



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

PDB ID : 4V84
Title : Crystal structure of a complex containing domain 3 of CrPV IGR IRES RNA bound to the 70S ribosome.
Authors : Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.
Deposited on : 2010-12-13
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

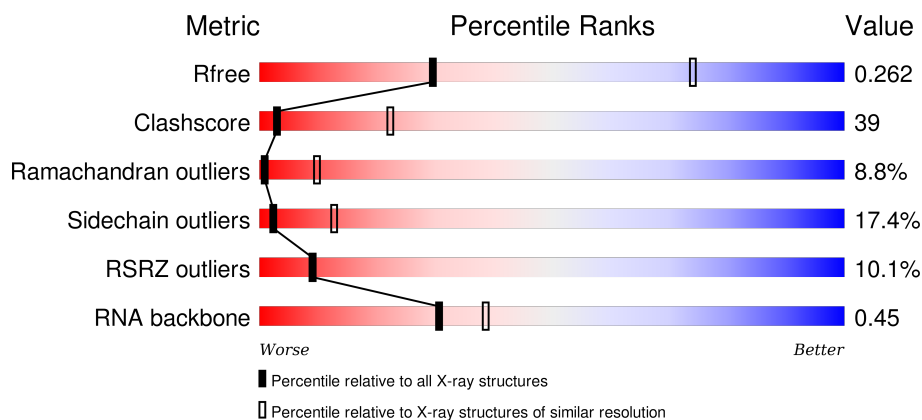
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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 ≥ 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	1506	<div> <div>4%</div> <div>20%</div> <div>63%</div> <div>16%</div> <div>.</div> </div>
1	CA	1506	<div> <div>7%</div> <div>19%</div> <div>64%</div> <div>18%</div> </div>
2	AB	234	<div> <div>20%</div> <div>33%</div> <div>53%</div> <div>13%</div> </div>
2	CB	234	<div> <div>21%</div> <div>32%</div> <div>56%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	208	
4	CD	208	
5	AE	151	
5	CE	151	
6	AF	101	
6	CF	101	
7	AG	155	
7	CG	155	
8	AH	138	
8	CH	138	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	119	
11	CK	119	
12	AL	124	
12	CL	124	
13	AM	116	
13	CM	116	
14	AN	60	
14	CN	60	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	83	
16	CP	83	
17	AQ	99	
17	CQ	99	
18	AR	70	
18	CR	70	
19	AS	78	
19	CS	78	
20	AT	99	
20	CT	99	
21	AU	24	
21	CU	24	
22	AV	43	
22	CV	43	
23	BA	2879	
23	DA	2879	
24	BB	119	
24	DB	119	
25	BC	271	
25	DC	271	
26	BD	204	
26	DD	204	
27	BE	202	
27	DE	202	

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Mol	Chain	Length	Quality of chain
28	BF	181	
28	DF	181	
29	BG	159	
29	DG	159	
30	BH	145	
30	DH	145	
31	BI	65	
31	DI	65	
32	BJ	137	
32	DJ	137	
33	BK	122	
33	DK	122	
34	BL	146	
34	DL	146	
35	BM	136	
35	DM	136	
36	BN	117	
36	DN	117	
37	BO	98	
37	DO	98	
38	BP	137	
38	DP	137	
39	BQ	116	
39	DQ	116	
40	BR	101	

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Mol	Chain	Length	Quality of chain
40	DR	101	
41	BS	112	
41	DS	112	
42	BT	92	
42	DT	92	
43	BU	100	
43	DU	100	
44	BV	188	
44	DV	188	
45	BW	76	
45	DW	76	
46	BX	88	
46	DX	88	
47	BY	62	
47	DY	62	
48	BZ	59	
48	DZ	59	
49	B1	30	
49	D1	30	
50	B2	52	
50	D2	52	
51	B3	44	
51	D3	44	
52	B4	48	
52	D4	48	

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Mol	Chain	Length	Quality of chain
53	B5	63	
53	D5	63	

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
54	MG	AA	1601	-	-	-	X
54	MG	AA	1603	-	-	-	X
54	MG	AA	1621	-	-	-	X
54	MG	AA	1622	-	-	-	X
54	MG	AA	1624	-	-	-	X
54	MG	AA	1630	-	-	-	X
54	MG	AA	1636	-	-	-	X
54	MG	AA	1637	-	-	-	X
54	MG	AA	1647	-	-	-	X
54	MG	AA	1650	-	-	-	X
54	MG	AA	1679	-	-	-	X
54	MG	AA	1682	-	-	-	X
54	MG	AA	1695	-	-	-	X
54	MG	AA	1707	-	-	-	X
54	MG	AA	1713	-	-	-	X
54	MG	AA	1714	-	-	-	X
54	MG	AA	1721	-	-	-	X
54	MG	AA	1723	-	-	-	X
54	MG	AA	1728	-	-	-	X
54	MG	AA	1731	-	-	-	X
54	MG	AA	1742	-	-	-	X
54	MG	AA	1752	-	-	-	X
54	MG	BA	2901	-	-	-	X
54	MG	BA	2903	-	-	-	X
54	MG	BA	2904	-	-	-	X
54	MG	BA	2908	-	-	-	X
54	MG	BA	2909	-	-	-	X
54	MG	BA	2910	-	-	-	X
54	MG	BA	2911	-	-	-	X
54	MG	BA	2913	-	-	-	X
54	MG	BA	2914	-	-	-	X
54	MG	BA	2916	-	-	-	X
54	MG	BA	2917	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	2918	-	-	-	X
54	MG	BA	2920	-	-	-	X
54	MG	BA	2921	-	-	-	X
54	MG	BA	2922	-	-	-	X
54	MG	BA	2924	-	-	-	X
54	MG	BA	2925	-	-	-	X
54	MG	BA	2930	-	-	-	X
54	MG	BA	2931	-	-	-	X
54	MG	BA	2940	-	-	-	X
54	MG	BA	2941	-	-	-	X
54	MG	BA	2943	-	-	-	X
54	MG	BA	2952	-	-	-	X
54	MG	BA	2961	-	-	-	X
54	MG	BA	2967	-	-	-	X
54	MG	BA	2968	-	-	-	X
54	MG	BA	2970	-	-	-	X
54	MG	BA	2979	-	-	-	X
54	MG	BA	2980	-	-	-	X
54	MG	BA	2982	-	-	-	X
54	MG	BA	2998	-	-	-	X
54	MG	BA	2999	-	-	-	X
54	MG	BA	3004	-	-	-	X
54	MG	BA	3006	-	-	-	X
54	MG	BA	3019	-	-	-	X
54	MG	BA	3027	-	-	-	X
54	MG	BA	3046	-	-	-	X
54	MG	BA	3052	-	-	-	X
54	MG	BA	3088	-	-	-	X
54	MG	BA	3090	-	-	-	X
54	MG	BA	3091	-	-	-	X
54	MG	BA	3097	-	-	-	X
54	MG	BA	3118	-	-	-	X
54	MG	BA	3151	-	-	-	X
54	MG	BA	3152	-	-	-	X
54	MG	BA	3179	-	-	-	X
54	MG	BA	3180	-	-	-	X
54	MG	BA	3181	-	-	-	X
54	MG	BA	3182	-	-	-	X
54	MG	BA	3184	-	-	-	X
54	MG	BA	3185	-	-	-	X
54	MG	BA	3186	-	-	-	X
54	MG	BA	3188	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3192	-	-	-	X
54	MG	BA	3204	-	-	-	X
54	MG	BA	3208	-	-	-	X
54	MG	BA	3220	-	-	-	X
54	MG	BA	3222	-	-	-	X
54	MG	BA	3226	-	-	-	X
54	MG	BA	3232	-	-	-	X
54	MG	BA	3242	-	-	-	X
54	MG	BA	3256	-	-	-	X
54	MG	BA	3257	-	-	-	X
54	MG	BA	3268	-	-	-	X
54	MG	BA	3270	-	-	-	X
54	MG	BA	3277	-	-	-	X
54	MG	BA	3284	-	-	-	X
54	MG	CA	1607	-	-	-	X
54	MG	CA	1609	-	-	-	X
54	MG	CA	1612	-	-	-	X
54	MG	CA	1617	-	-	-	X
54	MG	CA	1672	-	-	-	X
54	MG	CA	1691	-	-	-	X
54	MG	CA	1692	-	-	-	X
54	MG	CA	1698	-	-	-	X
54	MG	CA	1703	-	-	-	X
54	MG	CA	1715	-	-	-	X
54	MG	CA	1717	-	-	-	X
54	MG	DA	2901	-	-	-	X
54	MG	DA	2902	-	-	-	X
54	MG	DA	2904	-	-	-	X
54	MG	DA	2905	-	-	-	X
54	MG	DA	2906	-	-	-	X
54	MG	DA	2907	-	-	-	X
54	MG	DA	2908	-	-	-	X
54	MG	DA	2909	-	-	-	X
54	MG	DA	2911	-	-	-	X
54	MG	DA	2914	-	-	-	X
54	MG	DA	2915	-	-	-	X
54	MG	DA	2916	-	-	-	X
54	MG	DA	2917	-	-	-	X
54	MG	DA	2918	-	-	-	X
54	MG	DA	2921	-	-	-	X
54	MG	DA	2927	-	-	-	X
54	MG	DA	2932	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	2933	-	-	-	X
54	MG	DA	2934	-	-	-	X
54	MG	DA	2943	-	-	-	X
54	MG	DA	2944	-	-	-	X
54	MG	DA	2950	-	-	-	X
54	MG	DA	2955	-	-	-	X
54	MG	DA	2959	-	-	-	X
54	MG	DA	2965	-	-	-	X
54	MG	DA	2966	-	-	-	X
54	MG	DA	2968	-	-	-	X
54	MG	DA	2971	-	-	-	X
54	MG	DA	2976	-	-	-	X
54	MG	DA	2978	-	-	-	X
54	MG	DA	2989	-	-	-	X
54	MG	DA	2999	-	-	-	X
54	MG	DA	3000	-	-	-	X
54	MG	DA	3003	-	-	-	X
54	MG	DA	3012	-	-	-	X
54	MG	DA	3022	-	-	-	X
54	MG	DA	3023	-	-	-	X
54	MG	DA	3024	-	-	-	X
54	MG	DA	3033	-	-	-	X
54	MG	DA	3034	-	-	-	X
54	MG	DA	3036	-	-	-	X
54	MG	DA	3039	-	-	-	X
54	MG	DA	3047	-	-	-	X
54	MG	DA	3066	-	-	-	X
54	MG	DA	3070	-	-	-	X
54	MG	DA	3072	-	-	-	X
54	MG	DA	3079	-	-	-	X
54	MG	DA	3082	-	-	-	X
54	MG	DA	3083	-	-	-	X
54	MG	DA	3101	-	-	-	X
54	MG	DA	3105	-	-	-	X
54	MG	DA	3149	-	-	-	X
54	MG	DA	3154	-	-	-	X
54	MG	DA	3165	-	-	-	X
54	MG	DA	3174	-	-	-	X
54	MG	DA	3188	-	-	-	X
54	MG	DA	3190	-	-	-	X
54	MG	DA	3191	-	-	-	X
54	MG	DA	3192	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3198	-	-	-	X
54	MG	DA	3201	-	-	-	X
54	MG	DA	3202	-	-	-	X
54	MG	DA	3208	-	-	-	X
54	MG	DA	3214	-	-	-	X
54	MG	DA	3215	-	-	-	X
54	MG	DA	3216	-	-	-	X
54	MG	DA	3223	-	-	-	X
54	MG	DA	3228	-	-	-	X
54	MG	DA	3232	-	-	-	X
54	MG	DA	3241	-	-	-	X
54	MG	DA	3251	-	-	-	X
54	MG	DA	3259	-	-	-	X
54	MG	DA	3272	-	-	-	X
54	MG	DA	3274	-	-	-	X
54	MG	DA	3298	-	-	-	X
54	MG	DA	3304	-	-	-	X
54	MG	DA	3306	-	-	-	X
54	MG	DA	3310	-	-	-	X
54	MG	DA	3313	-	-	-	X
54	MG	DA	3324	-	-	-	X
54	MG	DG	201	-	-	-	X

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 282142 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 ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	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	0
			1156	729	218	205	4			
5	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	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	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			
13	CM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	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	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			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	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 21 is a protein called domain 3 of CrPV IGR IRES RNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			
21	CU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	34	Total	C	N	O	P	0	0	0
			719	323	125	238	33			
22	CV	34	Total	C	N	O	P	0	0	0
			719	323	125	238	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2760	Total	C	N	O	P	0	0	0
			59440	26455	11114	19112	2759			
23	DA	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1142	U	C	SEE REMARK 999	GB AE017221.1
BA	2825	U	G	SEE REMARK 999	GB AE017221.1
DA	1142	U	C	SEE REMARK 999	GB AE017221.1
DA	2825	U	G	SEE REMARK 999	GB AE017221.1

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	DC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
26	DD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
27	DE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
28	DF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
29	DG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
30	DH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BI	32	Total	C	N	O	0	0	0
			254	157	49	48			
31	DI	32	Total	C	N	O	0	0	0
			254	157	49	48			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
32	DJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
33	DK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
34	DL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
35	DM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BN	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	DN	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BO	98	Total	C	N	O	0	0	0
			771	486	154	131			
37	DO	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			
38	DP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			
39	DQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	PHE	DELETION	UNP Q72L76
DQ	?	-	PHE	DELETION	UNP Q72L76

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	DR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
41	DS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O		0	0	0
			726	471	131	124				
42	DT	92	Total	C	N	O		0	0	0
			726	471	131	124				

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
43	DU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			
44	DV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
45	DW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	88	Total	C	N	O	0	0	0
			695	435	141	119			
46	DX	88	Total	C	N	O	0	0	0
			695	435	141	119			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
47	DY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
48	DZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
49	D1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
50	D2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	D3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
52	D4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
53	D5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	17	Total	Mg	0	0
			17	17		
54	DE	1	Total	Mg	0	0
			1	1		
54	BA	408	Total	Mg	0	0
			408	408		
54	CA	140	Total	Mg	0	0
			140	140		
54	DG	1	Total	Mg	0	0
			1	1		
54	CV	1	Total	Mg	0	0
			1	1		
54	AV	4	Total	Mg	0	0
			4	4		
54	D2	1	Total	Mg	0	0
			1	1		
54	DA	436	Total	Mg	0	0
			436	436		
54	B2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CP	1	Total 1	Mg 1	0	0
54	AA	163	Total 163	Mg 163	0	0
54	D4	1	Total 1	Mg 1	0	0
54	BK	1	Total 1	Mg 1	0	0
54	AD	1	Total 1	Mg 1	0	0
54	DB	17	Total 17	Mg 17	0	0

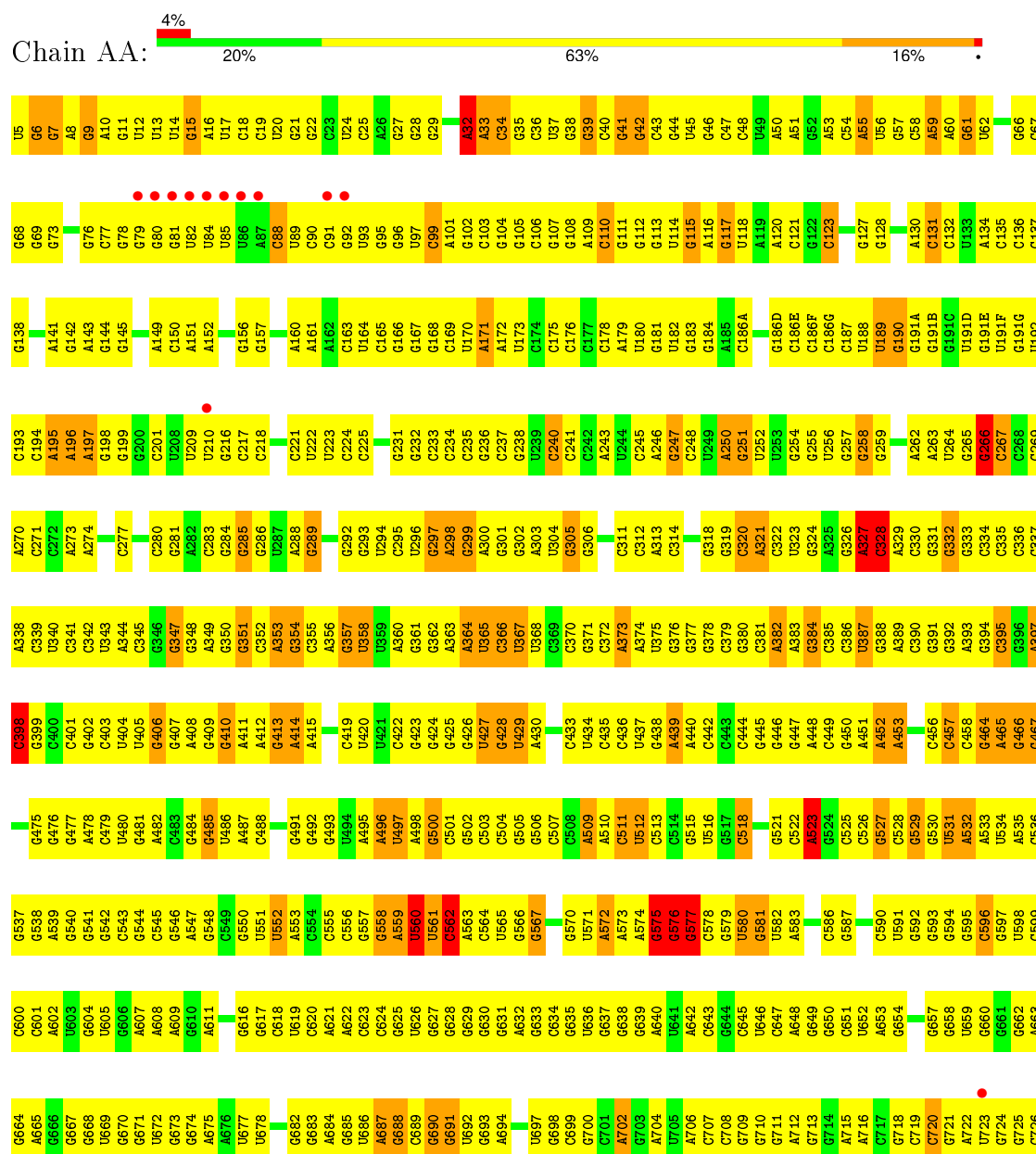
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

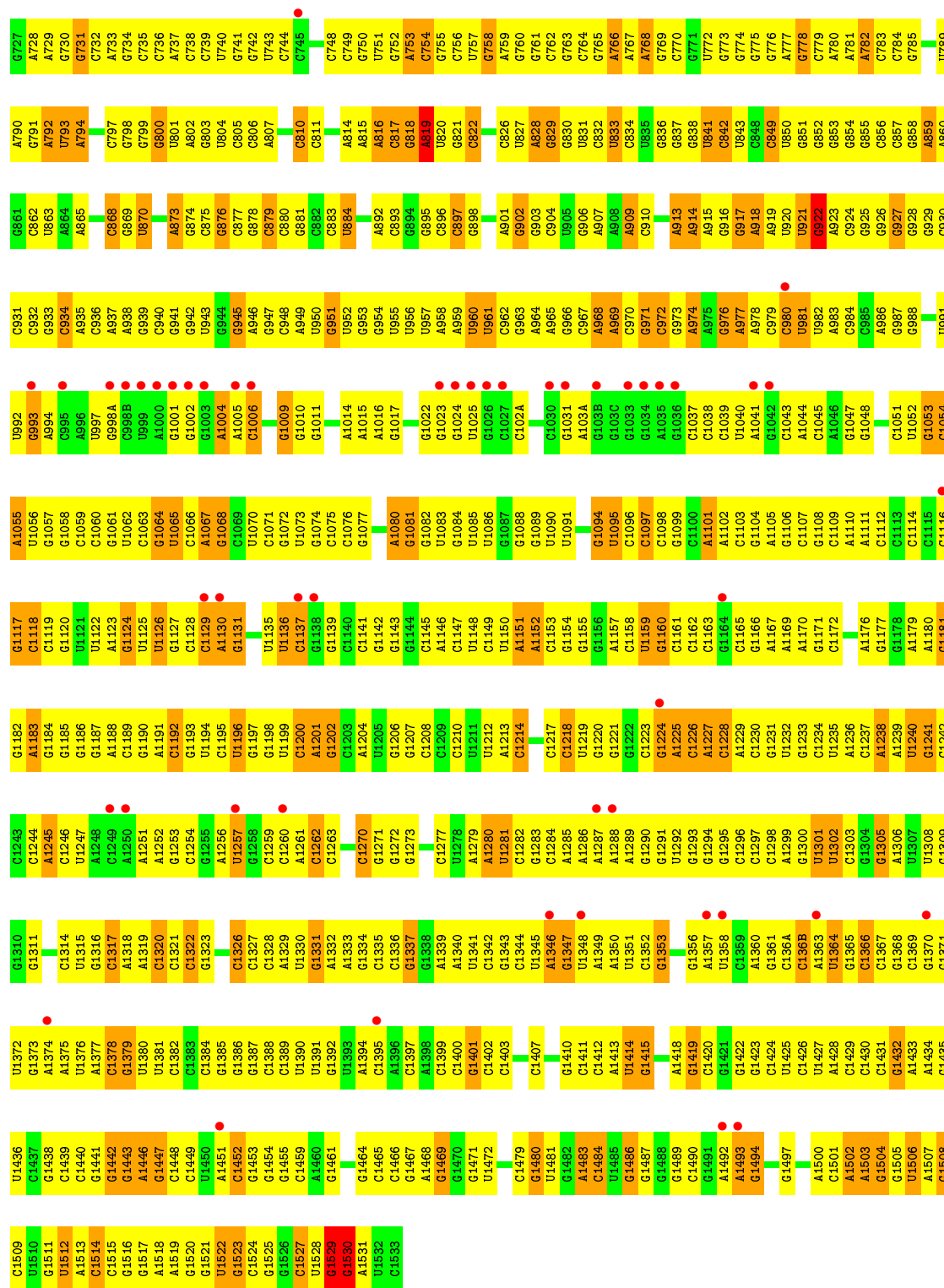
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CN	1	Total 1	Zn 1	0	0
55	AD	1	Total 1	Zn 1	0	0
55	CD	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0

3 Residue-property plots

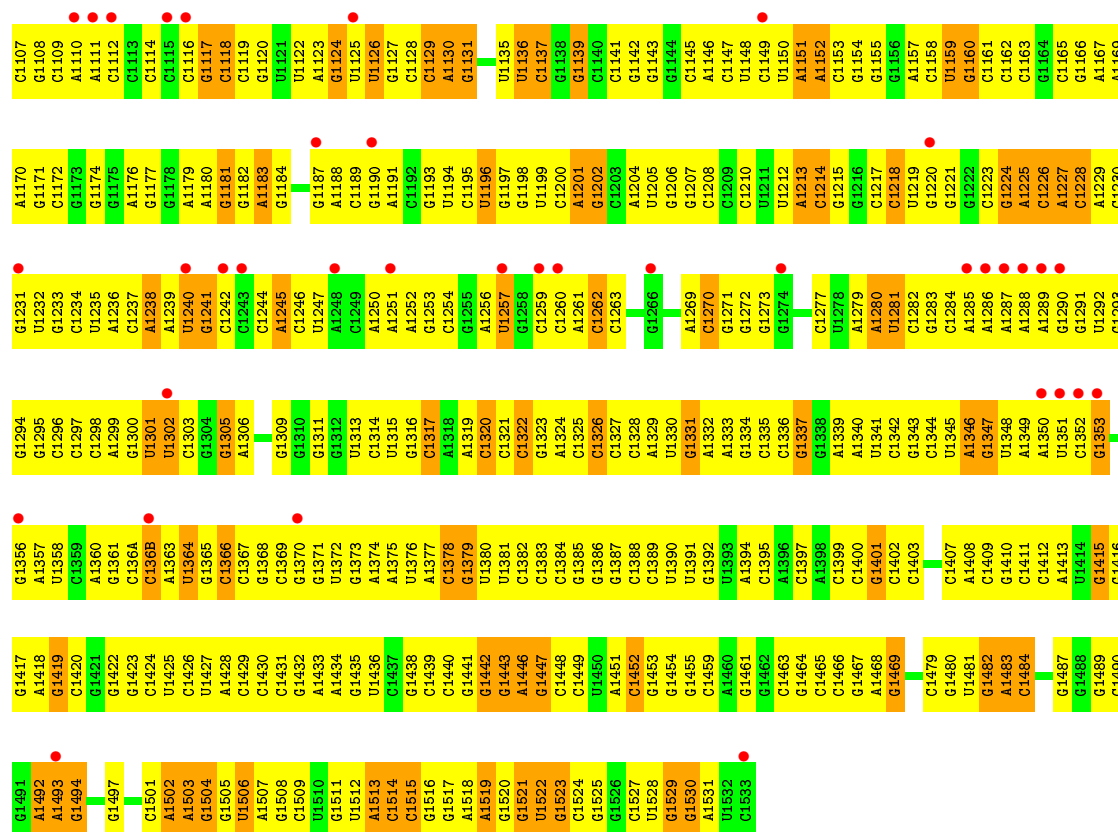
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ribosomal RNA 16S

