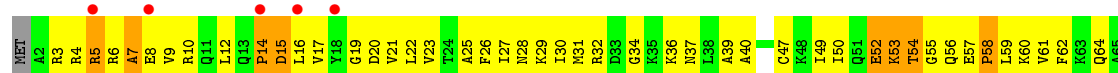




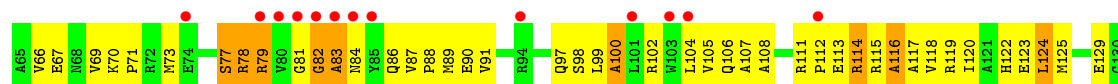
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



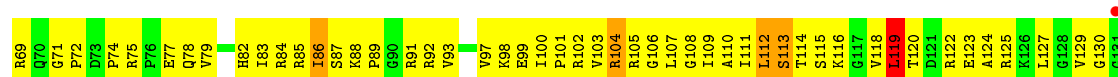
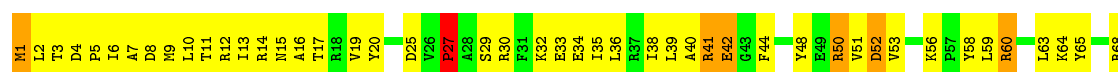
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 8: 30S RIBOSOMAL PROTEIN S8



E132  
L133  
I134  
C135  
E136  
V137  
W138

• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH: 

M1 L2 T3 D4 P6 I6 A7 D8 M9 L10 T11 T12 I13 R14 N15 A16 T17 R18 R19 V19 Y20 S23 T24 D25 V26 V27 A28 S29 R30 F31 K32 E33 E34 I35 I36 R37 I38 I39 A40 R41 E42 G43 F44 G47 R50 V51 D52 Y58 L59 R60 V61 Y62 I63 K64 Y65 R68

R69 Q70 G71 P72 D73 P74 R75 R76 E77 Q78 V79 R82 I83 R84 R85 I86 S87 R88 P89 G90 R91 R92 V93 V94 V95 G96 R97 R98 E99 I100 P101 R102 V103 R104 R105 G106 L107 G108 I109 A110 A111 I112 S113 T114 S115 K116 G117 V118 I119 T120 D121 R122 E123 A124 L127 G128 V129 R130

G131 E132  
L133  
I134  
C135  
E136  
V137  
W138

• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI: 

MET E2 Q3 Y4 Y5 G6 T7 G8 R9 R10 K11 A12 A13 V14 A15 R16 R17 V18 F18 L19 R20 V26 T27 R28 V29 G30 Q31 D32 F33 R34 E35 Y36 F37 Q38 G39 L40 V41 R42 A43 V44 A45 A46 L47 E48 P49 L50 V53 D54 A55 L56 G57 H58 F59 D60 A61 Y62 I63 T64 V65

R66 G67 G68 G69 K70 S71 G72 Q73 I74 A75 A76 I77 K78 L79 G80 R81 A82 R83 A84 L85 V86 Q87 Y88 R89 V90 D91 Y92 R93 A94 R95 R96 R97 R98 F99 G100 F101 L102 T103 R104 D105 A106 R107 E110 R111 K112 K113 Y114 H117 K118 A119 R120 R121 R122 A123 P124 Q124 Y125 S126 I127

R128

• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI: 

MET E2 Q3 Y4 Y5 G6 T7 G8 R9 R10 K11 A12 A13 V14 A15 R16 R17 V18 F18 L19 R20 K25 V26 T27 R28 V29 G30 Q31 D32 F33 R34 E35 Y36 F37 Q38 G39 L40 V41 R42 A43 V44 A45 A46 L47 E48 P49 L50 V53 D54 A55 L56 G57 H58 F59 D60 A61 Y62 I63 T64

V65 R66 G67 G68 G69 K70 S71 G72 Q73 I74 A75 A76 I77 K78 L79 G80 R81 A82 R83 A84 L85 V86 Q87 Y88 R89 V90 D91 Y92 R93 A94 R95 R96 R97 R98 F99 G100 F101 L102 T103 R104 D105 A106 R107 E110 R111 K112 K113 Y114 H117 K118 A119 R120 R121 R122 A123 P124 Q124 Y125 S126 I127

S126  
K127  
R128

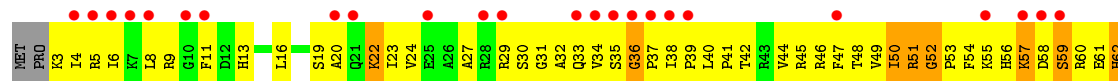
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ: 

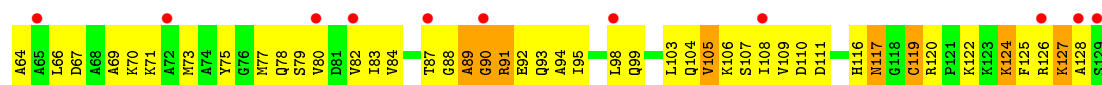
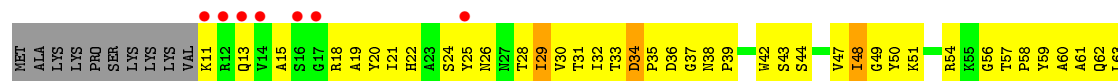
MET P90 K3 I4 R5 I6 K7 L8 R9 G10 F11 D12 H13 K14 T15 S19 A20 A21 Q22 L23 I24 V24 E25 A26 A27 R28 R29 S30 G31 A32 Q33 Q34 S35 G36 P37 I38 P39 L40 P41 T42 R43 V44 R45 R46 F47 T48 V49 I50 R51 G52 P53 F54 K55 H56 K57 D58 S59 R60 E61



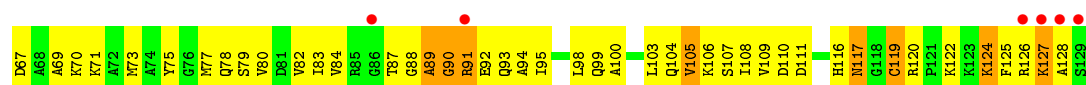
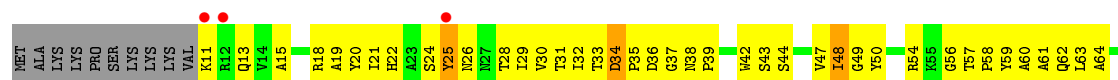
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



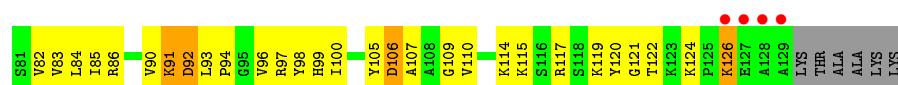
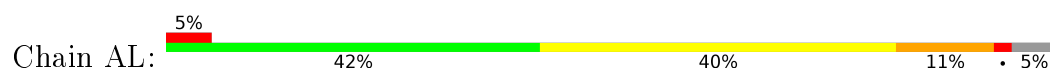
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

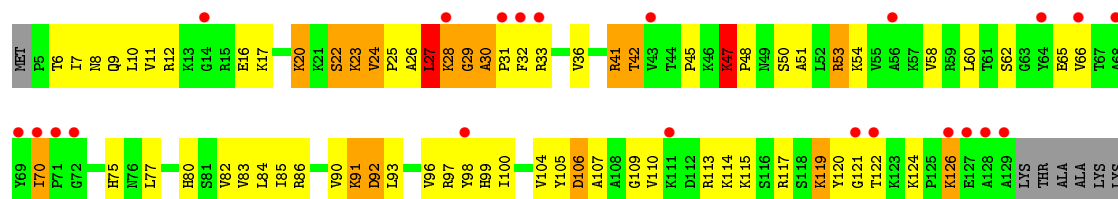


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

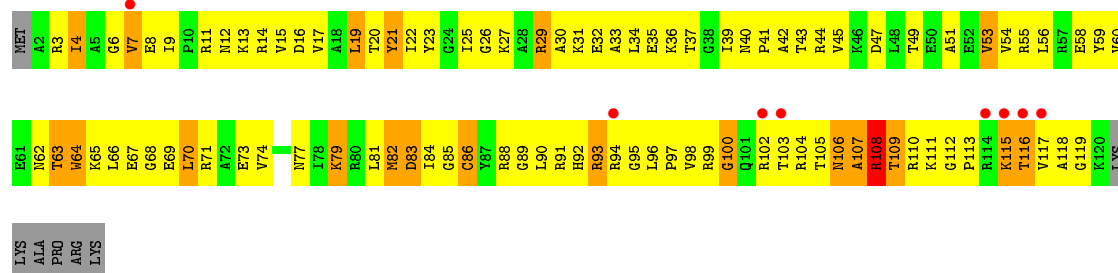


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

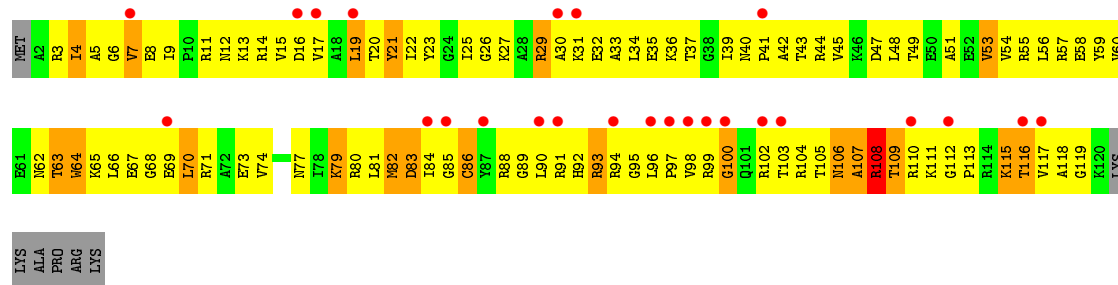




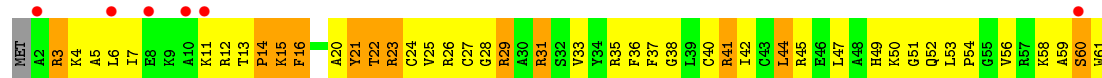
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

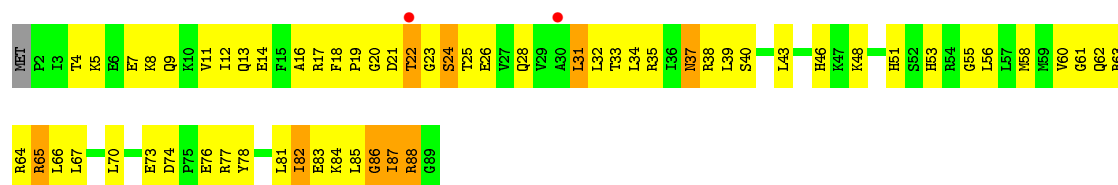


• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

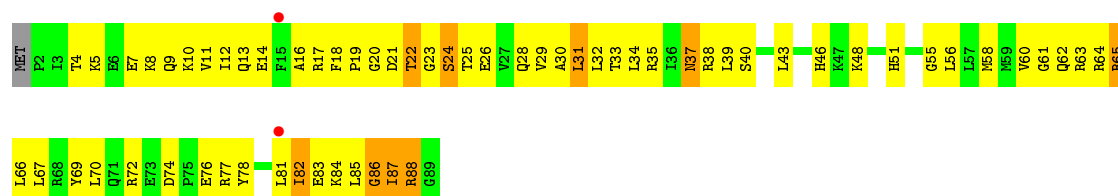


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

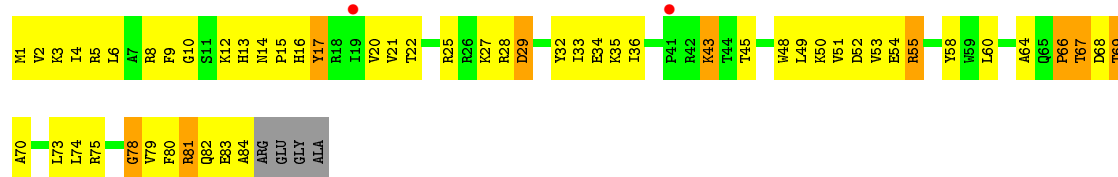




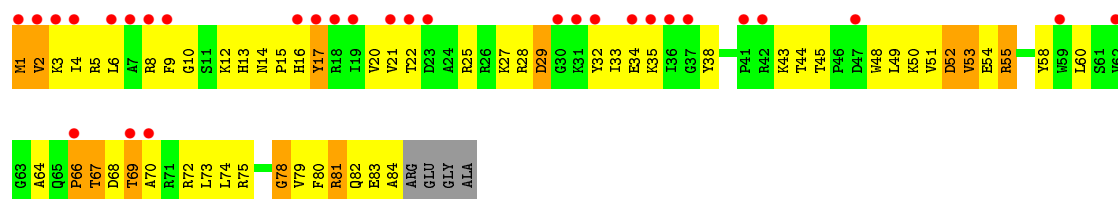
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



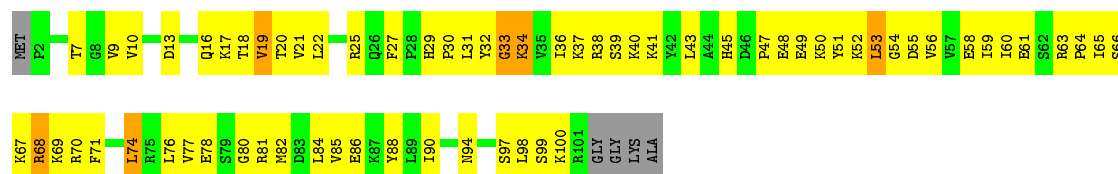
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

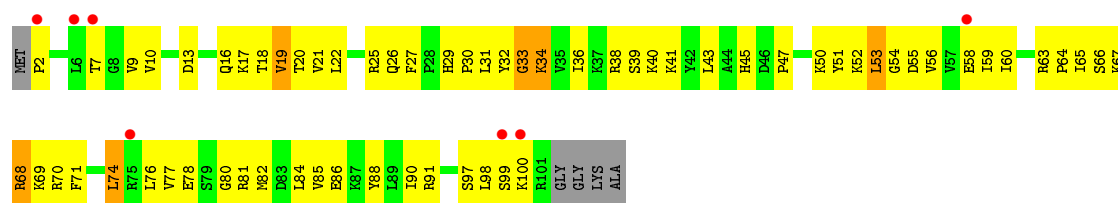


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

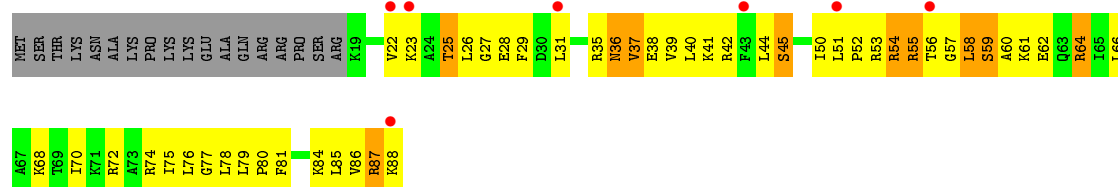


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

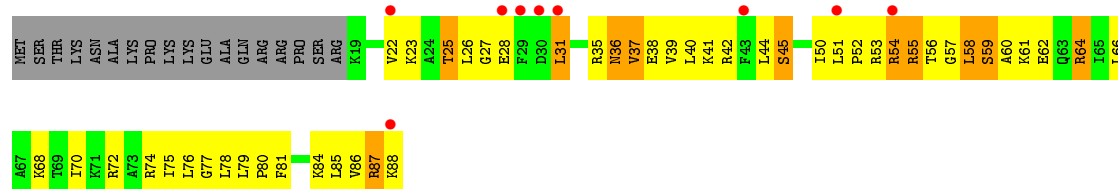




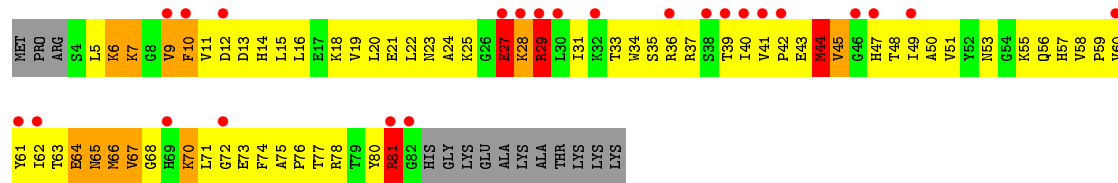
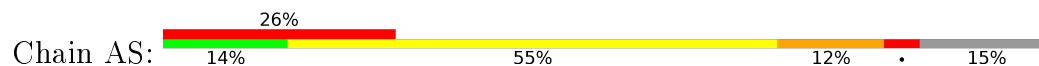
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



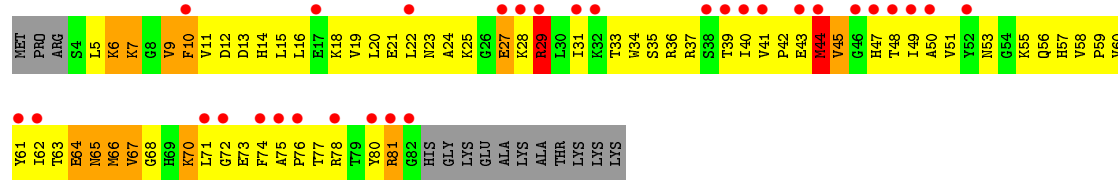
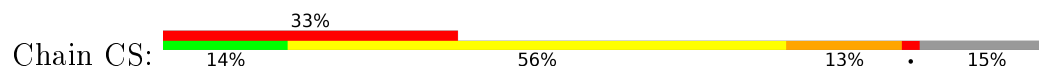
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

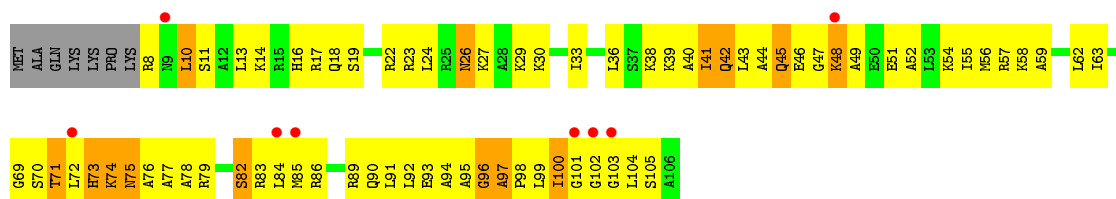


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

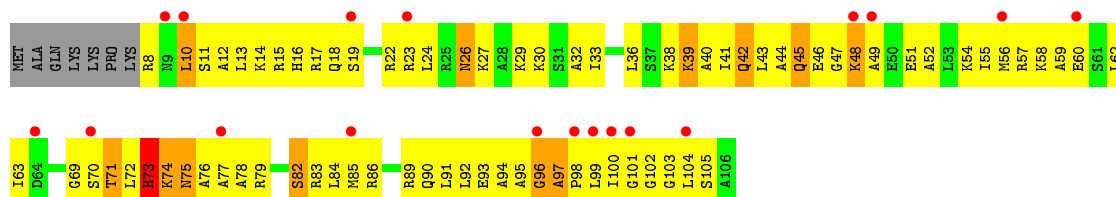


• Molecule 20: 30S RIBOSOMAL PROTEIN S20





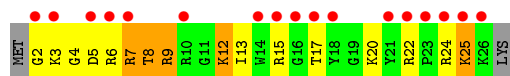
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



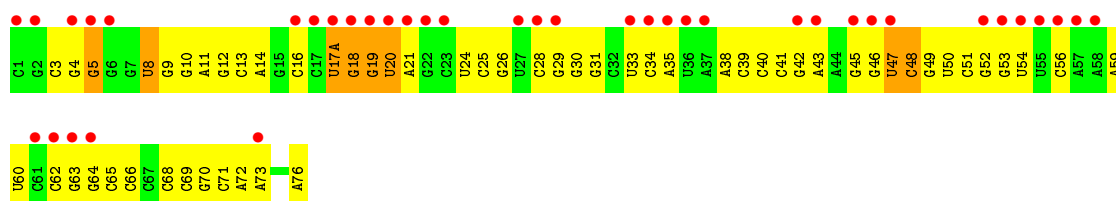
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



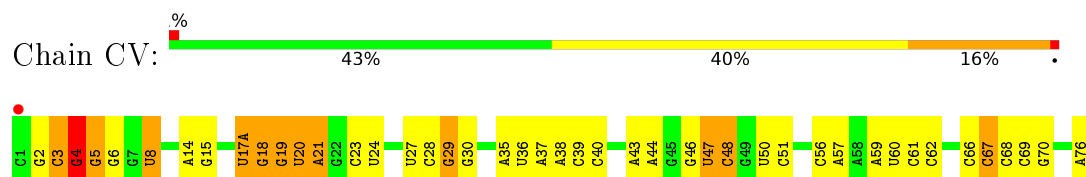
• Molecule 22: RNA (77-MER)



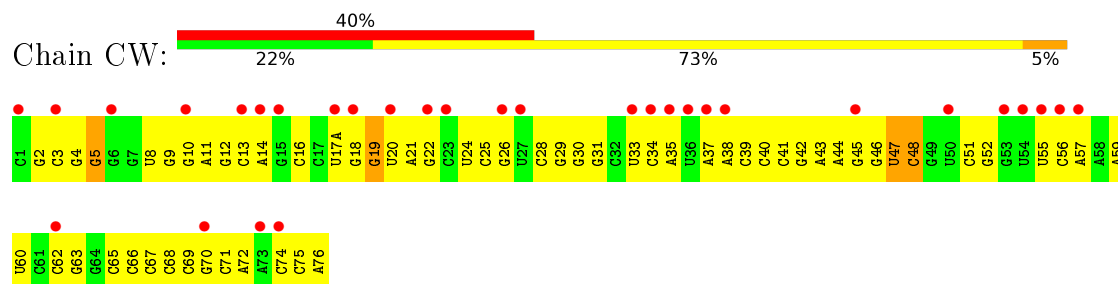
• Molecule 23: RNA (77-MER)



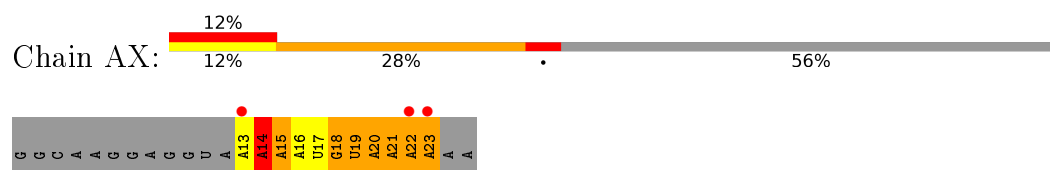
- Molecule 23: RNA (77-MER)



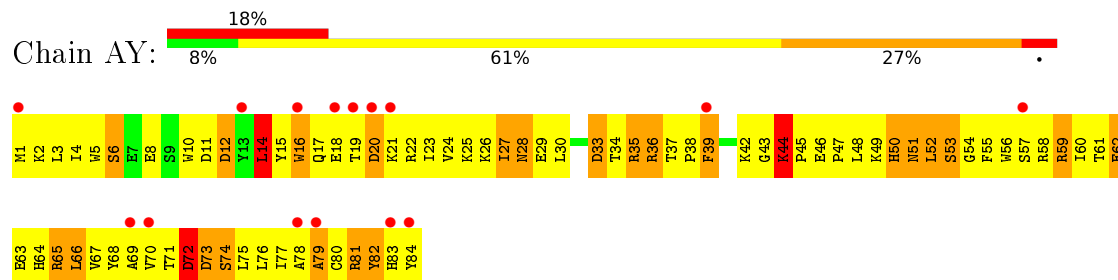
- Molecule 23: RNA (77-MER)