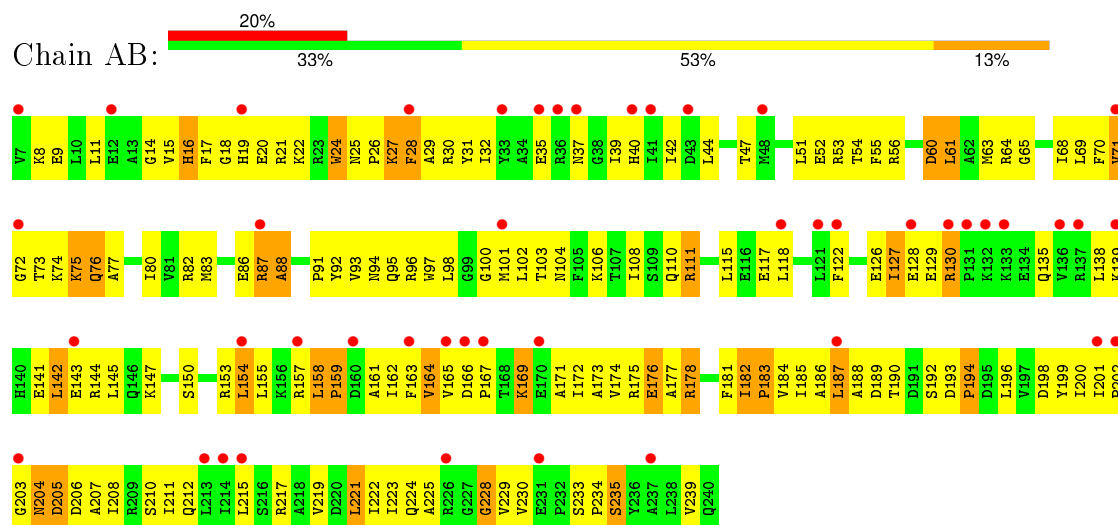




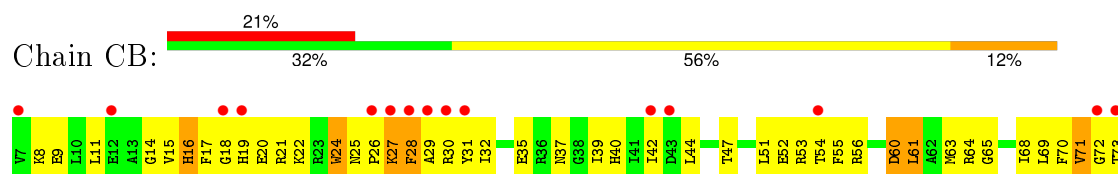
U65	C135	U192	C268	G333	A393	G458	G529	C589	G649	G713	G778	G851	G922	A983	G1046
G66	C136	C193	C269	C334	G394	G464	G530	C590	G650	G714	C779	G852	A923	C984	G1047
C67	C137	C194	C270	C335	G395	G465	U531	U591	U651	A715	A781	G853	A924	C985	G1048
G68	G138	A195	C271	C336	C396	G466	A532	G592	U652	A716	A782	G854	G926	A986	C1051
G69		A196	C272	C337	A397	G467	U533	G593	G653		G763	G855	G927	G987	C1052
G73	A141	A197	A273	A338	C398	A468	U534	G594	G654	G719	G764	G856	G928	G988	C1053
C74	G142	G198	A274	C339	C399	G474	A535	G595	G655	G720	G765	C857	G929	U991	C1054
C75	A143	G199		U340	C400	G475	C536	C596	G657	G721	G785	G858	G930	U992	C1055
G76	A144	G200	C277	U341	C401	G476	G537	G597	G658	A722	A789	A859	C931	U993	C1056
C77	G145	C201	C278	C342	G402	G477	U538	U598	U659	G723	A790	A860	C932	G993	C1057
G78		U208	A279	U343	C403	A478	A539	U599	G660	G724	G791	G861	C933	A994	C1058
G79	A149	U209	C280	C344	U404	G479	G540	C600	G661	G725	G792	G862	C934		C1059
G80	A150	U210	C281	C345	U405	U480	G541	C601	G662	G726	A792	U863	A935		C1060
G81	A151	G216	A282	G346	G406	G481	G542	A602	A663	G727	U793	A864	C936		C1061
U82	A152	C217	C283	G347	G407	A482	C543	G603	G664	G728	A794	A865	A937		C1062
U84		C218	G284	G348	G408	G483	C544	G604	A665	A729		A866	A938		C1063
U85	G156		G285	A349	G409	G484	C545	U605	G666	G730	G798	C868	C939		C1064
U86	G157	C221	G286	A350	G410	G485	C546	G606	G667	G731	G799	C869	C940		C1065
A87	G158	U222	U287	G351	A411	U486	A547	A607	G668	C732	G800	U870	C941		C1066
C88	G159	U223	C288	C352	A412	A487	G548	A608	U669	A733	U801	U871	G942		C1067
U89	G160	C224	G289	C353	G413	C488	C549	A609	G670	G734	A802	A872	U943		C1068
C90	A161	C225	C290	C354	A414	G489	G550	G610	G671	C735	G803	A873	G944		C1069
C91	A162		G292	C355	A415	G490	U551	A611	U672	C736	U804	A874	G945		C1070
G92	G163		G293	A356	C419	G491	U552	C612	G673	G737	C805	C875	G946		C1071
U93	U164	G231	U294	G357	U420	G492	A553	G613	G674	C738	C806	G876	G947		C1072
G95	C165	C232	C295	U358	U421	G493	C555	A614	A675	C739	A807	C877	G948		C1073
G96	G166	C233	G296	U359	U422	U494	C556	C615	A676	U740	C810	C878	G949		C1074
U97	G167	C234	U297	G360	U423	U495	C557	G616	A677	G741	C811	C879	U950		C1075
C99	G168	C235	A298	G361	G423	A496	G558	G617	U678	G742	G818	C880	U951		C1076
A101	C169	G236	G299	G362	G424	U497	G559	C618	G679	U743	G819	C881	U952		C1077
G102	G170	C238	A300	A363	G425	A498	A559	U619	C680	C744	A814	C882	G953		C1078
C103	A171	U239	G301	A364	G426	G500	U560	C620	C681		A815	C883	G954		C1079
G104	U172	C240	G302	U365	U427	C501	U561	A621	G682	G745	A816	C884	U955		C1080
C105	U173	C241	A303	C366	G428	G502	C562	A622	G683	C749	C817		U956		C1081
G106	C174	C242	U304	U367	U429	A503	A563	C623	A684	U751	G818	A892	U957		C1082
G107	C175	A243	G305	U368	A430	C504	C564	C624	G685	U752	A819	C893	U958		C1083
G108	G176	U244	G306	G369	A431	G505	U565	G625	U686	G753	U820		U959		C1084
A109	C177	C245	C307	C370	A432	G506	G566	U626	A687	A753	G821		U960		C1085
C110	C178	A246			U433	C507	G567	G627	G688	C754	C822		U961		C1086
G111	A179	G247	C311	G371	U434	C508	G568	G628	C689	G755			U962		C1087
G112	U180	C248	A312	A373	C435	A509	C569	G629	G690	C756	G825		C997		C1088
G113	G181	U249	A313	A374	C436	A510	G570	C630	G691	U757	C826		C998		C1089
U114	U182	G251	C314	U375	U437	C511	U571	G631	U692	G758	U827		C999		C1090
G115	G183	G252	G317	G376	U438	U512	A572	A632	G693	A759	A828		A900		C1091
A116		U253	G318	C377	A439	C513	A573	G633	A694	G760	G829		A901		C1092
U117	G186D	U254	G319	G378	A440	C514	A574	C634	A695	G761	G830		A902		C1093
U118	C186E	G255	G319	C379		G515	G575	G635	A696	G762	U831		A907		C1094
A119	C186F	G256	C320	G380	C444	U516	G576	U636	U697	C763	U832		A908		C1095
C120	C186G	G257	A321	C381	G445	G517	G577	G637	G698	G764	U833		A909		C1096
C121	C187	C257	C322	A382	G446	C518	C578	G638	C699	G765	C834		C910		C1097
G122	U188	G258	U323	A383	G447	C519	C579	G639		A766	U835		C911		C1098
C123	U189	G259	G324	G384	A448	A520	U580	A640	A702	A767	G836		A913		C1099
	G190	C260	A325	C385	C449	G521	U582	G641		A768	G837		A914		C1100
G127	G191A	U261	G326	C386	G450	C522	G583	A642	A706	U772	G838		A915		C1101
G128	G191B	A262	A327	U387	A451	A523	U584	C643	C707	G773	U839		A916		C1102
	G191C	A263	C328	G388	A452	G524	G584	G644	C708	G774	U840		A917		C1103
A130	U191D	U264	A329	A389	A453	C525	G585	C645	G709	G775	U841		A918		C1104
C131	G191E	G265	C330	G390	C456	C526	G586	U646	G710	G776	C842		A919		C1105
C132	U191F	G266	G331	G391	G457	G527	G587	C647	G711	A777	U843		U920		C1106
	G191G	C267	G332	G392		C528	G588	A648	A712		U850		U921		

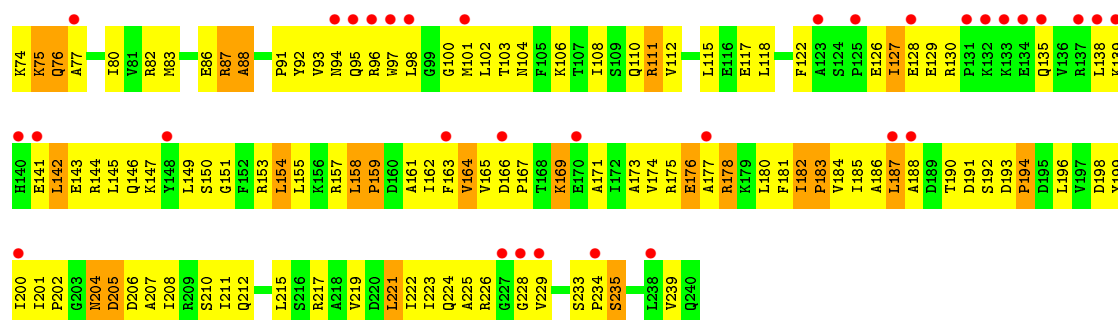


• Molecule 2: 30S ribosomal protein S2

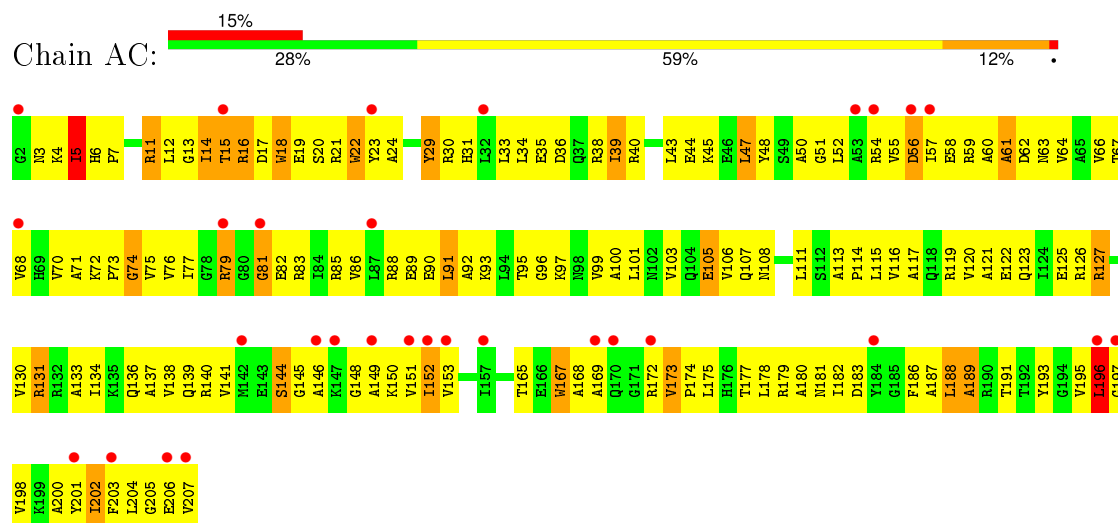


• Molecule 2: 30S ribosomal protein S2

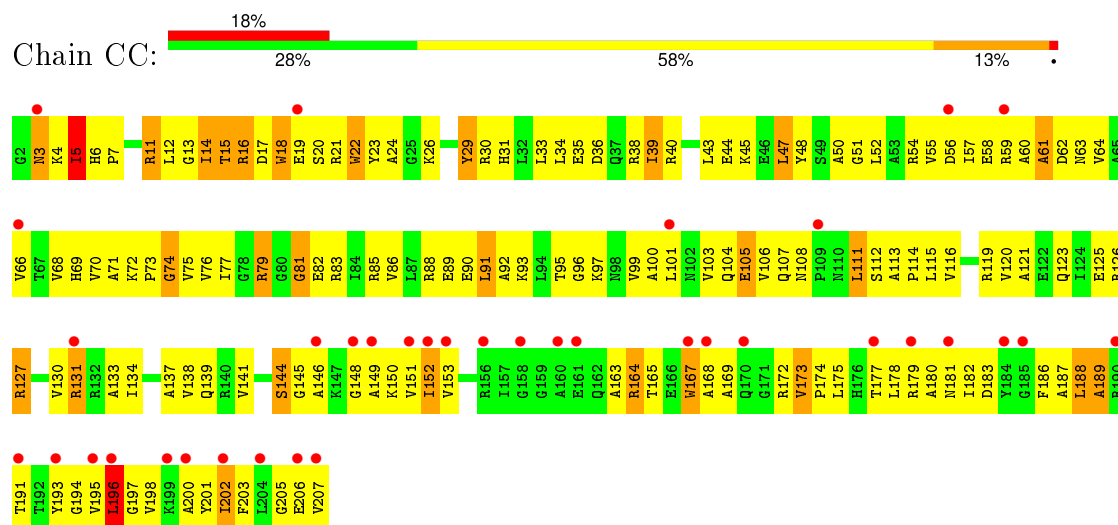




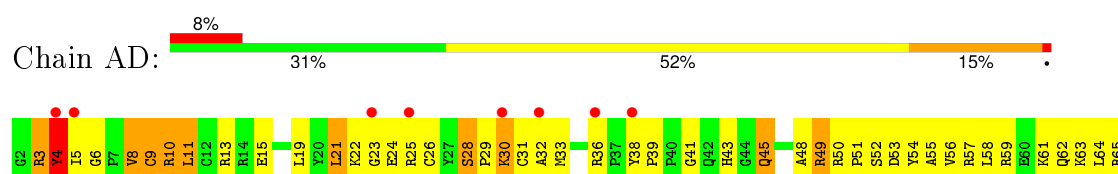
• Molecule 3: 30S ribosomal protein S3



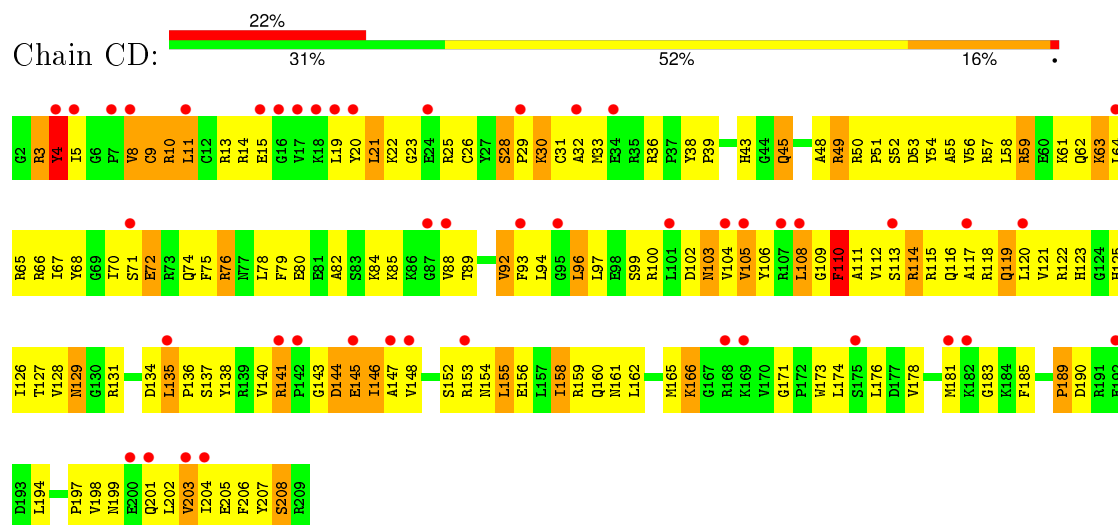
• Molecule 3: 30S ribosomal protein S3



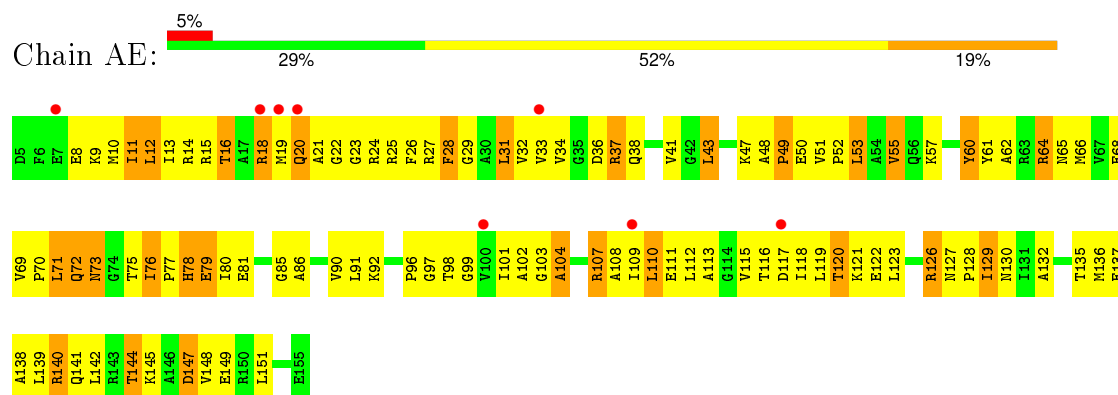
• Molecule 4: 30S ribosomal protein S4



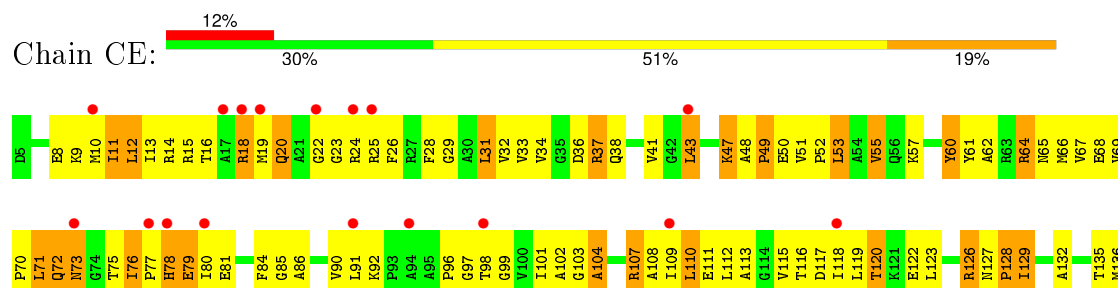
- Molecule 4: 30S ribosomal protein S4

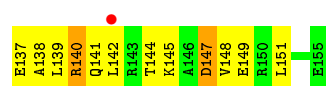


- Molecule 5: 30S ribosomal protein S5

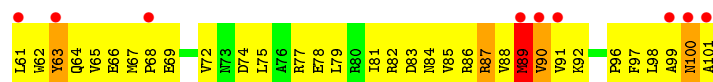


- Molecule 5: 30S ribosomal protein S5

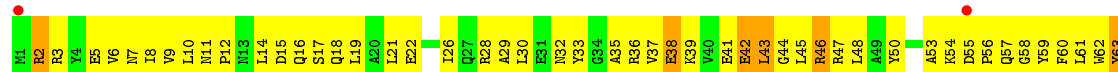




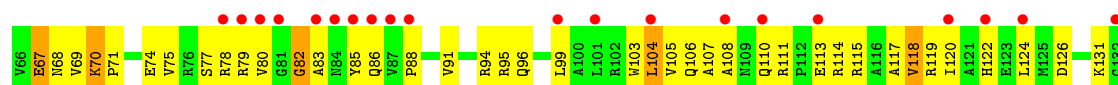
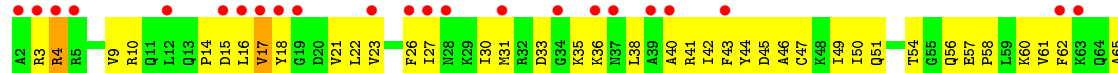
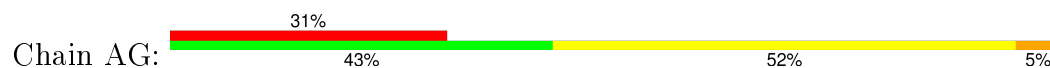
• Molecule 6: 30S ribosomal protein S6



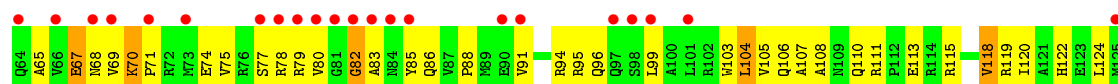
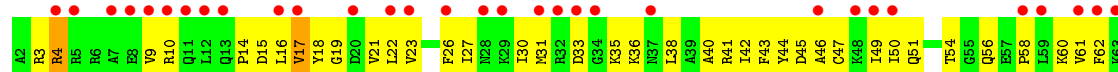
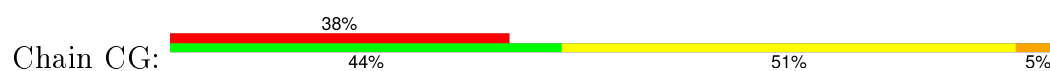
• Molecule 6: 30S ribosomal protein S6

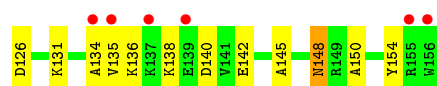


• Molecule 7: 30S ribosomal protein S7

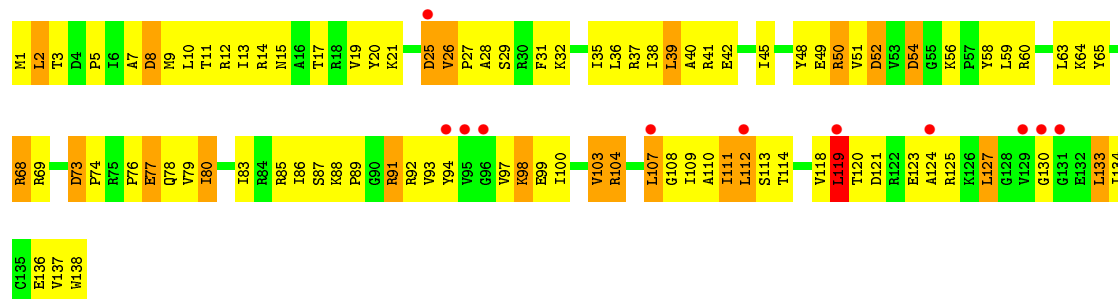


• Molecule 7: 30S ribosomal protein S7

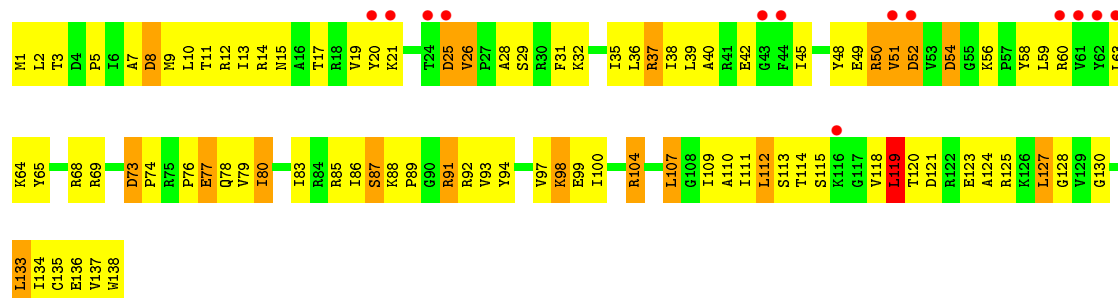




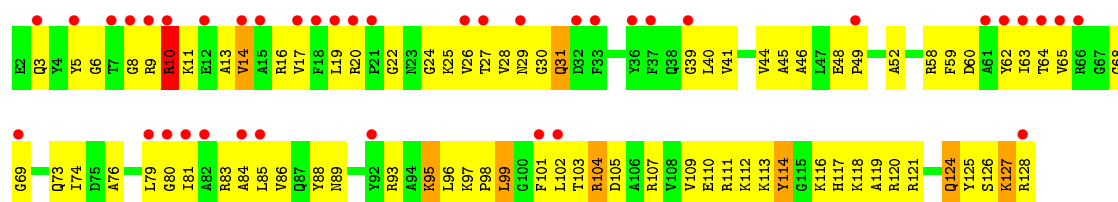
- Molecule 8: 30S ribosomal protein S8



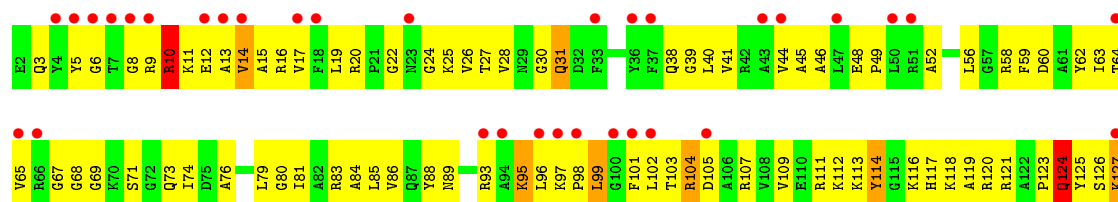
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

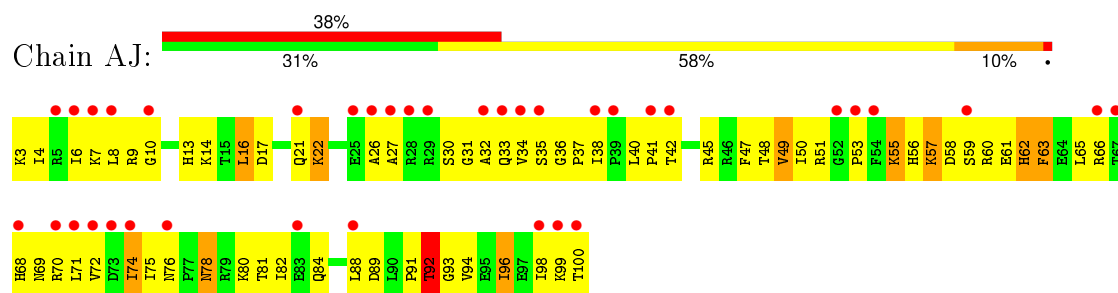


- Molecule 9: 30S ribosomal protein S9

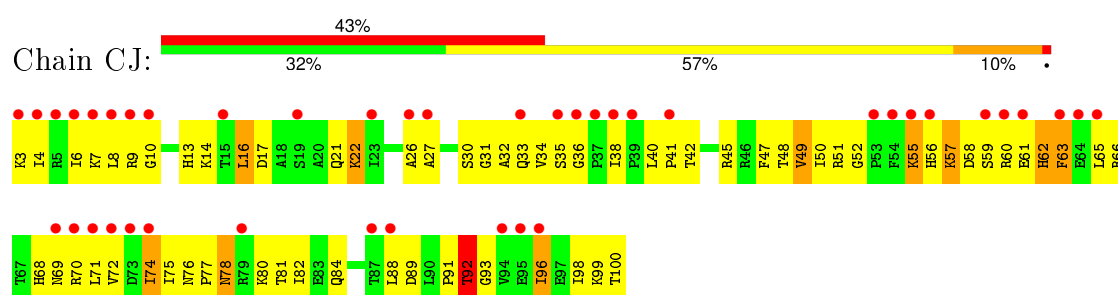


R128

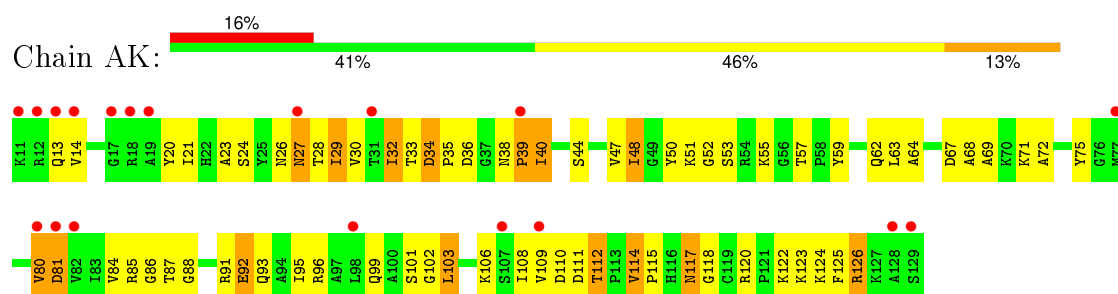
- Molecule 10: 30S ribosomal protein S10



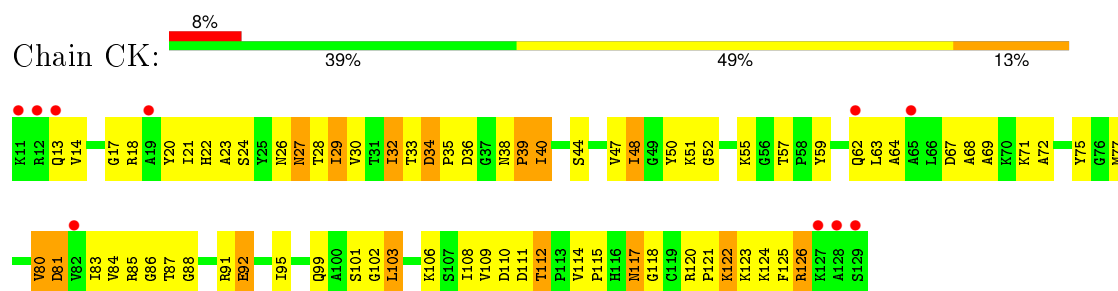
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

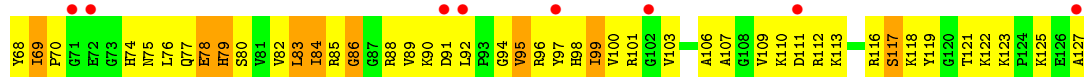


- Molecule 12: 30S ribosomal protein S12

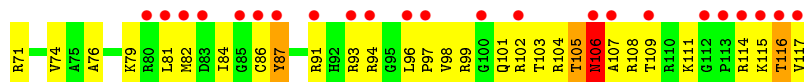




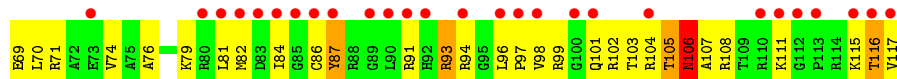
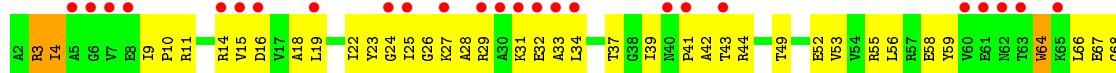
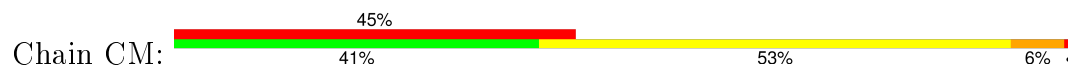
• Molecule 12: 30S ribosomal protein S12



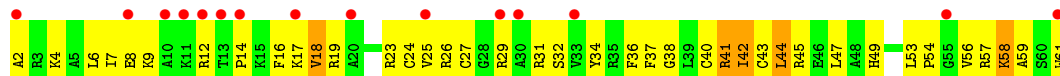
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

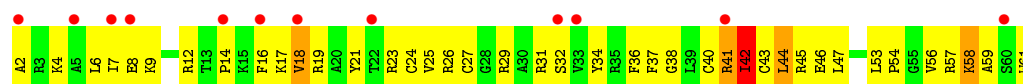


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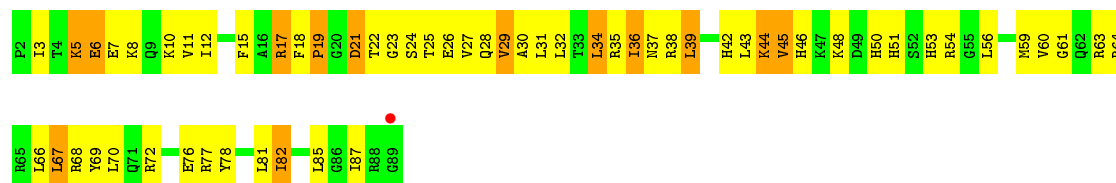


• Molecule 14: 30S ribosomal protein S14 type Z

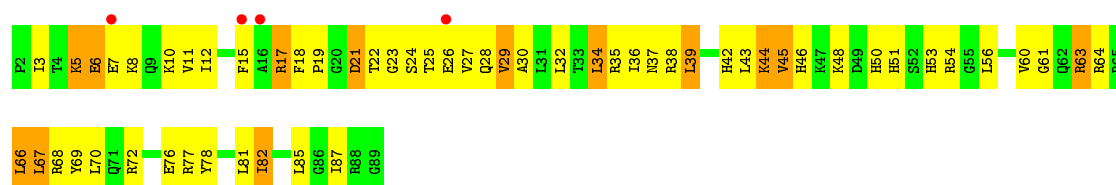




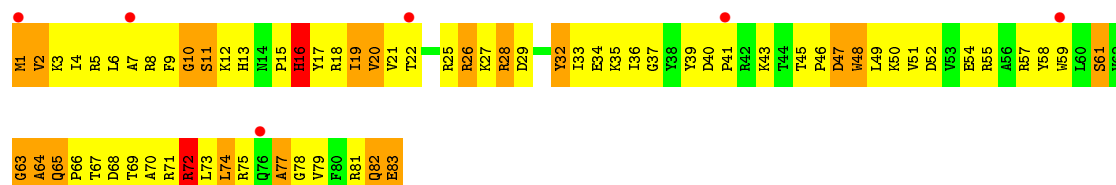
• Molecule 15: 30S ribosomal protein S15



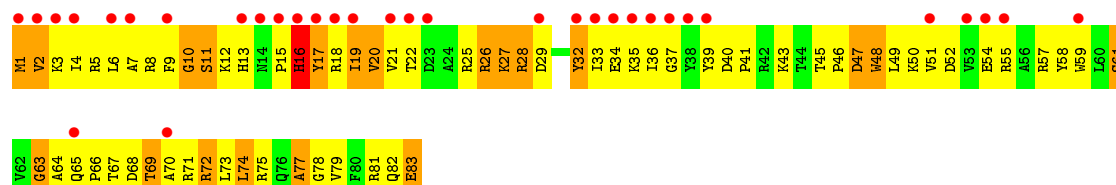
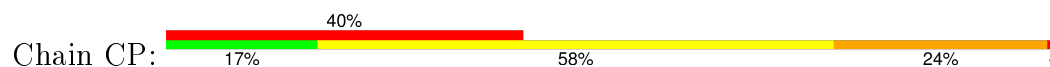
• Molecule 15: 30S ribosomal protein S15



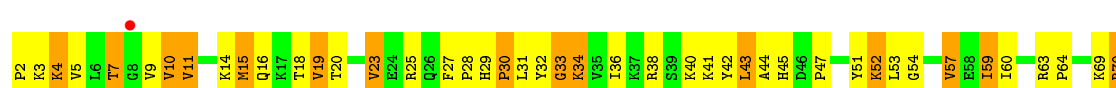
• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16

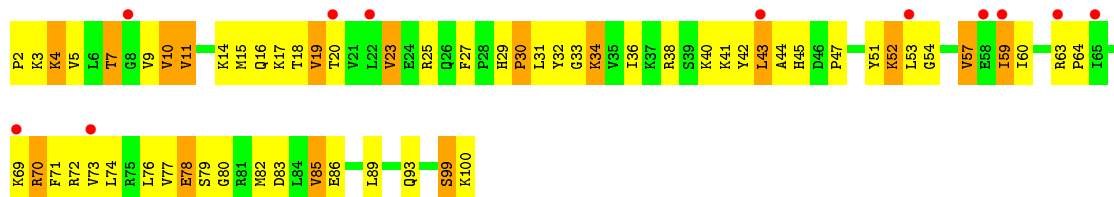
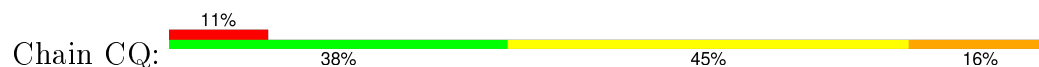


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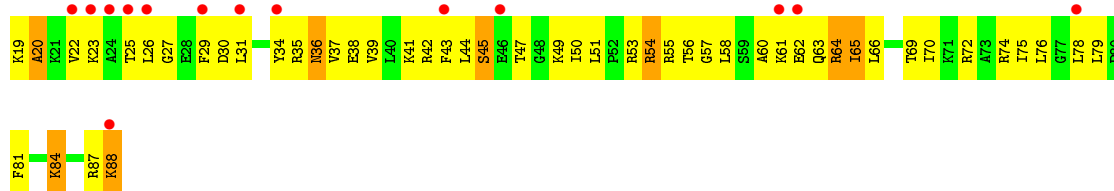




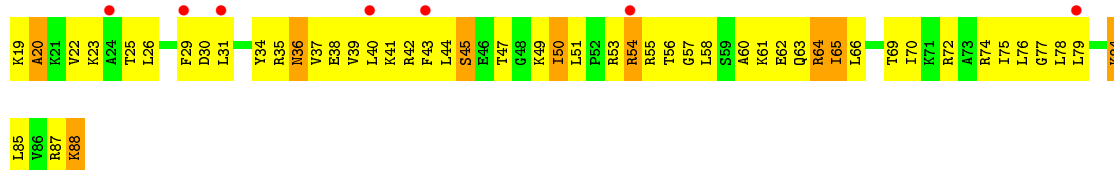
- Molecule 17: 30S ribosomal protein S17



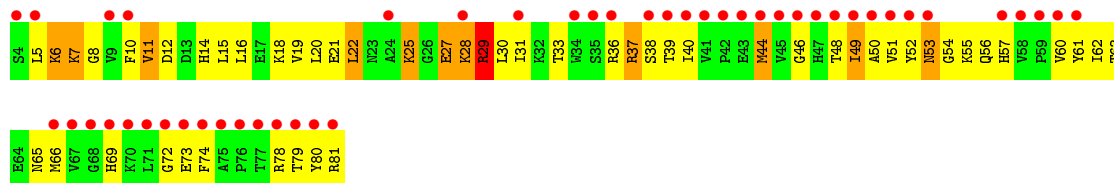
- Molecule 18: 30S ribosomal protein S18



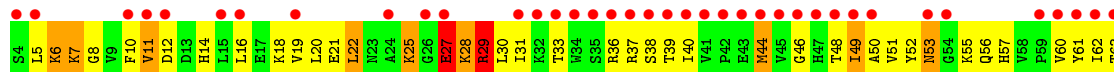
- Molecule 18: 30S ribosomal protein S18

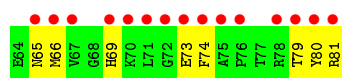


- Molecule 19: 30S ribosomal protein S19

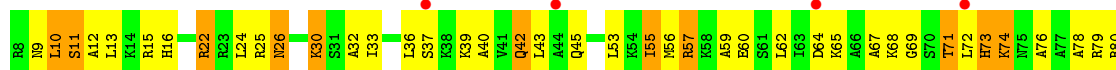
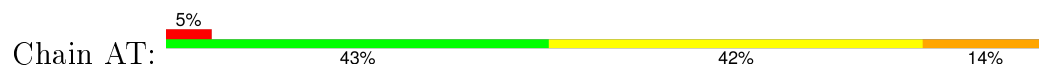


- Molecule 19: 30S ribosomal protein S19

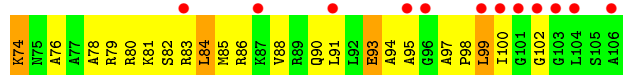
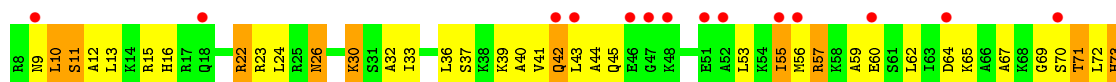
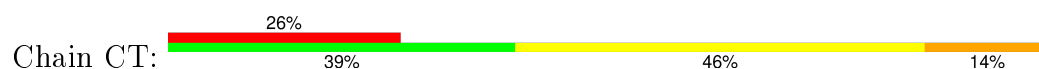




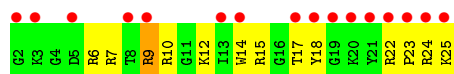
- Molecule 20: 30S ribosomal protein Thx



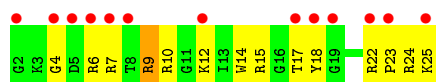
- Molecule 20: 30S ribosomal protein Thx



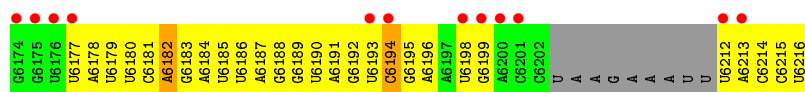
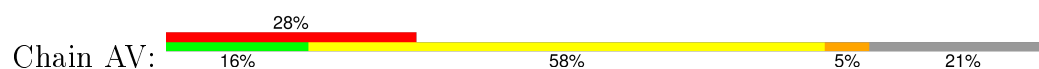
- Molecule 21: domain 3 of CrPV IGR IRES RNA



- Molecule 21: domain 3 of CrPV IGR IRES RNA

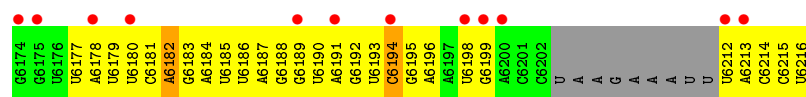


- Molecule 22: RNA (34-MER)

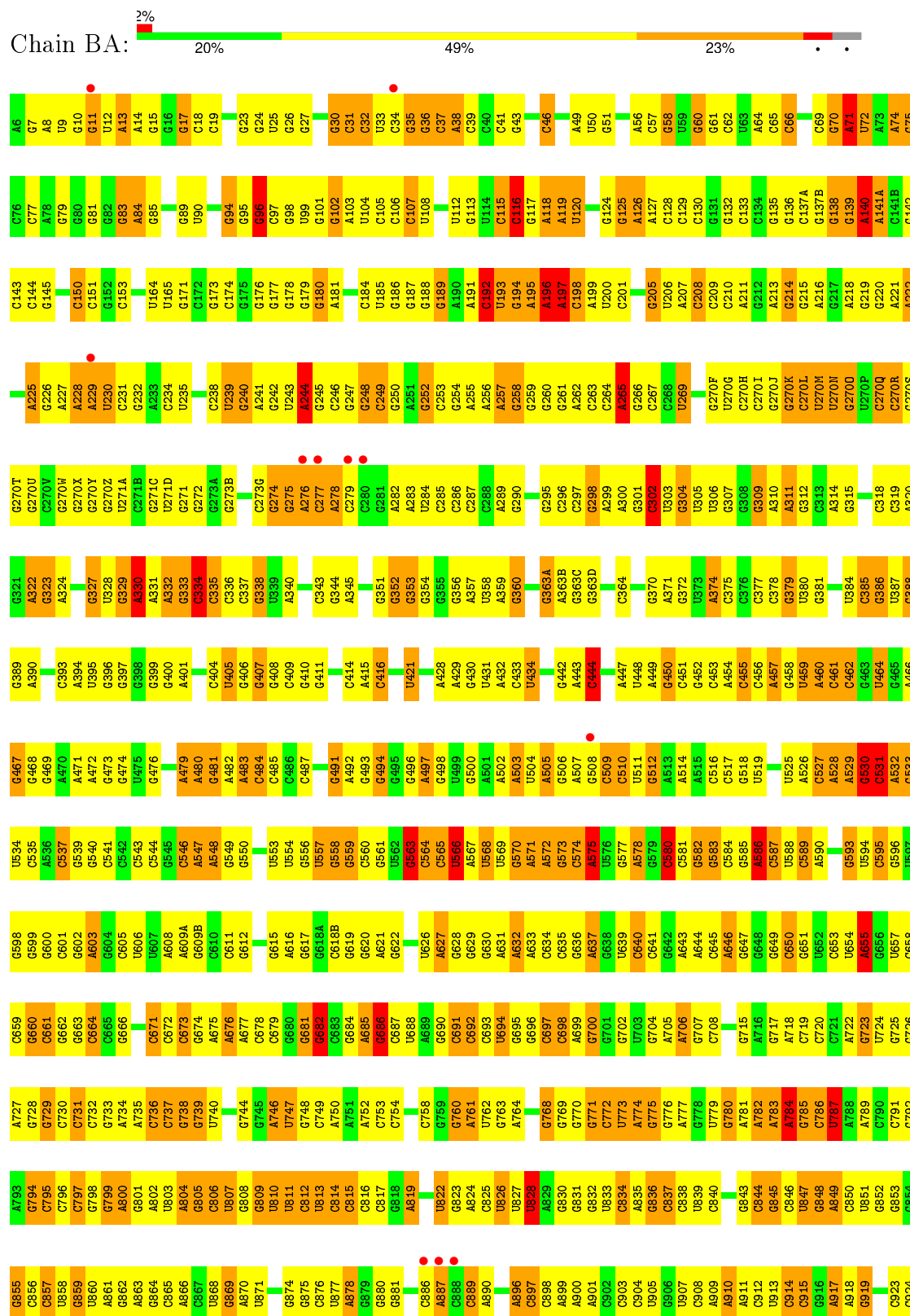


- Molecule 22: RNA (34-MER)



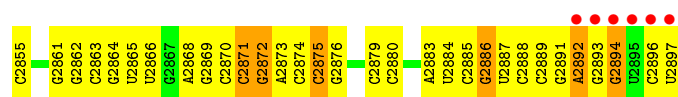


• Molecule 23: 23S ribosomal RNA

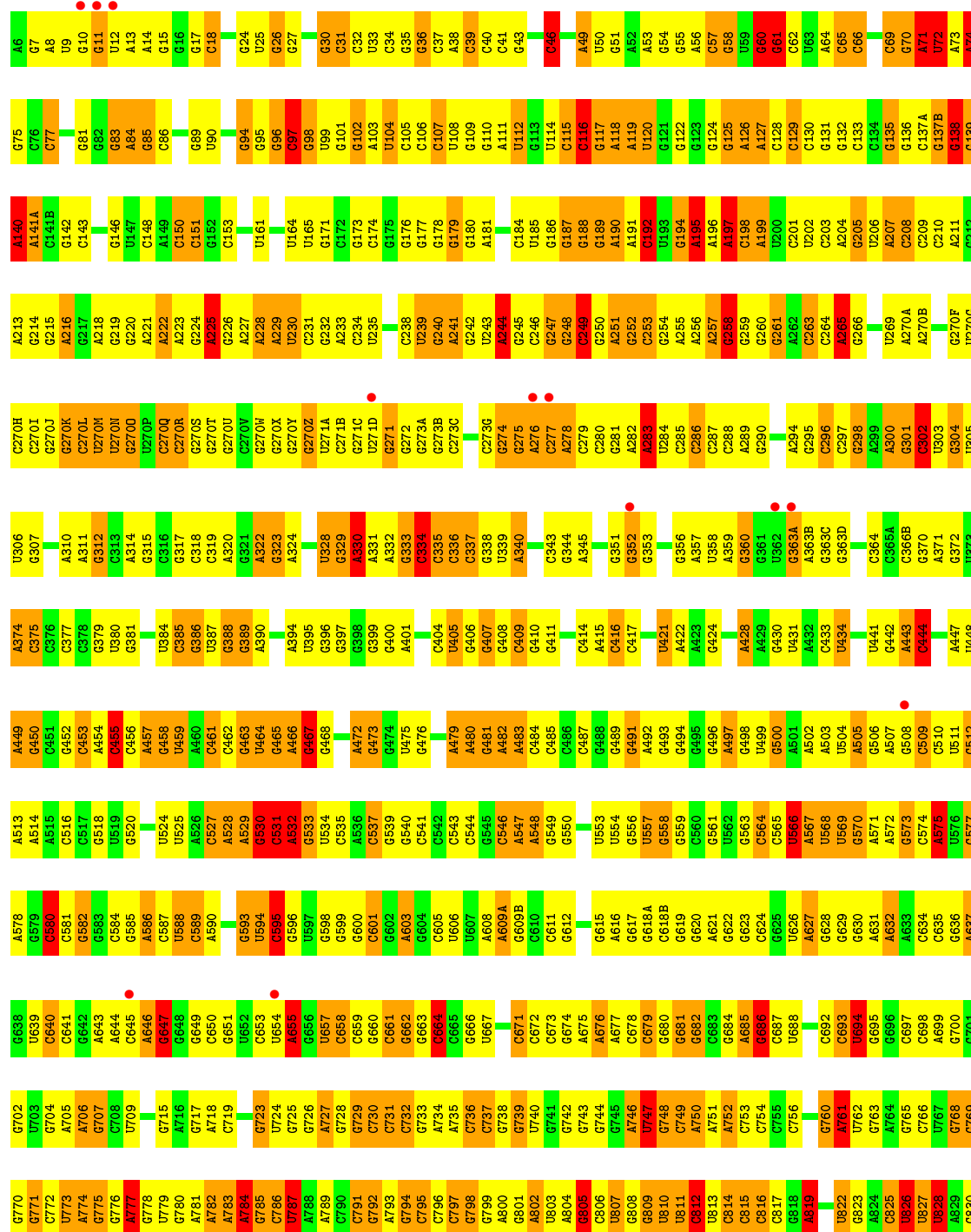
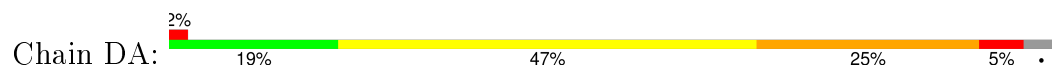


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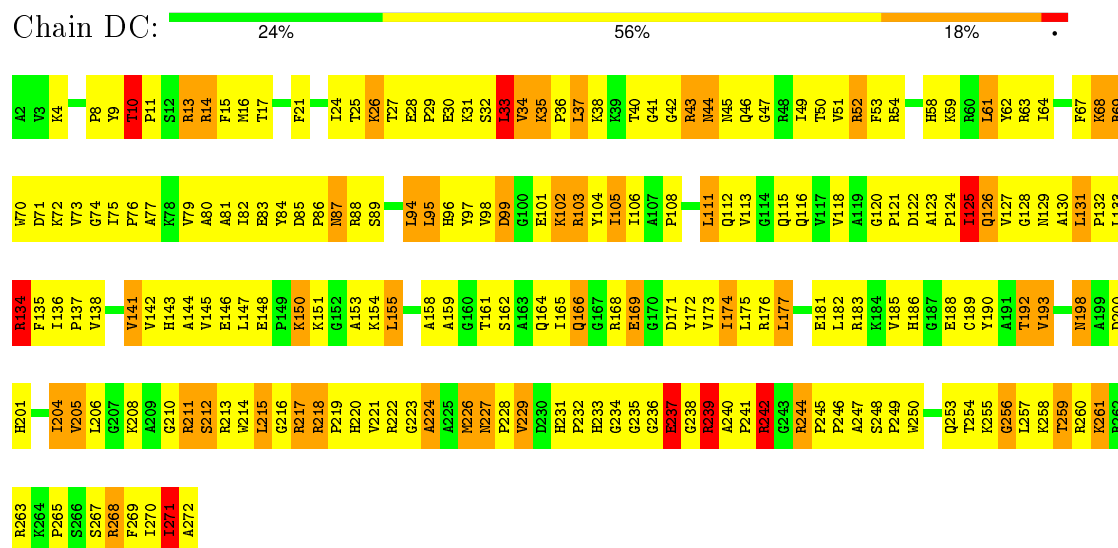
• Molecule 23: 23S ribosomal RNA

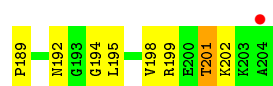


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G1742	C1662	A1603	G1538	A1473	G1414	A1353	C1293	C1222	C1158	A	A1032	G972	U907	U839
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- Molecule 25: 50S ribosomal protein L2





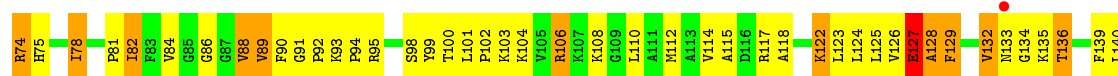
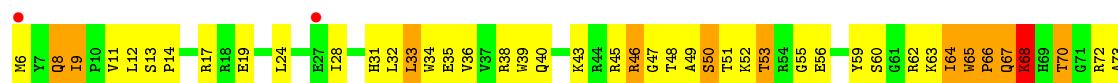
- Molecule 27: 50S ribosomal protein L4

Chain BE: 35% 47% 18%



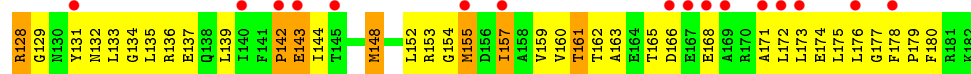
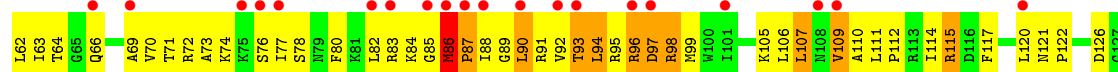
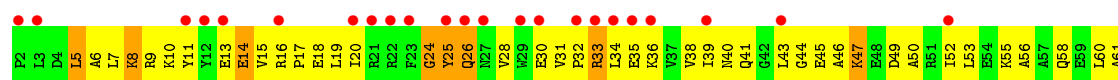
- Molecule 27: 50S ribosomal protein L4