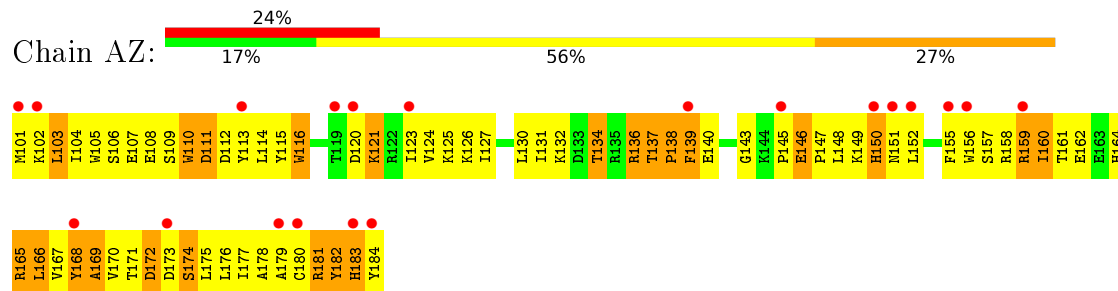
- Molecule 24: 5'-R(\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*AP\*GP\*GP\*UP\*AP\*AP\*AP\*AP\*AP\*UP\*G U2M A2M A2MP\*AP\*AP\*AP\*A)-3'



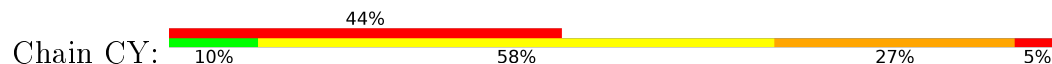
- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

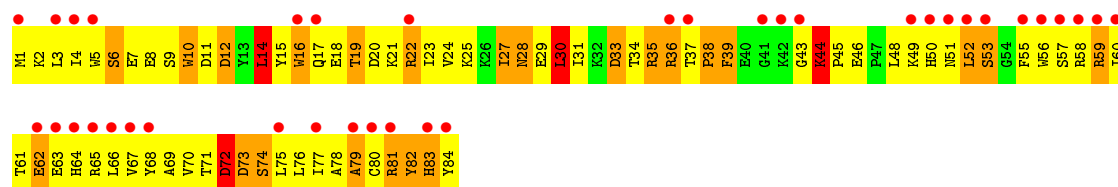


- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

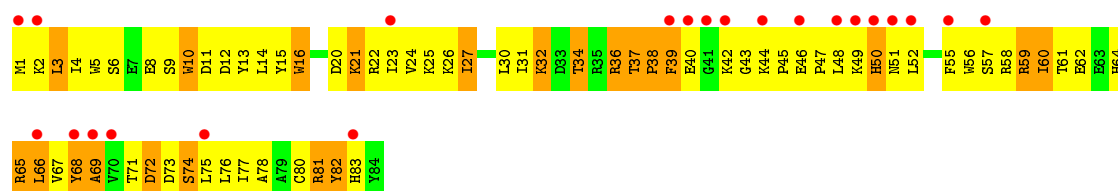


- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

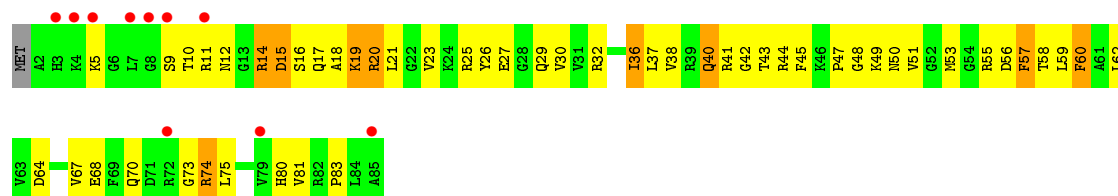




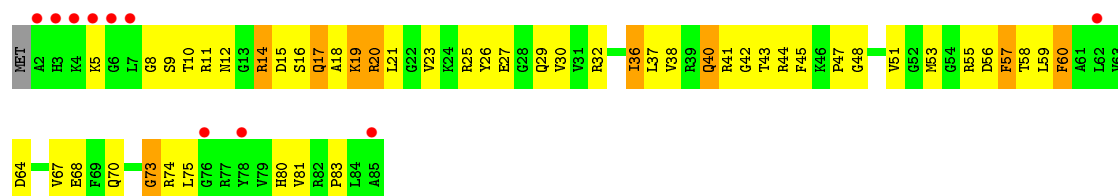
● Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM



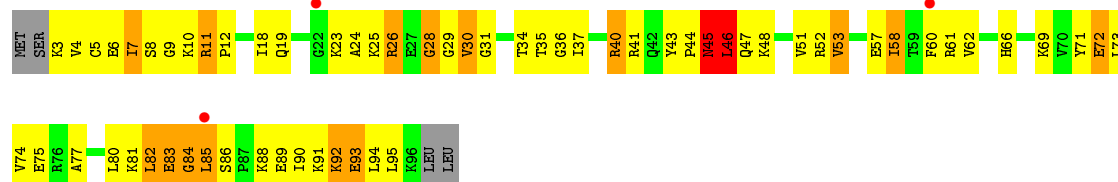
● Molecule 26: 50S RIBOSOMAL PROTEIN L27



● Molecule 26: 50S RIBOSOMAL PROTEIN L27

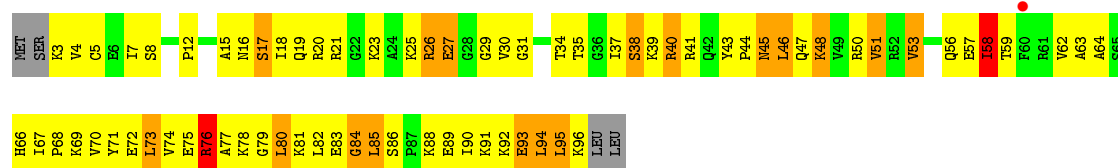


● Molecule 27: 50S RIBOSOMAL PROTEIN L28

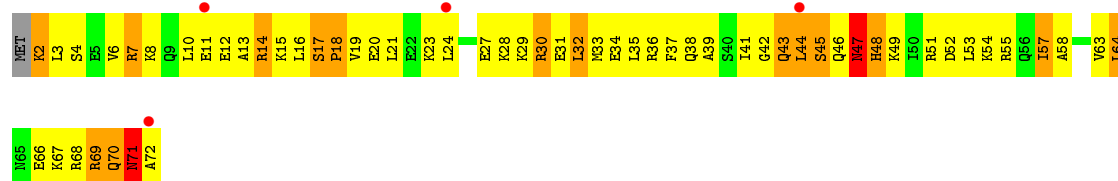


● Molecule 27: 50S RIBOSOMAL PROTEIN L28





• Molecule 28: 50S RIBOSOMAL PROTEIN L29



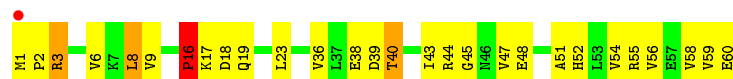
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



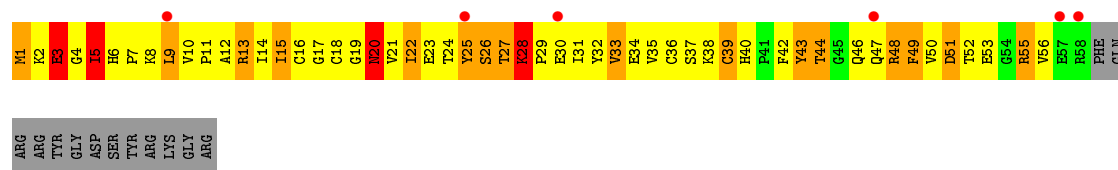
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



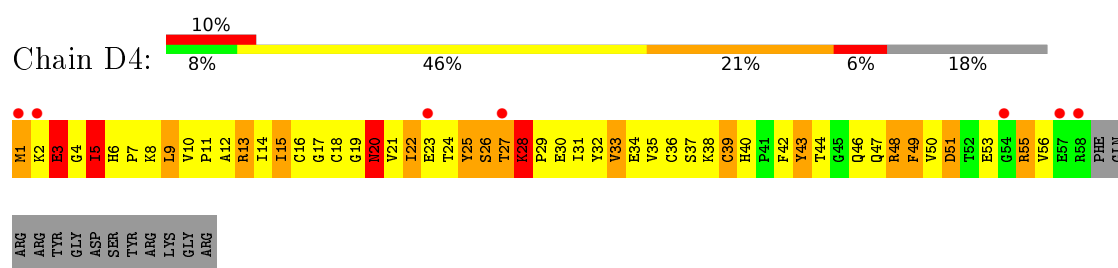
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



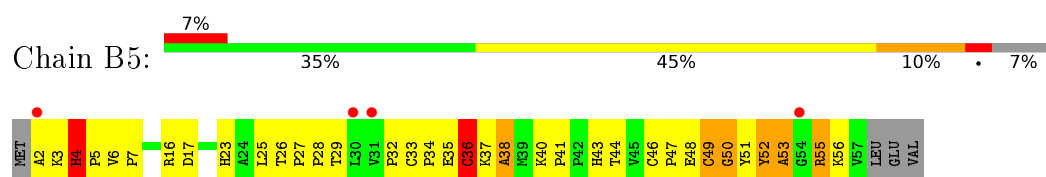
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



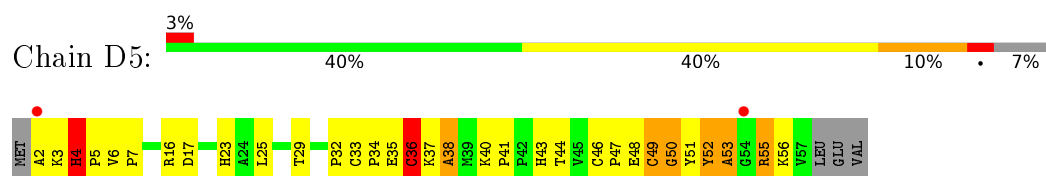
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



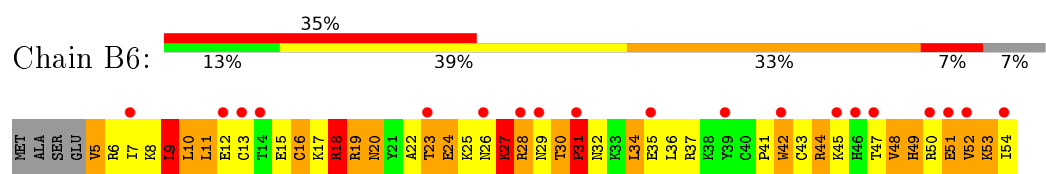
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



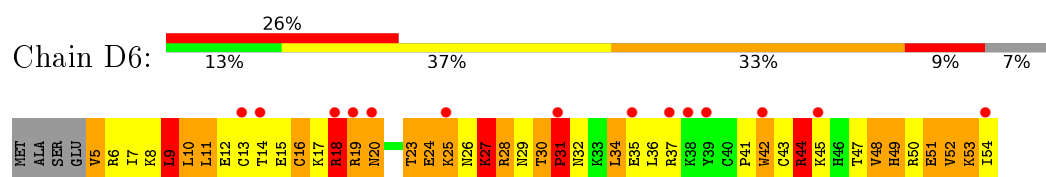
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



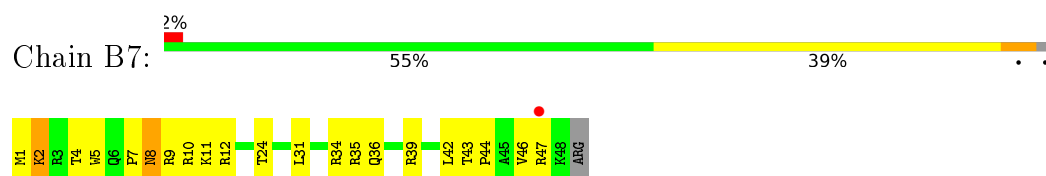
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



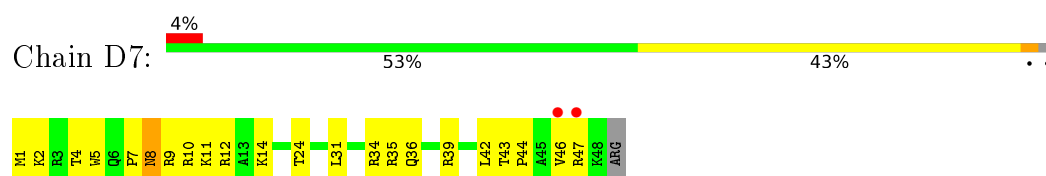
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



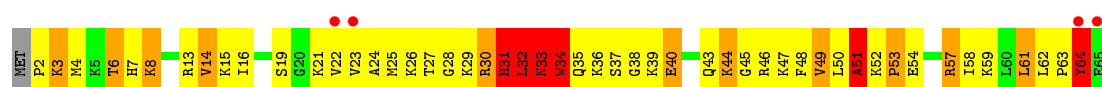
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



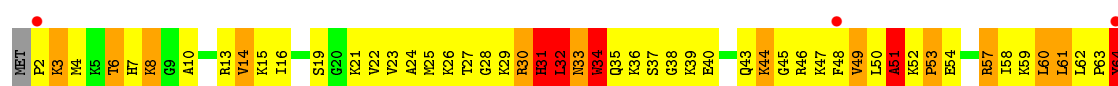
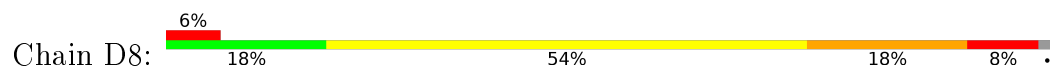
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



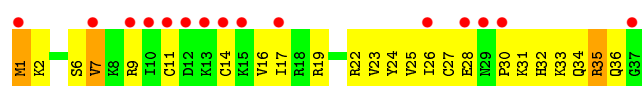
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



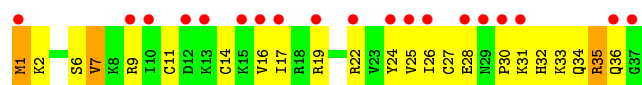
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



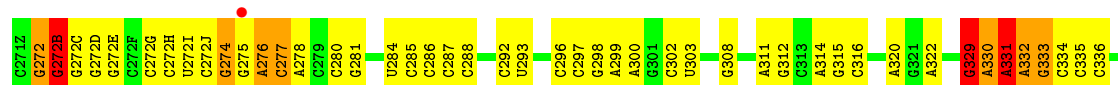
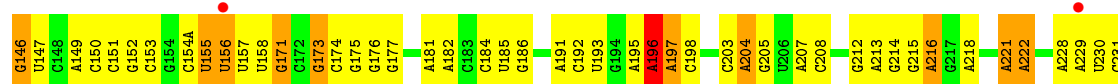
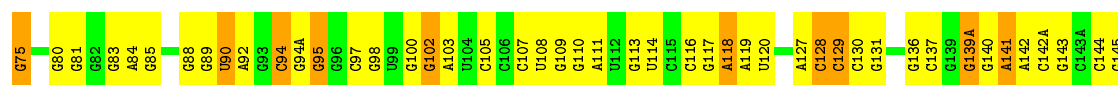
• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 36: RNA (2848-MER)

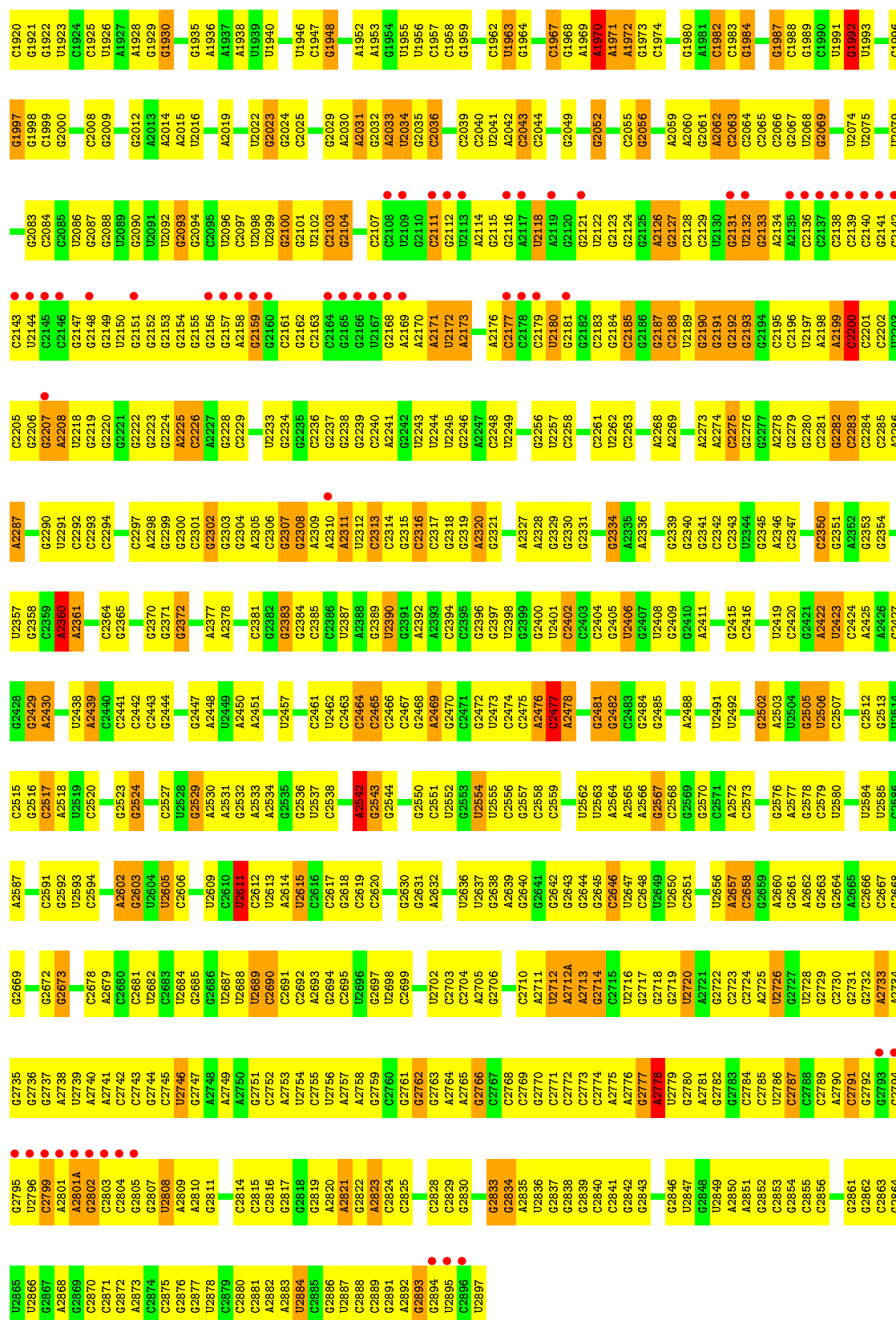




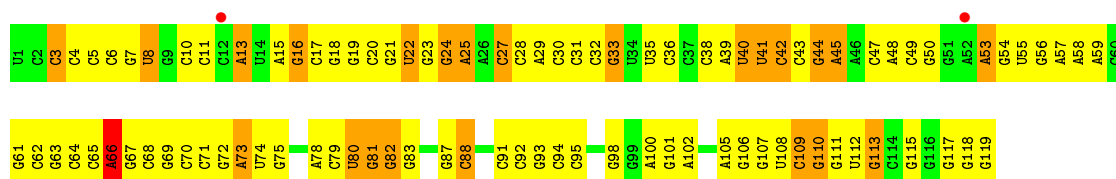
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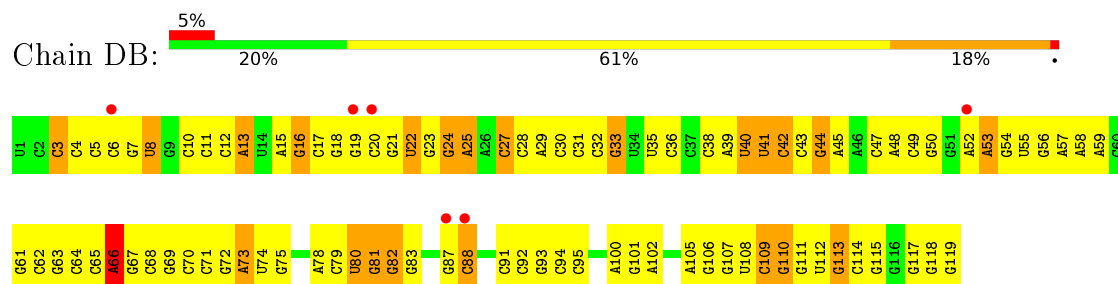
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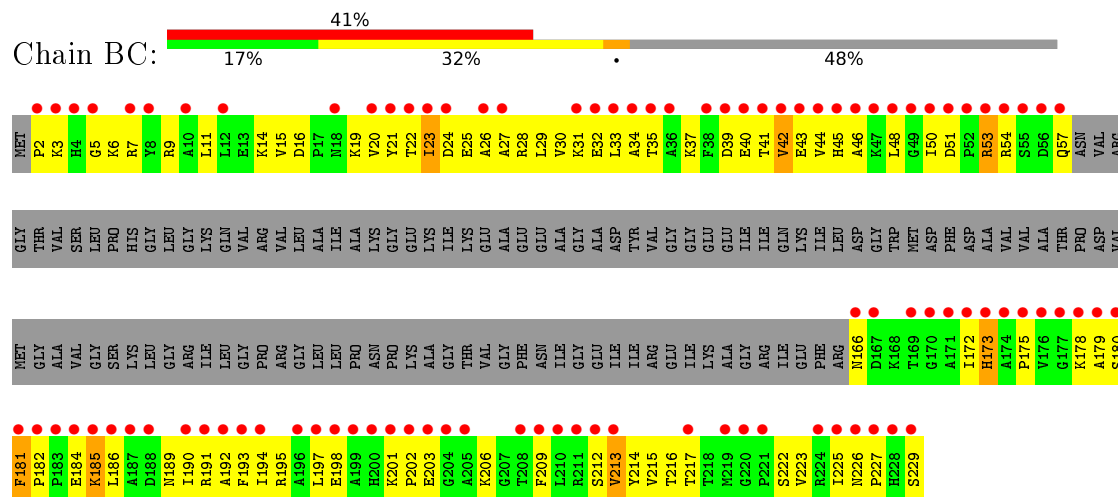
• Molecule 37: RNA (119-MER)



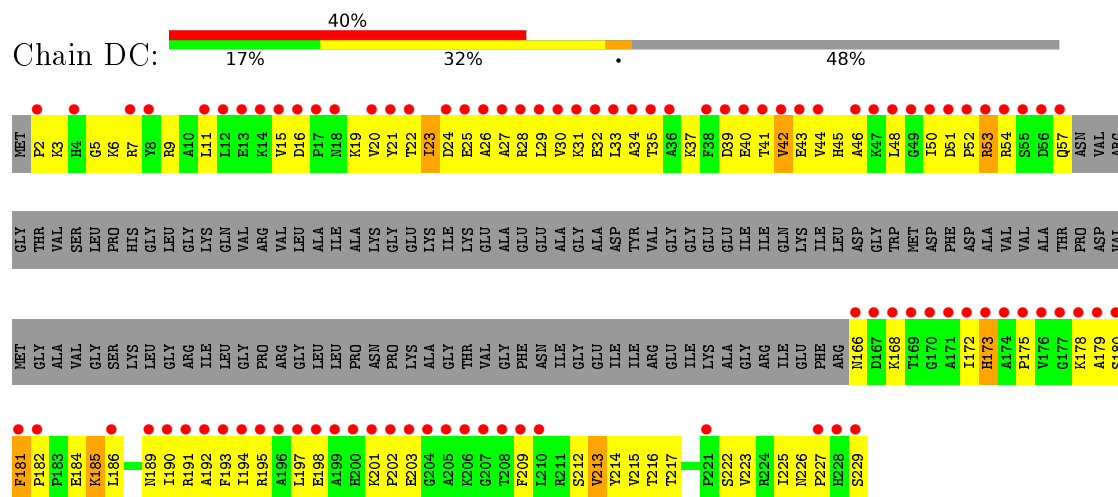
• Molecule 37: RNA (119-MER)