Chain DE: 2% 34% 48% 16%



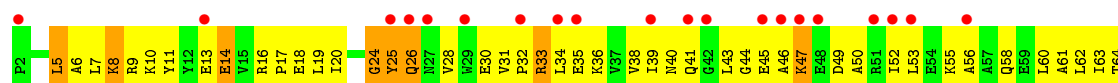
- Molecule 28: 50S ribosomal protein L5

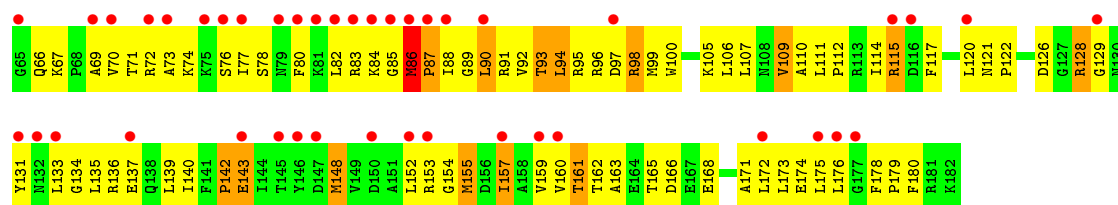
Chain BF: 33% 30% 56% 14%



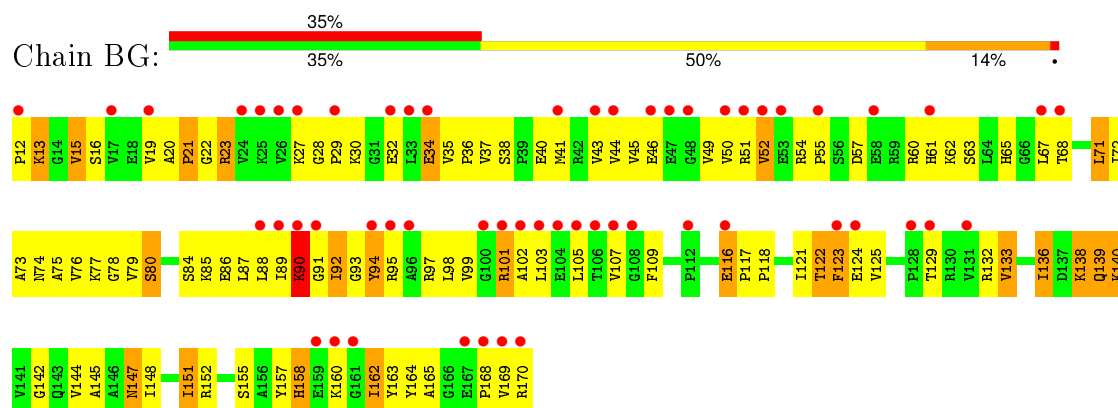
- Molecule 28: 50S ribosomal protein L5

Chain DF: 34% 30% 57% 12%

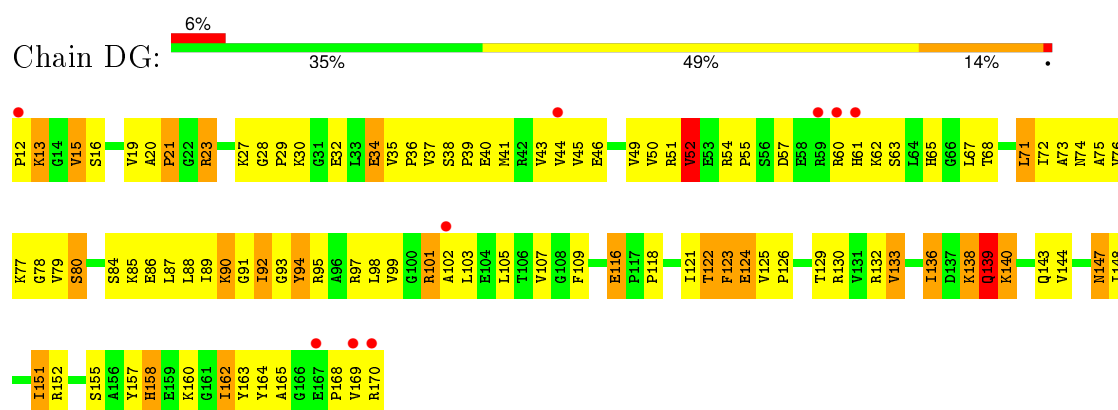




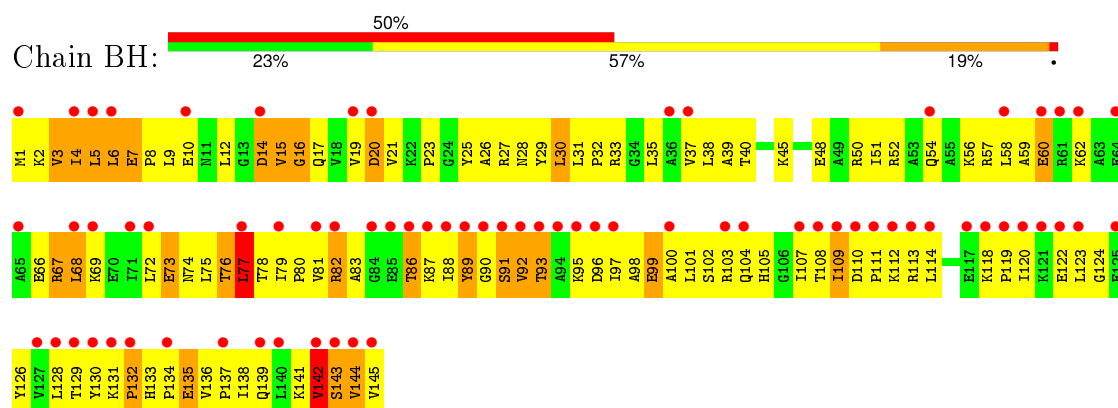
• Molecule 29: 50S ribosomal protein L6



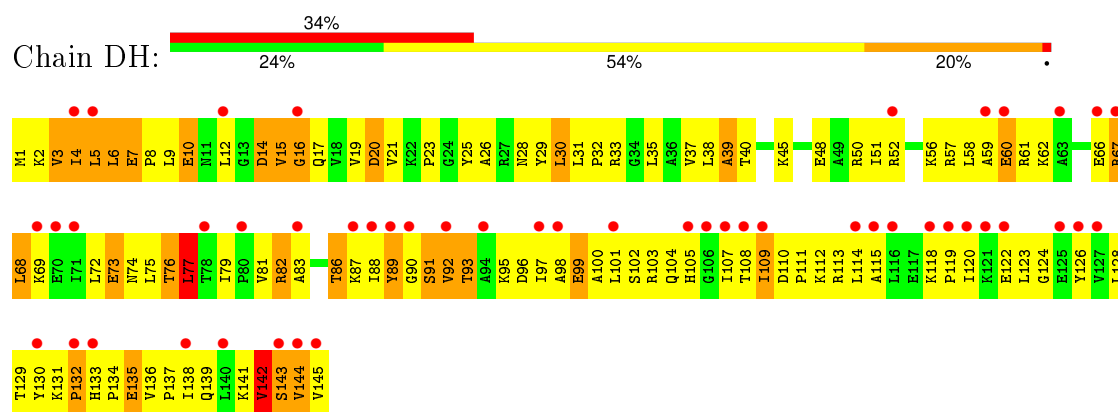
• Molecule 29: 50S ribosomal protein L6



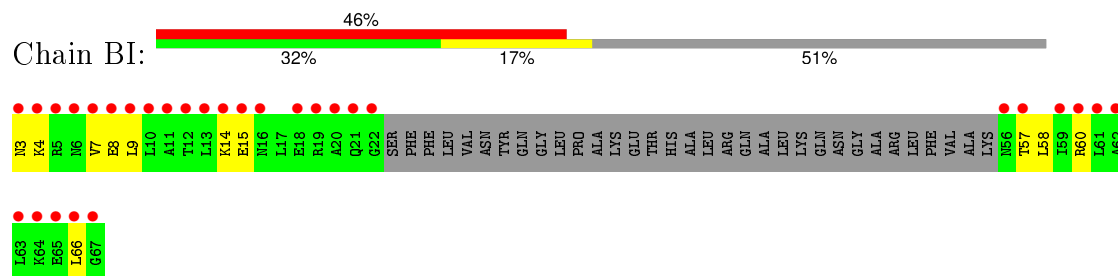
• Molecule 30: 50S ribosomal protein L9



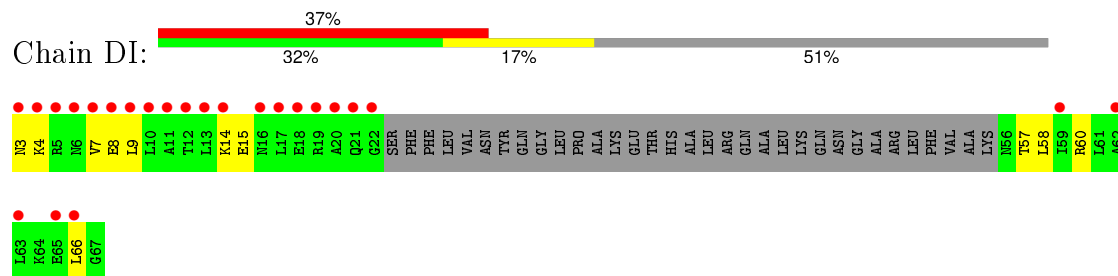
• Molecule 30: 50S ribosomal protein L9



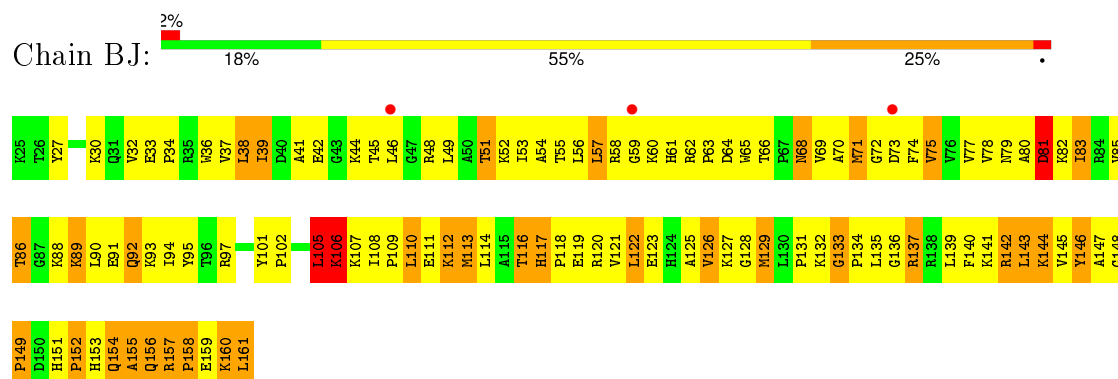
• Molecule 31: 50S ribosomal protein L10



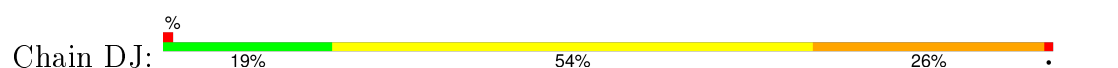
• Molecule 31: 50S ribosomal protein L10

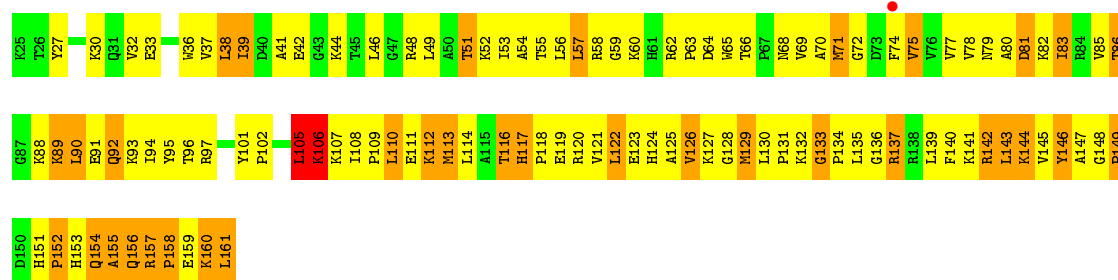


• Molecule 32: 50S ribosomal protein L13



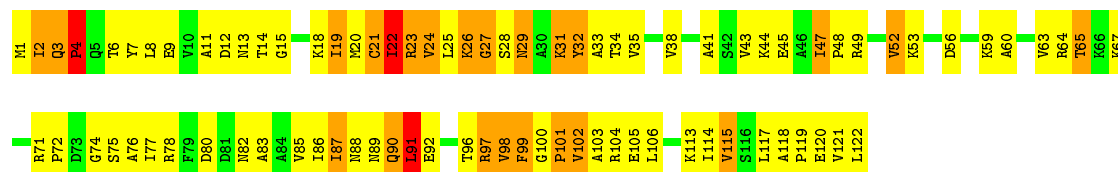
• Molecule 32: 50S ribosomal protein L13





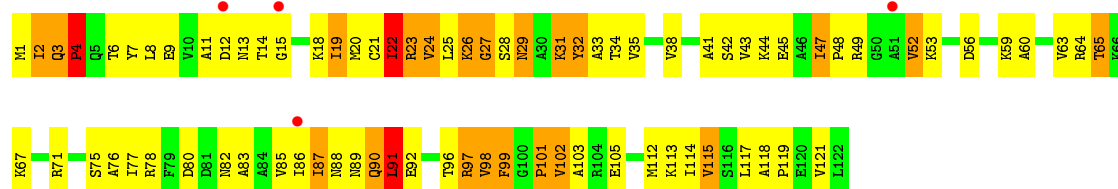
- Molecule 33: 50S ribosomal protein L14

Chain BK: 30% 49% 18%



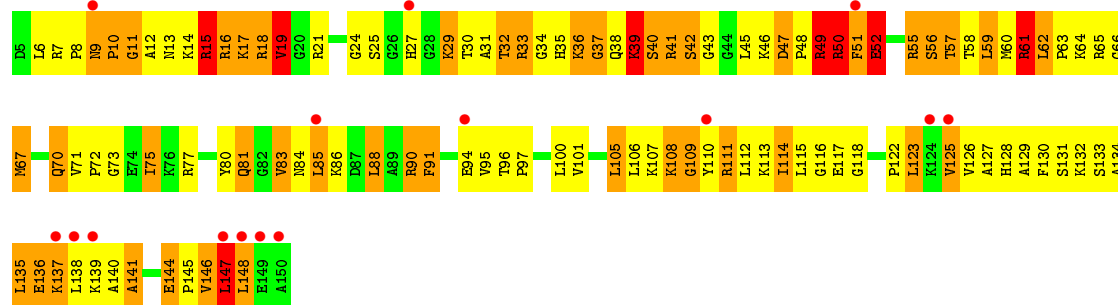
- Molecule 33: 50S ribosomal protein L14

Chain DK: 3% 34% 46% 17%



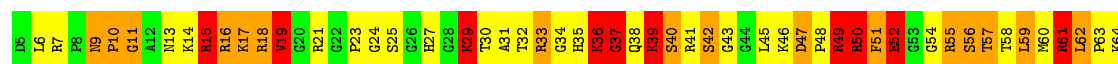
- Molecule 34: 50S ribosomal protein L15

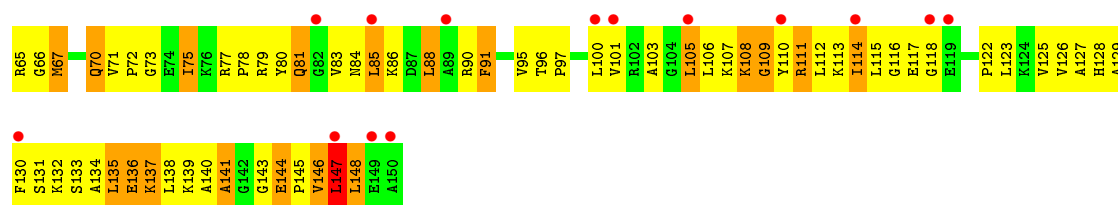
Chain BL: 10% 23% 42% 30% 5%



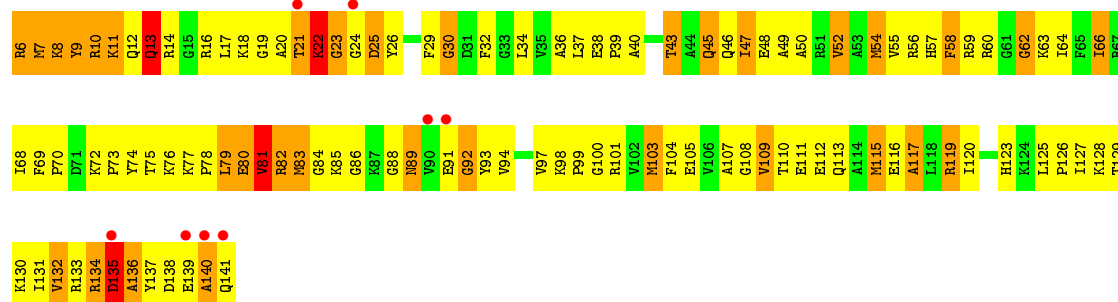
- Molecule 34: 50S ribosomal protein L15

Chain DL: 10% 21% 48% 24% 8%

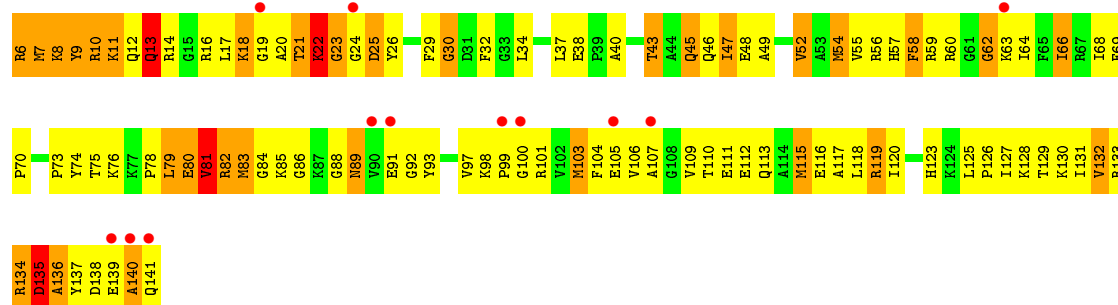




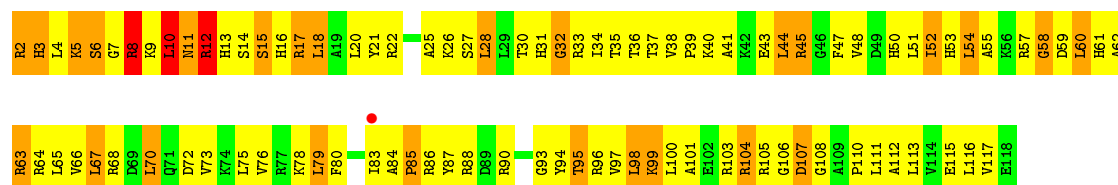
• Molecule 35: 50S ribosomal protein L16



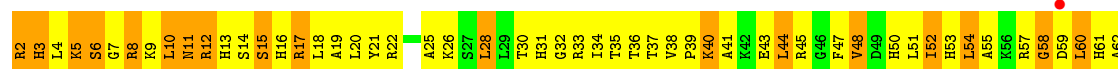
• Molecule 35: 50S ribosomal protein L16

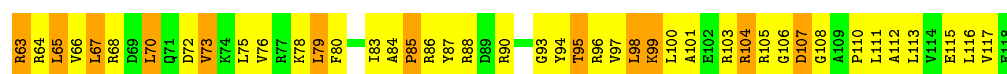


• Molecule 36: 50S ribosomal protein L17

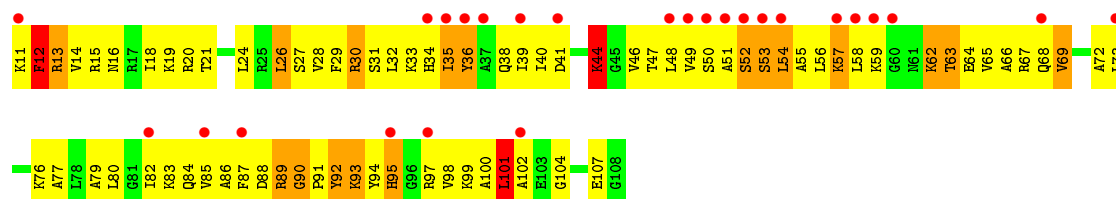


• Molecule 36: 50S ribosomal protein L17

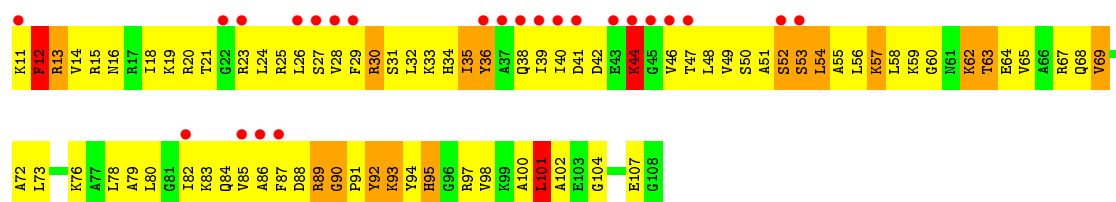




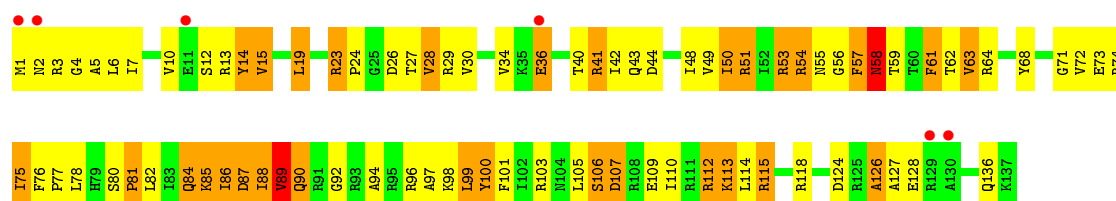
• Molecule 37: 50S ribosomal protein L18



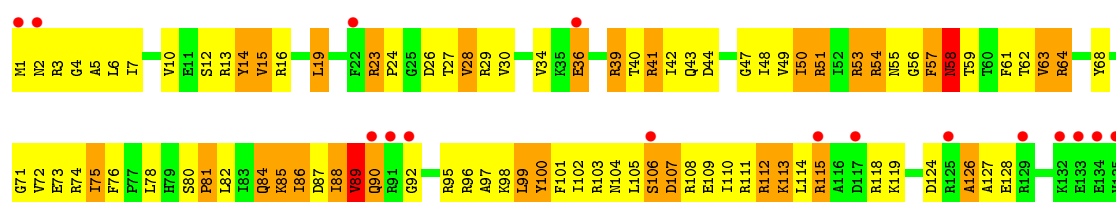
• Molecule 37: 50S ribosomal protein L18



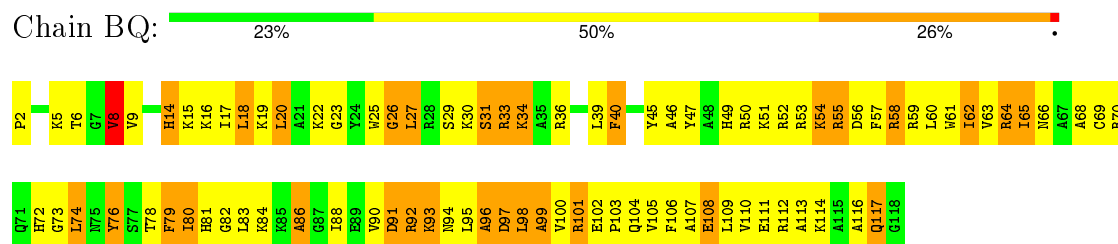
• Molecule 38: 50S ribosomal protein L19



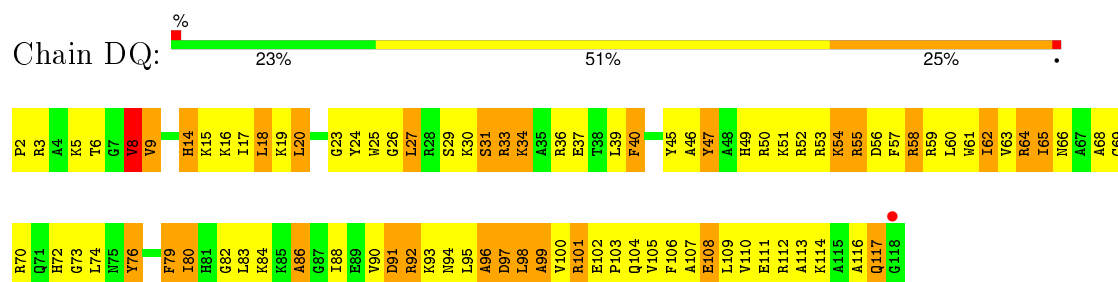
• Molecule 38: 50S ribosomal protein L19



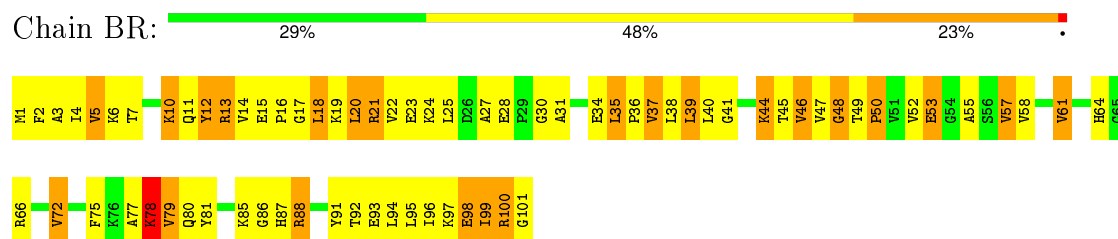
• Molecule 39: 50S ribosomal protein L20



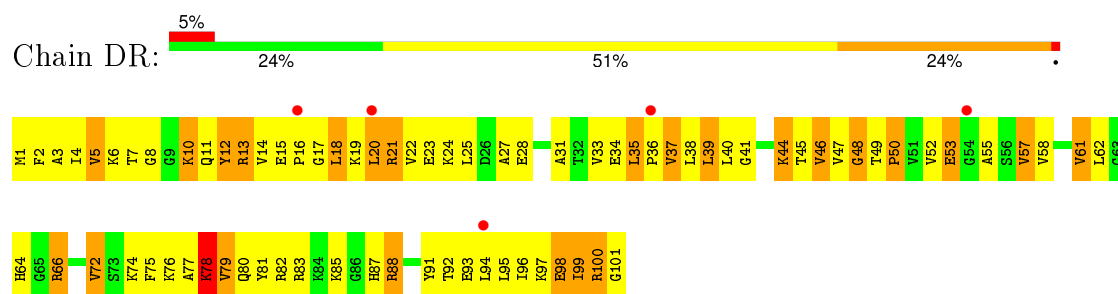
- Molecule 39: 50S ribosomal protein L20



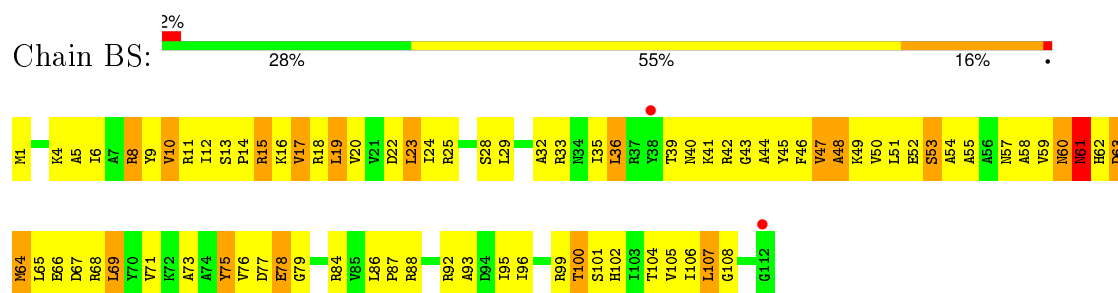
- Molecule 40: 50S ribosomal protein L21



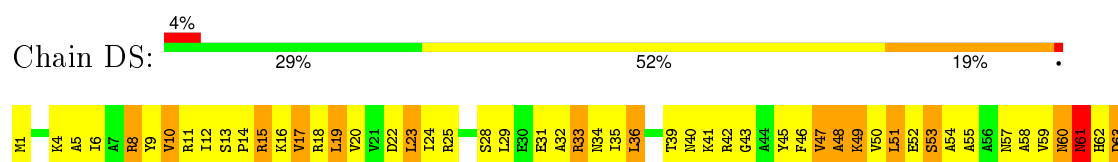
- Molecule 40: 50S ribosomal protein L21



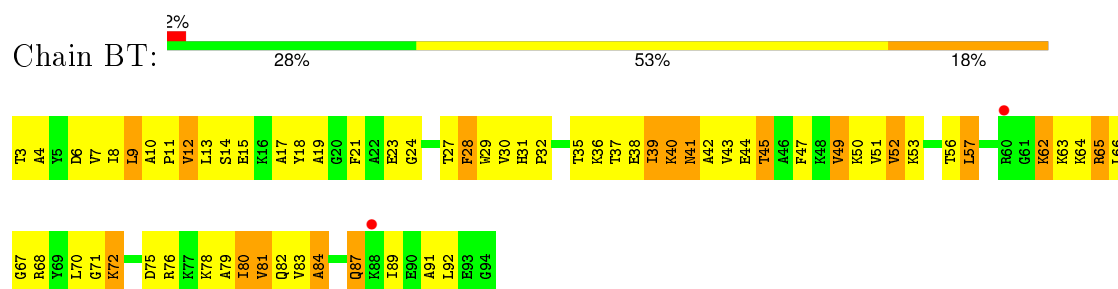
- Molecule 41: 50S ribosomal protein L22



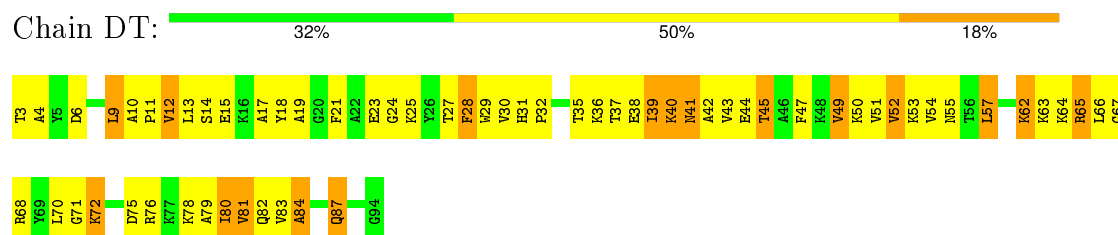
- Molecule 41: 50S ribosomal protein L22



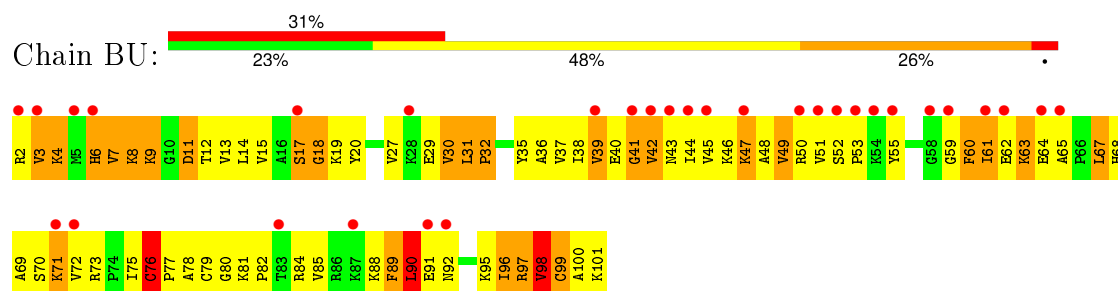
- Molecule 42: 50S ribosomal protein L23



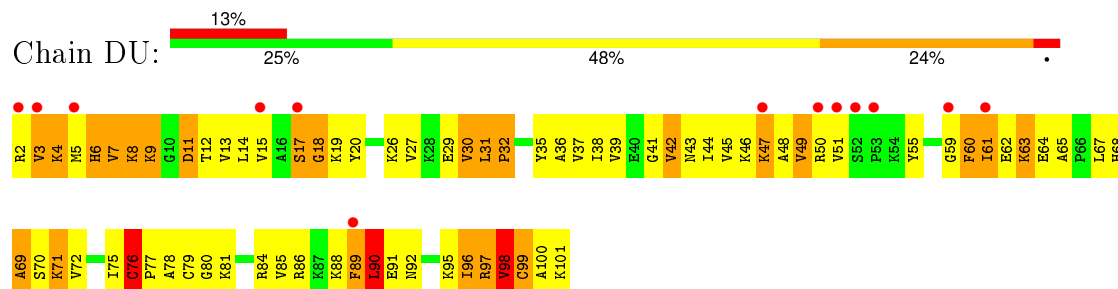
- Molecule 42: 50S ribosomal protein L23



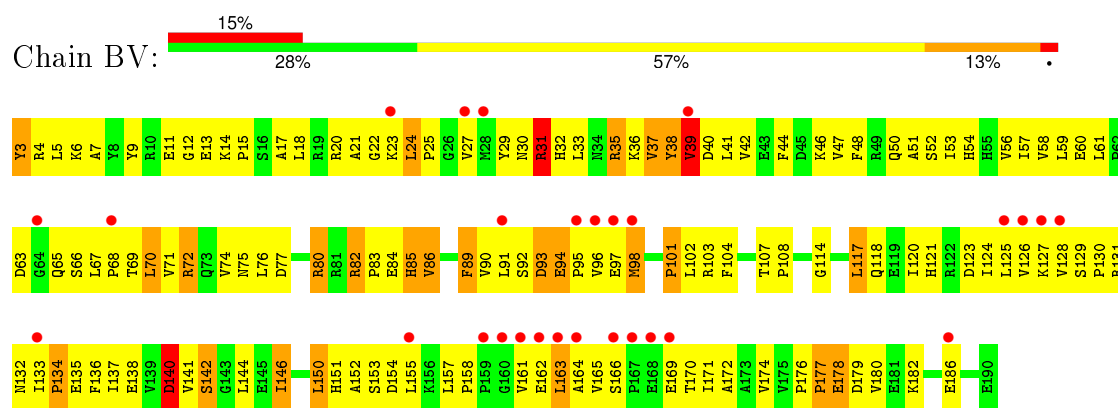
- Molecule 43: 50S ribosomal protein L24



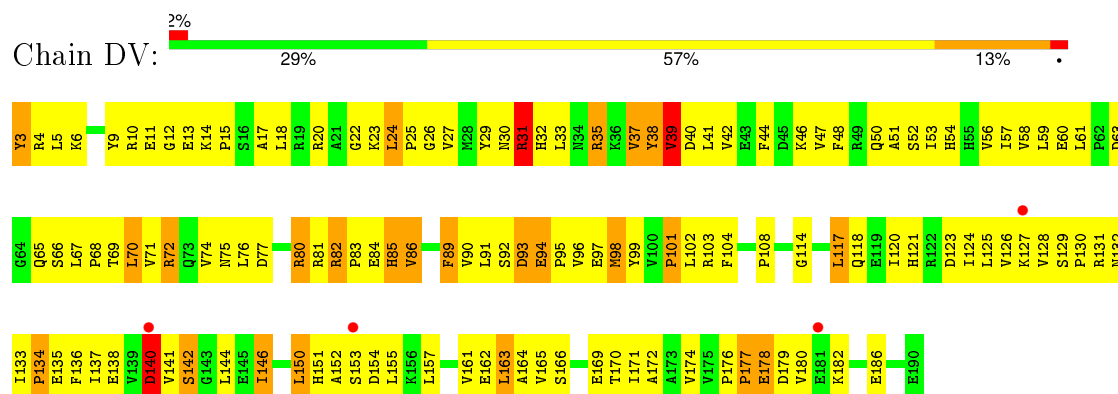
- Molecule 43: 50S ribosomal protein L24



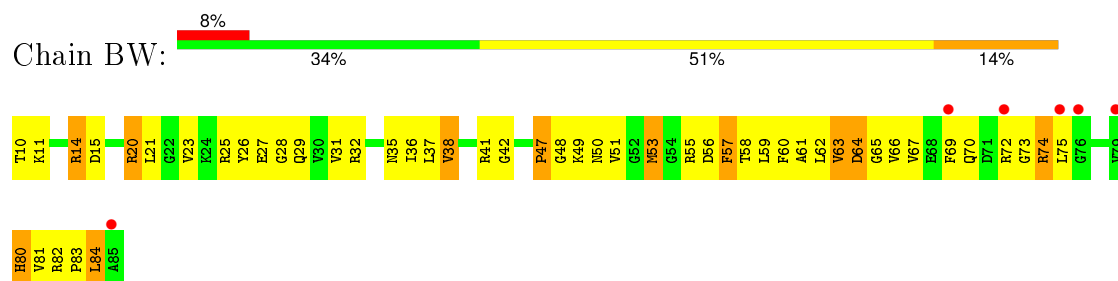
- Molecule 44: 50S ribosomal protein L25



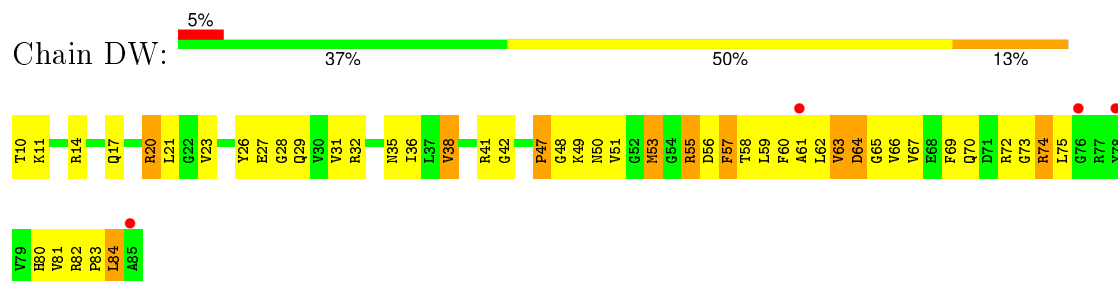
- Molecule 44: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L27

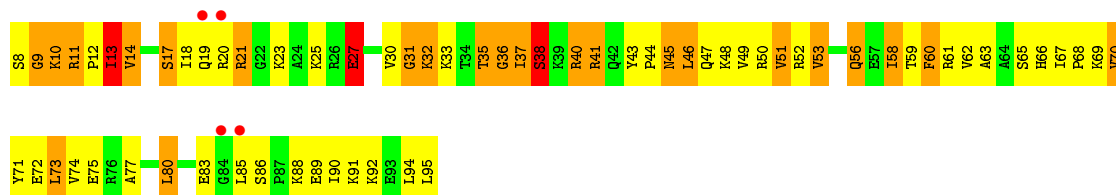


- Molecule 45: 50S ribosomal protein L27

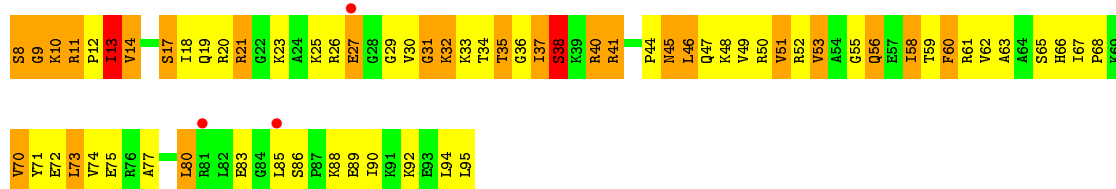


- Molecule 46: 50S ribosomal protein L28





- Molecule 46: 50S ribosomal protein L28



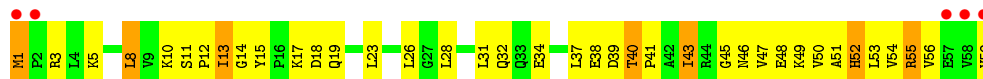
- Molecule 47: 50S ribosomal protein L29



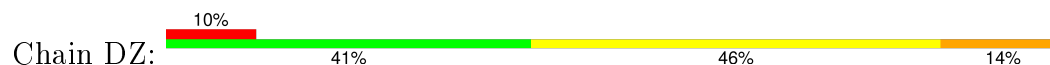
- Molecule 47: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L30

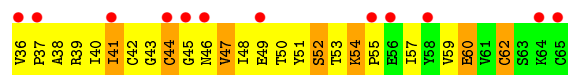
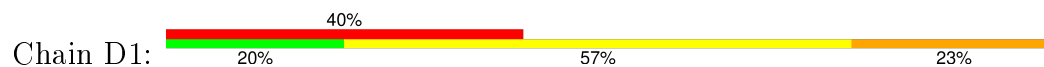


- Molecule 49: 50S ribosomal protein L31

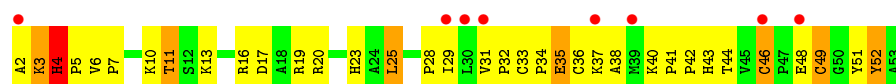




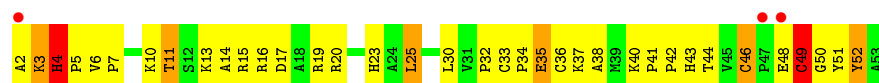
- Molecule 49: 50S ribosomal protein L31



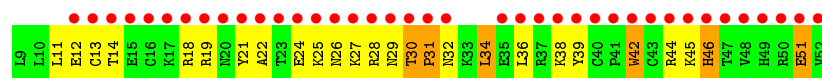
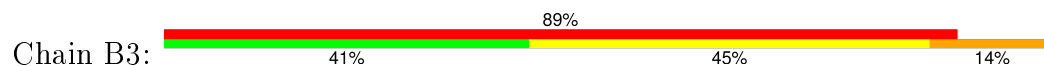
- Molecule 50: 50S ribosomal protein L32



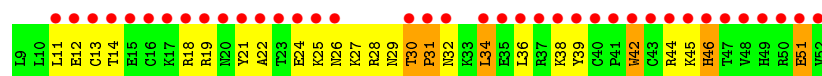
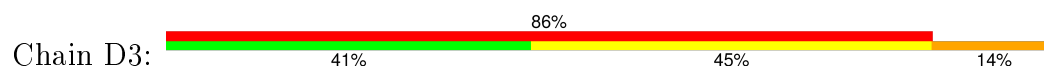
- Molecule 50: 50S ribosomal protein L32



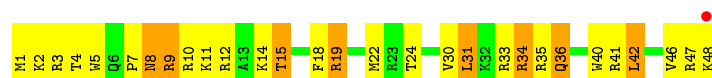
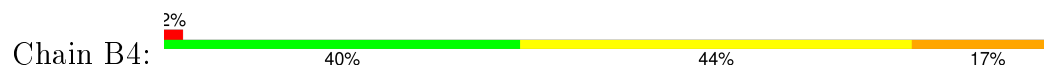
- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L34





- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.69Å 451.66Å 614.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 3.40 49.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.52-3.40) 97.6 (49.52-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.228 , 0.266 0.223 , 0.262	Depositor DCC
R_{free} test set	7680 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 106.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 775950 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	282142	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.63	4/36238 (0.0%)	1.02	99/56561 (0.2%)
1	CA	0.57	0/36238	0.96	75/56561 (0.1%)
2	AB	0.31	0/1936	0.51	0/2609
2	CB	0.28	0/1936	0.50	0/2609
3	AC	0.31	0/1637	0.47	0/2205
3	CC	0.29	0/1637	0.47	0/2205
4	AD	0.41	0/1733	0.59	0/2318
4	CD	0.34	0/1733	0.56	0/2318
5	AE	0.41	0/1172	0.61	0/1576
5	CE	0.36	0/1172	0.57	0/1576
6	AF	0.33	0/856	0.57	0/1154
6	CF	0.37	0/856	0.59	0/1154
7	AG	0.27	0/1276	0.46	0/1709
7	CG	0.27	0/1276	0.46	0/1709
8	AH	0.39	0/1136	0.61	0/1527
8	CH	0.33	0/1136	0.58	0/1527
9	AI	0.29	0/1029	0.45	0/1378
9	CI	0.27	0/1029	0.45	0/1378
10	AJ	0.28	0/808	0.48	0/1085
10	CJ	0.27	0/808	0.46	0/1085
11	AK	0.39	0/900	0.59	0/1213
11	CK	0.41	0/900	0.61	0/1213
12	AL	0.47	0/987	0.70	1/1320 (0.1%)
12	CL	0.44	0/987	0.68	0/1320
13	AM	0.25	0/939	0.44	0/1258
13	CM	0.24	0/939	0.44	0/1258
14	AN	0.31	0/501	0.50	0/664
14	CN	0.31	0/501	0.52	0/664
15	AO	0.39	0/745	0.57	0/992
15	CO	0.37	0/745	0.56	0/992
16	AP	0.42	0/717	0.62	0/963
16	CP	0.34	0/717	0.59	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	0/837	0.60	0/1117
17	CQ	0.37	0/837	0.56	0/1117
18	AR	0.38	0/579	0.61	0/768
18	CR	0.37	0/579	0.60	0/768
19	AS	0.25	0/643	0.43	0/865
19	CS	0.25	0/643	0.42	0/865
20	AT	0.38	0/764	0.57	0/1006
20	CT	0.33	0/764	0.54	0/1006
21	AU	0.23	0/213	0.43	0/277
21	CU	0.24	0/213	0.42	0/277
22	AV	0.43	0/802	0.68	0/1245
22	CV	0.43	0/802	0.69	0/1245
23	BA	1.07	153/66570 (0.2%)	1.48	1344/103918 (1.3%)
23	DA	1.19	253/66575 (0.4%)	1.59	1756/103930 (1.7%)
24	BB	0.58	0/2853	1.00	9/4451 (0.2%)
24	DB	0.59	0/2853	1.04	3/4451 (0.1%)
25	BC	0.71	1/2155 (0.0%)	0.90	3/2905 (0.1%)
25	DC	0.74	1/2155 (0.0%)	0.91	5/2905 (0.2%)
26	BD	0.58	0/1597	0.77	0/2153
26	DD	0.62	1/1597 (0.1%)	0.81	0/2153
27	BE	0.63	0/1622	0.77	0/2194
27	DE	0.67	0/1622	0.78	0/2194
28	BF	0.28	0/1500	0.49	0/2017
28	DF	0.28	0/1500	0.49	0/2017
29	BG	0.32	0/1246	0.58	0/1682
29	DG	0.44	0/1246	0.64	0/1682
30	BH	0.33	0/1148	0.56	0/1552
30	DH	0.38	0/1148	0.56	0/1552
31	BI	0.25	0/252	0.44	0/333
31	DI	0.27	0/252	0.46	0/333
32	BJ	0.56	0/1124	0.75	0/1515
32	DJ	0.59	0/1124	0.76	0/1515
33	BK	0.57	0/942	0.76	0/1268
33	DK	0.61	0/942	0.77	0/1268
34	BL	0.74	1/1131 (0.1%)	1.01	1/1504 (0.1%)
34	DL	0.75	2/1131 (0.2%)	1.03	5/1504 (0.3%)
35	BM	0.61	0/1099	0.83	2/1468 (0.1%)
35	DM	0.60	0/1099	0.83	1/1468 (0.1%)
36	BN	0.59	0/974	0.85	0/1302
36	DN	0.59	0/974	0.83	1/1302 (0.1%)
37	BO	0.36	0/779	0.58	0/1036
37	DO	0.39	0/779	0.61	0/1036
38	BP	0.50	0/1158	0.68	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DP	0.51	0/1158	0.69	0/1544
39	BQ	0.63	0/970	0.81	0/1290
39	DQ	0.67	0/970	0.81	0/1290
40	BR	0.58	0/790	0.73	1/1057 (0.1%)
40	DR	0.61	0/790	0.74	1/1057 (0.1%)
41	BS	0.63	0/902	0.78	0/1209
41	DS	0.66	0/902	0.76	0/1209
42	BT	0.64	0/740	0.79	0/993
42	DT	0.74	0/740	0.84	0/993
43	BU	0.53	0/789	0.76	0/1051
43	DU	0.56	0/789	0.76	0/1051
44	BV	0.36	0/1524	0.57	0/2068
44	DV	0.38	0/1524	0.57	0/2068
45	BW	0.50	0/613	0.71	0/816
45	DW	0.52	0/613	0.72	0/816
46	BX	0.73	0/702	0.98	2/932 (0.2%)
46	DX	0.82	0/702	1.04	2/932 (0.2%)
47	BY	0.55	0/523	0.87	1/690 (0.1%)
47	DY	0.72	0/523	0.98	3/690 (0.4%)
48	BZ	0.52	0/473	0.68	0/634
48	DZ	0.50	0/473	0.65	0/634
49	B1	0.23	0/229	0.40	0/309
49	D1	0.22	0/229	0.41	0/309
50	B2	0.61	0/419	0.80	0/567
50	D2	0.58	0/419	0.79	0/567
51	B3	0.28	0/388	0.46	0/518
51	D3	0.27	0/388	0.46	0/518
52	B4	0.72	0/427	0.89	0/561
52	D4	0.84	0/427	1.05	1/561 (0.2%)
53	B5	0.68	0/516	0.88	0/679
53	D5	0.69	0/516	0.88	1/679 (0.1%)
All	All	0.85	416/305211 (0.1%)	1.21	3317/456064 (0.7%)

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
25	DC	0	1
27	BE	0	1
27	DE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	BL	0	5
34	DL	0	5
35	BM	0	1
35	DM	0	1
36	BN	0	1
36	DN	0	1
39	BQ	0	2
39	DQ	0	2
All	All	0	21

The worst 5 of 416 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DA	774	A	N9-C4	-13.87	1.29	1.37
23	DA	1332	G	N9-C4	-11.99	1.28	1.38
23	DA	1602	U	C4-O4	11.31	1.32	1.23
23	BA	1332	G	N9-C4	-11.02	1.29	1.38
23	DA	2249	U	C4-O4	10.67	1.32	1.23

The worst 5 of 3317 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DA	761	A	N1-C6-N6	30.82	137.09	118.60
23	BA	761	A	N1-C6-N6	25.08	133.65	118.60
23	DA	1332	G	N3-C4-N9	-24.42	111.35	126.00
23	DA	1332	G	N3-C4-C5	23.85	140.52	128.60
23	BA	1332	G	N3-C4-N9	-22.46	112.52	126.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BE	47	GLY	Peptide
34	BL	29	LYS	Peptide
34	BL	37	GLY	Peptide
34	BL	39	LYS	Peptide
34	BL	9	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32372	0	16339	1680	0
1	CA	32372	0	16339	1784	0
2	AB	1901	0	1951	173	0
2	CB	1901	0	1951	180	0
3	AC	1613	0	1677	180	0
3	CC	1613	0	1677	186	0
4	AD	1703	0	1764	192	0
4	CD	1703	0	1764	182	1
5	AE	1156	0	1213	141	0
5	CE	1156	0	1213	141	0
6	AF	843	0	857	96	1
6	CF	843	0	857	93	0
7	AG	1257	0	1296	95	0
7	CG	1257	0	1296	92	0
8	AH	1116	0	1177	133	0
8	CH	1116	0	1177	140	0
9	AI	1011	0	1043	100	0
9	CI	1011	0	1043	112	0
10	AJ	795	0	840	93	0
10	CJ	795	0	840	92	0
11	AK	885	0	904	76	0
11	CK	885	0	904	72	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	139	0
13	AM	929	0	987	83	0
13	CM	929	0	987	83	0
14	AN	492	0	530	49	0
14	CN	492	0	532	61	0
15	AO	734	0	771	66	0
15	CO	734	0	771	60	0
16	AP	701	0	720	96	0
16	CP	701	0	720	90	0
17	AQ	824	0	893	66	0
17	CQ	824	0	893	77	0
18	AR	574	0	644	70	0
18	CR	574	0	644	70	0
19	AS	630	0	652	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	630	0	652	60	0
20	AT	762	0	859	64	0
20	CT	762	0	859	70	0
21	AU	209	0	221	16	0
21	CU	209	0	221	17	0
22	AV	719	0	366	58	0
22	CV	719	0	366	57	0
23	BA	59440	0	29964	2618	0
23	DA	59442	0	29965	2593	0
24	BB	2551	0	1295	147	0
24	DB	2551	0	1295	148	0
25	BC	2105	0	2182	353	0
25	DC	2105	0	2182	347	0
26	BD	1564	0	1629	224	0
26	DD	1564	0	1629	224	0
27	BE	1587	0	1632	147	0
27	DE	1587	0	1632	155	0
28	BF	1475	0	1537	155	0
28	DF	1475	0	1537	150	0
29	BG	1223	0	1282	114	0
29	DG	1223	0	1282	121	0
30	BH	1133	0	1220	131	0
30	DH	1133	0	1220	133	0
31	BI	254	0	275	8	0
31	DI	254	0	275	8	0
32	BJ	1097	0	1168	170	0
32	DJ	1097	0	1168	158	0
33	BK	932	0	994	97	0
33	DK	932	0	994	100	0
34	BL	1114	0	1187	270	0
34	DL	1114	0	1187	279	0
35	BM	1079	0	1127	170	0
35	DM	1079	0	1127	172	0
36	BN	960	0	1021	153	0
36	DN	960	0	1021	142	0
37	BO	771	0	832	95	0
37	DO	771	0	832	100	0
38	BP	1144	0	1211	129	0
38	DP	1144	0	1211	132	0
39	BQ	953	0	1013	150	0
39	DQ	953	0	1013	155	0
40	BR	779	0	852	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DR	779	0	852	128	0
41	BS	891	0	951	106	0
41	DS	891	0	951	110	0
42	BT	726	0	778	88	0
42	DT	726	0	778	92	0
43	BU	776	0	870	138	0
43	DU	776	0	870	139	0
44	BV	1492	0	1513	174	0
44	DV	1492	0	1513	171	0
45	BW	605	0	628	71	0
45	DW	605	0	628	63	0
46	BX	695	0	764	112	0
46	DX	695	0	764	106	0
47	BY	521	0	575	81	0
47	DY	521	0	575	81	0
48	BZ	468	0	523	46	0
48	DZ	468	0	523	46	0
49	B1	226	0	225	23	0
49	D1	226	0	225	24	0
50	B2	405	0	420	61	0
50	D2	405	0	420	64	0
51	B3	381	0	391	25	0
51	D3	381	0	391	26	0
52	B4	419	0	467	50	0
52	D4	419	0	467	48	0
53	B5	508	0	576	111	0
53	D5	508	0	576	110	0
54	AA	163	0	0	0	0
54	AD	1	0	0	0	0
54	AV	4	0	0	0	0
54	B2	1	0	0	0	0
54	BA	408	0	0	0	0
54	BB	17	0	0	0	0
54	BK	1	0	0	0	0
54	CA	140	0	0	0	0
54	CP	1	0	0	0	0
54	CV	1	0	0	0	0
54	D2	1	0	0	0	0
54	D4	1	0	0	0	0
54	DA	436	0	0	0	0
54	DB	17	0	0	0	0
54	DE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DG	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
All	All	282142	0	191729	18333	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 18333 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)
34:DL:59:LEU:HA	34:DL:61:ARG:NE	1.55	1.20
34:DL:57:THR:HG23	34:DL:59:LEU:HD22	1.22	1.20
35:BM:81:VAL:O	35:BM:82:ARG:HG2	1.39	1.19
34:BL:57:THR:HG23	34:BL:59:LEU:HD22	1.21	1.19
52:D4:8:ASN:C	52:D4:8:ASN:HD22	1.42	1.18