• Molecule 38: 50S RIBOSOMAL PROTEIN L1



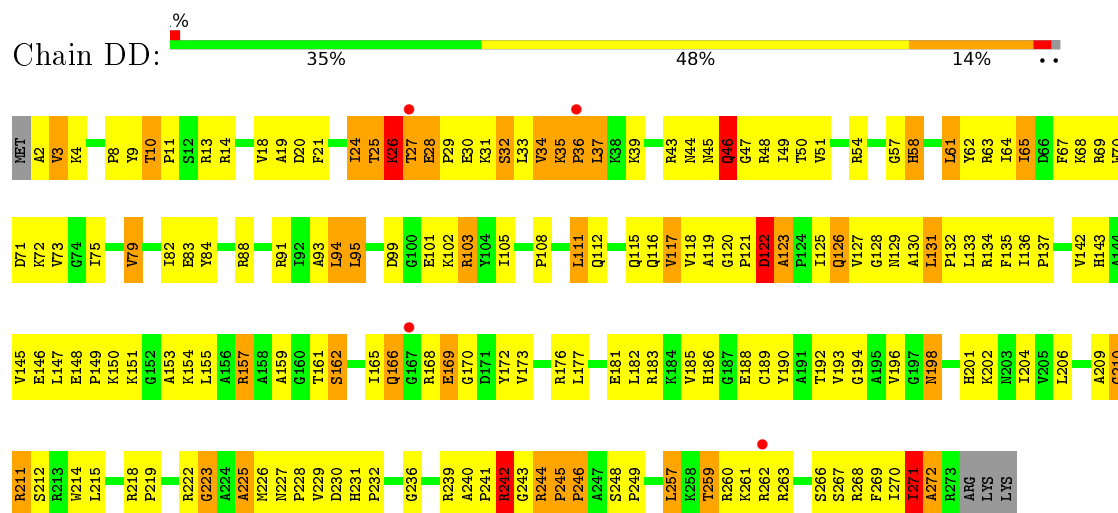
• Molecule 38: 50S RIBOSOMAL PROTEIN L1



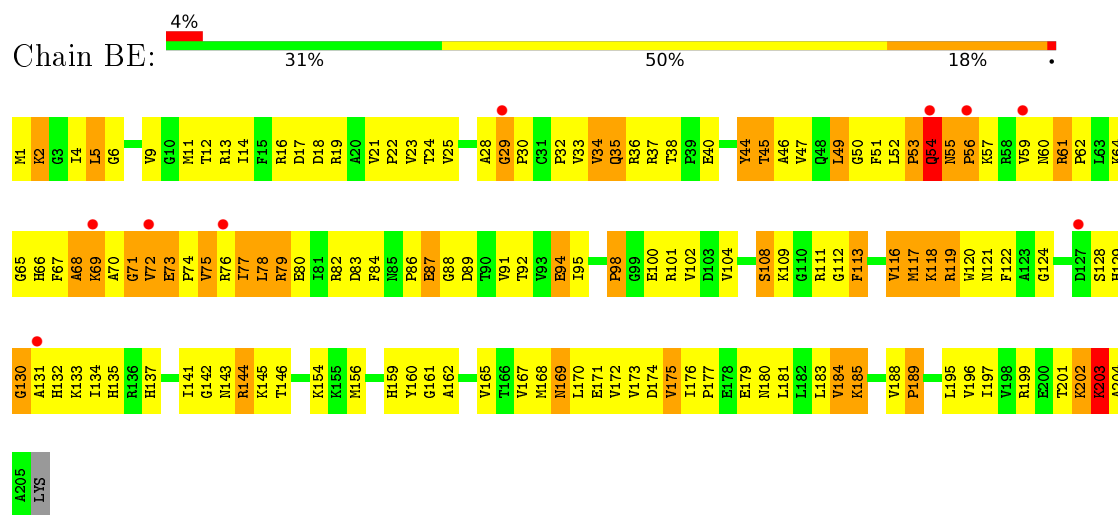
• Molecule 39: 50S RIBOSOMAL PROTEIN L2



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

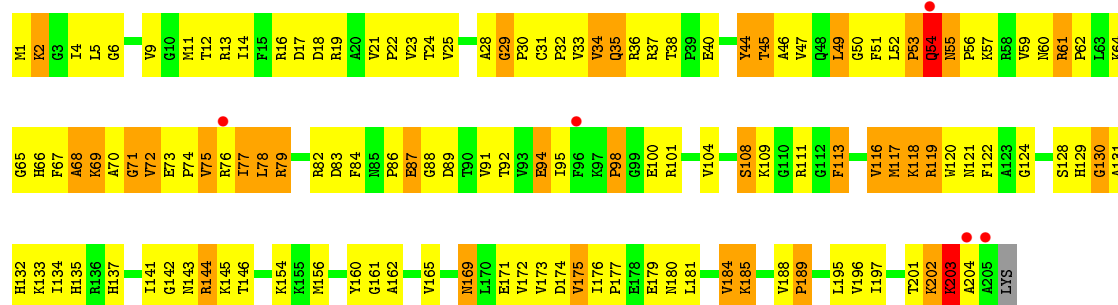


• Molecule 40: 50S RIBOSOMAL PROTEIN L3



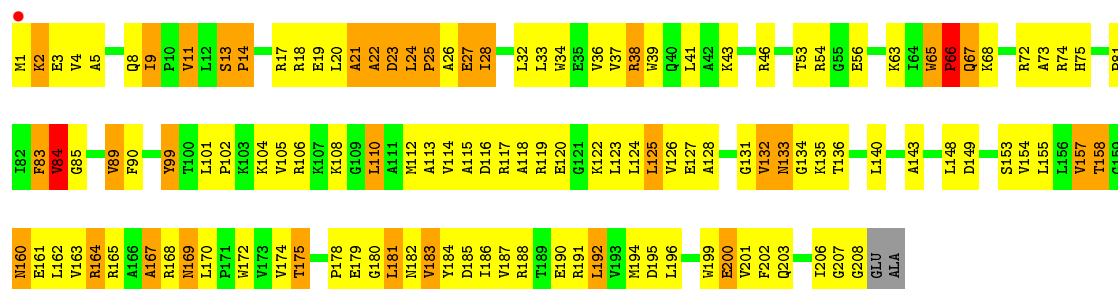
• Molecule 40: 50S RIBOSOMAL PROTEIN L3





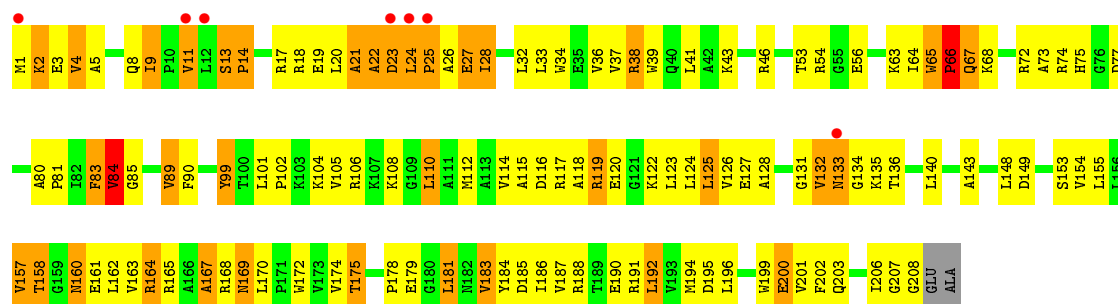
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF: 39% 44% 16% ..



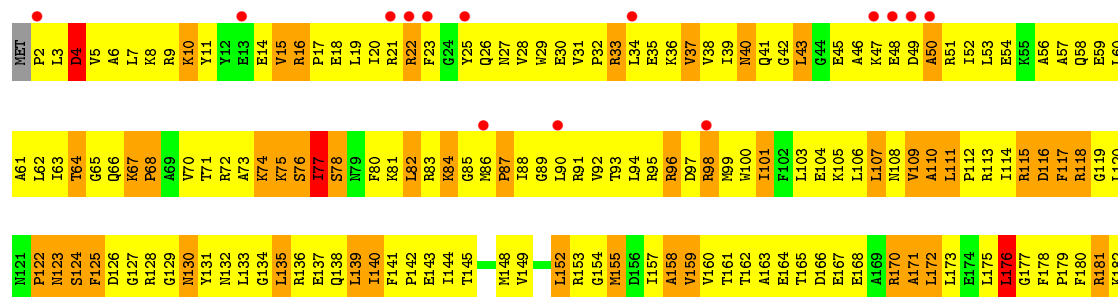
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain DF: 3% 39% 43% 17% ..

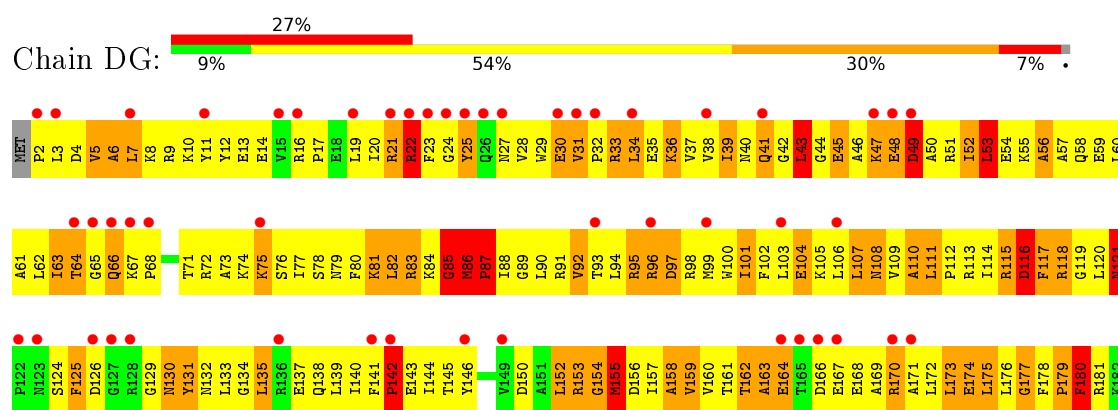


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

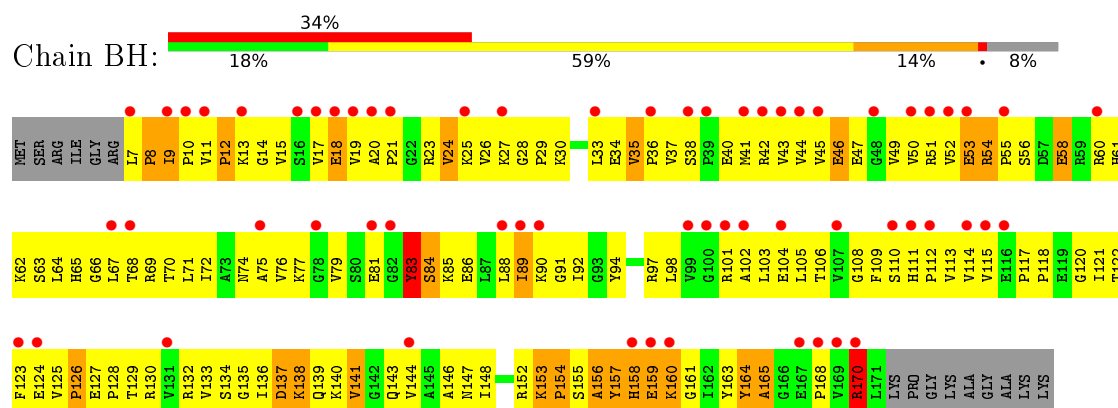
Chain BG: 8% 9% 64% 25% ..



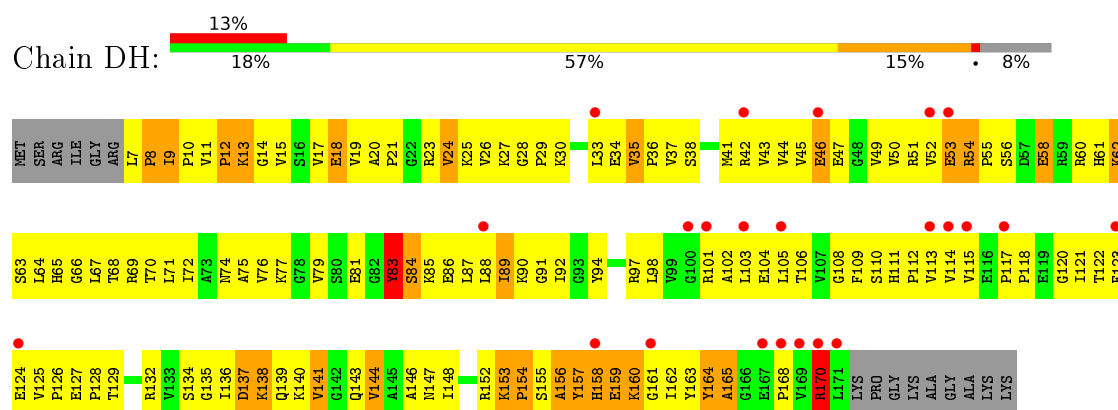
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



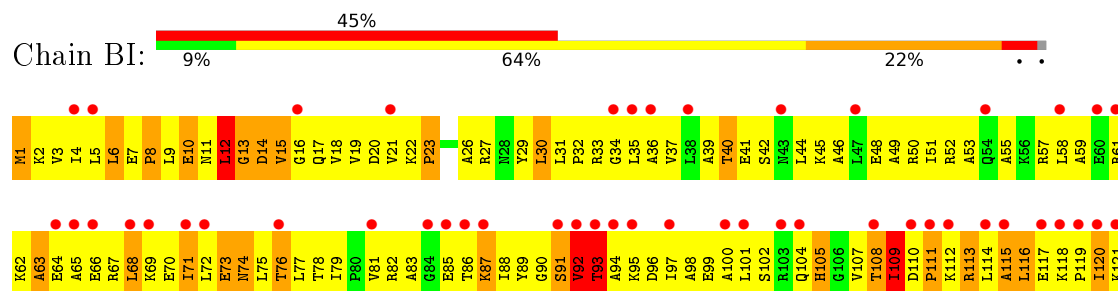
## • Molecule 43: 50S RIBOSOMAL PROTEIN L6

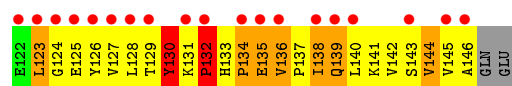


## • Molecule 43: 50S RIBOSOMAL PROTEIN L6

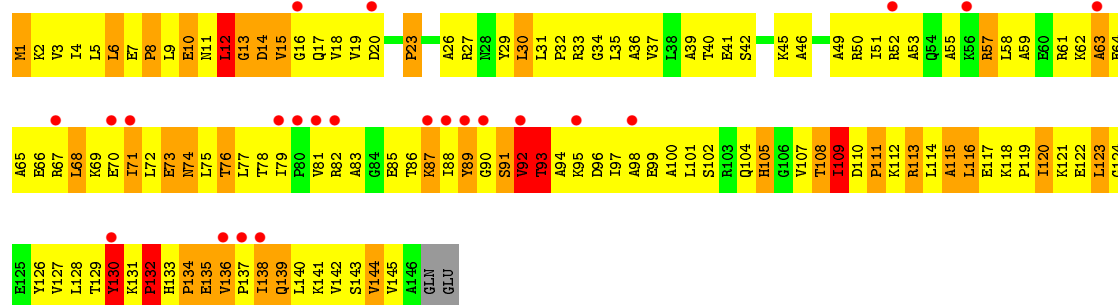
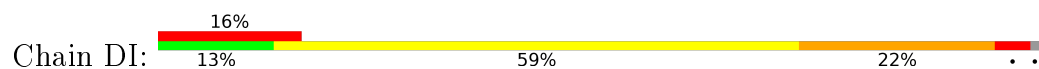


## • Molecule 44: 50S RIBOSOMAL PROTEIN L9

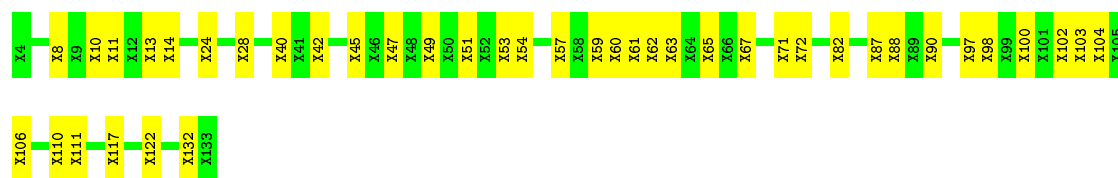




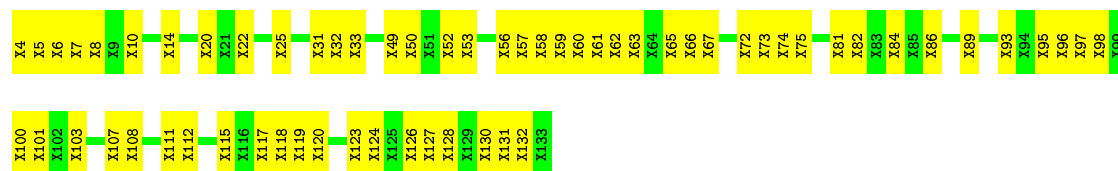
• Molecule 44: 50S RIBOSOMAL PROTEIN L9



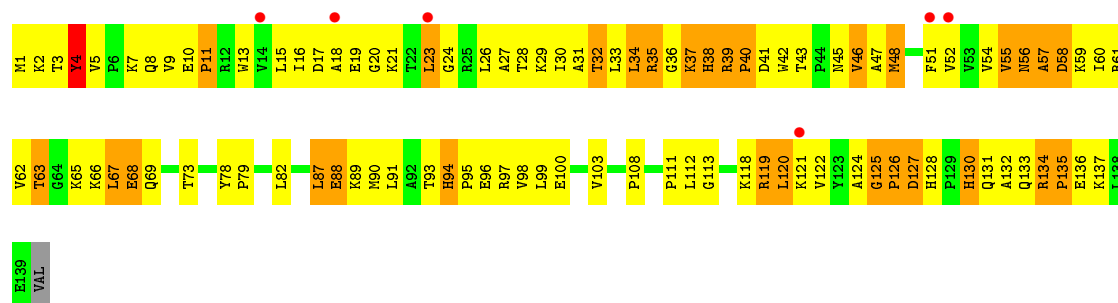
• Molecule 45: 50S RIBOSOMAL PROTEIN L10



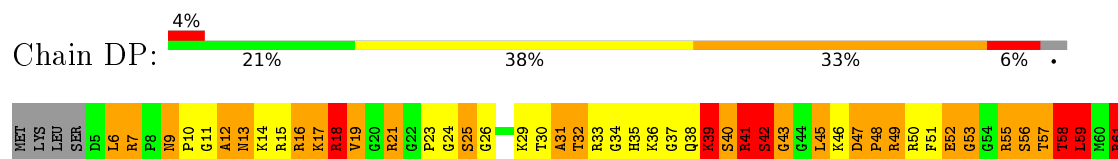
• Molecule 45: 50S RIBOSOMAL PROTEIN L10

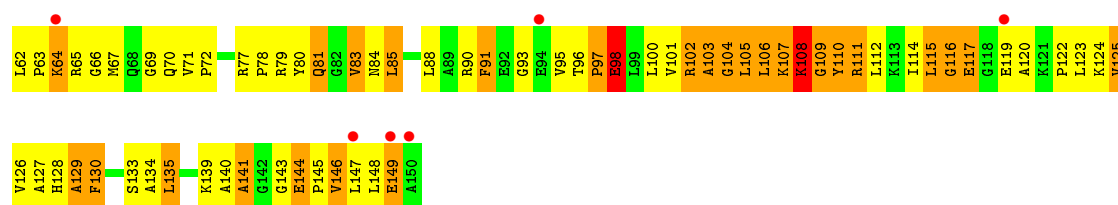


• Molecule 46: 50S RIBOSOMAL PROTEIN L13

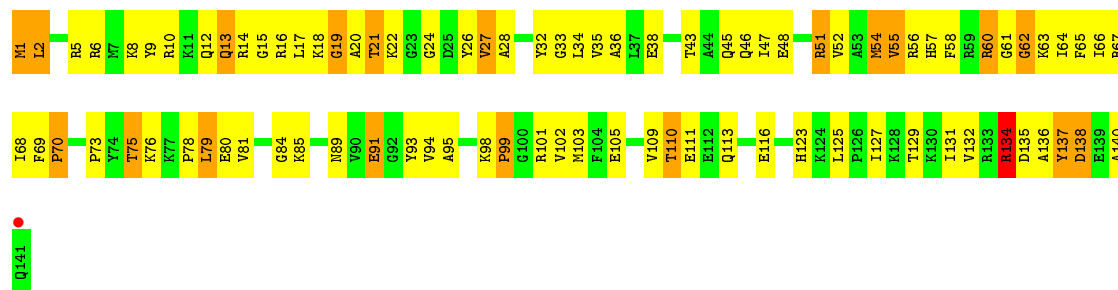


• Molecule 46: 50S RIBOSOMAL PROTEIN L13

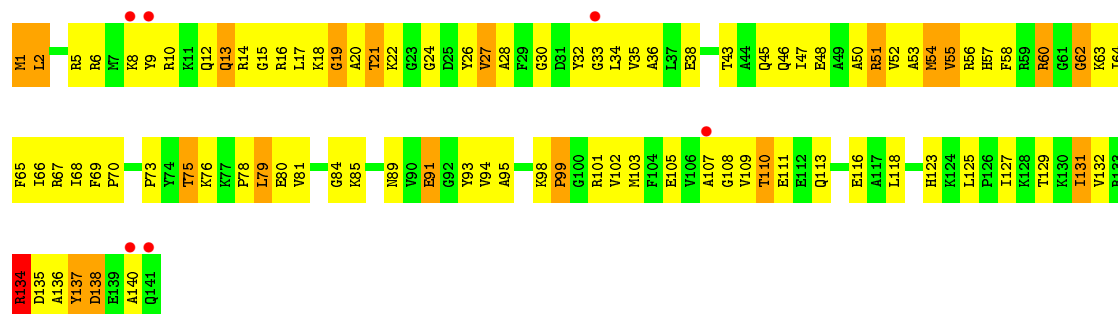




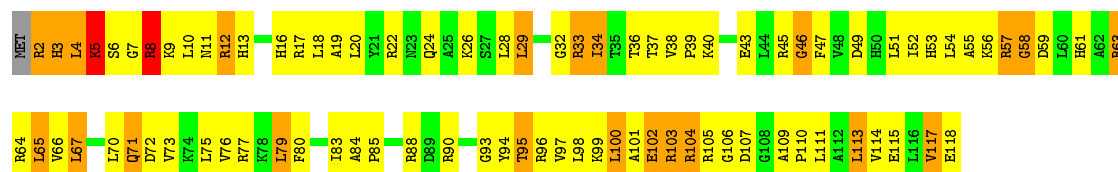
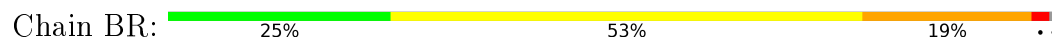
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



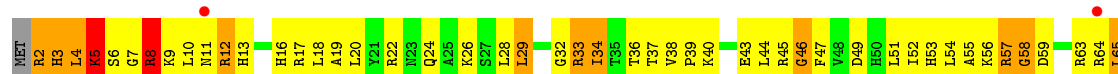
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

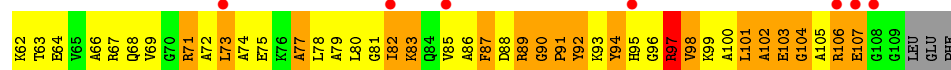
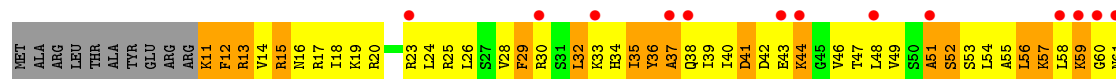


• Molecule 50: 50S RIBOSOMAL PROTEIN L17

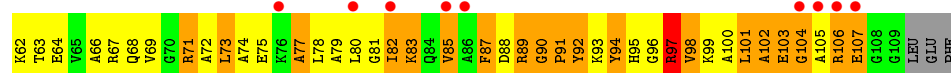
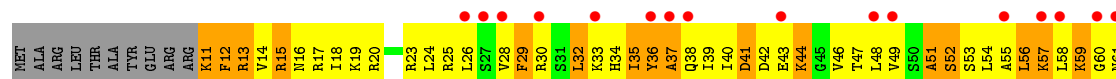




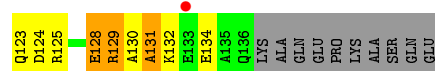
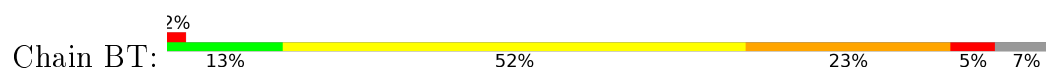
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