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)
6:AF:15:ASP:OD1	4:CD:20:TYR:OH[4_555]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	232/234 (99%)	172 (74%)	40 (17%)	20 (9%)	1 10
2	CB	232/234 (99%)	173 (75%)	38 (16%)	21 (9%)	1 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/206 (99%)	136 (67%)	43 (21%)	25 (12%)	0	5
3	CC	204/206 (99%)	134 (66%)	45 (22%)	25 (12%)	0	5
4	AD	206/208 (99%)	152 (74%)	38 (18%)	16 (8%)	1	12
4	CD	206/208 (99%)	151 (73%)	40 (19%)	15 (7%)	1	14
5	AE	149/151 (99%)	103 (69%)	34 (23%)	12 (8%)	1	11
5	CE	149/151 (99%)	104 (70%)	34 (23%)	11 (7%)	1	14
6	AF	99/101 (98%)	71 (72%)	17 (17%)	11 (11%)	0	6
6	CF	99/101 (98%)	71 (72%)	18 (18%)	10 (10%)	1	7
7	AG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	5	37
7	CG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	5	37
8	AH	136/138 (99%)	97 (71%)	29 (21%)	10 (7%)	1	14
8	CH	136/138 (99%)	98 (72%)	28 (21%)	10 (7%)	1	14
9	AI	125/127 (98%)	91 (73%)	31 (25%)	3 (2%)	7	44
9	CI	125/127 (98%)	89 (71%)	32 (26%)	4 (3%)	5	38
10	AJ	96/98 (98%)	72 (75%)	20 (21%)	4 (4%)	3	29
10	CJ	96/98 (98%)	74 (77%)	18 (19%)	4 (4%)	3	29
11	AK	117/119 (98%)	83 (71%)	29 (25%)	5 (4%)	3	29
11	CK	117/119 (98%)	82 (70%)	30 (26%)	5 (4%)	3	29
12	AL	122/124 (98%)	78 (64%)	28 (23%)	16 (13%)	0	4
12	CL	122/124 (98%)	80 (66%)	27 (22%)	15 (12%)	0	5
13	AM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	4	35
13	CM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	4	35
14	AN	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	2	23
14	CN	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	2	23
15	AO	86/88 (98%)	62 (72%)	17 (20%)	7 (8%)	1	11
15	CO	86/88 (98%)	61 (71%)	19 (22%)	6 (7%)	1	15
16	AP	81/83 (98%)	46 (57%)	24 (30%)	11 (14%)	0	3
16	CP	81/83 (98%)	46 (57%)	25 (31%)	10 (12%)	0	5
17	AQ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	14
17	CQ	97/99 (98%)	75 (77%)	16 (16%)	6 (6%)	2	18
18	AR	68/70 (97%)	40 (59%)	19 (28%)	9 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	68/70 (97%)	41 (60%)	18 (26%)	9 (13%)	0	4
19	AS	76/78 (97%)	51 (67%)	21 (28%)	4 (5%)	2	22
19	CS	76/78 (97%)	50 (66%)	21 (28%)	5 (7%)	1	16
20	AT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	1	14
20	CT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	1	14
21	AU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	3	27
21	CU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	3	27
25	BC	269/271 (99%)	213 (79%)	36 (13%)	20 (7%)	1	14
25	DC	269/271 (99%)	210 (78%)	39 (14%)	20 (7%)	1	14
26	BD	202/204 (99%)	154 (76%)	34 (17%)	14 (7%)	1	15
26	DD	202/204 (99%)	155 (77%)	32 (16%)	15 (7%)	1	14
27	BE	200/202 (99%)	152 (76%)	32 (16%)	16 (8%)	1	12
27	DE	200/202 (99%)	155 (78%)	30 (15%)	15 (8%)	1	13
28	BF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	1	16
28	DF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	1	16
29	BG	157/159 (99%)	112 (71%)	35 (22%)	10 (6%)	2	17
29	DG	157/159 (99%)	111 (71%)	36 (23%)	10 (6%)	2	17
30	BH	143/145 (99%)	95 (66%)	29 (20%)	19 (13%)	0	4
30	DH	143/145 (99%)	91 (64%)	31 (22%)	21 (15%)	0	3
31	BI	28/65 (43%)	25 (89%)	3 (11%)	0	100	100
31	DI	28/65 (43%)	25 (89%)	3 (11%)	0	100	100
32	BJ	135/137 (98%)	97 (72%)	26 (19%)	12 (9%)	1	9
32	DJ	135/137 (98%)	97 (72%)	24 (18%)	14 (10%)	1	7
33	BK	120/122 (98%)	100 (83%)	11 (9%)	9 (8%)	1	13
33	DK	120/122 (98%)	98 (82%)	14 (12%)	8 (7%)	1	16
34	BL	144/146 (99%)	87 (60%)	31 (22%)	26 (18%)	0	1
34	DL	144/146 (99%)	86 (60%)	35 (24%)	23 (16%)	0	2
35	BM	134/136 (98%)	86 (64%)	28 (21%)	20 (15%)	0	2
35	DM	134/136 (98%)	86 (64%)	30 (22%)	18 (13%)	0	4
36	BN	115/117 (98%)	91 (79%)	13 (11%)	11 (10%)	1	8
36	DN	115/117 (98%)	90 (78%)	15 (13%)	10 (9%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	96/98 (98%)	57 (59%)	23 (24%)	16 (17%)	0	2
37	DO	96/98 (98%)	54 (56%)	25 (26%)	17 (18%)	0	2
38	BP	135/137 (98%)	101 (75%)	18 (13%)	16 (12%)	0	5
38	DP	135/137 (98%)	100 (74%)	19 (14%)	16 (12%)	0	5
39	BQ	114/116 (98%)	78 (68%)	22 (19%)	14 (12%)	0	5
39	DQ	114/116 (98%)	82 (72%)	20 (18%)	12 (10%)	1	7
40	BR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	9
40	DR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	9
41	BS	110/112 (98%)	88 (80%)	17 (16%)	5 (4%)	3	27
41	DS	110/112 (98%)	87 (79%)	17 (16%)	6 (6%)	2	21
42	BT	90/92 (98%)	69 (77%)	16 (18%)	5 (6%)	2	21
42	DT	90/92 (98%)	67 (74%)	18 (20%)	5 (6%)	2	21
43	BU	98/100 (98%)	55 (56%)	24 (24%)	19 (19%)	0	1
43	DU	98/100 (98%)	58 (59%)	21 (21%)	19 (19%)	0	1
44	BV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	1	9
44	DV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	1	9
45	BW	74/76 (97%)	61 (82%)	10 (14%)	3 (4%)	3	30
45	DW	74/76 (97%)	60 (81%)	10 (14%)	4 (5%)	2	22
46	BX	86/88 (98%)	57 (66%)	16 (19%)	13 (15%)	0	2
46	DX	86/88 (98%)	54 (63%)	19 (22%)	13 (15%)	0	2
47	BY	60/62 (97%)	45 (75%)	8 (13%)	7 (12%)	0	5
47	DY	60/62 (97%)	41 (68%)	12 (20%)	7 (12%)	0	5
48	BZ	57/59 (97%)	49 (86%)	7 (12%)	1 (2%)	11	50
48	DZ	57/59 (97%)	50 (88%)	6 (10%)	1 (2%)	11	50
49	B1	28/30 (93%)	15 (54%)	7 (25%)	6 (21%)	0	1
49	D1	28/30 (93%)	15 (54%)	7 (25%)	6 (21%)	0	1
50	B2	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	12
50	D2	50/52 (96%)	39 (78%)	7 (14%)	4 (8%)	1	12
51	B3	42/44 (96%)	26 (62%)	11 (26%)	5 (12%)	0	5
51	D3	42/44 (96%)	26 (62%)	11 (26%)	5 (12%)	0	5
52	B4	46/48 (96%)	42 (91%)	3 (6%)	1 (2%)	8	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	D4	46/48 (96%)	42 (91%)	3 (6%)	1 (2%)	8	46
53	B5	61/63 (97%)	43 (70%)	12 (20%)	6 (10%)	1	8
53	D5	61/63 (97%)	44 (72%)	10 (16%)	7 (12%)	0	5
All	All	11192/11458 (98%)	8080 (72%)	2125 (19%)	987 (9%)	1	10

5 of 987 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	204	ASN
3	AC	189	ALA
3	AC	196	LEU
4	AD	28	SER
4	AD	30	LYS

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	202/202 (100%)	178 (88%)	24 (12%)	6	29
2	CB	202/202 (100%)	179 (89%)	23 (11%)	7	31
3	AC	160/160 (100%)	146 (91%)	14 (9%)	12	46
3	CC	160/160 (100%)	145 (91%)	15 (9%)	11	42
4	AD	180/180 (100%)	150 (83%)	30 (17%)	3	14
4	CD	180/180 (100%)	150 (83%)	30 (17%)	3	14
5	AE	116/116 (100%)	92 (79%)	24 (21%)	1	7
5	CE	116/116 (100%)	94 (81%)	22 (19%)	2	9
6	AF	90/90 (100%)	82 (91%)	8 (9%)	12	45
6	CF	90/90 (100%)	83 (92%)	7 (8%)	16	52
7	AG	126/126 (100%)	121 (96%)	5 (4%)	38	75
7	CG	126/126 (100%)	121 (96%)	5 (4%)	38	75
8	AH	119/119 (100%)	102 (86%)	17 (14%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	104 (87%)	15 (13%)	5	27
9	AI	98/98 (100%)	88 (90%)	10 (10%)	9	38
9	CI	98/98 (100%)	88 (90%)	10 (10%)	9	38
10	AJ	88/88 (100%)	78 (89%)	10 (11%)	7	31
10	CJ	88/88 (100%)	78 (89%)	10 (11%)	7	31
11	AK	90/90 (100%)	75 (83%)	15 (17%)	3	14
11	CK	90/90 (100%)	76 (84%)	14 (16%)	3	18
12	AL	104/104 (100%)	83 (80%)	21 (20%)	1	7
12	CL	104/104 (100%)	83 (80%)	21 (20%)	1	7
13	AM	94/94 (100%)	87 (93%)	7 (7%)	17	55
13	CM	94/94 (100%)	87 (93%)	7 (7%)	17	55
14	AN	49/49 (100%)	45 (92%)	4 (8%)	14	50
14	CN	49/49 (100%)	45 (92%)	4 (8%)	14	50
15	AO	79/79 (100%)	69 (87%)	10 (13%)	5	26
15	CO	79/79 (100%)	69 (87%)	10 (13%)	5	26
16	AP	72/72 (100%)	57 (79%)	15 (21%)	1	6
16	CP	72/72 (100%)	56 (78%)	16 (22%)	1	5
17	AQ	94/94 (100%)	78 (83%)	16 (17%)	2	14
17	CQ	94/94 (100%)	79 (84%)	15 (16%)	3	16
18	AR	61/61 (100%)	58 (95%)	3 (5%)	31	70
18	CR	61/61 (100%)	58 (95%)	3 (5%)	31	70
19	AS	69/69 (100%)	60 (87%)	9 (13%)	5	25
19	CS	69/69 (100%)	60 (87%)	9 (13%)	5	25
20	AT	76/76 (100%)	65 (86%)	11 (14%)	4	21
20	CT	76/76 (100%)	65 (86%)	11 (14%)	4	21
21	AU	19/19 (100%)	19 (100%)	0	100	100
21	CU	19/19 (100%)	19 (100%)	0	100	100
25	BC	213/213 (100%)	164 (77%)	49 (23%)	1	4
25	DC	213/213 (100%)	162 (76%)	51 (24%)	1	4
26	BD	165/165 (100%)	129 (78%)	36 (22%)	1	6
26	DD	165/165 (100%)	129 (78%)	36 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BE	161/161 (100%)	124 (77%)	37 (23%)	1	4
27	DE	161/161 (100%)	124 (77%)	37 (23%)	1	4
28	BF	155/155 (100%)	132 (85%)	23 (15%)	4	20
28	DF	155/155 (100%)	134 (86%)	21 (14%)	5	24
29	BG	132/132 (100%)	108 (82%)	24 (18%)	2	11
29	DG	132/132 (100%)	107 (81%)	25 (19%)	2	9
30	BH	122/122 (100%)	103 (84%)	19 (16%)	3	18
30	DH	122/122 (100%)	103 (84%)	19 (16%)	3	18
31	BI	27/53 (51%)	25 (93%)	2 (7%)	17	55
31	DI	27/53 (51%)	25 (93%)	2 (7%)	17	55
32	BJ	116/116 (100%)	84 (72%)	32 (28%)	0	3
32	DJ	116/116 (100%)	85 (73%)	31 (27%)	0	3
33	BK	100/100 (100%)	78 (78%)	22 (22%)	1	5
33	DK	100/100 (100%)	78 (78%)	22 (22%)	1	5
34	BL	112/112 (100%)	75 (67%)	37 (33%)	0	2
34	DL	112/112 (100%)	76 (68%)	36 (32%)	0	2
35	BM	106/106 (100%)	82 (77%)	24 (23%)	1	5
35	DM	106/106 (100%)	81 (76%)	25 (24%)	1	4
36	BN	100/100 (100%)	75 (75%)	25 (25%)	1	4
36	DN	100/100 (100%)	76 (76%)	24 (24%)	1	4
37	BO	77/77 (100%)	63 (82%)	14 (18%)	2	11
37	DO	77/77 (100%)	63 (82%)	14 (18%)	2	11
38	BP	121/121 (100%)	96 (79%)	25 (21%)	1	7
38	DP	121/121 (100%)	94 (78%)	27 (22%)	1	5
39	BQ	92/92 (100%)	71 (77%)	21 (23%)	1	5
39	DQ	92/92 (100%)	71 (77%)	21 (23%)	1	5
40	BR	82/82 (100%)	63 (77%)	19 (23%)	1	4
40	DR	82/82 (100%)	61 (74%)	21 (26%)	0	3
41	BS	91/91 (100%)	65 (71%)	26 (29%)	0	2
41	DS	91/91 (100%)	65 (71%)	26 (29%)	0	2
42	BT	74/74 (100%)	60 (81%)	14 (19%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DT	74/74 (100%)	60 (81%)	14 (19%)	2	9
43	BU	84/84 (100%)	66 (79%)	18 (21%)	1	6
43	DU	84/84 (100%)	67 (80%)	17 (20%)	1	7
44	BV	163/163 (100%)	142 (87%)	21 (13%)	5	26
44	DV	163/163 (100%)	141 (86%)	22 (14%)	5	24
45	BW	61/61 (100%)	52 (85%)	9 (15%)	4	20
45	DW	61/61 (100%)	53 (87%)	8 (13%)	5	25
46	BX	73/73 (100%)	50 (68%)	23 (32%)	0	2
46	DX	73/73 (100%)	50 (68%)	23 (32%)	0	2
47	BY	58/58 (100%)	46 (79%)	12 (21%)	1	7
47	DY	58/58 (100%)	46 (79%)	12 (21%)	1	7
48	BZ	51/51 (100%)	43 (84%)	8 (16%)	3	18
48	DZ	51/51 (100%)	43 (84%)	8 (16%)	3	18
49	B1	27/27 (100%)	26 (96%)	1 (4%)	41	77
49	D1	27/27 (100%)	26 (96%)	1 (4%)	41	77
50	B2	45/45 (100%)	40 (89%)	5 (11%)	8	33
50	D2	45/45 (100%)	39 (87%)	6 (13%)	5	24
51	B3	43/43 (100%)	38 (88%)	5 (12%)	7	31
51	D3	43/43 (100%)	38 (88%)	5 (12%)	7	31
52	B4	41/41 (100%)	29 (71%)	12 (29%)	0	2
52	D4	41/41 (100%)	28 (68%)	13 (32%)	0	2
53	B5	53/53 (100%)	42 (79%)	11 (21%)	1	6
53	D5	53/53 (100%)	43 (81%)	10 (19%)	2	9
All	All	9462/9514 (100%)	7811 (83%)	1651 (17%)	2	13

5 of 1651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BW	63	VAL
7	CG	67	GLU
42	DT	81	VAL
46	BX	73	LEU
2	CB	117	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 245 such sidechains are listed below:

Mol	Chain	Res	Type
46	BX	45	ASN
7	CG	13	GLN
44	DV	121	HIS
47	BY	56	GLN
2	CB	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	293 (19%)	14 (0%)
1	CA	1505/1506 (99%)	294 (19%)	14 (0%)
22	AV	32/43 (74%)	3 (9%)	0
22	CV	32/43 (74%)	3 (9%)	0
23	BA	2755/2879 (95%)	584 (21%)	27 (0%)
23	DA	2757/2879 (95%)	589 (21%)	29 (1%)
24	BB	118/119 (99%)	26 (22%)	0
24	DB	118/119 (99%)	27 (22%)	0
All	All	8822/9094 (97%)	1819 (20%)	84 (0%)

5 of 1819 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 84 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2433	A
1	CA	793	U
23	DA	2272	U
23	BA	2542	A
1	CA	327	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1198 ligands modelled in this entry, 1198 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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1506/1506 (100%)	0.40	63 (4%) 40 35	51, 122, 245, 498	0
1	CA	1506/1506 (100%)	0.47	98 (6%) 22 21	51, 126, 251, 414	0
2	AB	234/234 (100%)	1.11	46 (19%) 1 2	113, 174, 244, 298	0
2	CB	234/234 (100%)	0.92	48 (20%) 1 1	111, 177, 259, 325	0
3	AC	206/206 (100%)	0.82	30 (14%) 3 3	106, 160, 225, 263	0
3	CC	206/206 (100%)	0.85	37 (17%) 2 2	105, 161, 226, 271	0
4	AD	208/208 (100%)	0.56	17 (8%) 14 13	90, 142, 199, 247	0
4	CD	208/208 (100%)	1.22	46 (22%) 1 1	94, 146, 220, 300	0
5	AE	151/151 (100%)	0.40	8 (5%) 30 27	73, 114, 172, 272	0
5	CE	151/151 (100%)	0.65	18 (11%) 6 6	73, 117, 188, 252	0
6	AF	101/101 (100%)	0.82	17 (16%) 2 2	83, 135, 192, 270	0
6	CF	101/101 (100%)	0.26	5 (4%) 32 29	79, 131, 184, 246	0
7	AG	155/155 (100%)	1.31	48 (30%) 1 1	118, 187, 237, 333	0
7	CG	155/155 (100%)	1.77	59 (38%) 0 1	119, 187, 237, 286	0
8	AH	138/138 (100%)	0.53	11 (7%) 15 14	77, 121, 166, 199	0
8	CH	138/138 (100%)	0.70	13 (9%) 11 11	81, 123, 167, 219	0
9	AI	127/127 (100%)	1.70	40 (31%) 1 1	119, 225, 289, 345	0
9	CI	127/127 (100%)	1.75	34 (26%) 1 1	121, 225, 286, 354	0
10	AJ	98/98 (100%)	1.92	37 (37%) 0 1	118, 198, 278, 356	0
10	CJ	98/98 (100%)	2.03	42 (42%) 0 0	122, 197, 264, 351	0
11	AK	119/119 (100%)	0.71	19 (15%) 3 3	71, 111, 171, 263	0
11	CK	119/119 (100%)	0.45	10 (8%) 14 13	74, 111, 178, 264	0
12	AL	124/124 (100%)	0.52	6 (4%) 34 31	67, 107, 165, 268	0
12	CL	124/124 (100%)	0.89	19 (15%) 3 3	70, 109, 178, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	116/116 (100%)	1.29	34 (29%) 1 1	134, 213, 299, 335	0
13	CM	116/116 (100%)	2.18	52 (44%) 0 0	135, 214, 309, 362	0
14	AN	60/60 (100%)	1.49	15 (25%) 1 1	114, 166, 217, 235	0
14	CN	60/60 (100%)	1.25	12 (20%) 1 2	116, 167, 227, 281	0
15	AO	88/88 (100%)	0.17	1 (1%) 82 77	66, 108, 159, 227	0
15	CO	88/88 (100%)	0.45	4 (4%) 37 33	67, 110, 166, 241	0
16	AP	83/83 (100%)	0.63	6 (7%) 18 17	84, 118, 174, 214	0
16	CP	83/83 (100%)	1.84	33 (39%) 0 0	87, 123, 177, 210	0
17	AQ	99/99 (100%)	0.30	2 (2%) 68 62	78, 112, 169, 216	0
17	CQ	99/99 (100%)	0.78	11 (11%) 7 7	79, 116, 166, 215	0
18	AR	70/70 (100%)	1.01	14 (20%) 1 2	84, 128, 183, 284	0
18	CR	70/70 (100%)	0.63	7 (10%) 9 9	82, 128, 192, 232	0
19	AS	78/78 (100%)	2.97	47 (60%) 0 0	152, 210, 275, 321	0
19	CS	78/78 (100%)	3.24	53 (67%) 0 0	151, 216, 291, 350	0
20	AT	99/99 (100%)	0.62	5 (5%) 32 28	86, 134, 203, 241	0
20	CT	99/99 (100%)	1.21	26 (26%) 1 1	92, 136, 212, 269	0
21	AU	24/24 (100%)	2.89	16 (66%) 0 0	160, 225, 264, 322	0
21	CU	24/24 (100%)	3.00	13 (54%) 0 0	163, 218, 265, 364	0
22	AV	34/43 (79%)	1.59	12 (35%) 0 1	89, 196, 324, 362	0
22	CV	34/43 (79%)	2.13	12 (35%) 0 1	92, 198, 333, 339	0
23	BA	2760/2879 (95%)	0.03	55 (1%) 68 62	27, 65, 180, 398	0
23	DA	2760/2879 (95%)	0.09	48 (1%) 73 67	25, 63, 178, 410	0
24	BB	119/119 (100%)	0.24	5 (4%) 40 35	77, 129, 182, 232	0
24	DB	119/119 (100%)	0.23	6 (5%) 32 29	78, 129, 184, 236	0
25	BC	271/271 (100%)	-0.06	3 (1%) 82 77	25, 58, 109, 175	0
25	DC	271/271 (100%)	-0.01	0 100 100	18, 57, 109, 177	0
26	BD	204/204 (100%)	0.45	17 (8%) 14 13	36, 73, 146, 341	0
26	DD	204/204 (100%)	0.45	9 (4%) 38 34	33, 71, 145, 347	0
27	BE	202/202 (100%)	-0.04	1 (0%) 91 89	31, 73, 155, 246	0
27	DE	202/202 (100%)	0.20	5 (2%) 61 55	25, 73, 155, 192	0
28	BF	181/181 (100%)	1.57	59 (32%) 1 1	102, 182, 254, 314	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	181/181 (100%)	1.55	62 (34%) 0 1	104, 185, 268, 331	0
29	BG	159/159 (100%)	1.65	56 (35%) 0 1	85, 143, 221, 343	0
29	DG	159/159 (100%)	0.61	9 (5%) 27 25	79, 136, 186, 235	0
30	BH	145/145 (100%)	3.27	72 (49%) 0 0	67, 243, 391, 482	0
30	DH	145/145 (100%)	1.90	49 (33%) 0 1	64, 236, 379, 480	0
31	BI	32/65 (49%)	6.02	30 (93%) 0 0	171, 246, 347, 355	0
31	DI	32/65 (49%)	3.39	24 (75%) 0 0	168, 253, 310, 334	0
32	BJ	137/137 (100%)	0.15	3 (2%) 65 60	51, 81, 142, 201	0
32	DJ	137/137 (100%)	0.07	1 (0%) 89 85	52, 81, 146, 194	0
33	BK	122/122 (100%)	0.09	0 100 100	42, 70, 111, 150	0
33	DK	122/122 (100%)	0.23	4 (3%) 50 45	41, 69, 111, 162	0
34	BL	146/146 (100%)	0.65	15 (10%) 9 8	34, 97, 166, 309	0
34	DL	146/146 (100%)	0.56	14 (9%) 10 10	32, 97, 163, 293	0
35	BM	136/136 (100%)	0.35	8 (5%) 26 23	49, 89, 199, 370	0
35	DM	136/136 (100%)	0.58	12 (8%) 12 12	48, 88, 205, 406	0
36	BN	117/117 (100%)	0.35	1 (0%) 85 81	45, 73, 137, 249	0
36	DN	117/117 (100%)	0.24	1 (0%) 85 81	43, 73, 134, 235	0
37	BO	98/98 (100%)	1.31	26 (26%) 1 1	82, 137, 197, 223	0
37	DO	98/98 (100%)	1.05	24 (24%) 1 1	80, 136, 190, 215	0
38	BP	137/137 (100%)	0.16	6 (4%) 38 34	58, 93, 185, 250	0
38	DP	137/137 (100%)	0.45	18 (13%) 5 4	55, 92, 190, 273	0
39	BQ	116/116 (100%)	-0.04	0 100 100	35, 75, 124, 239	0
39	DQ	116/116 (100%)	-0.19	1 (0%) 85 81	26, 74, 126, 248	0
40	BR	101/101 (100%)	0.15	0 100 100	41, 105, 164, 264	0
40	DR	101/101 (100%)	0.60	5 (4%) 32 29	41, 110, 156, 259	0
41	BS	112/112 (100%)	0.10	2 (1%) 71 65	44, 59, 137, 254	0
41	DS	112/112 (100%)	0.14	5 (4%) 37 33	43, 59, 134, 255	0
42	BT	92/92 (100%)	0.03	2 (2%) 65 60	45, 77, 129, 170	0
42	DT	92/92 (100%)	0.19	0 100 100	36, 73, 127, 169	0
43	BU	100/100 (100%)	1.69	31 (31%) 1 1	62, 104, 257, 396	0
43	DU	100/100 (100%)	1.43	13 (13%) 5 4	61, 102, 251, 408	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	188/188 (100%)	0.79	28 (14%) 3 3	83, 138, 195, 245	0
44	DV	188/188 (100%)	0.32	4 (2%) 67 61	83, 139, 194, 230	0
45	BW	76/76 (100%)	0.49	6 (7%) 15 14	58, 84, 139, 261	0
45	DW	76/76 (100%)	0.62	4 (5%) 30 27	59, 84, 135, 256	0
46	BX	88/88 (100%)	0.43	4 (4%) 37 33	37, 74, 153, 322	0
46	DX	88/88 (100%)	0.49	3 (3%) 49 44	39, 70, 153, 326	0
47	BY	62/62 (100%)	0.32	6 (9%) 10 10	57, 98, 209, 292	0
47	DY	62/62 (100%)	0.85	7 (11%) 7 7	51, 96, 212, 328	0
48	BZ	59/59 (100%)	0.85	5 (8%) 13 13	43, 81, 156, 299	0
48	DZ	59/59 (100%)	1.08	6 (10%) 9 9	45, 85, 157, 305	0
49	B1	30/30 (100%)	2.79	20 (66%) 0 0	184, 253, 295, 311	0
49	D1	30/30 (100%)	2.09	12 (40%) 0 0	183, 261, 306, 358	0
50	B2	52/52 (100%)	0.50	8 (15%) 3 3	26, 71, 187, 233	0
50	D2	52/52 (100%)	0.03	3 (5%) 26 24	21, 72, 197, 229	0
51	B3	44/44 (100%)	8.21	39 (88%) 0 0	139, 249, 299, 320	0
51	D3	44/44 (100%)	9.38	38 (86%) 0 0	141, 245, 312, 333	0
52	B4	48/48 (100%)	0.09	1 (2%) 67 61	33, 43, 93, 194	0
52	D4	48/48 (100%)	0.02	1 (2%) 67 61	21, 41, 91, 200	0
53	B5	63/63 (100%)	0.17	1 (1%) 74 69	45, 68, 131, 215	0
53	D5	63/63 (100%)	0.29	4 (6%) 23 22	45, 70, 132, 216	0
All	All	20230/20552 (98%)	0.58	2048 (10%) 9 9	18, 104, 241, 498	0

The worst 5 of 2048 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	D3	47	THR	31.3
51	B3	41	PRO	26.6
43	DU	52	SER	25.3
51	B3	40	CYS	24.3
51	B3	13	CYS	24.2

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

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	BA	3222	1/1	0.92	1.17	87.35	91,91,91,91	0
54	MG	CA	1612	1/1	0.86	0.93	81.46	58,58,58,58	0
54	MG	DA	3223	1/1	0.85	0.61	56.85	45,45,45,45	0
54	MG	BA	3284	1/1	0.86	0.89	54.14	85,85,85,85	0
54	MG	BA	3046	1/1	0.98	0.92	45.19	87,87,87,87	0
54	MG	DA	3216	1/1	0.90	0.62	44.76	46,46,46,46	0
54	MG	BA	3019	1/1	0.75	0.65	44.61	58,58,58,58	0
54	MG	CA	1692	1/1	0.90	0.80	40.04	78,78,78,78	0
54	MG	DA	3191	1/1	0.99	0.48	35.59	24,24,24,24	0
54	MG	AA	1752	1/1	0.87	0.93	35.09	81,81,81,81	0
54	MG	DA	2932	1/1	0.81	0.53	32.74	38,38,38,38	0
54	MG	DA	2934	1/1	0.94	0.44	29.96	25,25,25,25	0
54	MG	DA	3190	1/1	0.99	0.44	29.54	27,27,27,27	0
54	MG	BA	3268	1/1	0.81	0.77	29.22	58,58,58,58	0
54	MG	DA	3202	1/1	0.81	0.66	27.71	44,44,44,44	0
54	MG	BA	3027	1/1	0.71	0.51	26.34	62,62,62,62	0
54	MG	AA	1621	1/1	0.77	0.61	26.08	74,74,74,74	0
54	MG	DA	2955	1/1	0.95	0.45	24.73	40,40,40,40	0
54	MG	BA	2924	1/1	0.95	0.45	23.35	47,47,47,47	0
54	MG	DA	2999	1/1	0.57	0.43	23.14	76,76,76,76	0
54	MG	DA	2907	1/1	0.98	0.47	21.13	7,7,7,7	0
54	MG	DA	2911	1/1	0.96	0.40	21.11	7,7,7,7	0
54	MG	DA	3241	1/1	0.89	0.51	20.02	54,54,54,54	0
54	MG	AA	1630	1/1	0.91	0.37	19.13	70,70,70,70	0
54	MG	DA	2904	1/1	0.95	0.46	19.12	4,4,4,4	0
54	MG	BA	2941	1/1	0.95	0.64	18.77	50,50,50,50	0
54	MG	BA	3088	1/1	0.92	0.55	18.69	73,73,73,73	0
54	MG	BA	3185	1/1	0.95	0.24	18.51	56,56,56,56	0
54	MG	DA	3024	1/1	0.72	0.39	17.66	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	2902	1/1	0.98	0.40	17.51	10,10,10,10	0
54	MG	BA	2911	1/1	0.97	0.47	17.42	23,23,23,23	0
54	MG	DA	2905	1/1	0.95	0.38	17.19	9,9,9,9	0
54	MG	BA	2910	1/1	0.97	0.53	17.07	27,27,27,27	0
54	MG	BA	2903	1/1	0.99	0.39	16.87	14,14,14,14	0
54	MG	BA	2961	1/1	0.90	0.38	16.69	43,43,43,43	0
54	MG	DA	3228	1/1	0.85	0.46	16.56	51,51,51,51	0
54	MG	DA	2959	1/1	0.79	0.39	16.47	56,56,56,56	0
54	MG	DA	3208	1/1	0.96	0.41	16.45	49,49,49,49	0
54	MG	BA	3182	1/1	0.96	0.51	15.84	20,20,20,20	0
54	MG	BA	2952	1/1	0.97	0.28	15.70	38,38,38,38	0
54	MG	BA	2970	1/1	0.90	0.58	15.47	45,45,45,45	0
54	MG	DA	2933	1/1	0.95	0.47	15.32	30,30,30,30	0
54	MG	BA	2920	1/1	0.95	0.35	15.19	28,28,28,28	0
54	MG	BA	2921	1/1	0.94	0.39	15.18	21,21,21,21	0
54	MG	BA	2918	1/1	0.98	0.35	15.07	17,17,17,17	0
54	MG	BA	3006	1/1	0.58	0.51	14.92	77,77,77,77	0
54	MG	DA	3165	1/1	0.80	0.62	14.88	71,71,71,71	0
54	MG	DA	3274	1/1	0.85	0.39	14.87	62,62,62,62	0
54	MG	AA	1682	1/1	0.84	0.40	14.64	85,85,85,85	0
54	MG	BA	2931	1/1	0.87	0.47	14.53	32,32,32,32	0
54	MG	DA	3324	1/1	0.58	0.51	14.33	78,78,78,78	0
54	MG	BA	3004	1/1	0.71	1.27	13.59	74,74,74,74	0
54	MG	BA	2909	1/1	0.95	0.41	13.58	24,24,24,24	0
54	MG	BA	3192	1/1	0.94	0.58	13.48	52,52,52,52	0
54	MG	DA	3251	1/1	0.72	0.37	13.33	63,63,63,63	0
54	MG	AA	1622	1/1	0.97	0.81	13.23	88,88,88,88	0
54	MG	DA	3259	1/1	0.85	0.53	13.20	108,108,108,108	0
54	MG	BA	3220	1/1	0.81	0.33	13.11	56,56,56,56	0
54	MG	BA	2967	1/1	0.95	0.41	13.10	24,24,24,24	0
54	MG	DA	3012	1/1	0.84	0.38	13.02	45,45,45,45	0
54	MG	BA	2968	1/1	0.87	0.47	12.76	51,51,51,51	0
54	MG	DA	3232	1/1	0.95	0.34	12.74	39,39,39,39	0
54	MG	DA	2915	1/1	0.91	0.47	12.72	14,14,14,14	0
54	MG	BA	3188	1/1	0.77	0.38	12.69	45,45,45,45	0
54	MG	DA	3149	1/1	0.81	0.45	12.64	74,74,74,74	0
54	MG	DA	3188	1/1	0.98	0.51	12.31	9,9,9,9	0
54	MG	DA	3047	1/1	0.84	0.34	12.26	66,66,66,66	0
54	MG	DA	3066	1/1	0.89	0.47	12.23	85,85,85,85	0
54	MG	DA	2921	1/1	0.98	0.42	12.17	17,17,17,17	0
54	MG	BA	3232	1/1	0.97	0.40	12.04	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1679	1/1	0.85	0.58	11.91	78,78,78,78	0
54	MG	DA	2906	1/1	0.98	0.41	11.68	27,27,27,27	0
54	MG	AA	1742	1/1	0.93	0.42	11.66	87,87,87,87	0
54	MG	BA	2901	1/1	0.98	0.40	11.46	23,23,23,23	0
54	MG	BA	2917	1/1	0.97	0.41	11.32	8,8,8,8	0
54	MG	DA	3000	1/1	0.97	0.36	11.30	35,35,35,35	0
54	MG	DA	2943	1/1	0.95	0.41	11.26	32,32,32,32	0
54	MG	DA	2909	1/1	0.97	0.41	11.21	5,5,5,5	0
54	MG	BA	3256	1/1	0.89	0.39	10.99	79,79,79,79	0
54	MG	DA	3272	1/1	0.87	0.43	10.87	41,41,41,41	0
54	MG	DA	3174	1/1	0.64	0.51	10.81	42,42,42,42	0
54	MG	BA	3179	1/1	0.96	0.48	10.76	19,19,19,19	0
54	MG	AA	1728	1/1	0.94	0.89	10.71	105,105,105,105	0
54	MG	BA	3270	1/1	0.92	0.30	10.63	61,61,61,61	0
54	MG	DA	2976	1/1	0.98	0.30	10.61	37,37,37,37	0
54	MG	BA	2914	1/1	0.93	0.43	10.61	31,31,31,31	0
54	MG	AA	1601	1/1	0.96	0.44	10.38	31,31,31,31	0
54	MG	BA	3091	1/1	0.83	0.40	10.23	56,56,56,56	0
54	MG	DA	2918	1/1	0.99	0.35	10.22	15,15,15,15	0
54	MG	AA	1723	1/1	0.79	0.51	10.19	81,81,81,81	0
54	MG	BA	2943	1/1	0.97	0.37	10.14	42,42,42,42	0
54	MG	DA	3215	1/1	0.94	0.45	10.10	39,39,39,39	0
54	MG	DA	3079	1/1	0.90	0.33	9.98	38,38,38,38	0
54	MG	BA	3226	1/1	0.76	0.42	9.84	81,81,81,81	0
54	MG	DA	2989	1/1	0.94	0.34	9.62	45,45,45,45	0
54	MG	BA	3097	1/1	0.89	0.30	9.42	53,53,53,53	0
54	MG	DA	2914	1/1	0.94	0.46	9.41	27,27,27,27	0
54	MG	DA	3198	1/1	0.97	0.29	9.38	26,26,26,26	0
54	MG	BA	3181	1/1	0.98	0.53	9.30	22,22,22,22	0
54	MG	CA	1715	1/1	0.88	0.36	9.25	74,74,74,74	0
54	MG	BA	2930	1/1	0.98	0.34	8.96	34,34,34,34	0
54	MG	AA	1603	1/1	0.93	0.32	8.81	35,35,35,35	0
54	MG	AA	1636	1/1	0.96	0.44	8.28	76,76,76,76	0
54	MG	BA	3184	1/1	0.96	0.32	8.16	42,42,42,42	0
54	MG	AA	1714	1/1	0.89	0.34	7.76	58,58,58,58	0
54	MG	BA	3151	1/1	0.97	0.71	7.54	56,56,56,56	0
54	MG	DA	3022	1/1	0.94	0.32	7.48	60,60,60,60	0
54	MG	BA	2904	1/1	0.97	0.39	7.46	13,13,13,13	0
54	MG	DA	3313	1/1	0.34	0.27	7.43	107,107,107,107	0
54	MG	BA	2940	1/1	0.96	0.30	7.40	29,29,29,29	0
54	MG	CA	1672	1/1	0.83	0.30	7.31	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3039	1/1	0.97	0.29	7.29	48,48,48,48	0
54	MG	BA	3118	1/1	0.75	0.44	7.26	109,109,109,109	0
54	MG	DA	3306	1/1	0.89	0.31	7.15	51,51,51,51	0
54	MG	BA	3257	1/1	0.92	0.32	7.07	64,64,64,64	0
54	MG	DA	3082	1/1	0.84	0.41	6.92	70,70,70,70	0
54	MG	BA	3277	1/1	0.95	0.27	6.88	71,71,71,71	0
54	MG	DA	3101	1/1	0.76	0.76	6.77	72,72,72,72	0
54	MG	DA	3214	1/1	0.95	0.34	6.40	46,46,46,46	0
54	MG	DA	3083	1/1	0.91	0.24	6.32	67,67,67,67	0
54	MG	DG	201	1/1	0.07	0.44	6.32	101,101,101,101	0
54	MG	CA	1609	1/1	0.92	0.23	6.32	93,93,93,93	0
54	MG	BA	3204	1/1	0.81	0.35	6.29	74,74,74,74	0
54	MG	BA	2913	1/1	0.97	0.33	6.19	16,16,16,16	0
54	MG	DA	3033	1/1	0.46	0.46	6.11	101,101,101,101	0
54	MG	AA	1637	1/1	0.89	0.45	6.07	61,61,61,61	0
54	MG	BA	2925	1/1	0.99	0.27	5.97	29,29,29,29	0
54	MG	DA	2965	1/1	0.93	0.39	5.87	57,57,57,57	0
54	MG	DA	2944	1/1	0.97	0.36	5.77	35,35,35,35	0
54	MG	DA	3298	1/1	0.78	0.68	5.64	79,79,79,79	0
54	MG	BA	3242	1/1	0.85	0.35	5.60	44,44,44,44	0
54	MG	BA	2999	1/1	0.94	0.24	5.41	45,45,45,45	0
54	MG	DA	3003	1/1	0.85	0.36	5.28	41,41,41,41	0
54	MG	BA	2908	1/1	0.96	0.47	5.10	18,18,18,18	0
54	MG	DA	3154	1/1	0.88	0.33	5.10	94,94,94,94	0
54	MG	DA	2901	1/1	0.96	0.46	5.00	7,7,7,7	0
54	MG	AA	1695	1/1	0.78	0.38	4.93	83,83,83,83	0
54	MG	DA	3023	1/1	0.85	0.24	4.91	49,49,49,49	0
54	MG	DA	2968	1/1	0.95	0.27	4.86	56,56,56,56	0
54	MG	CA	1617	1/1	0.95	0.34	4.84	90,90,90,90	0
54	MG	DA	3105	1/1	0.47	0.52	4.62	75,75,75,75	0
54	MG	DA	2966	1/1	0.96	0.35	4.61	70,70,70,70	0
54	MG	DA	3304	1/1	0.95	0.25	4.57	59,59,59,59	0
54	MG	BA	2979	1/1	0.94	0.25	4.48	40,40,40,40	0
54	MG	DA	2927	1/1	0.91	0.23	4.44	22,22,22,22	0
54	MG	BA	3090	1/1	0.82	0.34	4.42	69,69,69,69	0
54	MG	DA	3070	1/1	0.88	0.27	4.40	70,70,70,70	0
54	MG	DA	3310	1/1	0.89	0.27	4.35	52,52,52,52	0
54	MG	BA	2922	1/1	0.97	0.46	4.21	25,25,25,25	0
54	MG	AA	1721	1/1	0.90	0.55	4.16	66,66,66,66	0
54	MG	BA	3180	1/1	0.97	0.27	4.13	26,26,26,26	0
54	MG	BA	2998	1/1	0.96	0.22	4.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	2916	1/1	0.95	0.43	4.07	38,38,38,38	0
54	MG	DA	3192	1/1	0.94	0.29	4.06	30,30,30,30	0
54	MG	CA	1607	1/1	0.87	0.27	4.01	52,52,52,52	0
54	MG	BA	2982	1/1	0.93	0.31	3.83	41,41,41,41	0
54	MG	BA	3186	1/1	0.97	0.32	3.81	52,52,52,52	0
54	MG	DA	2978	1/1	0.93	0.28	3.67	44,44,44,44	0
54	MG	AA	1624	1/1	0.96	0.36	3.64	67,67,67,67	0
54	MG	BA	3208	1/1	0.82	0.24	3.39	48,48,48,48	0
54	MG	DA	3034	1/1	0.84	0.29	3.37	65,65,65,65	0
54	MG	AA	1707	1/1	0.87	0.29	3.28	100,100,100,100	0
54	MG	DA	2971	1/1	0.97	0.23	3.25	47,47,47,47	0
54	MG	CA	1691	1/1	0.71	0.42	3.19	85,85,85,85	0
54	MG	BA	2980	1/1	0.91	0.26	3.09	40,40,40,40	0
54	MG	CA	1703	1/1	0.60	0.35	3.06	108,108,108,108	0
54	MG	DA	3072	1/1	0.79	0.60	2.99	73,73,73,73	0
54	MG	BA	3052	1/1	0.96	0.24	2.86	56,56,56,56	0
54	MG	AA	1713	1/1	0.73	0.30	2.70	93,93,93,93	0
54	MG	DA	3036	1/1	0.89	0.34	2.69	51,51,51,51	0
54	MG	DA	2950	1/1	0.92	0.20	2.53	29,29,29,29	0
54	MG	AA	1647	1/1	0.90	0.24	2.52	85,85,85,85	0
54	MG	AA	1731	1/1	0.86	0.27	2.42	76,76,76,76	0
54	MG	BA	3152	1/1	0.91	0.21	2.31	75,75,75,75	0
54	MG	CA	1698	1/1	0.75	0.30	2.31	117,117,117,117	0
54	MG	CA	1717	1/1	0.69	0.27	2.27	84,84,84,84	0
54	MG	AA	1650	1/1	0.88	0.29	2.26	103,103,103,103	0
54	MG	DA	2916	1/1	0.89	0.27	2.14	22,22,22,22	0
54	MG	DA	2908	1/1	0.98	0.26	2.14	24,24,24,24	0
54	MG	DA	2917	1/1	0.99	0.25	2.13	22,22,22,22	0
54	MG	DA	3201	1/1	0.85	0.44	1.88	72,72,72,72	0
54	MG	BA	3255	1/1	0.75	0.21	1.81	57,57,57,57	0
54	MG	DA	3277	1/1	0.89	0.31	1.76	52,52,52,52	0
54	MG	DA	3037	1/1	0.67	0.18	1.68	77,77,77,77	0
54	MG	DA	3195	1/1	0.98	0.26	1.66	51,51,51,51	0
54	MG	BA	3102	1/1	0.95	0.27	1.54	69,69,69,69	0
54	MG	DA	3007	1/1	0.89	0.19	1.50	43,43,43,43	0
54	MG	BA	2938	1/1	0.97	0.20	1.38	10,10,10,10	0
54	MG	AA	1755	1/1	0.83	0.32	1.32	103,103,103,103	0
54	MG	AA	1628	1/1	0.96	0.38	1.23	62,62,62,62	0
54	MG	DA	3067	1/1	0.96	0.20	1.22	63,63,63,63	0
54	MG	BA	3017	1/1	0.89	0.21	1.13	69,69,69,69	0
54	MG	AA	1740	1/1	0.87	0.34	1.08	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1686	1/1	0.95	0.25	1.00	60,60,60,60	0
54	MG	DA	2967	1/1	0.94	0.35	0.97	54,54,54,54	0
54	MG	CA	1604	1/1	0.94	0.23	0.95	59,59,59,59	0
54	MG	BA	3234	1/1	0.95	0.22	0.79	61,61,61,61	0
54	MG	BA	3153	1/1	0.99	0.30	0.72	67,67,67,67	0
54	MG	BA	3065	1/1	0.92	0.20	0.68	61,61,61,61	0
54	MG	DA	2991	1/1	0.91	0.24	0.64	31,31,31,31	0
54	MG	AA	1612	1/1	0.81	0.25	0.63	64,64,64,64	0
54	MG	DA	2980	1/1	0.95	0.18	0.60	63,63,63,63	0
54	MG	DA	3025	1/1	0.92	0.16	0.59	69,69,69,69	0
54	MG	AA	1754	1/1	0.42	0.22	0.59	110,110,110,110	0
54	MG	CA	1603	1/1	0.94	0.27	0.58	48,48,48,48	0
54	MG	D2	101	1/1	0.87	0.27	0.57	66,66,66,66	0
54	MG	BA	2986	1/1	0.63	0.23	0.56	67,67,67,67	0
54	MG	CA	1610	1/1	0.79	0.28	0.51	77,77,77,77	0
54	MG	DA	3118	1/1	0.93	0.25	0.50	62,62,62,62	0
54	MG	BA	3011	1/1	0.97	0.15	0.50	83,83,83,83	0
54	MG	DA	2984	1/1	0.98	0.20	0.48	66,66,66,66	0
54	MG	CA	1629	1/1	0.98	0.24	0.43	106,106,106,106	0
54	MG	BA	2949	1/1	0.94	0.18	0.38	47,47,47,47	0
54	MG	BA	2915	1/1	0.94	0.17	0.20	4,4,4,4	0
54	MG	BA	2995	1/1	0.91	0.20	0.14	47,47,47,47	0
54	MG	BA	3055	1/1	0.93	0.17	0.08	60,60,60,60	0
54	MG	DA	2939	1/1	0.92	0.17	0.07	40,40,40,40	0
54	MG	DE	301	1/1	0.88	0.24	-0.01	44,44,44,44	0
54	MG	BA	2975	1/1	0.84	0.19	-0.12	37,37,37,37	0
54	MG	CA	1664	1/1	0.94	0.20	-0.16	82,82,82,82	0
54	MG	BK	201	1/1	0.68	0.19	-0.19	91,91,91,91	0
54	MG	DA	3221	1/1	0.89	0.18	-0.27	68,68,68,68	0
54	MG	DA	2964	1/1	0.94	0.20	-0.32	34,34,34,34	0
54	MG	CA	1638	1/1	0.90	0.19	-0.34	65,65,65,65	0
54	MG	DA	2990	1/1	0.97	0.20	-0.37	35,35,35,35	0
54	MG	BA	3243	1/1	0.88	0.17	-0.40	82,82,82,82	0
54	MG	AA	1615	1/1	0.95	0.15	-0.51	42,42,42,42	0
54	MG	DB	203	1/1	0.84	0.19	-0.55	82,82,82,82	0
54	MG	AA	1662	1/1	0.93	0.23	-0.60	53,53,53,53	0
54	MG	AA	1619	1/1	0.95	0.16	-0.64	80,80,80,80	0
54	MG	AA	1607	1/1	0.97	0.21	-0.65	54,54,54,54	0
54	MG	AA	1652	1/1	0.93	0.20	-0.69	89,89,89,89	0
55	ZN	AD	301	1/1	0.99	0.27	-0.69	80,80,80,80	0
54	MG	BA	3010	1/1	0.95	0.15	-0.72	37,37,37,37	0
54	MG	DA	2982	1/1	0.90	0.20	-0.77	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3030	1/1	0.86	0.15	-0.77	57,57,57,57	0
54	MG	AA	1716	1/1	0.91	0.16	-0.90	120,120,120,120	0
54	MG	DA	2994	1/1	0.87	0.13	-0.97	67,67,67,67	0
54	MG	BA	2973	1/1	0.94	0.15	-1.00	61,61,61,61	0
54	MG	BA	3227	1/1	0.95	0.15	-1.06	48,48,48,48	0
54	MG	CA	1608	1/1	0.84	0.11	-1.11	61,61,61,61	0
54	MG	CA	1725	1/1	0.31	0.17	-1.12	105,105,105,105	0
54	MG	BA	3307	1/1	0.93	0.14	-1.14	68,68,68,68	0
54	MG	DA	3018	1/1	0.90	0.13	-1.20	73,73,73,73	0
54	MG	DA	2969	1/1	0.96	0.18	-1.27	42,42,42,42	0
54	MG	BA	2962	1/1	0.90	0.17	-1.28	17,17,17,17	0
54	MG	AA	1739	1/1	0.76	0.15	-1.32	129,129,129,129	0
54	MG	AD	302	1/1	0.56	0.18	-1.33	87,87,87,87	0
54	MG	BA	3263	1/1	0.45	0.23	-1.42	80,80,80,80	0
54	MG	AA	1725	1/1	0.92	0.20	-1.46	72,72,72,72	0
54	MG	AA	1632	1/1	0.92	0.11	-1.48	68,68,68,68	0
54	MG	DA	2951	1/1	0.99	0.18	-1.64	38,38,38,38	0
55	ZN	CD	301	1/1	0.96	0.24	-1.75	131,131,131,131	0
55	ZN	CN	101	1/1	0.96	0.10	-1.76	144,144,144,144	0
54	MG	BA	2991	1/1	0.88	0.16	-1.76	36,36,36,36	0
54	MG	BA	3252	1/1	0.87	0.12	-1.83	92,92,92,92	0
54	MG	BB	210	1/1	0.82	0.10	-1.86	100,100,100,100	0
54	MG	BA	3138	1/1	0.83	0.14	-1.91	100,100,100,100	0
54	MG	CA	1624	1/1	0.90	0.13	-1.93	66,66,66,66	0
54	MG	DB	204	1/1	0.94	0.07	-2.34	75,75,75,75	0
54	MG	BA	2969	1/1	0.80	0.15	-2.37	37,37,37,37	0
54	MG	AA	1604	1/1	0.96	0.12	-2.52	57,57,57,57	0
54	MG	BB	207	1/1	0.90	0.11	-2.68	105,105,105,105	0
54	MG	BA	3251	1/1	0.96	0.10	-2.70	64,64,64,64	0
54	MG	CA	1719	1/1	0.97	0.13	-3.12	78,78,78,78	0
54	MG	DA	2975	1/1	0.89	0.07	-3.50	58,58,58,58	0
54	MG	AA	1618	1/1	0.67	0.09	-3.67	91,91,91,91	0
54	MG	DA	3006	1/1	0.87	0.12	-3.88	74,74,74,74	0
54	MG	DA	2974	1/1	0.92	0.08	-3.91	46,46,46,46	0
54	MG	CA	1666	1/1	0.93	0.08	-3.92	116,116,116,116	0
54	MG	AA	1736	1/1	0.97	0.13	-5.40	79,79,79,79	0
54	MG	DA	2958	1/1	0.96	0.16	-6.56	2,2,2,2	0
54	MG	DA	3026	1/1	0.92	0.08	-10.63	48,48,48,48	0
54	MG	AA	1654	1/1	0.90	0.30	-	76,76,76,76	0
54	MG	DA	3276	1/1	0.84	0.17	-	128,128,128,128	0
54	MG	DB	212	1/1	0.64	0.14	-	70,70,70,70	0
54	MG	AA	1741	1/1	0.95	0.13	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3205	1/1	0.82	0.32	-	48,48,48,48	0
54	MG	AA	1668	1/1	0.94	0.08	-	90,90,90,90	0
54	MG	DA	3094	1/1	0.72	0.30	-	76,76,76,76	0
54	MG	DA	3312	1/1	0.72	0.54	-	66,66,66,66	0
54	MG	DA	3252	1/1	0.97	0.10	-	44,44,44,44	0
54	MG	CA	1705	1/1	0.66	0.24	-	54,54,54,54	0
54	MG	DA	2995	1/1	0.85	0.55	-	48,48,48,48	0
54	MG	DA	3020	1/1	0.94	0.17	-	63,63,63,63	0
54	MG	DA	3123	1/1	0.99	0.07	-	59,59,59,59	0
54	MG	BA	3114	1/1	0.70	0.67	-	78,78,78,78	0
54	MG	DA	3281	1/1	0.78	0.29	-	73,73,73,73	0
54	MG	DA	3004	1/1	0.85	0.33	-	67,67,67,67	0
54	MG	DA	2993	1/1	0.78	0.08	-	69,69,69,69	0
54	MG	BA	3249	1/1	0.92	0.24	-	37,37,37,37	0
54	MG	DA	3234	1/1	0.94	0.10	-	130,130,130,130	0
54	MG	DA	3099	1/1	0.89	0.18	-	81,81,81,81	0
54	MG	BA	3022	1/1	0.88	0.14	-	77,77,77,77	0
54	MG	AA	1672	1/1	0.98	0.46	-	101,101,101,101	0
54	MG	BA	2951	1/1	0.98	0.38	-	28,28,28,28	0
54	MG	DA	3109	1/1	0.87	0.31	-	54,54,54,54	0
54	MG	DA	2936	1/1	0.90	0.36	-	27,27,27,27	0
54	MG	DA	3226	1/1	0.59	0.49	-	80,80,80,80	0
54	MG	BA	3200	1/1	0.88	0.33	-	64,64,64,64	0
54	MG	CA	1648	1/1	0.41	0.34	-	64,64,64,64	0
54	MG	BA	3142	1/1	0.93	0.09	-	89,89,89,89	0
54	MG	BA	3302	1/1	0.79	0.30	-	121,121,121,121	0