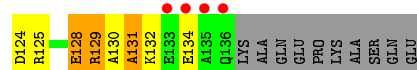
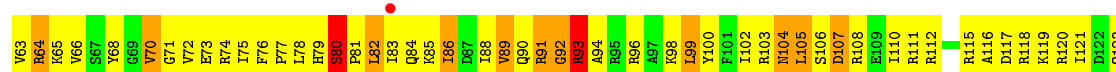
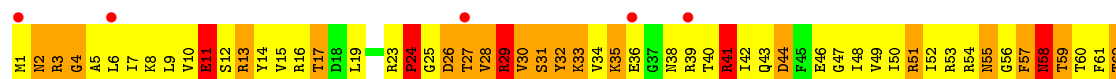
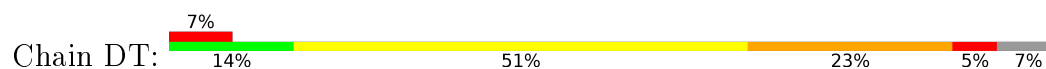
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



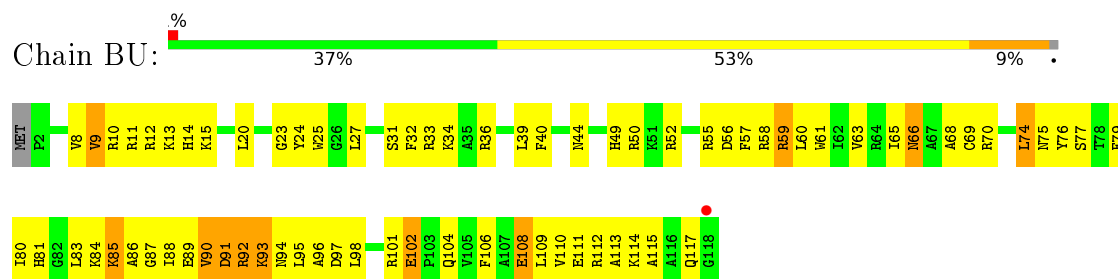
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



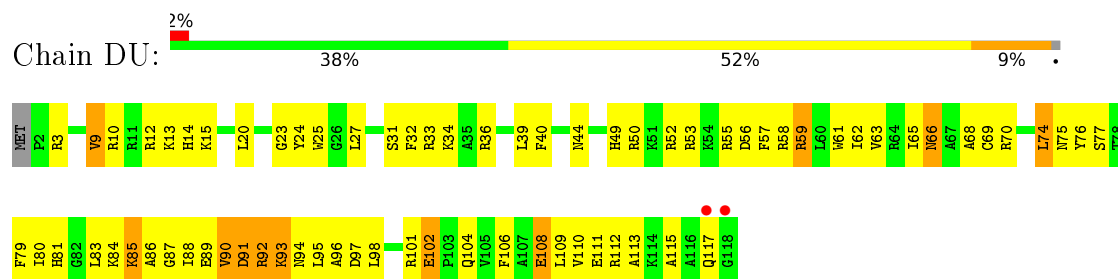
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



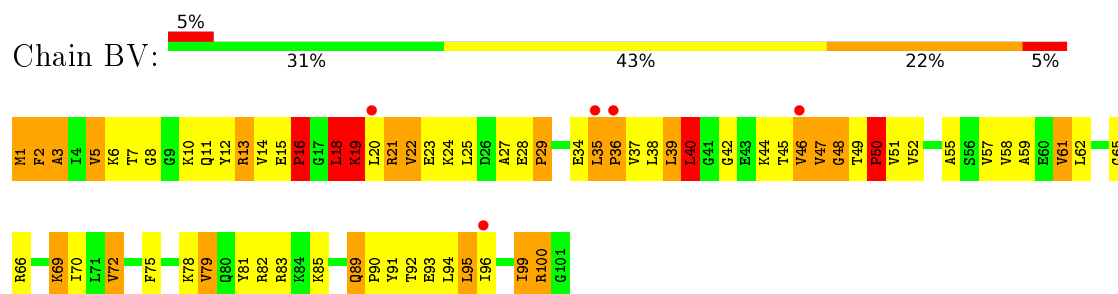
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



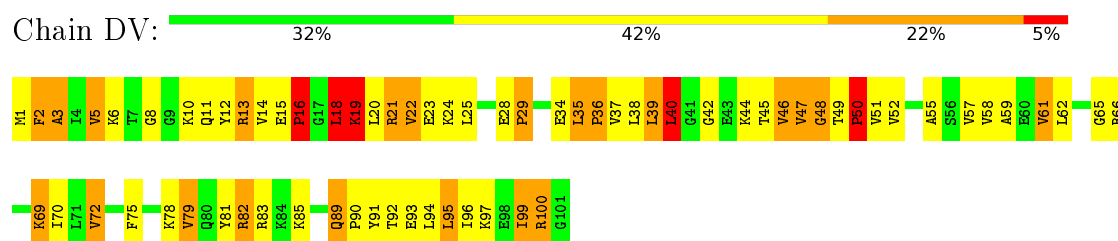
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



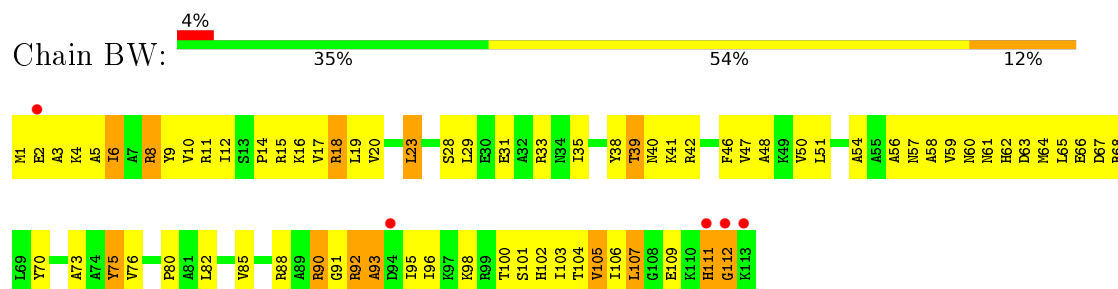
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



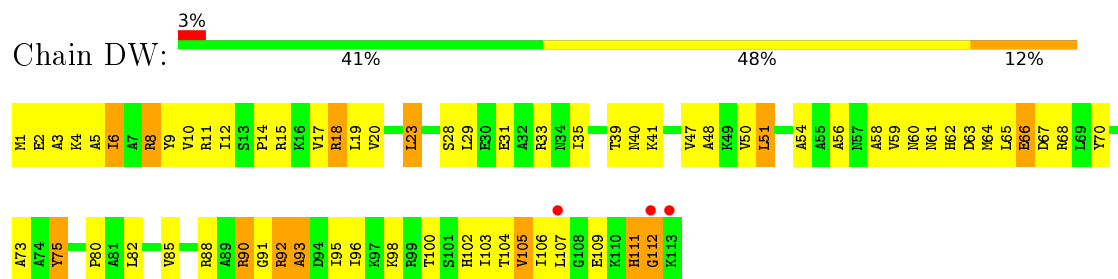
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



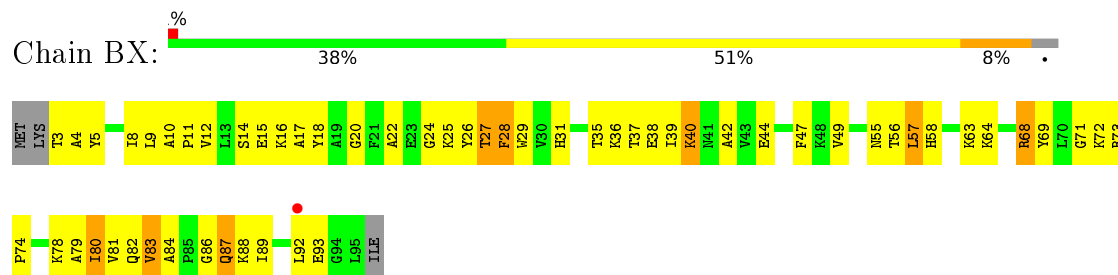
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



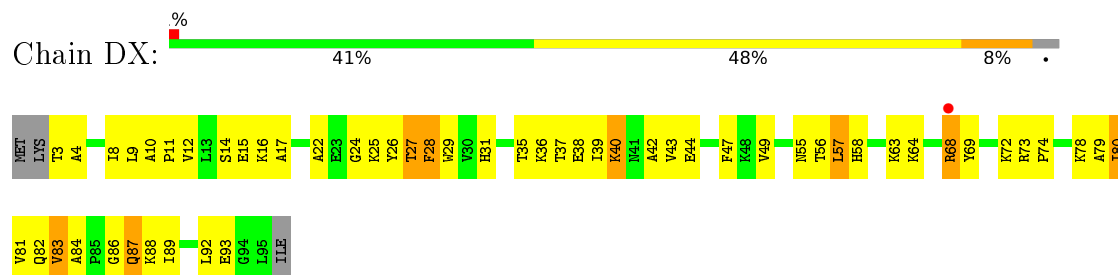
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



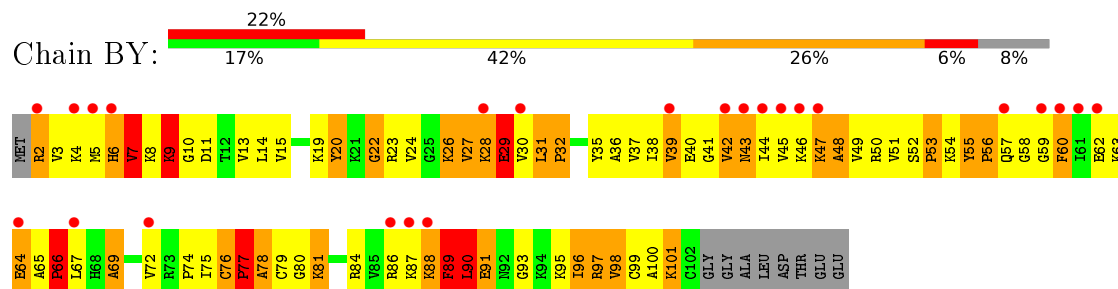
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



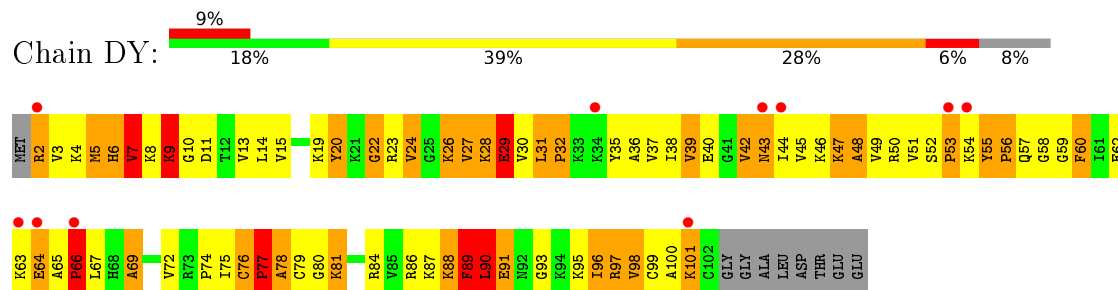
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



- Molecule 57: 50S RIBOSOMAL PROTEIN L24



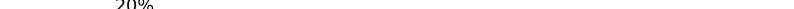
- Molecule 57: 50S RIBOSOMAL PROTEIN L24



[illegible]

Chain DZ: 

Chain	DZ
A184	I124
E185	L125
E186	V126
A187	K127
ALA	V128
ALA	S129
GLU	P130
VAL	R131
ALA	N132
GLU	I133
PRO	P134
GLU	E135
VAL	F136
ILE	I137
LYS	E138
LYS	V139
LYS	D140
LYS	V141
GLU	S142
GLU	G143
GLU	L144
GLU	E145
GLU	I146
GLU	G147
GLU	D148
GLU	S149
GLU	L150
GLU	H151
GLU	A152
GLU	S153
GLU	D154
GLU	L155
GLU	K156
GLU	L157
GLU	P158
GLU	P159
GLU	G160
GLU	V161
GLU	E162
GLU	L163
GLU	A164
GLU	V165
GLU	S166
GLU	P167
GLU	E168
GLU	E169
GLU	T170
GLU	I171
GLU	A172
GLU	V173
GLU	V174
GLU	V175
GLU	P176
GLU	P177
GLU	E178
GLU	D179
GLU	E180
GLU	E181
GLU	K182
GLU	L183
MET	P62
GLU	D63
GLU	G64
GLU	Y3
R4	G65
L5	S66
K6	L67
A7	P68
Y8	T69
R9	L70
R10	V71
E11	R72
G12	Q73
E13	V74
K14	M75
L15	L76
L16	D77
L17	K78
L18	R79
L19	R80
R20	R81
A21	R82
G22	R83
K23	H85
L24	H86
P25	D87
G26	D88
V27	F89
M28	V90
Y29	L91
N30	S92
R31	D93
H32	E94
L33	N95
N34	V96
R35	E97
K36	M98
V37	Y99
Y38	V100
V39	P101
D40	L102
L41	R103
V42	F104
E43	V105
F44	G106
D45	T107
K46	P108
V47	A109
F48	G110
R49	V111
Q50	R112
A51	A113
S52	G114
I53	G115
H54	V116
H55	E119
V56	I120
I57	H121
S58	L122
L59	D123
E60	L124
L61	L125

Chain CX: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.59Å 455.43Å 616.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.35 49.79 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.79-3.35) 99.7 (49.79-3.35)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.223 , 0.261 0.224 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	96.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 95.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	298206	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MG, OMU, A2M

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	0.43	1/36190 (0.0%)	0.69	13/56486 (0.0%)
1	CA	0.41	1/36190 (0.0%)	0.70	15/56486 (0.0%)
2	AB	0.33	0/1936	0.62	0/2611
2	CB	0.33	0/1936	0.61	0/2611
3	AC	0.33	0/1637	0.59	0/2207
3	CC	0.33	0/1637	0.59	0/2207
4	AD	0.38	0/1733	0.67	1/2318 (0.0%)
4	CD	0.35	0/1733	0.64	0/2318
5	AE	0.38	0/1163	0.67	0/1566
5	CE	0.37	0/1163	0.65	0/1566
6	AF	0.34	0/856	0.64	0/1154
6	CF	0.35	0/856	0.64	0/1154
7	AG	0.32	0/1276	0.55	0/1709
7	CG	0.30	0/1276	0.55	0/1709
8	AH	0.35	0/1136	0.69	0/1527
8	CH	0.33	0/1136	0.68	0/1527
9	AI	0.33	0/1027	0.60	0/1373
9	CI	0.32	0/1027	0.61	0/1373
10	AJ	0.35	0/808	0.62	0/1087
10	CJ	0.33	0/808	0.61	0/1087
11	AK	0.33	0/900	0.61	0/1213
11	CK	0.35	0/900	0.61	0/1213
12	AL	0.42	0/987	0.75	0/1322
12	CL	0.43	0/987	0.74	1/1322 (0.1%)
13	AM	0.33	0/943	0.84	3/1256 (0.2%)
13	CM	0.33	0/943	0.85	3/1256 (0.2%)
14	AN	0.36	0/501	0.94	3/664 (0.5%)
14	CN	0.37	0/501	0.92	3/664 (0.5%)
15	AO	0.36	0/745	0.61	0/992
15	CO	0.38	0/745	0.61	0/992
16	AP	0.39	0/717	0.63	0/965
16	CP	0.36	0/717	0.61	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.39	0/837	0.66	0/1119
17	CQ	0.37	0/837	0.65	0/1119
18	AR	0.37	0/579	1.06	3/768 (0.4%)
18	CR	0.36	0/579	0.97	3/768 (0.4%)
19	AS	0.43	0/643	0.92	3/867 (0.3%)
19	CS	0.51	0/643	0.98	3/867 (0.3%)
20	AT	0.35	0/765	0.61	0/1007
20	CT	0.32	0/765	0.60	0/1007
21	AU	0.46	0/213	0.61	0/279
21	CU	0.48	0/213	0.61	0/279
22	AV	0.49	0/1810	0.70	0/2821
23	AW	0.39	0/1832	0.69	0/2855
23	CV	0.44	0/1832	0.72	1/2855 (0.0%)
23	CW	0.37	0/1832	0.69	0/2855
24	AX	0.41	0/194	0.65	0/301
25	AY	0.41	0/742	0.63	1/1002 (0.1%)
25	AZ	0.40	0/743	0.63	0/1002
25	CY	0.48	0/742	0.69	2/1002 (0.2%)
25	CZ	0.47	0/743	0.64	0/1002
26	B0	0.39	0/671	0.68	0/892
26	D0	0.39	0/671	0.69	0/892
27	B1	0.43	0/739	0.81	1/983 (0.1%)
27	D1	0.47	0/739	0.78	0/983
28	B2	0.38	0/600	0.68	0/793
28	D2	0.47	0/600	0.76	1/793 (0.1%)
29	B3	0.38	0/473	0.65	0/636
29	D3	0.40	0/473	0.66	0/636
30	B4	0.39	0/461	0.70	0/623
30	D4	0.40	0/461	0.69	0/623
31	B5	0.51	0/442	0.86	0/598
31	D5	0.54	0/442	0.85	0/598
32	B6	0.46	0/440	0.83	0/586
32	D6	0.51	0/440	0.85	0/586
33	B7	0.48	0/418	0.68	0/552
33	D7	0.54	0/418	0.69	0/552
34	B8	0.57	0/516	0.97	4/681 (0.6%)
34	D8	0.56	0/516	0.97	5/681 (0.7%)
35	B9	0.36	0/310	0.61	0/407
35	D9	0.36	0/310	0.62	0/407
36	BA	0.53	5/68704 (0.0%)	0.74	50/107260 (0.0%)
36	DA	0.56	3/68704 (0.0%)	0.75	57/107260 (0.1%)
37	BB	0.39	0/2853	0.69	0/4451
37	DB	0.41	0/2853	0.70	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	BC	0.31	0/956	0.55	0/1288
38	DC	0.31	0/956	0.55	0/1288
39	BD	0.47	0/2155	0.82	2/2907 (0.1%)
39	DD	0.51	0/2155	0.83	3/2907 (0.1%)
40	BE	0.46	0/1597	0.78	1/2155 (0.0%)
40	DE	0.47	0/1597	0.78	1/2155 (0.0%)
41	BF	0.46	0/1659	0.76	1/2246 (0.0%)
41	DF	0.48	0/1659	0.76	1/2246 (0.0%)
42	BG	0.36	0/1498	0.66	0/2013
42	DG	0.42	0/1498	0.79	1/2013 (0.0%)
43	BH	0.38	0/1285	0.71	0/1741
43	DH	0.40	0/1285	0.72	0/1741
44	BI	0.37	0/1147	0.87	3/1553 (0.2%)
44	DI	0.39	0/1147	0.88	3/1553 (0.2%)
46	BN	0.42	0/1132	0.74	1/1527 (0.1%)
46	DN	0.43	0/1132	0.75	1/1527 (0.1%)
47	BO	0.45	0/943	0.69	0/1269
47	DO	0.41	0/943	0.67	0/1269
48	BP	0.53	0/1131	1.06	6/1504 (0.4%)
48	DP	0.55	0/1131	1.08	7/1504 (0.5%)
49	BQ	0.44	0/1134	0.68	0/1517
49	DQ	0.42	0/1134	0.68	0/1517
50	BR	0.42	0/974	0.77	2/1302 (0.2%)
50	DR	0.44	0/974	0.79	2/1302 (0.2%)
51	BS	0.40	0/779	0.69	0/1038
51	DS	0.41	0/779	0.69	0/1038
52	BT	0.48	0/1138	0.83	3/1521 (0.2%)
52	DT	0.45	0/1138	0.81	3/1521 (0.2%)
53	BU	0.44	0/975	0.75	0/1297
53	DU	0.47	0/975	0.75	0/1297
54	BV	0.42	0/790	0.73	0/1057
54	DV	0.46	0/790	0.75	0/1057
55	BW	0.44	0/907	0.72	0/1216
55	DW	0.46	0/907	0.74	0/1216
56	BX	0.44	0/740	0.69	0/995
56	DX	0.47	0/740	0.71	0/995
57	BY	0.51	0/789	0.79	1/1053 (0.1%)
57	DY	0.55	0/789	0.80	1/1053 (0.1%)
58	BZ	0.38	0/1500	0.71	0/2037
58	DZ	0.40	0/1500	0.74	1/2037 (0.0%)
59	CX	0.44	0/169	0.70	0/262
All	All	0.48	10/321535 (0.0%)	0.73	220/480333 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	15
1	CA	0	13
22	AV	0	1
23	CV	0	2
24	AX	0	1
36	BA	7	51
36	DA	7	58
37	BB	0	2
37	DB	0	2
59	CX	0	1
All	All	15	146

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BA	975(A)	G	O3'-P	-12.04	1.46	1.61
1	AA	413	G	O3'-P	-8.20	1.51	1.61
1	CA	413	G	O3'-P	-7.59	1.52	1.61
36	BA	783	A	C5-C6	-5.78	1.35	1.41
36	BA	2506	U	N1-C2	5.66	1.43	1.38

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AR	64	ARG	NE-CZ-NH2	-15.72	112.44	120.30
19	CS	81	ARG	NE-CZ-NH1	15.12	127.86	120.30
18	AR	64	ARG	NE-CZ-NH1	14.85	127.73	120.30
13	CM	29	ARG	NE-CZ-NH2	-13.53	113.53	120.30
13	CM	29	ARG	NE-CZ-NH1	13.37	126.99	120.30

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	115	G	C3'
36	BA	49	A	C3'
36	BA	331	A	C3'
36	BA	752	A	C3'
36	BA	1799	G	C3'

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	13	U	Sidechain
1	AA	254	G	Sidechain
1	AA	318	G	Sidechain
1	AA	436	C	Sidechain
1	AA	575	G	Sidechain

## 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	16317	1250	0
1	CA	32329	0	16317	1322	1
2	AB	1901	0	1951	294	0
2	CB	1901	0	1951	300	0
3	AC	1613	0	1677	234	0
3	CC	1613	0	1677	234	0
4	AD	1703	0	1766	193	0
4	CD	1703	0	1764	192	0
5	AE	1147	0	1207	140	0
5	CE	1147	0	1207	133	0
6	AF	843	0	857	109	0
6	CF	843	0	857	111	0
7	AG	1257	0	1296	134	0
7	CG	1257	0	1296	136	0
8	AH	1116	0	1177	129	0
8	CH	1116	0	1177	125	0
9	AI	1010	0	1035	149	0
9	CI	1010	0	1035	152	0
10	AJ	795	0	840	159	0
10	CJ	795	0	840	162	0
11	AK	885	0	904	107	0
11	CK	885	0	904	106	0
12	AL	971	0	1057	109	0
12	CL	971	0	1057	112	0
13	AM	938	0	991	143	0
13	CM	938	0	991	152	0
14	AN	492	0	530	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	531	70	0
15	AO	734	0	771	75	0
15	CO	734	0	771	70	0
16	AP	701	0	720	69	0
16	CP	701	0	720	78	0
17	AQ	824	0	891	75	0
17	CQ	824	0	891	73	0
18	AR	574	0	644	84	0
18	CR	574	0	644	82	0
19	AS	630	0	652	109	0
19	CS	630	0	652	106	0
20	AT	763	0	861	85	0
20	CT	763	0	861	95	0
21	AU	209	0	221	23	0
21	CU	209	0	221	25	0
22	AV	1641	0	839	55	0
23	AW	1640	0	837	57	0
23	CV	1640	0	837	55	0
23	CW	1640	0	837	66	0
24	AX	239	0	127	94	0
25	AY	722	0	713	147	0
25	AZ	723	0	710	110	0
25	CY	722	0	713	149	0
25	CZ	723	0	713	103	0
26	B0	662	0	688	79	0
26	D0	662	0	688	75	0
27	B1	732	0	808	87	0
27	D1	732	0	808	91	0
28	B2	598	0	653	88	0
28	D2	598	0	653	67	0
29	B3	468	0	523	27	0
29	D3	468	0	523	27	0
30	B4	451	0	449	126	0
30	D4	451	0	449	109	0
31	B5	428	0	445	65	0
31	D5	428	0	445	65	0
32	B6	433	0	461	109	0
32	D6	433	0	461	110	0
33	B7	410	0	454	29	0
33	D7	410	0	454	27	0
34	B8	508	0	576	119	0
34	D8	508	0	576	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B9	307	0	338	34	0
35	D9	307	0	338	31	0
36	BA	61341	0	30927	1970	0
36	DA	61341	0	30928	1950	0
37	BB	2551	0	1295	125	0
37	DB	2551	0	1295	119	0
38	BC	937	0	957	96	0
38	DC	937	0	957	101	0
39	BD	2105	0	2182	253	0
39	DD	2105	0	2182	266	0
40	BE	1564	0	1629	215	0
40	DE	1564	0	1629	213	0
41	BF	1624	0	1677	185	0
41	DF	1624	0	1677	168	0
42	BG	1474	0	1534	329	0
42	DG	1474	0	1534	389	0
43	BH	1260	0	1326	180	0
43	DH	1260	0	1326	175	0
44	BI	1132	0	1218	282	1
44	DI	1132	0	1218	279	0
45	BJ	651	0	177	28	0
45	DJ	651	0	174	64	0
46	BN	1105	0	1180	154	0
46	DN	1105	0	1180	160	0
47	BO	933	0	996	86	0
47	DO	933	0	996	97	0
48	BP	1114	0	1187	297	0
48	DP	1114	0	1187	294	0
49	BQ	1113	0	1171	105	0
49	DQ	1113	0	1171	112	0
50	BR	960	0	1021	139	0
50	DR	960	0	1021	130	0
51	BS	771	0	832	166	0
51	DS	771	0	832	173	0
52	BT	1124	0	1181	226	0
52	DT	1124	0	1181	211	0
53	BU	958	0	1014	125	0
53	DU	958	0	1015	123	0
54	BV	779	0	852	135	0
54	DV	779	0	852	139	0
55	BW	896	0	953	90	0
55	DW	896	0	953	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BX	726	0	778	74	0
56	DX	726	0	778	71	0
57	BY	776	0	870	182	0
57	DY	776	0	870	176	0
58	BZ	1468	0	1492	253	0
58	DZ	1468	0	1492	348	0
59	CX	217	0	116	77	0
60	AA	103	0	0	0	0
60	AL	1	0	0	0	0
60	AV	1	0	0	0	0
60	AX	1	0	0	0	0
60	B0	1	0	0	0	0
60	B1	2	0	0	0	0
60	B5	2	0	0	0	0
60	BA	236	0	0	0	0
60	BB	2	0	0	0	0
60	BF	1	0	0	0	0
60	BP	1	0	0	0	0
60	BX	1	0	0	0	0
60	CA	103	0	0	0	0
60	CG	1	0	0	0	0
60	CL	1	0	0	0	0
60	CV	2	0	0	0	0
60	D1	1	0	0	0	0
60	D5	1	0	0	0	0
60	DA	242	0	0	0	0
60	DB	1	0	0	0	0
60	DF	1	0	0	0	0
60	DR	1	0	0	0	0
60	DX	1	0	0	0	0
61	AD	1	0	0	2	0
61	AN	1	0	0	0	0
61	CD	1	0	0	1	0
61	CN	1	0	0	1	0
All	All	298206	0	202858	19519	1

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 39.

The worst 5 of 19519 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)
24:AX:19:OMU:CM2	25:AY:51:ASN:HD21	1.10	1.58
4:CD:26:CYS:SG	61:CD:301:ZN:ZN	1.01	1.49
1:AA:1493:A:C8	24:AX:20:A2M:HM'3	1.49	1.48
1:AA:1493:A:C8	24:AX:20:A2M:CM'	1.98	1.46
1:AA:1493:A:N7	24:AX:20:A2M:CM'	1.89	1.34

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BI:121:LYS:NZ	1:CA:358:U:OP1[4_555]	2.13	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	128 (55%)	77 (33%)	28 (12%)	0	3
2	CB	233/256 (91%)	129 (55%)	75 (32%)	29 (12%)	0	2
3	AC	205/239 (86%)	123 (60%)	54 (26%)	28 (14%)	0	2
3	CC	205/239 (86%)	125 (61%)	53 (26%)	27 (13%)	0	2
4	AD	206/209 (99%)	138 (67%)	52 (25%)	16 (8%)	1	9
4	CD	206/209 (99%)	139 (68%)	51 (25%)	16 (8%)	1	9
5	AE	149/162 (92%)	106 (71%)	31 (21%)	12 (8%)	1	9
5	CE	149/162 (92%)	107 (72%)	29 (20%)	13 (9%)	1	7
6	AF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	1	12
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	1	12
7	AG	153/156 (98%)	106 (69%)	30 (20%)	17 (11%)	0	4
7	CG	153/156 (98%)	106 (69%)	30 (20%)	17 (11%)	0	4
8	AH	136/138 (99%)	99 (73%)	25 (18%)	12 (9%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	1	6
9	AI	121/128 (94%)	82 (68%)	28 (23%)	11 (9%)	1	6
9	CI	121/128 (94%)	82 (68%)	28 (23%)	11 (9%)	1	6
10	AJ	97/105 (92%)	69 (71%)	21 (22%)	7 (7%)	1	11
10	CJ	97/105 (92%)	72 (74%)	18 (19%)	7 (7%)	1	11
11	AK	117/129 (91%)	84 (72%)	22 (19%)	11 (9%)	1	6
11	CK	117/129 (91%)	84 (72%)	22 (19%)	11 (9%)	1	6
12	AL	123/132 (93%)	87 (71%)	26 (21%)	10 (8%)	1	9
12	CL	123/132 (93%)	88 (72%)	25 (20%)	10 (8%)	1	9
13	AM	107/126 (85%)	71 (66%)	20 (19%)	16 (15%)	0	1
13	CM	107/126 (85%)	71 (66%)	20 (19%)	16 (15%)	0	1
14	AN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	1
14	CN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	1
15	AO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	12
15	CO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	12
16	AP	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	11
16	CP	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	11
17	AQ	98/105 (93%)	74 (76%)	19 (19%)	5 (5%)	2	21
17	CQ	98/105 (93%)	74 (76%)	19 (19%)	5 (5%)	2	21
18	AR	68/88 (77%)	41 (60%)	17 (25%)	10 (15%)	0	1
18	CR	68/88 (77%)	42 (62%)	16 (24%)	10 (15%)	0	1
19	AS	77/93 (83%)	45 (58%)	19 (25%)	13 (17%)	0	1
19	CS	77/93 (83%)	45 (58%)	19 (25%)	13 (17%)	0	1
20	AT	97/106 (92%)	59 (61%)	26 (27%)	12 (12%)	0	2
20	CT	97/106 (92%)	58 (60%)	26 (27%)	13 (13%)	0	2
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	2
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	1
25	AY	82/84 (98%)	53 (65%)	13 (16%)	16 (20%)	0	1
25	AZ	82/84 (98%)	54 (66%)	20 (24%)	8 (10%)	1	5
25	CY	82/84 (98%)	50 (61%)	16 (20%)	16 (20%)	0	1
25	CZ	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	3	22
26	D0	82/85 (96%)	67 (82%)	10 (12%)	5 (6%)	2	16
27	B1	92/98 (94%)	67 (73%)	12 (13%)	13 (14%)	0	2
27	D1	92/98 (94%)	66 (72%)	14 (15%)	12 (13%)	0	2
28	B2	69/72 (96%)	44 (64%)	14 (20%)	11 (16%)	0	1
28	D2	69/72 (96%)	45 (65%)	16 (23%)	8 (12%)	0	3
29	B3	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	5	33
29	D3	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	5	33
30	B4	56/71 (79%)	17 (30%)	24 (43%)	15 (27%)	0	0
30	D4	56/71 (79%)	17 (30%)	24 (43%)	15 (27%)	0	0
31	B5	54/60 (90%)	39 (72%)	8 (15%)	7 (13%)	0	2
31	D5	54/60 (90%)	39 (72%)	8 (15%)	7 (13%)	0	2
32	B6	48/54 (89%)	25 (52%)	7 (15%)	16 (33%)	0	0
32	D6	48/54 (89%)	26 (54%)	7 (15%)	15 (31%)	0	0
33	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	8	43
33	D7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
34	B8	62/65 (95%)	36 (58%)	16 (26%)	10 (16%)	0	1
34	D8	62/65 (95%)	36 (58%)	16 (26%)	10 (16%)	0	1
35	B9	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1	8
35	D9	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1	8
38	BC	116/229 (51%)	84 (72%)	26 (22%)	6 (5%)	2	20
38	DC	116/229 (51%)	85 (73%)	25 (22%)	6 (5%)	2	20
39	BD	270/276 (98%)	205 (76%)	37 (14%)	28 (10%)	1	4
39	DD	270/276 (98%)	202 (75%)	41 (15%)	27 (10%)	1	5
40	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	3
40	DE	203/206 (98%)	145 (71%)	35 (17%)	23 (11%)	0	3
41	BF	206/210 (98%)	155 (75%)	29 (14%)	22 (11%)	0	4
41	DF	206/210 (98%)	157 (76%)	26 (13%)	23 (11%)	0	3
42	BG	177/182 (97%)	105 (59%)	33 (19%)	39 (22%)	0	1
42	DG	177/182 (97%)	80 (45%)	47 (27%)	50 (28%)	0	0
43	BH	163/180 (91%)	98 (60%)	39 (24%)	26 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DH	163/180 (91%)	98 (60%)	38 (23%)	27 (17%)	0	1
44	BI	144/148 (97%)	76 (53%)	37 (26%)	31 (22%)	0	1
44	DI	144/148 (97%)	76 (53%)	37 (26%)	31 (22%)	0	1
46	BN	137/140 (98%)	96 (70%)	23 (17%)	18 (13%)	0	2
46	DN	137/140 (98%)	95 (69%)	25 (18%)	17 (12%)	0	2
47	BO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	7	40
47	DO	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	7	40
48	BP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0
48	DP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0
49	BQ	139/141 (99%)	109 (78%)	17 (12%)	13 (9%)	1	6
49	DQ	139/141 (99%)	107 (77%)	20 (14%)	12 (9%)	1	8
50	BR	115/118 (98%)	89 (77%)	14 (12%)	12 (10%)	1	4
50	DR	115/118 (98%)	89 (77%)	13 (11%)	13 (11%)	0	3
51	BS	97/112 (87%)	51 (53%)	23 (24%)	23 (24%)	0	0
51	DS	97/112 (87%)	50 (52%)	23 (24%)	24 (25%)	0	0
52	BT	134/146 (92%)	79 (59%)	28 (21%)	27 (20%)	0	1
52	DT	134/146 (92%)	79 (59%)	28 (21%)	27 (20%)	0	1
53	BU	115/118 (98%)	87 (76%)	22 (19%)	6 (5%)	2	20
53	DU	115/118 (98%)	87 (76%)	22 (19%)	6 (5%)	2	20
54	BV	99/101 (98%)	63 (64%)	21 (21%)	15 (15%)	0	1
54	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	2
55	BW	111/113 (98%)	91 (82%)	14 (13%)	6 (5%)	2	19
55	DW	111/113 (98%)	96 (86%)	9 (8%)	6 (5%)	2	19
56	BX	91/96 (95%)	71 (78%)	17 (19%)	3 (3%)	5	34
56	DX	91/96 (95%)	72 (79%)	16 (18%)	3 (3%)	5	34
57	BY	99/110 (90%)	42 (42%)	25 (25%)	32 (32%)	0	0
57	DY	99/110 (90%)	41 (41%)	26 (26%)	32 (32%)	0	0
58	BZ	183/206 (89%)	102 (56%)	40 (22%)	41 (22%)	0	0
58	DZ	183/206 (89%)	85 (46%)	58 (32%)	40 (22%)	0	1
All	All	11928/12922 (92%)	7972 (67%)	2431 (20%)	1525 (13%)	0	2

5 of 1525 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	10	LEU
2	AB	75	LYS
2	AB	123	ALA
2	AB	155	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	189 (94%)	13 (6%)	22	60
2	CB	202/220 (92%)	191 (95%)	11 (5%)	27	66
3	AC	160/188 (85%)	146 (91%)	14 (9%)	12	44
3	CC	160/188 (85%)	147 (92%)	13 (8%)	15	49
4	AD	180/181 (99%)	162 (90%)	18 (10%)	9	36
4	CD	180/181 (99%)	162 (90%)	18 (10%)	9	36
5	AE	115/123 (94%)	98 (85%)	17 (15%)	4	17
5	CE	115/123 (94%)	98 (85%)	17 (15%)	4	17
6	AF	90/90 (100%)	84 (93%)	6 (7%)	20	59
6	CF	90/90 (100%)	84 (93%)	6 (7%)	20	59
7	AG	126/127 (99%)	120 (95%)	6 (5%)	31	70
7	CG	126/127 (99%)	121 (96%)	5 (4%)	38	74
8	AH	119/119 (100%)	109 (92%)	10 (8%)	14	47
8	CH	119/119 (100%)	108 (91%)	11 (9%)	11	40
9	AI	98/99 (99%)	89 (91%)	9 (9%)	11	40
9	CI	98/99 (99%)	89 (91%)	9 (9%)	11	40
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	15	50
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	15	50
11	AK	90/99 (91%)	87 (97%)	3 (3%)	45	79
11	CK	90/99 (91%)	87 (97%)	3 (3%)	45	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/109 (95%)	95 (91%)	9 (9%)	13	45
12	CL	104/109 (95%)	95 (91%)	9 (9%)	13	45
13	AM	94/101 (93%)	83 (88%)	11 (12%)	7	28
13	CM	94/101 (93%)	83 (88%)	11 (12%)	7	28
14	AN	49/50 (98%)	46 (94%)	3 (6%)	23	62
14	CN	49/50 (98%)	46 (94%)	3 (6%)	23	62
15	AO	79/80 (99%)	73 (92%)	6 (8%)	16	53
15	CO	79/80 (99%)	73 (92%)	6 (8%)	16	53
16	AP	72/74 (97%)	65 (90%)	7 (10%)	10	38
16	CP	72/74 (97%)	65 (90%)	7 (10%)	10	38
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	28	66
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	28	66
18	AR	61/77 (79%)	61 (100%)	0	100	100
18	CR	61/77 (79%)	60 (98%)	1 (2%)	70	88
19	AS	69/80 (86%)	60 (87%)	9 (13%)	5	22
19	CS	69/80 (86%)	61 (88%)	8 (12%)	7	28
20	AT	76/82 (93%)	68 (90%)	8 (10%)	8	33
20	CT	76/82 (93%)	69 (91%)	7 (9%)	11	40
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	33
21	CU	19/22 (86%)	17 (90%)	2 (10%)	8	33
25	AY	78/78 (100%)	65 (83%)	13 (17%)	3	13
25	AZ	78/78 (100%)	57 (73%)	21 (27%)	0	2
25	CY	78/78 (100%)	64 (82%)	14 (18%)	2	10
25	CZ	78/78 (100%)	56 (72%)	22 (28%)	0	2
26	B0	66/67 (98%)	56 (85%)	10 (15%)	3	16
26	D0	66/67 (98%)	56 (85%)	10 (15%)	3	16
27	B1	78/83 (94%)	69 (88%)	9 (12%)	7	28
27	D1	78/83 (94%)	66 (85%)	12 (15%)	3	16
28	B2	66/67 (98%)	56 (85%)	10 (15%)	3	16
28	D2	66/67 (98%)	56 (85%)	10 (15%)	3	16
29	B3	51/52 (98%)	46 (90%)	5 (10%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	D3	51/52 (98%)	46 (90%)	5 (10%)	10	37
30	B4	51/63 (81%)	39 (76%)	12 (24%)	1	3
30	D4	51/63 (81%)	39 (76%)	12 (24%)	1	3
31	B5	47/52 (90%)	42 (89%)	5 (11%)	8	33
31	D5	47/52 (90%)	42 (89%)	5 (11%)	8	33
32	B6	49/52 (94%)	38 (78%)	11 (22%)	1	4
32	D6	49/52 (94%)	36 (74%)	13 (26%)	0	2
33	B7	40/42 (95%)	36 (90%)	4 (10%)	9	36
33	D7	40/42 (95%)	36 (90%)	4 (10%)	9	36
34	B8	53/55 (96%)	42 (79%)	11 (21%)	1	5
34	D8	53/55 (96%)	43 (81%)	10 (19%)	2	8
35	B9	34/34 (100%)	32 (94%)	2 (6%)	24	63
35	D9	34/34 (100%)	32 (94%)	2 (6%)	24	63
38	BC	99/181 (55%)	96 (97%)	3 (3%)	48	80
38	DC	99/181 (55%)	96 (97%)	3 (3%)	48	80
39	BD	213/218 (98%)	188 (88%)	25 (12%)	7	28
39	DD	213/218 (98%)	187 (88%)	26 (12%)	6	25
40	BE	165/166 (99%)	143 (87%)	22 (13%)	5	21
40	DE	165/166 (99%)	144 (87%)	21 (13%)	5	24
41	BF	165/166 (99%)	145 (88%)	20 (12%)	6	26
41	DF	165/166 (99%)	145 (88%)	20 (12%)	6	26
42	BG	155/156 (99%)	137 (88%)	18 (12%)	7	28
42	DG	155/156 (99%)	121 (78%)	34 (22%)	1	5
43	BH	137/148 (93%)	127 (93%)	10 (7%)	17	54
43	DH	137/148 (93%)	127 (93%)	10 (7%)	17	54
44	BI	122/124 (98%)	105 (86%)	17 (14%)	4	20
44	DI	122/124 (98%)	105 (86%)	17 (14%)	4	20
46	BN	117/119 (98%)	98 (84%)	19 (16%)	3	14
46	DN	117/119 (98%)	98 (84%)	19 (16%)	3	14
47	BO	100/100 (100%)	94 (94%)	6 (6%)	24	62
47	DO	100/100 (100%)	94 (94%)	6 (6%)	24	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BP	112/116 (97%)	84 (75%)	28 (25%)	1	3
48	DP	112/116 (97%)	84 (75%)	28 (25%)	1	3
49	BQ	110/111 (99%)	95 (86%)	15 (14%)	5	21
49	DQ	110/111 (99%)	95 (86%)	15 (14%)	5	21
50	BR	100/101 (99%)	83 (83%)	17 (17%)	2	12
50	DR	100/101 (99%)	83 (83%)	17 (17%)	2	12
51	BS	77/88 (88%)	60 (78%)	17 (22%)	1	4
51	DS	77/88 (88%)	60 (78%)	17 (22%)	1	4
52	BT	118/127 (93%)	98 (83%)	20 (17%)	2	12
52	DT	118/127 (93%)	99 (84%)	19 (16%)	3	14
53	BU	92/94 (98%)	83 (90%)	9 (10%)	10	37
53	DU	92/94 (98%)	83 (90%)	9 (10%)	10	37
54	BV	82/82 (100%)	61 (74%)	21 (26%)	0	3
54	DV	82/82 (100%)	62 (76%)	20 (24%)	1	3
55	BW	91/92 (99%)	78 (86%)	13 (14%)	4	19
55	DW	91/92 (99%)	77 (85%)	14 (15%)	3	16
56	BX	74/78 (95%)	68 (92%)	6 (8%)	15	49
56	DX	74/78 (95%)	68 (92%)	6 (8%)	15	49
57	BY	84/91 (92%)	67 (80%)	17 (20%)	1	6
57	DY	84/91 (92%)	67 (80%)	17 (20%)	1	6
58	BZ	162/179 (90%)	137 (85%)	25 (15%)	3	16
58	DZ	162/179 (90%)	131 (81%)	31 (19%)	2	7
All	All	10102/10740 (94%)	8871 (88%)	1231 (12%)	6	25

5 of 1231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	BX	27	THR
9	CI	95	LYS
53	DU	74	LEU
57	BY	60	PHE
3	CC	131	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 309 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	14	HIS
4	CD	123	HIS
50	DR	61	HIS
54	BV	11	GLN
2	CB	76	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	214 (14%)	30 (1%)
1	CA	1503/1504 (99%)	209 (13%)	31 (2%)
22	AV	76/77 (98%)	15 (19%)	0
23	AW	76/77 (98%)	10 (13%)	1 (1%)
23	CV	76/77 (98%)	12 (15%)	0
23	CW	76/77 (98%)	10 (13%)	1 (1%)
24	AX	10/25 (40%)	8 (80%)	1 (10%)
36	BA	2847/2848 (99%)	500 (17%)	49 (1%)
36	DA	2847/2848 (99%)	498 (17%)	47 (1%)
37	BB	118/119 (99%)	25 (21%)	2 (1%)
37	DB	118/119 (99%)	25 (21%)	2 (1%)
59	CX	9/10 (90%)	6 (66%)	2 (22%)
All	All	9259/9285 (99%)	1532 (16%)	166 (1%)

5 of 1532 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	30	U
1	AA	31	G
1	AA	32	A

5 of 166 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2439	A
1	CA	366	C
36	DA	2191	G
36	BA	2481	G
1	CA	60	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
22	5MU	AV	54	22	13,22,23	1.13	2 (15%)	16,32,35	4.83	3 (18%)
24	OMU	AX	19	24	14,22,23	1.27	3 (21%)	19,31,34	3.07	3 (15%)
24	A2M	AX	20	60,24	18,25,26	0.52	0	18,36,39	1.12	1 (5%)
24	A2M	AX	21	24	18,25,26	0.53	0	18,36,39	1.52	1 (5%)
59	OMU	CX	19	59	14,22,23	1.23	2 (14%)	19,31,34	3.01	3 (15%)
59	A2M	CX	20	59	18,25,26	0.53	0	18,36,39	1.02	1 (5%)
59	A2M	CX	21	59	18,25,26	0.53	0	18,36,39	0.44	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
22	5MU	AV	54	22	-	0/3/25/26	0/2/2/2
24	OMU	AX	19	24	-	0/5/27/28	0/2/2/2
24	A2M	AX	20	60,24	-	0/5/27/28	0/3/3/3
24	A2M	AX	21	24	-	0/5/27/28	0/3/3/3
59	OMU	CX	19	59	-	0/5/27/28	0/2/2/2
59	A2M	CX	20	59	-	0/5/27/28	0/3/3/3
59	A2M	CX	21	59	-	0/5/27/28	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	54	5MU	C6-C5	-2.10	1.34	1.40
24	AX	19	OMU	O2'-CM2	-2.08	1.34	1.42
24	AX	19	OMU	C6-N1	2.05	1.38	1.35
59	CX	19	OMU	C6-N1	2.07	1.38	1.35
22	AV	54	5MU	C4-N3	3.11	1.38	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	54	5MU	C5-C4-N3	-12.18	115.13	125.35
24	AX	21	A2M	CM'-O2'-C2'	-6.34	96.81	114.58
24	AX	20	A2M	CM'-O2'-C2'	-4.58	101.75	114.58
59	CX	20	A2M	CM'-O2'-C2'	-4.17	102.89	114.58
24	AX	19	OMU	CM2-O2'-C2'	-4.08	103.14	114.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	1	0
24	AX	19	OMU	14	0
24	AX	20	A2M	31	0
24	AX	21	A2M	21	0
59	CX	19	OMU	10	0
59	CX	20	A2M	30	0
59	CX	21	A2M	20	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 711 ligands modelled in this entry, 711 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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.

## 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	5
13	AM	5
9	AI	2
9	CI	2
42	DG	1
42	BG	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DG	112:PRO	C	113:ARG	N	5.57
1	CM	69:GLU	C	70:LEU	N	4.17
1	AM	69:GLU	C	70:LEU	N	4.16
1	CM	112:GLY	C	113:PRO	N	3.94
1	AM	112:GLY	C	113:PRO	N	3.93

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1504/1504 (100%)	0.04	31 (2%) 67 67	63, 109, 201, 216	0
1	CA	1504/1504 (100%)	0.23	45 (2%) 54 54	65, 139, 211, 216	0
2	AB	235/256 (91%)	0.53	27 (11%) 6 6	87, 146, 195, 216	0
2	CB	235/256 (91%)	0.61	27 (11%) 6 6	86, 165, 206, 216	0
3	AC	207/239 (86%)	0.42	13 (6%) 23 24	83, 143, 188, 216	0
3	CC	207/239 (86%)	0.99	39 (18%) 2 2	100, 164, 200, 216	0
4	AD	208/209 (99%)	0.09	1 (0%) 91 92	70, 104, 147, 167	0
4	CD	208/209 (99%)	0.82	27 (12%) 5 4	95, 151, 199, 216	0
5	AE	151/162 (93%)	0.35	4 (2%) 59 59	62, 102, 142, 216	0
5	CE	151/162 (93%)	0.91	22 (14%) 3 3	60, 125, 168, 210	0
6	AF	101/101 (100%)	0.16	4 (3%) 42 41	73, 128, 164, 183	0
6	CF	101/101 (100%)	-0.09	1 (0%) 84 85	63, 112, 156, 181	0
7	AG	155/156 (99%)	0.35	13 (8%) 14 13	91, 136, 181, 210	0
7	CG	155/156 (99%)	0.73	27 (17%) 2 2	91, 153, 194, 216	0
8	AH	138/138 (100%)	0.27	1 (0%) 89 89	73, 108, 147, 193	0
8	CH	138/138 (100%)	0.68	13 (9%) 11 11	89, 132, 183, 213	0
9	AI	127/128 (99%)	1.05	27 (21%) 1 1	95, 155, 190, 216	0
9	CI	127/128 (99%)	1.76	44 (34%) 0 1	113, 170, 211, 216	0
10	AJ	99/105 (94%)	1.43	27 (27%) 1 1	88, 159, 208, 216	0
10	CJ	99/105 (94%)	2.07	38 (38%) 0 1	122, 174, 215, 216	0
11	AK	119/129 (92%)	0.93	18 (15%) 3 3	70, 120, 170, 212	0
11	CK	119/129 (92%)	0.39	9 (7%) 17 17	70, 120, 167, 195	0
12	AL	125/132 (94%)	0.47	7 (5%) 28 27	60, 89, 139, 216	0
12	CL	125/132 (94%)	0.87	22 (17%) 2 2	77, 113, 157, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	119/126 (94%)	0.47	8 (6%) 21 21	80, 143, 183, 216	0
13	CM	119/126 (94%)	1.12	25 (21%) 1 1	97, 167, 210, 216	0
14	AN	60/61 (98%)	0.70	6 (10%) 9 10	84, 136, 187, 204	0
14	CN	60/61 (98%)	0.75	8 (13%) 4 4	92, 154, 192, 206	0
15	AO	88/89 (98%)	0.31	2 (2%) 64 64	66, 108, 148, 177	0
15	CO	88/89 (98%)	0.12	2 (2%) 64 64	70, 114, 149, 174	0
16	AP	84/88 (95%)	0.50	2 (2%) 62 62	70, 94, 143, 199	0
16	CP	84/88 (95%)	1.75	30 (35%) 0 1	99, 138, 175, 208	0
17	AQ	100/105 (95%)	0.15	0 100 100	70, 99, 129, 161	0
17	CQ	100/105 (95%)	0.55	7 (7%) 19 20	90, 125, 158, 179	0
18	AR	70/88 (79%)	0.85	7 (10%) 9 10	87, 128, 170, 181	0
18	CR	70/88 (79%)	0.87	9 (12%) 5 4	77, 118, 168, 186	0
19	AS	79/93 (84%)	1.43	24 (30%) 1 1	111, 163, 209, 216	0
19	CS	79/93 (84%)	2.10	31 (39%) 0 1	122, 169, 213, 216	0
20	AT	99/106 (93%)	0.46	8 (8%) 15 14	71, 107, 163, 187	0
20	CT	99/106 (93%)	1.06	18 (18%) 2 2	93, 143, 181, 216	0
21	AU	25/27 (92%)	2.36	12 (48%) 0 0	99, 143, 176, 193	0
21	CU	25/27 (92%)	3.23	17 (68%) 0 0	102, 155, 182, 191	0
22	AV	76/77 (98%)	-0.23	1 (1%) 79 80	71, 108, 162, 206	0
23	AW	77/77 (100%)	2.30	39 (50%) 0 0	151, 218, 220, 221	0
23	CV	77/77 (100%)	-0.12	1 (1%) 79 80	76, 126, 184, 211	0
23	CW	77/77 (100%)	1.84	31 (40%) 0 1	151, 218, 220, 221	0
24	AX	8/25 (32%)	1.89	3 (37%) 0 1	52, 100, 165, 180	0
25	AY	84/84 (100%)	1.09	15 (17%) 2 2	105, 142, 171, 199	0
25	AZ	84/84 (100%)	0.99	20 (23%) 1 1	121, 166, 197, 200	0
25	CY	84/84 (100%)	1.97	37 (44%) 0 1	103, 160, 194, 200	0
25	CZ	84/84 (100%)	1.30	22 (26%) 1 1	132, 182, 200, 200	0
26	B0	84/85 (98%)	0.62	10 (11%) 6 5	69, 103, 160, 207	0
26	D0	84/85 (98%)	1.02	10 (11%) 6 5	76, 107, 163, 198	0
27	B1	94/98 (95%)	0.31	3 (3%) 51 51	55, 87, 144, 208	0
27	D1	94/98 (95%)	0.31	1 (1%) 82 83	53, 83, 132, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	B2	71/72 (98%)	0.26	4 (5%) 28 27	81, 122, 156, 205	0
28	D2	71/72 (98%)	-0.12	3 (4%) 40 39	51, 84, 123, 188	0
29	B3	60/60 (100%)	0.97	8 (13%) 4 4	66, 97, 144, 212	0
29	D3	60/60 (100%)	0.29	1 (1%) 73 73	61, 93, 159, 199	0
30	B4	58/71 (81%)	0.28	6 (10%) 9 9	104, 171, 212, 216	0
30	D4	58/71 (81%)	0.83	7 (12%) 6 5	145, 180, 214, 216	0
31	B5	56/60 (93%)	0.18	4 (7%) 19 19	49, 92, 147, 216	0
31	D5	56/60 (93%)	0.01	2 (3%) 46 46	49, 83, 151, 216	0
32	B6	50/54 (92%)	1.81	19 (38%) 0 1	89, 132, 180, 183	0
32	D6	50/54 (92%)	1.36	14 (28%) 1 1	97, 140, 188, 210	0
33	B7	48/49 (97%)	0.09	1 (2%) 67 67	50, 73, 123, 163	0
33	D7	48/49 (97%)	0.11	2 (4%) 40 39	42, 57, 101, 161	0
34	B8	64/65 (98%)	0.47	4 (6%) 23 24	57, 85, 144, 170	0
34	D8	64/65 (98%)	0.45	4 (6%) 23 24	48, 85, 142, 210	0
35	B9	37/37 (100%)	2.08	15 (40%) 0 1	94, 118, 163, 186	0
35	D9	37/37 (100%)	2.16	19 (51%) 0 0	93, 119, 162, 173	0
36	BA	2848/2848 (100%)	0.09	103 (3%) 46 46	46, 88, 203, 216	0
36	DA	2848/2848 (100%)	0.09	92 (3%) 51 51	43, 82, 203, 216	0
37	BB	119/119 (100%)	-0.12	2 (1%) 73 73	88, 144, 195, 212	0
37	DB	119/119 (100%)	0.30	6 (5%) 32 32	90, 173, 210, 216	0
38	BC	120/229 (52%)	4.07	95 (79%) 0 0	139, 202, 216, 216	0
38	DC	120/229 (52%)	3.81	91 (75%) 0 0	145, 202, 216, 216	0
39	BD	272/276 (98%)	0.08	2 (0%) 89 89	45, 83, 120, 188	0
39	DD	272/276 (98%)	0.09	4 (1%) 76 77	45, 77, 113, 185	0
40	BE	205/206 (99%)	0.20	9 (4%) 38 37	50, 89, 166, 201	0
40	DE	205/206 (99%)	0.42	5 (2%) 62 62	37, 89, 146, 194	0
41	BF	208/210 (99%)	-0.05	1 (0%) 91 92	49, 88, 164, 216	0
41	DF	208/210 (99%)	0.08	7 (3%) 49 49	36, 82, 164, 211	0
42	BG	181/182 (99%)	0.49	14 (7%) 16 17	100, 143, 188, 212	0
42	DG	181/182 (99%)	1.30	50 (27%) 1 1	109, 171, 215, 216	0
43	BH	165/180 (91%)	1.67	61 (36%) 0 1	98, 166, 214, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	DH	165/180 (91%)	0.70	23 (13%) 4 3	67, 127, 186, 216	0
44	BI	146/148 (98%)	2.77	67 (45%) 0 0	84, 172, 216, 216	0
44	DI	146/148 (98%)	1.08	23 (15%) 3 3	69, 144, 211, 216	0
45	BJ	0/130	-	-	-	-
45	DJ	0/130	-	-	-	-
46	BN	139/140 (99%)	0.40	6 (4%) 39 38	63, 97, 149, 192	0
46	DN	139/140 (99%)	0.06	2 (1%) 78 79	54, 90, 144, 175	0
47	BO	122/122 (100%)	-0.02	0 100 100	48, 78, 111, 141	0
47	DO	122/122 (100%)	0.23	1 (0%) 87 88	60, 89, 121, 138	0
48	BP	146/150 (97%)	0.57	13 (8%) 12 12	51, 103, 161, 216	0
48	DP	146/150 (97%)	0.36	6 (4%) 41 40	51, 105, 162, 210	0
49	BQ	141/141 (100%)	0.05	1 (0%) 89 89	65, 96, 134, 209	0
49	DQ	141/141 (100%)	0.43	6 (4%) 39 38	67, 103, 149, 208	0
50	BR	117/118 (99%)	0.09	0 100 100	55, 89, 123, 137	0
50	DR	117/118 (99%)	0.32	4 (3%) 49 49	51, 84, 121, 145	0
51	BS	99/112 (88%)	1.03	20 (20%) 1 1	93, 141, 189, 208	0
51	DS	99/112 (88%)	1.27	25 (25%) 1 1	91, 154, 199, 216	0
52	BT	136/146 (93%)	0.19	3 (2%) 65 65	64, 97, 176, 216	0
52	DT	136/146 (93%)	0.41	10 (7%) 17 18	68, 110, 189, 215	0
53	BU	117/118 (99%)	-0.01	1 (0%) 85 87	53, 86, 139, 210	0
53	DU	117/118 (99%)	-0.07	2 (1%) 73 73	45, 75, 122, 215	0
54	BV	101/101 (100%)	0.28	5 (4%) 32 32	53, 109, 158, 206	0
54	DV	101/101 (100%)	0.08	0 100 100	38, 93, 133, 216	0
55	BW	113/113 (100%)	0.28	5 (4%) 38 37	55, 80, 132, 199	0
55	DW	113/113 (100%)	0.20	3 (2%) 58 58	40, 72, 121, 209	0
56	BX	93/96 (96%)	0.21	1 (1%) 82 83	63, 106, 136, 155	0
56	DX	93/96 (96%)	0.13	1 (1%) 82 83	55, 79, 117, 164	0
57	BY	101/110 (91%)	1.38	24 (23%) 1 1	62, 114, 180, 206	0
57	DY	101/110 (91%)	0.71	10 (9%) 9 10	56, 102, 168, 211	0
58	BZ	185/206 (89%)	0.52	19 (10%) 9 9	85, 131, 186, 216	0
58	DZ	185/206 (89%)	0.38	18 (9%) 10 11	88, 144, 202, 215	0
59	CX	7/10 (70%)	1.60	2 (28%) 1 1	110, 144, 193, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	21436/22467 (95%)	0.44	1852 (8%) 13 13	36, 111, 202, 221	0

The worst 5 of 1852 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	AL	129	ALA	19.7
44	BI	119	PRO	16.7
44	BI	100	ALA	15.9
44	DI	88	ILE	15.2
5	AE	155	GLU	14.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	A2M	AX	20	23/24	0.60	0.44	-	158,164,194,194	0
59	A2M	CX	21	23/24	0.87	0.29	-	177,179,187,190	0
24	A2M	AX	21	23/24	0.83	0.35	-	140,147,161,184	0
22	5MU	AV	54	21/22	0.93	0.23	-	114,133,152,153	0
59	OMU	CX	19	21/22	0.85	0.29	-	117,161,200,200	0
24	OMU	AX	19	21/22	0.85	0.29	-	99,130,198,198	0
59	A2M	CX	20	23/24	0.59	0.36	-	168,174,200,200	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	2943	1/1	0.95	0.80	130.55	56,56,56,56	0
60	MG	BA	2930	1/1	0.83	1.33	103.45	117,117,117,117	0
60	MG	DA	3096	1/1	0.43	1.00	91.96	124,124,124,124	0
60	MG	BA	3110	1/1	0.91	1.16	82.37	101,101,101,101	0
60	MG	BA	2918	1/1	0.93	0.87	68.06	64,64,64,64	0
60	MG	BA	2968	1/1	0.91	1.07	68.04	72,72,72,72	0
60	MG	BA	2955	1/1	0.82	1.12	66.44	109,109,109,109	0
60	MG	AA	1603	1/1	0.40	1.35	65.03	94,94,94,94	0
60	MG	DA	2917	1/1	0.98	0.86	56.12	58,58,58,58	0
60	MG	AA	1686	1/1	0.70	1.38	54.72	99,99,99,99	0
60	MG	BA	2942	1/1	0.81	0.86	51.96	107,107,107,107	0
60	MG	CA	1626	1/1	0.40	1.40	47.58	102,102,102,102	0
60	MG	DA	2935	1/1	0.81	0.81	46.76	68,68,68,68	0
60	MG	DA	2973	1/1	0.97	0.63	44.33	51,51,51,51	0
60	MG	DA	2974	1/1	0.96	0.71	43.83	92,92,92,92	0
60	MG	BA	2960	1/1	0.71	0.58	42.06	105,105,105,105	0
60	MG	BA	3098	1/1	0.57	0.68	42.00	89,89,89,89	0
60	MG	DA	3111	1/1	0.98	1.00	42.00	62,62,62,62	0
60	MG	DA	3083	1/1	0.76	1.09	41.52	112,112,112,112	0
60	MG	BA	3079	1/1	0.88	0.87	40.91	72,72,72,72	0
60	MG	CA	1656	1/1	0.98	0.60	40.46	90,90,90,90	0
60	MG	BA	3030	1/1	0.41	0.75	39.32	96,96,96,96	0
60	MG	BA	2933	1/1	0.94	0.66	36.98	77,77,77,77	0
60	MG	BA	2972	1/1	0.95	0.75	36.26	76,76,76,76	0
60	MG	BA	3133	1/1	0.96	1.12	35.21	73,73,73,73	0
60	MG	DA	2971	1/1	0.95	0.64	34.96	66,66,66,66	0
60	MG	DA	2965	1/1	0.71	0.58	32.59	96,96,96,96	0
60	MG	DA	2904	1/1	0.93	0.82	31.81	49,49,49,49	0
60	MG	DA	2929	1/1	0.71	0.70	31.70	94,94,94,94	0
60	MG	DA	3029	1/1	0.67	0.65	31.26	99,99,99,99	0
60	MG	DA	2932	1/1	0.93	0.60	31.05	64,64,64,64	0
60	MG	BA	2974	1/1	0.94	0.95	30.65	68,68,68,68	0
60	MG	BA	2912	1/1	0.97	0.78	30.65	71,71,71,71	0
60	MG	DA	2903	1/1	0.84	1.02	30.35	85,85,85,85	0
60	MG	DA	3005	1/1	0.97	0.58	29.87	53,53,53,53	0
60	MG	BA	3025	1/1	0.82	0.74	29.24	95,95,95,95	0
60	MG	AA	1702	1/1	0.96	0.76	28.84	74,74,74,74	0
60	MG	BA	2903	1/1	0.93	0.78	28.58	97,97,97,97	0
60	MG	BA	2945	1/1	0.90	0.93	28.51	73,73,73,73	0
60	MG	BA	2993	1/1	0.84	0.76	27.68	92,92,92,92	0
60	MG	CA	1622	1/1	0.76	0.51	27.46	93,93,93,93	0
60	MG	BA	2940	1/1	0.91	0.53	26.83	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	2996	1/1	0.79	1.05	26.71	106,106,106,106	0
60	MG	BA	2904	1/1	0.91	0.76	26.54	56,56,56,56	0
60	MG	DA	2995	1/1	0.91	0.74	25.72	75,75,75,75	0
60	MG	AA	1662	1/1	0.30	1.06	25.42	127,127,127,127	0
60	MG	DA	2911	1/1	0.97	0.57	25.06	62,62,62,62	0
60	MG	DA	2940	1/1	0.85	0.73	25.03	72,72,72,72	0
60	MG	DA	3065	1/1	0.93	0.90	24.98	75,75,75,75	0
60	MG	DA	2942	1/1	0.74	0.93	24.77	90,90,90,90	0
60	MG	BA	2922	1/1	0.97	0.49	24.32	53,53,53,53	0
60	MG	DA	3109	1/1	0.98	0.66	23.58	45,45,45,45	0
60	MG	AA	1617	1/1	0.84	0.46	23.48	104,104,104,104	0
60	MG	BA	2928	1/1	0.99	0.99	23.46	63,63,63,63	0
60	MG	DA	2978	1/1	0.89	0.53	22.85	85,85,85,85	0
60	MG	BA	2937	1/1	0.86	0.75	22.67	70,70,70,70	0
60	MG	DA	3075	1/1	0.85	0.36	22.53	75,75,75,75	0
60	MG	DA	2907	1/1	0.95	0.66	21.42	51,51,51,51	0
60	MG	DA	2967	1/1	0.97	0.66	21.17	51,51,51,51	0
60	MG	BA	3107	1/1	0.56	0.52	20.93	87,87,87,87	0
60	MG	BA	3038	1/1	0.80	0.34	20.80	90,90,90,90	0
60	MG	BA	2939	1/1	0.90	0.46	20.79	50,50,50,50	0
60	MG	DA	3077	1/1	0.67	0.60	20.56	96,96,96,96	0
60	MG	BA	2936	1/1	0.95	0.76	20.50	58,58,58,58	0
60	MG	AA	1623	1/1	0.13	0.66	20.32	100,100,100,100	0
60	MG	BA	3057	1/1	0.95	0.52	19.99	73,73,73,73	0
60	MG	BA	2934	1/1	0.99	0.47	19.88	55,55,55,55	0
60	MG	DA	2918	1/1	0.96	0.67	19.80	59,59,59,59	0
60	MG	BA	3122	1/1	0.88	0.74	19.69	84,84,84,84	0
60	MG	BA	2944	1/1	0.94	0.40	19.68	58,58,58,58	0
60	MG	BA	2969	1/1	0.82	0.45	19.58	61,61,61,61	0
60	MG	CA	1678	1/1	0.39	0.56	19.52	86,86,86,86	1
60	MG	BA	3100	1/1	0.57	0.47	19.36	117,117,117,117	0
60	MG	AA	1658	1/1	0.96	0.65	19.30	92,92,92,92	0
60	MG	DA	3094	1/1	0.72	0.45	19.14	87,87,87,87	0
60	MG	BA	2967	1/1	0.92	0.67	19.14	57,57,57,57	0
60	MG	BA	3015	1/1	0.75	0.55	18.66	94,94,94,94	0
60	MG	DA	2957	1/1	0.98	0.55	18.17	66,66,66,66	0
60	MG	AA	1671	1/1	0.83	1.00	17.64	96,96,96,96	0
60	MG	CA	1701	1/1	0.96	0.54	17.39	58,58,58,58	0
60	MG	DA	3067	1/1	0.98	0.50	17.27	52,52,52,52	0
60	MG	DA	2921	1/1	0.96	0.46	17.16	49,49,49,49	0
60	MG	DA	2909	1/1	0.96	0.68	17.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	2968	1/1	0.99	0.47	16.70	43,43,43,43	0
60	MG	CA	1628	1/1	0.86	0.42	16.66	66,66,66,66	0
60	MG	DA	2933	1/1	0.98	0.50	16.48	53,53,53,53	0
60	MG	D1	101	1/1	0.94	0.91	16.17	92,92,92,92	0
60	MG	DA	2927	1/1	0.98	0.79	16.05	52,52,52,52	0
60	MG	AA	1608	1/1	0.65	0.44	15.66	81,81,81,81	0
60	MG	DA	3092	1/1	0.93	0.47	15.44	86,86,86,86	0
60	MG	BA	3064	1/1	0.66	0.48	15.28	86,86,86,86	0
60	MG	DA	2914	1/1	0.93	0.42	15.04	49,49,49,49	0
60	MG	DA	3035	1/1	0.62	0.51	15.02	105,105,105,105	0
60	MG	BA	3003	1/1	0.98	0.66	14.99	68,68,68,68	0
60	MG	DA	2998	1/1	0.75	0.52	14.71	91,91,91,91	0
60	MG	DA	2996	1/1	0.82	0.37	14.61	63,63,63,63	0
60	MG	DR	201	1/1	0.69	1.02	13.99	117,117,117,117	0
60	MG	DA	3037	1/1	0.67	0.44	13.85	74,74,74,74	0
60	MG	BA	2921	1/1	0.84	0.34	13.58	98,98,98,98	0
60	MG	DA	3025	1/1	0.88	0.56	13.49	51,51,51,51	0
60	MG	AA	1628	1/1	0.89	0.49	13.46	87,87,87,87	0
60	MG	DA	3105	1/1	0.75	0.32	13.46	93,93,93,93	0
60	MG	BA	2909	1/1	0.90	0.50	13.33	64,64,64,64	0
60	MG	BA	2973	1/1	0.78	0.66	13.29	92,92,92,92	0
60	MG	BA	2949	1/1	0.78	0.48	13.24	77,77,77,77	0
60	MG	AA	1622	1/1	0.76	0.29	12.68	128,128,128,128	0
60	MG	BA	2995	1/1	0.38	0.43	12.57	105,105,105,105	0
60	MG	BA	2915	1/1	0.98	0.35	12.04	51,51,51,51	0
60	MG	DA	2972	1/1	0.69	0.60	12.00	100,100,100,100	0
60	MG	AA	1629	1/1	0.89	0.52	11.72	65,65,65,65	1
60	MG	BA	3027	1/1	0.94	0.56	11.66	51,51,51,51	0
60	MG	DA	2915	1/1	0.91	0.41	11.60	64,64,64,64	0
60	MG	BA	3078	1/1	0.77	0.33	11.27	104,104,104,104	0
60	MG	BA	2907	1/1	0.97	0.56	11.26	55,55,55,55	0
60	MG	DA	3042	1/1	0.83	0.35	10.97	81,81,81,81	0
60	MG	BA	2966	1/1	0.70	0.40	10.90	92,92,92,92	0
60	MG	DA	3038	1/1	0.94	0.62	10.86	77,77,77,77	0
60	MG	BA	3088	1/1	0.56	0.39	10.84	105,105,105,105	0
60	MG	BA	2919	1/1	0.87	0.50	10.50	75,75,75,75	0
60	MG	DA	3108	1/1	0.95	0.53	10.35	61,61,61,61	0
60	MG	BA	3077	1/1	0.92	0.37	10.17	84,84,84,84	0
60	MG	BA	3082	1/1	0.83	0.44	10.06	101,101,101,101	0
60	MG	DA	3074	1/1	0.90	0.70	9.96	96,96,96,96	0
60	MG	BA	3014	1/1	0.87	0.38	9.85	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	1652	1/1	0.40	0.35	9.71	103,103,103,103	1
60	MG	CA	1612	1/1	0.43	0.56	9.59	102,102,102,102	0
60	MG	BA	3102	1/1	0.54	0.52	9.27	108,108,108,108	0
60	MG	CA	1663	1/1	0.81	0.37	9.23	121,121,121,121	0
60	MG	DA	2950	1/1	0.94	0.36	9.01	55,55,55,55	0
60	MG	BA	3006	1/1	0.73	0.39	8.99	91,91,91,91	0
60	MG	CA	1655	1/1	0.84	0.68	8.80	111,111,111,111	0
60	MG	DA	2938	1/1	0.95	0.34	8.69	45,45,45,45	0
60	MG	DA	2979	1/1	0.86	0.32	8.26	57,57,57,57	0
60	MG	CA	1614	1/1	0.95	0.29	8.16	87,87,87,87	0
60	MG	AA	1605	1/1	0.96	0.33	7.84	66,66,66,66	0
60	MG	BA	2994	1/1	0.87	0.28	7.81	77,77,77,77	0
60	MG	AA	1616	1/1	0.97	0.40	7.69	84,84,84,84	0
60	MG	BA	2987	1/1	0.88	0.72	7.26	100,100,100,100	0
60	MG	B1	102	1/1	0.96	0.71	7.17	83,83,83,83	0
60	MG	BA	2954	1/1	0.93	0.34	7.06	66,66,66,66	0
60	MG	BA	3136	1/1	0.91	0.63	6.94	106,106,106,106	0
60	MG	DA	2994	1/1	0.90	0.60	6.83	52,52,52,52	0
60	MG	BA	3071	1/1	0.97	0.45	6.56	61,61,61,61	0
60	MG	DA	2937	1/1	0.97	0.33	6.48	45,45,45,45	0
60	MG	BA	2990	1/1	0.90	0.36	6.47	81,81,81,81	0
60	MG	DA	3022	1/1	0.69	0.31	6.33	81,81,81,81	0
60	MG	CA	1687	1/1	0.79	0.41	6.31	119,119,119,119	0
60	MG	DA	3052	1/1	0.97	0.27	6.30	57,57,57,57	0
60	MG	BA	3059	1/1	0.91	0.47	6.28	95,95,95,95	0
60	MG	DA	3103	1/1	0.45	0.32	6.27	82,82,82,82	0
60	MG	BA	2992	1/1	0.83	0.54	6.16	61,61,61,61	0
60	MG	BA	3135	1/1	0.94	0.47	5.93	83,83,83,83	0
60	MG	BA	3039	1/1	0.93	0.50	5.85	67,67,67,67	0
60	MG	BA	3016	1/1	0.83	0.23	5.40	102,102,102,102	0
60	MG	BF	301	1/1	0.73	0.55	5.33	100,100,100,100	0
60	MG	DA	2910	1/1	0.99	0.34	5.20	57,57,57,57	0
60	MG	CV	101	1/1	0.89	0.40	5.16	67,67,67,67	0
60	MG	AA	1635	1/1	0.78	0.30	4.91	111,111,111,111	0
60	MG	AA	1676	1/1	0.96	0.25	4.78	104,104,104,104	0
60	MG	AA	1680	1/1	0.97	0.30	4.71	75,75,75,75	0
60	MG	AA	1651	1/1	0.81	0.32	4.67	113,113,113,113	0
60	MG	BA	2916	1/1	0.91	0.30	4.64	71,71,71,71	0
60	MG	DA	2999	1/1	0.72	0.22	4.50	94,94,94,94	0
60	MG	BA	2946	1/1	0.92	0.29	4.50	66,66,66,66	0
60	MG	DA	3006	1/1	0.96	0.52	4.46	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	1613	1/1	0.76	0.41	4.04	89,89,89,89	0
60	MG	CA	1681	1/1	0.89	0.26	3.79	113,113,113,113	1
60	MG	BA	3047	1/1	0.85	0.21	3.77	105,105,105,105	0
60	MG	DA	3076	1/1	0.92	0.29	3.60	119,119,119,119	0
60	MG	DA	2946	1/1	0.96	0.32	3.41	57,57,57,57	0
60	MG	CA	1657	1/1	0.94	0.28	2.87	56,56,56,56	1
60	MG	BA	3104	1/1	0.87	0.24	2.84	115,115,115,115	0
60	MG	CA	1647	1/1	0.02	0.32	2.83	97,97,97,97	0
60	MG	AA	1620	1/1	0.84	0.24	2.77	134,134,134,134	0
60	MG	DA	3062	1/1	0.94	0.38	2.70	49,49,49,49	0
60	MG	DA	2958	1/1	0.92	0.23	2.63	96,96,96,96	0
60	MG	DA	3044	1/1	0.75	0.23	2.47	79,79,79,79	0
60	MG	DA	2941	1/1	0.95	0.24	2.39	45,45,45,45	0
60	MG	BA	3045	1/1	0.28	0.21	2.38	88,88,88,88	0
60	MG	DA	3040	1/1	0.95	0.40	2.32	64,64,64,64	0
60	MG	DA	3008	1/1	0.55	0.23	2.21	92,92,92,92	0
60	MG	DA	2943	1/1	0.94	0.25	2.18	59,59,59,59	0
60	MG	DA	2920	1/1	0.98	0.17	1.83	75,75,75,75	0
60	MG	BA	2910	1/1	0.99	0.25	1.63	75,75,75,75	0
60	MG	BA	3036	1/1	0.95	0.30	1.55	97,97,97,97	0
60	MG	DA	3001	1/1	0.84	0.28	1.48	69,69,69,69	0
60	MG	DA	3053	1/1	0.84	0.39	1.29	71,71,71,71	0
60	MG	CA	1630	1/1	0.94	0.18	1.18	105,105,105,105	0
60	MG	DF	301	1/1	0.62	0.30	1.10	100,100,100,100	0
60	MG	BA	3004	1/1	0.96	0.31	1.01	63,63,63,63	0
60	MG	BA	2951	1/1	0.93	0.22	0.84	63,63,63,63	0
60	MG	CA	1643	1/1	0.74	0.24	0.57	105,105,105,105	0
60	MG	BA	3105	1/1	0.85	0.16	0.42	68,68,68,68	0
60	MG	AA	1687	1/1	0.93	0.20	0.36	74,74,74,74	0
60	MG	DA	2997	1/1	0.88	0.18	0.29	79,79,79,79	0
60	MG	CA	1645	1/1	0.90	0.21	0.18	68,68,68,68	0
60	MG	BA	3043	1/1	0.72	0.23	0.17	83,83,83,83	0
60	MG	BA	2997	1/1	0.84	0.13	-0.17	79,79,79,79	0
60	MG	AA	1619	1/1	0.92	0.18	-0.40	72,72,72,72	0
60	MG	BP	201	1/1	0.93	0.21	-0.67	71,71,71,71	0
60	MG	DA	3101	1/1	0.84	0.12	-0.73	88,88,88,88	0
60	MG	DA	2947	1/1	0.93	0.18	-0.78	51,51,51,51	0
60	MG	CA	1608	1/1	0.81	0.17	-0.95	113,113,113,113	0
60	MG	CA	1632	1/1	0.76	0.15	-1.09	79,79,79,79	0
60	MG	CA	1616	1/1	0.74	0.17	-1.36	105,105,105,105	0
61	ZN	AD	301	1/1	0.98	0.17	-1.49	106,106,106,106	0
60	MG	DA	3017	1/1	0.73	0.12	-1.62	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	ZN	AN	101	1/1	0.94	0.04	-1.69	153,153,153,153	0
60	MG	CA	1648	1/1	0.92	0.13	-1.72	71,71,71,71	0
61	ZN	CN	101	1/1	0.92	0.04	-1.76	153,153,153,153	0
61	ZN	CD	301	1/1	0.94	0.10	-2.05	106,106,106,106	0
60	MG	CA	1651	1/1	0.94	0.10	-2.06	144,144,144,144	0
60	MG	DA	3016	1/1	0.88	0.16	-2.18	83,83,83,83	0
60	MG	CA	1609	1/1	0.76	0.14	-2.23	84,84,84,84	0
60	MG	CA	1683	1/1	0.94	0.13	-3.52	93,93,93,93	0
60	MG	AA	1673	1/1	0.91	0.09	-5.25	79,79,79,79	0
60	MG	CA	1634	1/1	0.53	0.34	-	122,122,122,122	0
60	MG	DA	3027	1/1	0.80	0.90	-	92,92,92,92	0
60	MG	AA	1694	1/1	0.96	0.54	-	102,102,102,102	0
60	MG	CA	1654	1/1	0.70	0.47	-	107,107,107,107	0
60	MG	BA	3115	1/1	0.70	0.84	-	85,85,85,85	0
60	MG	DA	3120	1/1	0.95	0.49	-	71,71,71,71	0
60	MG	BA	2958	1/1	0.98	0.18	-	76,76,76,76	0
60	MG	DA	3064	1/1	0.97	0.24	-	66,66,66,66	0
60	MG	DA	3045	1/1	0.84	0.97	-	104,104,104,104	0
60	MG	AA	1667	1/1	0.69	0.97	-	118,118,118,118	0
60	MG	DA	3028	1/1	0.94	0.56	-	123,123,123,123	0
60	MG	DA	2916	1/1	0.91	0.81	-	53,53,53,53	0
60	MG	BA	3000	1/1	0.95	0.46	-	52,52,52,52	1
60	MG	BA	3103	1/1	0.88	1.05	-	107,107,107,107	0
60	MG	BA	3090	1/1	0.68	1.40	-	123,123,123,123	0
60	MG	CA	1664	1/1	0.70	0.97	-	112,112,112,112	0
60	MG	DA	3107	1/1	0.94	0.68	-	59,59,59,59	0
60	MG	BA	3086	1/1	0.36	0.61	-	114,114,114,114	0
60	MG	CA	1684	1/1	0.88	0.38	-	101,101,101,101	0
60	MG	AA	1650	1/1	0.76	0.71	-	111,111,111,111	0
60	MG	CV	102	1/1	0.70	1.68	-	132,132,132,132	1
60	MG	DA	3059	1/1	0.89	1.06	-	110,110,110,110	0
60	MG	CA	1625	1/1	0.91	0.60	-	96,96,96,96	0
60	MG	DA	3141	1/1	0.59	0.67	-	92,92,92,92	0
60	MG	BA	2913	1/1	0.94	0.53	-	59,59,59,59	0
60	MG	DA	2905	1/1	0.93	0.45	-	59,59,59,59	0
60	MG	AA	1685	1/1	0.91	0.29	-	66,66,66,66	0
60	MG	DA	3104	1/1	0.78	0.64	-	118,118,118,118	0
60	MG	DA	3091	1/1	0.76	0.34	-	107,107,107,107	0
60	MG	DA	3118	1/1	0.83	0.64	-	73,73,73,73	0
60	MG	B1	101	1/1	0.77	0.56	-	113,113,113,113	0
60	MG	DA	3124	1/1	0.59	1.97	-	98,98,98,98	0
60	MG	AA	1670	1/1	0.71	1.40	-	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	3024	1/1	0.85	0.46	-	96,96,96,96	0
60	MG	DA	3055	1/1	0.62	0.26	-	106,106,106,106	0
60	MG	BA	3035	1/1	0.77	0.18	-	86,86,86,86	0
60	MG	DA	3081	1/1	0.45	0.57	-	104,104,104,104	0
60	MG	AA	1634	1/1	0.53	1.60	-	120,120,120,120	0
60	MG	DA	3046	1/1	0.72	0.84	-	76,76,76,76	0
60	MG	DA	2925	1/1	0.97	0.42	-	58,58,58,58	0
60	MG	CA	1692	1/1	0.05	0.67	-	117,117,117,117	0
60	MG	CA	1605	1/1	0.93	0.20	-	104,104,104,104	0
60	MG	DA	3050	1/1	0.94	1.43	-	105,105,105,105	0
60	MG	DA	3093	1/1	0.88	0.48	-	86,86,86,86	0
60	MG	BA	3060	1/1	0.79	0.87	-	83,83,83,83	0
60	MG	DA	3110	1/1	0.94	0.75	-	63,63,63,63	0
60	MG	AA	1645	1/1	0.25	1.24	-	99,99,99,99	0
60	MG	DA	3023	1/1	0.84	0.38	-	103,103,103,103	0
60	MG	DA	3030	1/1	0.93	0.32	-	101,101,101,101	0
60	MG	DA	3063	1/1	0.67	0.92	-	94,94,94,94	0
60	MG	AA	1646	1/1	0.36	0.97	-	125,125,125,125	0
60	MG	DA	3087	1/1	0.94	0.69	-	68,68,68,68	0
60	MG	CA	1689	1/1	0.78	0.69	-	75,75,75,75	0
60	MG	BA	2902	1/1	0.85	0.33	-	155,155,155,155	0
60	MG	CA	1696	1/1	0.71	1.18	-	162,162,162,162	0
60	MG	DA	3121	1/1	0.81	0.62	-	104,104,104,104	0
60	MG	BA	3072	1/1	0.86	0.85	-	89,89,89,89	0
60	MG	BA	2961	1/1	0.91	0.73	-	78,78,78,78	0
60	MG	AA	1615	1/1	0.88	0.95	-	84,84,84,84	0
60	MG	BA	2988	1/1	0.52	0.69	-	117,117,117,117	0
60	MG	AA	1693	1/1	0.80	0.96	-	119,119,119,119	0
60	MG	CA	1603	1/1	0.77	0.86	-	113,113,113,113	0
60	MG	DA	2963	1/1	0.82	0.53	-	70,70,70,70	0
60	MG	DA	2953	1/1	0.77	0.33	-	65,65,65,65	0
60	MG	BA	2991	1/1	0.92	0.48	-	122,122,122,122	0
60	MG	B5	101	1/1	0.94	0.42	-	76,76,76,76	0
60	MG	CA	1674	1/1	0.95	0.27	-	137,137,137,137	0
60	MG	BA	3091	1/1	0.90	0.45	-	79,79,79,79	0
60	MG	CA	1617	1/1	0.92	0.14	-	93,93,93,93	0
60	MG	DA	3132	1/1	0.77	0.58	-	120,120,120,120	0
60	MG	CA	1627	1/1	0.13	0.67	-	162,162,162,162	0
60	MG	BA	3022	1/1	0.72	0.46	-	125,125,125,125	0
60	MG	CA	1633	1/1	0.72	0.66	-	93,93,93,93	0
60	MG	CA	1638	1/1	0.92	0.37	-	81,81,81,81	0
60	MG	AA	1642	1/1	0.18	0.67	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	1696	1/1	0.92	0.82	-	90,90,90,90	0
60	MG	BB	201	1/1	0.45	1.05	-	84,84,84,84	0
60	MG	BA	3130	1/1	0.87	0.30	-	111,111,111,111	0
60	MG	DA	2944	1/1	0.99	0.41	-	74,74,74,74	0
60	MG	BA	3040	1/1	0.79	1.06	-	99,99,99,99	0
60	MG	AA	1700	1/1	0.93	1.33	-	111,111,111,111	0
60	MG	DA	3128	1/1	0.80	1.26	-	92,92,92,92	0
60	MG	CA	1672	1/1	0.25	0.89	-	109,109,109,109	0
60	MG	DA	3048	1/1	0.49	0.63	-	129,129,129,129	0
60	MG	DA	2923	1/1	0.96	0.29	-	52,52,52,52	0
60	MG	DA	3102	1/1	0.69	0.38	-	80,80,80,80	0
60	MG	BA	3013	1/1	0.87	0.30	-	72,72,72,72	0
60	MG	BA	3052	1/1	0.91	0.23	-	99,99,99,99	0
60	MG	AA	1636	1/1	0.64	0.76	-	142,142,142,142	0
60	MG	BA	2917	1/1	0.97	0.85	-	58,58,58,58	0
60	MG	AA	1674	1/1	0.76	0.97	-	87,87,87,87	1
60	MG	BA	3083	1/1	0.69	0.52	-	87,87,87,87	0
60	MG	BA	3018	1/1	0.69	1.54	-	109,109,109,109	0
60	MG	CA	1679	1/1	0.95	0.55	-	79,79,79,79	0
60	MG	CA	1703	1/1	0.81	0.31	-	107,107,107,107	0
60	MG	AV	101	1/1	0.77	0.57	-	83,83,83,83	1
60	MG	DA	3057	1/1	0.44	0.47	-	92,92,92,92	0
60	MG	BA	2929	1/1	0.94	0.71	-	65,65,65,65	0
60	MG	AA	1647	1/1	0.89	0.39	-	104,104,104,104	0
60	MG	BA	2920	1/1	0.76	1.17	-	98,98,98,98	0
60	MG	DA	3116	1/1	0.90	0.85	-	104,104,104,104	0
60	MG	AA	1654	1/1	0.96	0.50	-	139,139,139,139	0
60	MG	BA	2963	1/1	0.82	0.67	-	103,103,103,103	0
60	MG	AA	1703	1/1	0.90	1.31	-	102,102,102,102	0
60	MG	AA	1601	1/1	0.54	0.87	-	100,100,100,100	0
60	MG	BA	3020	1/1	0.67	0.63	-	103,103,103,103	0
60	MG	AA	1630	1/1	0.99	0.09	-	109,109,109,109	1
60	MG	B5	102	1/1	0.84	0.55	-	79,79,79,79	0
60	MG	DA	3026	1/1	0.95	0.35	-	78,78,78,78	0
60	MG	BA	3026	1/1	0.76	0.32	-	85,85,85,85	0
60	MG	DA	3089	1/1	0.80	1.22	-	92,92,92,92	0
60	MG	AA	1649	1/1	0.60	0.72	-	124,124,124,124	0
60	MG	BA	3066	1/1	0.77	0.99	-	113,113,113,113	0
60	MG	AA	1669	1/1	0.97	0.28	-	96,96,96,96	0
60	MG	CA	1635	1/1	0.94	0.12	-	98,98,98,98	0
60	MG	DA	2975	1/1	0.78	1.21	-	138,138,138,138	0
60	MG	DA	2936	1/1	0.93	0.24	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	3060	1/1	0.94	0.48	-	107,107,107,107	0
60	MG	BA	3029	1/1	0.85	0.33	-	139,139,139,139	0
60	MG	BA	3132	1/1	0.86	0.48	-	116,116,116,116	0
60	MG	BA	2976	1/1	0.81	0.50	-	66,66,66,66	0
60	MG	BA	3046	1/1	0.46	0.49	-	112,112,112,112	0
60	MG	BA	2901	1/1	0.32	0.30	-	145,145,145,145	0
60	MG	DA	3142	1/1	0.82	0.21	-	81,81,81,81	0
60	MG	AA	1633	1/1	-0.20	0.59	-	78,78,78,78	0
60	MG	BA	3063	1/1	0.36	0.63	-	136,136,136,136	0
60	MG	DA	3047	1/1	0.83	0.23	-	112,112,112,112	0
60	MG	AA	1691	1/1	0.56	0.38	-	96,96,96,96	0
60	MG	BA	2911	1/1	0.98	0.75	-	74,74,74,74	0
60	MG	DA	3058	1/1	0.51	0.49	-	104,104,104,104	0
60	MG	DA	3032	1/1	0.93	0.55	-	67,67,67,67	0
60	MG	DA	3003	1/1	0.71	0.90	-	69,69,69,69	1
60	MG	CA	1624	1/1	0.50	1.65	-	119,119,119,119	0
60	MG	AA	1688	1/1	0.83	1.13	-	113,113,113,113	0
60	MG	DA	3069	1/1	0.87	0.59	-	73,73,73,73	0
60	MG	CA	1658	1/1	0.59	0.38	-	93,93,93,93	0
60	MG	BA	3058	1/1	0.80	0.48	-	88,88,88,88	0
60	MG	DA	2939	1/1	0.98	0.51	-	41,41,41,41	0
60	MG	DA	3054	1/1	0.92	0.79	-	80,80,80,80	0
60	MG	DA	3119	1/1	0.93	0.89	-	75,75,75,75	0
60	MG	DA	3133	1/1	0.92	0.73	-	87,87,87,87	0
60	MG	DA	2969	1/1	0.70	0.83	-	84,84,84,84	0
60	MG	AA	1656	1/1	0.83	0.25	-	140,140,140,140	0
60	MG	DA	2961	1/1	0.82	0.60	-	90,90,90,90	0
60	MG	BA	3128	1/1	0.79	0.47	-	117,117,117,117	0
60	MG	DA	3019	1/1	0.57	0.88	-	112,112,112,112	0
60	MG	AA	1698	1/1	0.93	1.43	-	80,80,80,80	0
60	MG	AA	1681	1/1	0.84	0.92	-	99,99,99,99	0
60	MG	CA	1662	1/1	0.61	0.69	-	113,113,113,113	0
60	MG	BA	2952	1/1	0.83	0.83	-	87,87,87,87	0
60	MG	BA	2905	1/1	0.83	0.44	-	58,58,58,58	0
60	MG	BA	3044	1/1	0.93	0.78	-	108,108,108,108	0
60	MG	CA	1688	1/1	0.72	0.95	-	103,103,103,103	0
60	MG	DA	3043	1/1	0.79	0.30	-	96,96,96,96	0
60	MG	CA	1694	1/1	0.79	0.94	-	112,112,112,112	0
60	MG	CA	1686	1/1	0.59	0.54	-	94,94,94,94	0
60	MG	BA	3074	1/1	0.93	0.20	-	104,104,104,104	0
60	MG	DA	3024	1/1	0.74	0.73	-	106,106,106,106	0
60	MG	BA	2925	1/1	0.96	0.32	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	1698	1/1	0.43	1.20	-	145,145,145,145	0
60	MG	DA	2982	1/1	0.97	0.80	-	75,75,75,75	0
60	MG	BA	2983	1/1	0.79	0.34	-	108,108,108,108	0
60	MG	CA	1671	1/1	0.68	0.59	-	95,95,95,95	0
60	MG	DA	3126	1/1	0.94	0.79	-	76,76,76,76	0
60	MG	AA	1610	1/1	0.94	0.31	-	84,84,84,84	0
60	MG	DA	3072	1/1	0.73	0.41	-	102,102,102,102	0
60	MG	DB	201	1/1	0.73	0.43	-	69,69,69,69	0
60	MG	BA	2957	1/1	0.93	0.38	-	63,63,63,63	0
60	MG	BA	3037	1/1	0.84	0.82	-	79,79,79,79	0
60	MG	DA	3004	1/1	0.54	0.52	-	113,113,113,113	0
60	MG	CA	1621	1/1	0.95	0.13	-	96,96,96,96	0
60	MG	DA	2956	1/1	0.82	0.48	-	63,63,63,63	0
60	MG	BA	3127	1/1	0.96	0.42	-	84,84,84,84	0
60	MG	AA	1697	1/1	0.94	1.11	-	127,127,127,127	0
60	MG	DA	3099	1/1	0.47	0.62	-	108,108,108,108	0
60	MG	BA	3028	1/1	0.91	0.46	-	89,89,89,89	0
60	MG	DA	3039	1/1	0.74	0.68	-	85,85,85,85	0
60	MG	BA	3119	1/1	0.94	0.98	-	99,99,99,99	0
60	MG	AA	1640	1/1	0.83	0.51	-	64,64,64,64	1
60	MG	BA	2927	1/1	0.91	0.67	-	59,59,59,59	0
60	MG	BA	2953	1/1	0.86	1.12	-	113,113,113,113	0
60	MG	DA	2987	1/1	0.93	0.18	-	86,86,86,86	0
60	MG	AA	1613	1/1	0.84	1.48	-	114,114,114,114	0
60	MG	DA	2924	1/1	0.92	0.23	-	87,87,87,87	0
60	MG	BA	2980	1/1	0.94	0.61	-	82,82,82,82	0
60	MG	DA	3082	1/1	0.35	0.78	-	77,77,77,77	0
60	MG	DA	3068	1/1	0.67	1.08	-	102,102,102,102	0
60	MG	BA	2979	1/1	0.96	0.22	-	103,103,103,103	0
60	MG	AA	1663	1/1	0.86	0.77	-	83,83,83,83	0
60	MG	BA	3124	1/1	0.67	0.85	-	120,120,120,120	0
60	MG	BA	3096	1/1	0.74	0.33	-	84,84,84,84	0
60	MG	DA	3014	1/1	0.72	0.78	-	77,77,77,77	0
60	MG	AA	1679	1/1	0.97	0.61	-	100,100,100,100	0
60	MG	BA	3112	1/1	0.99	0.64	-	47,47,47,47	0
60	MG	BA	2932	1/1	0.87	0.36	-	61,61,61,61	0
60	MG	BA	3092	1/1	0.90	0.57	-	82,82,82,82	0
60	MG	BA	3034	1/1	0.96	0.15	-	82,82,82,82	0
60	MG	BA	3041	1/1	0.95	0.52	-	71,71,71,71	0
60	MG	BA	3084	1/1	0.45	0.86	-	126,126,126,126	0
60	MG	DA	2981	1/1	0.85	0.83	-	105,105,105,105	0
60	MG	DA	2912	1/1	0.98	0.52	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	1615	1/1	0.86	0.70	-	127,127,127,127	0
60	MG	DA	2948	1/1	0.93	0.63	-	60,60,60,60	0
60	MG	AA	1660	1/1	0.65	0.31	-	105,105,105,105	0
60	MG	DA	2960	1/1	0.86	0.66	-	59,59,59,59	0
60	MG	CA	1644	1/1	0.61	0.68	-	94,94,94,94	0
60	MG	BA	2998	1/1	0.90	0.63	-	88,88,88,88	0
60	MG	AA	1611	1/1	0.90	0.22	-	82,82,82,82	0
60	MG	CA	1677	1/1	0.56	0.86	-	88,88,88,88	0
60	MG	DA	3114	1/1	0.52	0.76	-	96,96,96,96	0
60	MG	AA	1695	1/1	0.78	0.36	-	105,105,105,105	0
60	MG	AA	1602	1/1	0.97	0.59	-	131,131,131,131	0
60	MG	BA	3019	1/1	0.84	0.39	-	74,74,74,74	0
60	MG	AA	1684	1/1	0.94	0.86	-	103,103,103,103	0
60	MG	BA	2908	1/1	0.71	1.25	-	103,103,103,103	0
60	MG	DA	2990	1/1	0.46	0.65	-	88,88,88,88	0
60	MG	BA	2984	1/1	0.81	0.85	-	95,95,95,95	0
60	MG	DA	2955	1/1	0.95	0.26	-	54,54,54,54	0
60	MG	AL	201	1/1	0.96	0.41	-	125,125,125,125	1
60	MG	BA	2959	1/1	0.95	0.48	-	59,59,59,59	0
60	MG	DA	3131	1/1	0.89	0.80	-	102,102,102,102	0
60	MG	AA	1690	1/1	0.92	0.82	-	96,96,96,96	0
60	MG	AA	1618	1/1	-0.31	0.38	-	121,121,121,121	0
60	MG	BA	2975	1/1	0.75	0.31	-	92,92,92,92	0
60	MG	BA	3117	1/1	0.95	0.49	-	72,72,72,72	0
60	MG	AA	1657	1/1	0.88	0.34	-	121,121,121,121	0
60	MG	CA	1618	1/1	0.72	0.55	-	83,83,83,83	0
60	MG	AA	1648	1/1	0.87	0.72	-	92,92,92,92	0
60	MG	AA	1638	1/1	0.37	0.13	-	139,139,139,139	1
60	MG	DA	3117	1/1	0.55	0.92	-	123,123,123,123	0
60	MG	BA	3125	1/1	0.84	0.46	-	91,91,91,91	0
60	MG	BA	3089	1/1	0.36	0.53	-	155,155,155,155	0
60	MG	AA	1641	1/1	0.58	0.59	-	93,93,93,93	0
60	MG	BA	3050	1/1	0.95	0.82	-	116,116,116,116	0
60	MG	DA	2951	1/1	0.80	1.03	-	91,91,91,91	0
60	MG	CA	1637	1/1	0.26	0.57	-	141,141,141,141	0
60	MG	D5	101	1/1	0.85	0.36	-	56,56,56,56	0
60	MG	AA	1653	1/1	0.96	0.40	-	94,94,94,94	0
60	MG	BA	3042	1/1	0.81	0.46	-	78,78,78,78	0
60	MG	DA	3112	1/1	0.89	0.81	-	83,83,83,83	0
60	MG	BA	2977	1/1	0.48	1.11	-	107,107,107,107	0
60	MG	BA	3080	1/1	0.73	0.58	-	115,115,115,115	0
60	MG	DA	2954	1/1	0.96	0.25	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	3088	1/1	0.64	0.80	-	110,110,110,110	0
60	MG	CA	1680	1/1	0.74	0.64	-	148,148,148,148	0
60	MG	AA	1689	1/1	0.72	0.27	-	98,98,98,98	0
60	MG	DA	3041	1/1	0.31	2.16	-	154,154,154,154	0
60	MG	AA	1632	1/1	0.88	0.77	-	75,75,75,75	0
60	MG	AA	1672	1/1	0.68	1.39	-	136,136,136,136	0
60	MG	AA	1699	1/1	0.80	0.64	-	109,109,109,109	0
60	MG	CA	1602	1/1	0.92	0.14	-	92,92,92,92	0
60	MG	CA	1669	1/1	0.81	0.28	-	113,113,113,113	0
60	MG	DA	3079	1/1	0.98	0.15	-	131,131,131,131	0
60	MG	BA	3005	1/1	0.94	0.70	-	85,85,85,85	0
60	MG	DA	3122	1/1	0.47	1.24	-	79,79,79,79	0
60	MG	DA	3137	1/1	0.65	0.58	-	121,121,121,121	0
60	MG	BA	3095	1/1	0.93	0.20	-	97,97,97,97	0
60	MG	DA	2993	1/1	0.91	0.31	-	79,79,79,79	0
60	MG	CA	1660	1/1	0.81	0.84	-	95,95,95,95	0
60	MG	BA	2981	1/1	0.96	0.15	-	88,88,88,88	0
60	MG	CA	1702	1/1	0.63	1.22	-	96,96,96,96	0
60	MG	BA	2982	1/1	0.78	0.26	-	100,100,100,100	0
60	MG	DA	2959	1/1	0.97	0.62	-	61,61,61,61	0
60	MG	AA	1666	1/1	0.94	0.27	-	84,84,84,84	0
60	MG	CA	1641	1/1	0.73	1.46	-	94,94,94,94	0
60	MG	BA	3053	1/1	0.47	0.81	-	122,122,122,122	0
60	MG	CA	1668	1/1	0.47	0.32	-	93,93,93,93	0
60	MG	CA	1653	1/1	0.66	0.61	-	127,127,127,127	0
60	MG	DA	2949	1/1	0.75	0.91	-	102,102,102,102	0
60	MG	BA	3075	1/1	0.86	0.19	-	100,100,100,100	0
60	MG	DA	3073	1/1	0.93	0.56	-	87,87,87,87	0
60	MG	DA	2931	1/1	0.94	0.44	-	52,52,52,52	0
60	MG	BA	2978	1/1	0.93	0.81	-	134,134,134,134	0
60	MG	CA	1665	1/1	0.50	0.60	-	111,111,111,111	1
60	MG	AA	1659	1/1	0.92	1.13	-	113,113,113,113	0
60	MG	BA	3069	1/1	0.94	0.18	-	87,87,87,87	0
60	MG	BA	2947	1/1	0.98	0.65	-	88,88,88,88	0
60	MG	DA	3031	1/1	0.68	0.83	-	92,92,92,92	0
60	MG	BA	3049	1/1	0.84	0.44	-	65,65,65,65	0
60	MG	BA	3065	1/1	0.93	1.01	-	122,122,122,122	0
60	MG	BA	3134	1/1	0.95	0.73	-	75,75,75,75	0
60	MG	AA	1621	1/1	0.87	0.38	-	95,95,95,95	0
60	MG	DA	3018	1/1	0.51	0.42	-	114,114,114,114	0
60	MG	DA	3095	1/1	0.91	0.34	-	98,98,98,98	0
60	MG	DA	2977	1/1	0.97	0.15	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	2980	1/1	0.83	1.16	-	111,111,111,111	0
60	MG	BA	3109	1/1	0.72	0.59	-	101,101,101,101	0
60	MG	CA	1629	1/1	0.76	0.98	-	95,95,95,95	0
60	MG	DA	2919	1/1	0.95	0.85	-	73,73,73,73	0
60	MG	BA	3017	1/1	0.12	0.65	-	117,117,117,117	0
60	MG	DA	3051	1/1	0.98	0.29	-	56,56,56,56	0
60	MG	BA	2935	1/1	0.99	0.50	-	110,110,110,110	0
60	MG	DA	2992	1/1	0.85	0.38	-	75,75,75,75	0
60	MG	DA	2901	1/1	0.40	0.79	-	136,136,136,136	0
60	MG	DA	3086	1/1	0.83	0.55	-	78,78,78,78	0
60	MG	BA	3009	1/1	0.89	0.97	-	117,117,117,117	0
60	MG	DA	2908	1/1	0.90	0.93	-	83,83,83,83	0
60	MG	BA	2931	1/1	0.90	0.41	-	72,72,72,72	0
60	MG	DA	2984	1/1	0.86	0.60	-	120,120,120,120	0
60	MG	CA	1642	1/1	0.87	1.27	-	97,97,97,97	0
60	MG	DA	3123	1/1	0.96	0.63	-	82,82,82,82	0
60	MG	BA	3010	1/1	0.96	0.43	-	88,88,88,88	0
60	MG	DA	3033	1/1	0.88	0.19	-	100,100,100,100	0
60	MG	AX	101	1/1	0.94	0.74	-	96,96,96,96	0
60	MG	DA	2934	1/1	0.98	0.40	-	86,86,86,86	0
60	MG	BA	3033	1/1	0.96	0.41	-	92,92,92,92	0
60	MG	DA	3100	1/1	0.70	0.82	-	113,113,113,113	0
60	MG	BA	3055	1/1	0.85	0.62	-	87,87,87,87	0
60	MG	DA	3021	1/1	0.87	0.28	-	81,81,81,81	0
60	MG	DA	3106	1/1	0.59	0.78	-	143,143,143,143	0
60	MG	DA	2966	1/1	0.98	0.69	-	48,48,48,48	0
60	MG	BA	2956	1/1	0.94	0.61	-	64,64,64,64	0
60	MG	DA	3078	1/1	0.87	0.71	-	122,122,122,122	0
60	MG	CA	1675	1/1	0.80	0.31	-	122,122,122,122	0
60	MG	BA	3067	1/1	0.94	0.22	-	93,93,93,93	0
60	MG	BA	3087	1/1	0.88	0.96	-	112,112,112,112	0
60	MG	DA	3002	1/1	0.77	0.36	-	95,95,95,95	0
60	MG	AA	1614	1/1	0.78	0.58	-	98,98,98,98	0
60	MG	BA	2970	1/1	0.70	1.24	-	86,86,86,86	0
60	MG	CA	1649	1/1	0.96	0.11	-	82,82,82,82	0
60	MG	BB	202	1/1	0.89	0.89	-	117,117,117,117	0
60	MG	BA	3023	1/1	0.88	1.15	-	79,79,79,79	0
60	MG	BA	3054	1/1	0.93	0.41	-	94,94,94,94	0
60	MG	AA	1677	1/1	0.68	0.24	-	114,114,114,114	0
60	MG	BA	3073	1/1	0.79	0.29	-	100,100,100,100	0
60	MG	DA	3007	1/1	0.84	0.26	-	82,82,82,82	0
60	MG	DA	3138	1/1	0.91	0.42	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	3000	1/1	0.83	0.52	-	77,77,77,77	0
60	MG	DA	3098	1/1	0.61	0.61	-	107,107,107,107	0
60	MG	DA	2983	1/1	0.92	0.32	-	93,93,93,93	0
60	MG	DA	2962	1/1	0.74	0.48	-	89,89,89,89	0
60	MG	CA	1601	1/1	0.63	0.87	-	86,86,86,86	0
60	MG	BA	2938	1/1	0.87	0.30	-	67,67,67,67	0
60	MG	CA	1673	1/1	0.94	0.48	-	116,116,116,116	0
60	MG	AA	1627	1/1	0.38	1.23	-	101,101,101,101	0
60	MG	DA	3090	1/1	0.66	0.69	-	106,106,106,106	0
60	MG	AA	1626	1/1	0.94	0.17	-	99,99,99,99	0
60	MG	DA	3085	1/1	0.78	0.51	-	86,86,86,86	0
60	MG	AA	1631	1/1	0.88	0.69	-	87,87,87,87	0
60	MG	BA	2999	1/1	0.91	0.77	-	121,121,121,121	0
60	MG	BA	3108	1/1	0.70	0.48	-	102,102,102,102	0
60	MG	DA	2926	1/1	0.96	0.74	-	47,47,47,47	0
60	MG	DA	3080	1/1	0.69	0.75	-	130,130,130,130	0
60	MG	DA	2902	1/1	0.95	0.15	-	152,152,152,152	0
60	MG	AA	1665	1/1	0.39	2.52	-	121,121,121,121	0
60	MG	CG	201	1/1	0.65	0.53	-	83,83,83,83	1
60	MG	BA	2964	1/1	0.93	0.42	-	80,80,80,80	0
60	MG	AA	1612	1/1	0.18	1.12	-	102,102,102,102	0
60	MG	CA	1652	1/1	0.82	0.79	-	148,148,148,148	0
60	MG	BA	2948	1/1	0.91	0.35	-	67,67,67,67	0
60	MG	AA	1624	1/1	0.71	0.65	-	111,111,111,111	0
60	MG	BA	3062	1/1	0.81	0.62	-	89,89,89,89	0
60	MG	CA	1691	1/1	0.57	1.45	-	105,105,105,105	0
60	MG	BA	3097	1/1	0.34	0.37	-	88,88,88,88	0
60	MG	BA	2926	1/1	0.97	0.41	-	58,58,58,58	0
60	MG	DA	3136	1/1	0.84	0.22	-	94,94,94,94	0
60	MG	DA	3061	1/1	0.74	0.45	-	94,94,94,94	0
60	MG	BA	3120	1/1	0.77	0.51	-	111,111,111,111	0
60	MG	AA	1639	1/1	0.85	0.41	-	98,98,98,98	1
60	MG	BA	2965	1/1	0.75	0.40	-	111,111,111,111	0
60	MG	CA	1646	1/1	0.88	0.55	-	119,119,119,119	0
60	MG	DA	3013	1/1	0.82	0.98	-	89,89,89,89	0
60	MG	DA	3134	1/1	0.88	0.73	-	89,89,89,89	0
60	MG	AA	1609	1/1	0.81	0.86	-	106,106,106,106	0
60	MG	CA	1619	1/1	0.98	0.10	-	67,67,67,67	0
60	MG	AA	1655	1/1	0.93	0.36	-	94,94,94,94	1
60	MG	DA	3066	1/1	0.98	0.52	-	102,102,102,102	0
60	MG	BA	3002	1/1	0.75	1.08	-	97,97,97,97	0
60	MG	BA	3129	1/1	0.73	0.63	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	1606	1/1	0.55	0.49	-	118,118,118,118	0
60	MG	CA	1636	1/1	0.76	0.51	-	90,90,90,90	0
60	MG	AA	1625	1/1	0.79	0.46	-	85,85,85,85	0
60	MG	DA	3010	1/1	0.59	0.59	-	92,92,92,92	0
60	MG	DX	101	1/1	0.73	0.73	-	72,72,72,72	1
60	MG	DA	2988	1/1	0.96	0.22	-	111,111,111,111	0
60	MG	DA	3139	1/1	0.97	0.87	-	69,69,69,69	0
60	MG	DA	3070	1/1	0.70	0.83	-	79,79,79,79	0
60	MG	BA	3113	1/1	0.74	0.34	-	126,126,126,126	0
60	MG	DA	3015	1/1	0.87	0.48	-	76,76,76,76	0
60	MG	DA	2928	1/1	0.96	0.41	-	42,42,42,42	0
60	MG	B0	101	1/1	0.82	0.50	-	98,98,98,98	0
60	MG	CA	1682	1/1	0.86	0.15	-	151,151,151,151	0
60	MG	BA	3111	1/1	0.91	0.93	-	103,103,103,103	0
60	MG	BA	3099	1/1	0.96	0.25	-	117,117,117,117	0
60	MG	BA	2986	1/1	0.95	0.63	-	81,81,81,81	0
60	MG	BA	2914	1/1	0.96	0.39	-	83,83,83,83	0
60	MG	CA	1607	1/1	-0.06	0.42	-	101,101,101,101	0
60	MG	BA	3094	1/1	0.05	0.97	-	100,100,100,100	0
60	MG	DA	2991	1/1	0.48	0.42	-	126,126,126,126	0
60	MG	DA	2986	1/1	0.48	0.76	-	87,87,87,87	0
60	MG	BA	3048	1/1	0.98	0.27	-	87,87,87,87	0
60	MG	DA	2970	1/1	0.91	0.13	-	47,47,47,47	0
60	MG	DA	3115	1/1	0.60	0.50	-	162,162,162,162	0
60	MG	BA	2906	1/1	0.93	0.40	-	100,100,100,100	0
60	MG	AA	1678	1/1	0.86	0.54	-	121,121,121,121	0
60	MG	BA	3012	1/1	0.68	1.21	-	91,91,91,91	0
60	MG	CA	1623	1/1	0.72	0.20	-	82,82,82,82	0
60	MG	CA	1690	1/1	0.55	0.80	-	100,100,100,100	0
60	MG	DA	3020	1/1	0.89	0.23	-	50,50,50,50	0
60	MG	CA	1659	1/1	0.66	0.35	-	104,104,104,104	1
60	MG	DA	3084	1/1	0.98	0.21	-	103,103,103,103	0
60	MG	BA	3008	1/1	0.74	0.67	-	96,96,96,96	0
60	MG	DA	3036	1/1	0.95	0.51	-	59,59,59,59	0
60	MG	BA	3021	1/1	0.89	0.14	-	79,79,79,79	0
60	MG	CA	1670	1/1	0.75	0.09	-	153,153,153,153	0
60	MG	AA	1604	1/1	0.65	0.39	-	132,132,132,132	0
60	MG	BA	3123	1/1	0.77	0.60	-	80,80,80,80	0
60	MG	BA	3118	1/1	0.82	1.49	-	110,110,110,110	0
60	MG	BA	3070	1/1	0.94	0.86	-	118,118,118,118	0
60	MG	BA	3031	1/1	0.88	0.85	-	108,108,108,108	0
60	MG	DA	2952	1/1	0.98	0.47	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	2922	1/1	0.92	0.41	-	59,59,59,59	0
60	MG	CA	1640	1/1	-0.11	1.19	-	102,102,102,102	0
60	MG	BA	3131	1/1	0.90	0.59	-	79,79,79,79	0
60	MG	CA	1650	1/1	0.36	1.29	-	127,127,127,127	0
60	MG	CA	1604	1/1	0.62	0.71	-	115,115,115,115	0
60	MG	DA	3125	1/1	0.78	0.40	-	72,72,72,72	0
60	MG	DA	3097	1/1	0.69	0.54	-	112,112,112,112	0
60	MG	BA	2962	1/1	0.94	0.76	-	64,64,64,64	0
60	MG	AA	1668	1/1	0.92	0.61	-	109,109,109,109	0
60	MG	AA	1661	1/1	0.76	0.96	-	94,94,94,94	0
60	MG	BA	2924	1/1	0.98	0.27	-	52,52,52,52	0
60	MG	BX	101	1/1	0.83	1.30	-	110,110,110,110	1
60	MG	AA	1682	1/1	0.96	0.39	-	98,98,98,98	0
60	MG	BA	3011	1/1	0.75	0.77	-	106,106,106,106	0
60	MG	DA	2906	1/1	0.97	0.33	-	67,67,67,67	0
60	MG	BA	3056	1/1	0.93	0.27	-	55,55,55,55	0
60	MG	BA	3085	1/1	0.81	0.58	-	118,118,118,118	0
60	MG	DA	2913	1/1	0.92	0.49	-	70,70,70,70	0
60	MG	CL	201	1/1	0.93	0.51	-	87,87,87,87	1
60	MG	DA	2989	1/1	0.93	0.58	-	79,79,79,79	0
60	MG	CA	1666	1/1	-0.01	0.59	-	137,137,137,137	1
60	MG	AA	1683	1/1	0.93	0.43	-	89,89,89,89	0
60	MG	BA	3001	1/1	0.33	0.20	-	157,157,157,157	0
60	MG	AA	1644	1/1	0.98	0.09	-	141,141,141,141	0
60	MG	CA	1611	1/1	0.83	0.42	-	97,97,97,97	0
60	MG	BA	2985	1/1	0.62	0.36	-	87,87,87,87	0
60	MG	CA	1693	1/1	0.95	0.55	-	65,65,65,65	0
60	MG	BA	2989	1/1	0.93	0.68	-	87,87,87,87	0
60	MG	AA	1692	1/1	0.93	1.16	-	101,101,101,101	0
60	MG	DA	3009	1/1	-0.07	0.87	-	168,168,168,168	0
60	MG	CA	1661	1/1	0.92	0.42	-	81,81,81,81	0
60	MG	DA	3049	1/1	0.90	0.50	-	85,85,85,85	0
60	MG	DA	2930	1/1	0.96	0.47	-	55,55,55,55	0
60	MG	BA	3126	1/1	0.56	1.74	-	131,131,131,131	0
60	MG	DA	3129	1/1	0.96	0.28	-	113,113,113,113	0
60	MG	DA	3056	1/1	0.73	0.47	-	126,126,126,126	0
60	MG	AA	1607	1/1	0.92	0.16	-	107,107,107,107	0
60	MG	DA	2976	1/1	0.99	0.67	-	53,53,53,53	0
60	MG	CA	1639	1/1	0.59	0.37	-	99,99,99,99	0
60	MG	DA	3034	1/1	0.78	0.29	-	72,72,72,72	0
60	MG	DA	3071	1/1	0.54	0.86	-	123,123,123,123	0
60	MG	BA	2971	1/1	0.84	0.13	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	1631	1/1	0.80	0.98	-	111,111,111,111	0
60	MG	CA	1667	1/1	0.46	1.44	-	83,83,83,83	1
60	MG	AA	1675	1/1	0.51	0.43	-	93,93,93,93	0
60	MG	AA	1637	1/1	0.84	0.55	-	99,99,99,99	0
60	MG	BA	3093	1/1	0.55	0.79	-	99,99,99,99	0
60	MG	CA	1685	1/1	0.74	0.34	-	115,115,115,115	0
60	MG	BA	3114	1/1	0.68	1.61	-	130,130,130,130	0
60	MG	BA	3032	1/1	0.76	0.70	-	98,98,98,98	0
60	MG	CA	1676	1/1	0.92	0.32	-	119,119,119,119	0
60	MG	DA	3140	1/1	0.96	0.69	-	77,77,77,77	0
60	MG	AA	1606	1/1	0.57	1.07	-	98,98,98,98	0
60	MG	CA	1697	1/1	0.84	0.87	-	126,126,126,126	0
60	MG	DA	2945	1/1	0.93	0.22	-	57,57,57,57	0
60	MG	DA	3135	1/1	0.61	1.44	-	103,103,103,103	0
60	MG	CA	1699	1/1	0.74	0.38	-	134,134,134,134	0
60	MG	BA	2941	1/1	0.95	0.58	-	49,49,49,49	0
60	MG	DA	2964	1/1	0.15	1.25	-	109,109,109,109	0
60	MG	BA	3007	1/1	0.68	0.32	-	125,125,125,125	0
60	MG	AA	1664	1/1	0.87	0.26	-	90,90,90,90	0
60	MG	BA	2923	1/1	0.96	0.50	-	78,78,78,78	0
60	MG	DA	3011	1/1	0.87	0.38	-	88,88,88,88	0
60	MG	BA	3068	1/1	0.87	1.40	-	103,103,103,103	0
60	MG	BA	3081	1/1	0.78	0.64	-	103,103,103,103	0
60	MG	BA	3061	1/1	0.93	0.62	-	71,71,71,71	0
60	MG	BA	3076	1/1	0.84	0.57	-	108,108,108,108	0
60	MG	CA	1610	1/1	0.86	0.20	-	116,116,116,116	0
60	MG	BA	3101	1/1	0.21	0.83	-	123,123,123,123	0
60	MG	DA	3130	1/1	0.91	1.39	-	115,115,115,115	0
60	MG	BA	3051	1/1	0.35	0.75	-	72,72,72,72	0
60	MG	DA	2985	1/1	0.89	0.27	-	85,85,85,85	0
60	MG	BA	3116	1/1	0.90	0.27	-	91,91,91,91	0
60	MG	BA	3106	1/1	0.70	0.74	-	97,97,97,97	0
60	MG	AA	1701	1/1	0.90	0.65	-	71,71,71,71	0
60	MG	AA	1643	1/1	0.51	0.65	-	106,106,106,106	0
60	MG	CA	1620	1/1	0.94	1.10	-	115,115,115,115	0
60	MG	DA	3127	1/1	0.87	1.23	-	112,112,112,112	0
60	MG	CA	1700	1/1	0.63	0.52	-	113,113,113,113	0
60	MG	BA	3121	1/1	0.63	0.47	-	112,112,112,112	0
60	MG	DA	3012	1/1	0.98	0.30	-	53,53,53,53	0
60	MG	BA	2950	1/1	0.83	0.93	-	81,81,81,81	0
60	MG	CA	1695	1/1	0.93	0.73	-	80,80,80,80	0
60	MG	DA	3113	1/1	0.94	0.49	-	96,96,96,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.