54	MG	BA	3167	1/1	0.98	0.14	-	50,50,50,50	0
54	MG	BA	3209	1/1	0.94	0.27	-	69,69,69,69	0
54	MG	AA	1631	1/1	0.90	0.31	-	70,70,70,70	0
54	MG	AA	1692	1/1	0.90	0.33	-	84,84,84,84	0
54	MG	BA	3223	1/1	0.90	0.23	-	54,54,54,54	0
54	MG	CA	1615	1/1	0.98	0.26	-	51,51,51,51	0
54	MG	DA	3053	1/1	0.96	0.27	-	61,61,61,61	0
54	MG	BA	3106	1/1	0.94	0.21	-	70,70,70,70	0
54	MG	DA	3189	1/1	0.86	0.25	-	37,37,37,37	0
54	MG	BA	3292	1/1	0.93	0.19	-	72,72,72,72	0
54	MG	BA	3293	1/1	0.96	0.20	-	86,86,86,86	0
54	MG	CA	1676	1/1	0.91	0.36	-	82,82,82,82	0
54	MG	BA	3043	1/1	0.93	0.30	-	70,70,70,70	0
54	MG	DA	3144	1/1	0.96	0.16	-	72,72,72,72	0
54	MG	AA	1735	1/1	0.90	0.20	-	104,104,104,104	0
54	MG	DA	3142	1/1	0.80	0.18	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3128	1/1	0.85	0.20	-	114,114,114,114	0
54	MG	DA	3284	1/1	0.05	0.33	-	134,134,134,134	0
54	MG	AA	1719	1/1	0.80	0.28	-	78,78,78,78	0
54	MG	AA	1620	1/1	0.98	0.23	-	56,56,56,56	0
54	MG	BB	201	1/1	0.90	0.35	-	56,56,56,56	0
54	MG	AA	1697	1/1	0.86	0.36	-	80,80,80,80	0
54	MG	BA	3197	1/1	0.86	0.37	-	57,57,57,57	0
54	MG	DA	3235	1/1	0.53	0.62	-	90,90,90,90	0
54	MG	AA	1756	1/1	0.92	0.20	-	106,106,106,106	0
54	MG	BA	3175	1/1	0.82	0.35	-	85,85,85,85	0
54	MG	DA	3263	1/1	0.78	0.35	-	63,63,63,63	0
54	MG	BA	3266	1/1	0.84	0.19	-	98,98,98,98	0
54	MG	DA	2938	1/1	0.74	0.27	-	66,66,66,66	0
54	MG	CA	1620	1/1	0.86	0.11	-	79,79,79,79	0
54	MG	DA	3273	1/1	0.93	0.29	-	85,85,85,85	0
54	MG	DA	3222	1/1	0.67	0.54	-	70,70,70,70	0
54	MG	DA	3139	1/1	0.93	0.28	-	60,60,60,60	0
54	MG	AA	1655	1/1	0.87	0.72	-	72,72,72,72	0
54	MG	BA	2958	1/1	0.90	0.32	-	42,42,42,42	0
54	MG	DA	3238	1/1	0.62	0.29	-	58,58,58,58	0
54	MG	BA	3168	1/1	0.87	0.20	-	76,76,76,76	0
54	MG	AA	1685	1/1	0.81	0.16	-	106,106,106,106	0
54	MG	BA	2966	1/1	0.88	0.09	-	75,75,75,75	0
54	MG	BA	2987	1/1	0.92	0.28	-	59,59,59,59	0
54	MG	BA	3264	1/1	0.98	0.14	-	116,116,116,116	0
54	MG	DB	210	1/1	0.95	0.06	-	74,74,74,74	0
54	MG	BA	2953	1/1	0.98	0.16	-	37,37,37,37	0
54	MG	BA	3304	1/1	0.98	0.06	-	124,124,124,124	0
54	MG	DA	3078	1/1	0.58	0.60	-	79,79,79,79	0
54	MG	BB	212	1/1	0.89	0.14	-	89,89,89,89	0
54	MG	DA	3106	1/1	0.95	0.37	-	67,67,67,67	0
54	MG	DA	3200	1/1	0.56	0.11	-	87,87,87,87	0
54	MG	DB	202	1/1	0.97	0.59	-	64,64,64,64	0
54	MG	CA	1645	1/1	0.87	0.64	-	72,72,72,72	0
54	MG	BB	213	1/1	0.82	0.65	-	84,84,84,84	0
54	MG	DA	3293	1/1	0.97	0.10	-	67,67,67,67	0
54	MG	DA	3199	1/1	0.72	0.71	-	38,38,38,38	0
54	MG	AA	1711	1/1	0.93	0.56	-	53,53,53,53	0
54	MG	DA	2985	1/1	0.96	0.38	-	48,48,48,48	0
54	MG	DA	3315	1/1	0.92	0.16	-	52,52,52,52	0
54	MG	BA	3267	1/1	0.78	0.47	-	86,86,86,86	0
54	MG	AV	6302	1/1	0.79	0.48	-	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1681	1/1	0.88	0.42	-	81,81,81,81	0
54	MG	DA	3233	1/1	0.95	0.42	-	57,57,57,57	0
54	MG	BA	3248	1/1	0.85	0.16	-	77,77,77,77	0
54	MG	BA	3214	1/1	0.98	0.41	-	53,53,53,53	0
54	MG	DB	213	1/1	0.95	0.45	-	63,63,63,63	0
54	MG	BA	3131	1/1	0.90	0.26	-	67,67,67,67	0
54	MG	BA	3093	1/1	0.76	0.34	-	83,83,83,83	0
54	MG	DA	2970	1/1	0.80	0.19	-	67,67,67,67	0
54	MG	AA	1681	1/1	0.84	0.16	-	99,99,99,99	0
54	MG	BA	3018	1/1	0.92	0.31	-	68,68,68,68	0
54	MG	DA	3320	1/1	0.87	0.41	-	58,58,58,58	0
54	MG	DA	3085	1/1	0.77	0.13	-	89,89,89,89	0
54	MG	BA	3083	1/1	0.74	0.30	-	87,87,87,87	0
54	MG	BA	3143	1/1	0.81	0.51	-	84,84,84,84	0
54	MG	DA	3197	1/1	0.96	0.34	-	28,28,28,28	0
54	MG	BA	3233	1/1	0.97	0.23	-	52,52,52,52	0
54	MG	BB	211	1/1	0.86	0.49	-	112,112,112,112	0
54	MG	BA	3007	1/1	0.91	0.19	-	55,55,55,55	0
54	MG	BA	3290	1/1	0.93	0.27	-	42,42,42,42	0
54	MG	CA	1647	1/1	0.91	0.28	-	77,77,77,77	0
54	MG	AA	1718	1/1	0.64	0.63	-	98,98,98,98	0
54	MG	BA	3273	1/1	0.96	0.16	-	83,83,83,83	0
54	MG	DA	2998	1/1	0.92	0.39	-	68,68,68,68	0
54	MG	DA	3264	1/1	0.89	0.24	-	61,61,61,61	0
54	MG	BA	3301	1/1	0.85	0.65	-	66,66,66,66	0
54	MG	AA	1634	1/1	0.91	0.19	-	70,70,70,70	0
54	MG	BA	3166	1/1	0.90	0.40	-	74,74,74,74	0
54	MG	DA	3131	1/1	0.82	0.45	-	66,66,66,66	0
54	MG	AA	1700	1/1	0.73	0.56	-	98,98,98,98	0
54	MG	CA	1738	1/1	0.86	0.51	-	81,81,81,81	0
54	MG	DA	3071	1/1	0.81	0.38	-	64,64,64,64	0
54	MG	BA	3135	1/1	0.91	0.23	-	77,77,77,77	0
54	MG	BA	2993	1/1	0.92	0.24	-	58,58,58,58	0
54	MG	AA	1724	1/1	0.96	0.29	-	85,85,85,85	0
54	MG	DA	3255	1/1	0.98	0.15	-	101,101,101,101	0
54	MG	DA	2961	1/1	0.98	0.15	-	29,29,29,29	0
54	MG	DA	3224	1/1	0.90	0.17	-	72,72,72,72	0
54	MG	BA	2976	1/1	0.88	0.47	-	70,70,70,70	0
54	MG	DA	3231	1/1	0.82	0.70	-	60,60,60,60	0
54	MG	BA	3172	1/1	0.65	0.68	-	102,102,102,102	0
54	MG	DA	3153	1/1	0.93	0.28	-	85,85,85,85	0
54	MG	CA	1706	1/1	0.84	0.53	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1748	1/1	0.89	0.15	-	96,96,96,96	0
54	MG	BA	3297	1/1	0.91	0.52	-	67,67,67,67	0
54	MG	BA	3049	1/1	0.88	0.14	-	86,86,86,86	0
54	MG	BA	3230	1/1	0.92	0.51	-	44,44,44,44	0
54	MG	BA	3288	1/1	0.87	0.62	-	62,62,62,62	0
54	MG	BA	3021	1/1	0.95	0.19	-	60,60,60,60	0
54	MG	DA	3217	1/1	0.97	0.12	-	56,56,56,56	0
54	MG	BA	3199	1/1	0.93	0.63	-	68,68,68,68	0
54	MG	AA	1661	1/1	0.72	0.41	-	65,65,65,65	0
54	MG	DA	3145	1/1	0.88	0.42	-	70,70,70,70	0
54	MG	DA	2946	1/1	0.94	0.55	-	24,24,24,24	0
54	MG	DA	3302	1/1	0.60	0.56	-	77,77,77,77	0
54	MG	DA	3060	1/1	0.91	0.21	-	87,87,87,87	0
54	MG	AA	1626	1/1	0.76	0.15	-	62,62,62,62	0
54	MG	DA	3301	1/1	0.90	0.30	-	80,80,80,80	0
54	MG	BA	3241	1/1	0.88	0.25	-	60,60,60,60	0
54	MG	BB	216	1/1	0.84	0.18	-	79,79,79,79	0
54	MG	DA	2992	1/1	0.89	0.18	-	46,46,46,46	0
54	MG	CA	1700	1/1	0.81	0.50	-	65,65,65,65	0
54	MG	DA	3249	1/1	0.67	0.36	-	56,56,56,56	0
54	MG	BA	2956	1/1	0.98	0.45	-	35,35,35,35	0
54	MG	BA	3229	1/1	0.80	0.28	-	62,62,62,62	0
54	MG	DA	3311	1/1	0.79	0.15	-	95,95,95,95	0
54	MG	BA	3057	1/1	0.94	0.43	-	63,63,63,63	0
54	MG	CA	1626	1/1	0.97	0.33	-	65,65,65,65	0
54	MG	BA	3028	1/1	0.94	0.46	-	62,62,62,62	0
54	MG	BB	217	1/1	0.83	0.15	-	78,78,78,78	0
54	MG	BA	3269	1/1	0.93	0.23	-	63,63,63,63	0
54	MG	CA	1702	1/1	0.91	0.70	-	68,68,68,68	0
54	MG	DA	3250	1/1	0.92	0.37	-	74,74,74,74	0
54	MG	DA	3048	1/1	0.98	0.09	-	66,66,66,66	0
54	MG	AA	1657	1/1	0.89	0.31	-	101,101,101,101	0
54	MG	BA	3205	1/1	0.93	0.23	-	38,38,38,38	0
54	MG	DA	3056	1/1	0.96	0.19	-	48,48,48,48	0
54	MG	DA	3029	1/1	0.82	0.23	-	70,70,70,70	0
54	MG	AA	1758	1/1	0.87	0.14	-	73,73,73,73	0
54	MG	BA	3206	1/1	0.94	0.10	-	60,60,60,60	0
54	MG	CA	1644	1/1	0.98	0.45	-	77,77,77,77	0
54	MG	CA	1633	1/1	0.88	0.48	-	102,102,102,102	0
54	MG	CA	1730	1/1	0.95	0.08	-	122,122,122,122	0
54	MG	DA	3331	1/1	0.97	0.19	-	52,52,52,52	0
54	MG	CA	1614	1/1	0.75	0.33	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3209	1/1	0.52	0.58	-	80,80,80,80	0
54	MG	BA	3189	1/1	0.65	0.44	-	88,88,88,88	0
54	MG	DA	3236	1/1	0.96	0.59	-	63,63,63,63	0
54	MG	DA	3084	1/1	0.93	0.11	-	146,146,146,146	0
54	MG	BB	202	1/1	0.97	0.24	-	75,75,75,75	0
54	MG	DA	3316	1/1	0.72	0.24	-	97,97,97,97	0
54	MG	CA	1670	1/1	0.96	0.47	-	128,128,128,128	0
54	MG	CA	1680	1/1	0.92	0.32	-	58,58,58,58	0
54	MG	DA	3146	1/1	0.91	0.13	-	95,95,95,95	0
54	MG	BA	3036	1/1	0.73	0.24	-	92,92,92,92	0
54	MG	BA	3201	1/1	0.86	0.20	-	80,80,80,80	0
54	MG	CA	1655	1/1	0.94	0.22	-	80,80,80,80	0
54	MG	BA	3296	1/1	0.98	0.16	-	47,47,47,47	0
54	MG	BA	3236	1/1	0.51	0.31	-	119,119,119,119	0
54	MG	BA	2964	1/1	0.90	0.47	-	30,30,30,30	0
54	MG	DA	3040	1/1	0.92	0.36	-	41,41,41,41	0
54	MG	BA	3219	1/1	0.69	0.80	-	66,66,66,66	0
54	MG	CA	1696	1/1	0.60	0.18	-	133,133,133,133	0
54	MG	AA	1703	1/1	0.94	0.15	-	83,83,83,83	0
54	MG	AA	1759	1/1	0.95	0.13	-	81,81,81,81	0
54	MG	BA	3144	1/1	0.90	0.34	-	75,75,75,75	0
54	MG	AA	1611	1/1	0.96	0.27	-	49,49,49,49	0
54	MG	DA	3134	1/1	0.77	0.16	-	71,71,71,71	0
54	MG	BA	3070	1/1	0.96	0.24	-	75,75,75,75	0
54	MG	AA	1644	1/1	0.85	0.27	-	53,53,53,53	0
54	MG	BA	3126	1/1	0.90	0.15	-	54,54,54,54	0
54	MG	DA	3180	1/1	0.90	0.26	-	77,77,77,77	0
54	MG	BA	3262	1/1	0.83	0.39	-	60,60,60,60	0
54	MG	AA	1704	1/1	0.84	0.20	-	81,81,81,81	0
54	MG	DA	3015	1/1	0.96	0.22	-	74,74,74,74	0
54	MG	CA	1684	1/1	0.80	0.14	-	117,117,117,117	0
54	MG	DA	3161	1/1	0.82	0.29	-	74,74,74,74	0
54	MG	DA	3074	1/1	0.81	0.31	-	64,64,64,64	0
54	MG	BA	3170	1/1	0.95	0.12	-	64,64,64,64	0
54	MG	DA	3148	1/1	0.91	0.23	-	99,99,99,99	0
54	MG	BA	2950	1/1	0.98	0.18	-	32,32,32,32	0
54	MG	BA	3124	1/1	0.89	0.30	-	89,89,89,89	0
54	MG	AA	1640	1/1	0.77	0.44	-	106,106,106,106	0
54	MG	DA	3046	1/1	0.91	0.09	-	76,76,76,76	0
54	MG	CP	101	1/1	0.78	0.17	-	96,96,96,96	0
54	MG	CA	1662	1/1	0.87	0.76	-	86,86,86,86	0
54	MG	AA	1751	1/1	0.90	0.18	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3254	1/1	0.92	0.52	-	79,79,79,79	0
54	MG	DA	3156	1/1	0.98	0.18	-	78,78,78,78	0
54	MG	DA	3124	1/1	0.92	0.09	-	90,90,90,90	0
54	MG	CA	1699	1/1	0.85	0.72	-	71,71,71,71	0
54	MG	DB	205	1/1	0.92	0.10	-	79,79,79,79	0
54	MG	BA	3054	1/1	0.85	0.18	-	46,46,46,46	0
54	MG	AA	1753	1/1	0.80	0.34	-	102,102,102,102	0
54	MG	AA	1677	1/1	0.85	0.44	-	64,64,64,64	0
54	MG	AA	1649	1/1	0.80	0.37	-	89,89,89,89	0
54	MG	BA	3291	1/1	0.79	0.28	-	68,68,68,68	0
54	MG	BB	208	1/1	0.88	0.47	-	109,109,109,109	0
54	MG	BA	3213	1/1	0.61	0.25	-	101,101,101,101	0
54	MG	DA	3030	1/1	0.67	0.41	-	71,71,71,71	0
54	MG	BA	2965	1/1	0.99	0.27	-	47,47,47,47	0
54	MG	DB	211	1/1	0.94	0.15	-	109,109,109,109	0
54	MG	BA	3077	1/1	0.97	0.09	-	75,75,75,75	0
54	MG	BA	3287	1/1	0.78	0.44	-	74,74,74,74	0
54	MG	AA	1629	1/1	0.88	0.36	-	72,72,72,72	0
54	MG	AA	1669	1/1	0.64	0.33	-	110,110,110,110	0
54	MG	DA	3052	1/1	0.93	0.16	-	107,107,107,107	0
54	MG	BA	3271	1/1	0.52	0.17	-	91,91,91,91	0
54	MG	BA	3113	1/1	0.87	0.29	-	71,71,71,71	0
54	MG	BA	3087	1/1	0.96	0.10	-	69,69,69,69	0
54	MG	BA	3110	1/1	0.75	0.14	-	86,86,86,86	0
54	MG	CA	1735	1/1	0.84	0.27	-	61,61,61,61	0
54	MG	DA	3176	1/1	0.94	0.24	-	83,83,83,83	0
54	MG	BA	2972	1/1	0.95	0.35	-	49,49,49,49	0
54	MG	BA	3061	1/1	0.79	0.21	-	91,91,91,91	0
54	MG	CA	1630	1/1	0.95	0.33	-	70,70,70,70	0
54	MG	BA	3157	1/1	0.78	0.29	-	68,68,68,68	0
54	MG	BA	3014	1/1	0.90	0.20	-	47,47,47,47	0
54	MG	AA	1720	1/1	0.78	0.23	-	69,69,69,69	0
54	MG	DA	2949	1/1	0.97	0.54	-	41,41,41,41	0
54	MG	DA	3292	1/1	0.96	0.47	-	33,33,33,33	0
54	MG	CA	1605	1/1	0.96	0.21	-	56,56,56,56	0
54	MG	BA	2929	1/1	0.98	0.45	-	37,37,37,37	0
54	MG	DA	3282	1/1	0.88	0.14	-	96,96,96,96	0
54	MG	DA	2913	1/1	0.92	0.41	-	17,17,17,17	0
54	MG	BA	3278	1/1	0.69	0.29	-	115,115,115,115	0
54	MG	DA	3168	1/1	0.64	0.46	-	94,94,94,94	0
54	MG	CA	1634	1/1	0.87	0.26	-	60,60,60,60	0
54	MG	AA	1702	1/1	0.56	1.09	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1743	1/1	0.98	0.47	-	83,83,83,83	0
54	MG	BA	2902	1/1	0.99	0.46	-	16,16,16,16	0
54	MG	BA	3058	1/1	0.94	0.12	-	114,114,114,114	0
54	MG	BA	3276	1/1	0.93	0.21	-	65,65,65,65	0
54	MG	DA	2928	1/1	0.95	0.22	-	43,43,43,43	0
54	MG	CA	1622	1/1	0.93	0.23	-	79,79,79,79	0
54	MG	DA	2926	1/1	0.97	0.23	-	43,43,43,43	0
54	MG	DA	3013	1/1	0.84	0.26	-	44,44,44,44	0
54	MG	BA	3041	1/1	0.87	0.23	-	67,67,67,67	0
54	MG	DA	3323	1/1	0.50	0.34	-	69,69,69,69	0
54	MG	DA	3050	1/1	0.71	0.09	-	105,105,105,105	0
54	MG	DA	2983	1/1	0.54	0.27	-	70,70,70,70	0
54	MG	BA	3001	1/1	0.90	0.30	-	59,59,59,59	0
54	MG	CA	1625	1/1	0.92	0.10	-	94,94,94,94	0
54	MG	AA	1676	1/1	0.84	0.15	-	63,63,63,63	0
54	MG	DA	3043	1/1	0.61	0.69	-	70,70,70,70	0
54	MG	DA	3151	1/1	0.95	0.37	-	82,82,82,82	0
54	MG	DA	2942	1/1	0.93	0.29	-	39,39,39,39	0
54	MG	CA	1688	1/1	0.53	0.35	-	99,99,99,99	0
54	MG	DA	3129	1/1	0.92	0.43	-	63,63,63,63	0
54	MG	DA	3260	1/1	0.87	0.50	-	102,102,102,102	0
54	MG	CA	1651	1/1	0.94	0.09	-	99,99,99,99	0
54	MG	BA	3237	1/1	0.94	0.14	-	60,60,60,60	0
54	MG	BA	3103	1/1	0.73	0.30	-	88,88,88,88	0
54	MG	AA	1613	1/1	0.96	0.15	-	47,47,47,47	0
54	MG	DA	3289	1/1	0.81	0.53	-	92,92,92,92	0
54	MG	BA	3169	1/1	0.87	0.51	-	75,75,75,75	0
54	MG	DA	3009	1/1	0.88	0.48	-	49,49,49,49	0
54	MG	BA	2971	1/1	0.84	0.34	-	65,65,65,65	0
54	MG	BA	3078	1/1	0.80	0.10	-	83,83,83,83	0
54	MG	AA	1667	1/1	0.83	0.51	-	61,61,61,61	0
54	MG	DA	3299	1/1	0.80	0.34	-	68,68,68,68	0
54	MG	BA	3100	1/1	0.85	0.07	-	77,77,77,77	0
54	MG	DA	3248	1/1	0.92	0.30	-	75,75,75,75	0
54	MG	DA	3054	1/1	0.94	0.32	-	75,75,75,75	0
54	MG	BA	3127	1/1	0.88	0.76	-	56,56,56,56	0
54	MG	CA	1623	1/1	0.92	0.48	-	99,99,99,99	0
54	MG	AA	1627	1/1	0.94	0.12	-	85,85,85,85	0
54	MG	BA	3053	1/1	0.97	0.20	-	67,67,67,67	0
54	MG	CA	1663	1/1	0.74	0.28	-	86,86,86,86	0
54	MG	CA	1671	1/1	0.81	0.24	-	74,74,74,74	0
54	MG	CA	1635	1/1	0.94	0.23	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1658	1/1	0.79	0.42	-	110,110,110,110	0
54	MG	BA	3253	1/1	0.78	0.35	-	76,76,76,76	0
54	MG	DA	3230	1/1	0.84	0.21	-	63,63,63,63	0
54	MG	DA	3132	1/1	0.90	0.07	-	70,70,70,70	0
54	MG	DA	3076	1/1	0.90	0.16	-	63,63,63,63	0
54	MG	BA	3235	1/1	0.94	0.13	-	62,62,62,62	0
54	MG	BA	3174	1/1	0.98	0.20	-	84,84,84,84	0
54	MG	DA	3322	1/1	-0.12	0.38	-	95,95,95,95	0
54	MG	BA	3259	1/1	0.71	0.38	-	75,75,75,75	0
54	MG	DA	3185	1/1	0.74	0.32	-	108,108,108,108	0
54	MG	AA	1763	1/1	0.76	0.13	-	96,96,96,96	0
54	MG	DB	216	1/1	0.72	0.36	-	88,88,88,88	0
54	MG	BA	3063	1/1	0.93	0.23	-	56,56,56,56	0
54	MG	DA	3314	1/1	0.93	0.54	-	102,102,102,102	0
54	MG	DA	3183	1/1	0.98	0.09	-	83,83,83,83	0
54	MG	BA	2945	1/1	0.98	0.22	-	72,72,72,72	0
54	MG	BA	3039	1/1	0.87	0.19	-	94,94,94,94	0
54	MG	CA	1685	1/1	0.72	0.60	-	106,106,106,106	0
54	MG	BA	3244	1/1	0.94	0.78	-	47,47,47,47	0
54	MG	AA	1684	1/1	0.88	0.38	-	95,95,95,95	0
54	MG	DA	3011	1/1	0.91	0.14	-	99,99,99,99	0
54	MG	BA	3173	1/1	0.87	0.51	-	80,80,80,80	0
54	MG	CA	1728	1/1	0.88	0.54	-	82,82,82,82	0
54	MG	DA	3096	1/1	0.97	0.37	-	40,40,40,40	0
54	MG	DA	2930	1/1	0.98	0.15	-	36,36,36,36	0
54	MG	AA	1674	1/1	0.85	0.49	-	79,79,79,79	0
54	MG	DA	3268	1/1	0.83	0.42	-	81,81,81,81	0
54	MG	BA	3089	1/1	0.95	0.29	-	59,59,59,59	0
54	MG	AA	1663	1/1	0.88	0.12	-	70,70,70,70	0
54	MG	DA	3001	1/1	0.94	0.12	-	56,56,56,56	0
54	MG	BA	3308	1/1	0.75	0.48	-	94,94,94,94	0
54	MG	DA	3055	1/1	0.09	0.85	-	93,93,93,93	0
54	MG	DA	2935	1/1	0.93	0.61	-	30,30,30,30	0
54	MG	AA	1690	1/1	0.88	0.09	-	117,117,117,117	0
54	MG	AA	1708	1/1	0.95	0.15	-	101,101,101,101	0
54	MG	B2	101	1/1	0.86	0.54	-	64,64,64,64	0
54	MG	DA	3179	1/1	0.93	0.19	-	68,68,68,68	0
54	MG	AA	1664	1/1	0.84	0.61	-	103,103,103,103	0
54	MG	CA	1723	1/1	0.83	0.24	-	141,141,141,141	0
54	MG	BA	3282	1/1	0.85	0.37	-	62,62,62,62	0
54	MG	BA	3231	1/1	0.96	0.16	-	22,22,22,22	0
54	MG	BA	3306	1/1	0.77	0.38	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3040	1/1	0.94	0.26	-	58,58,58,58	0
54	MG	BA	3245	1/1	0.98	0.29	-	54,54,54,54	0
54	MG	BA	3085	1/1	0.90	0.28	-	68,68,68,68	0
54	MG	CA	1643	1/1	0.95	0.13	-	58,58,58,58	0
54	MG	DA	3150	1/1	0.95	0.21	-	62,62,62,62	0
54	MG	DA	3294	1/1	0.87	0.28	-	61,61,61,61	0
54	MG	DA	2945	1/1	0.88	0.61	-	41,41,41,41	0
54	MG	AA	1609	1/1	0.92	0.63	-	70,70,70,70	0
54	MG	BA	3216	1/1	0.97	0.19	-	65,65,65,65	0
54	MG	BA	3218	1/1	0.75	0.67	-	75,75,75,75	0
54	MG	DA	3171	1/1	0.93	0.27	-	61,61,61,61	0
54	MG	CA	1695	1/1	0.97	0.37	-	80,80,80,80	0
54	MG	CA	1683	1/1	0.72	0.31	-	91,91,91,91	0
54	MG	CA	1613	1/1	0.95	0.24	-	87,87,87,87	0
54	MG	BA	3299	1/1	0.77	0.28	-	80,80,80,80	0
54	MG	AA	1639	1/1	0.86	0.35	-	79,79,79,79	0
54	MG	CA	1632	1/1	0.77	0.27	-	79,79,79,79	0
54	MG	AA	1643	1/1	0.86	0.33	-	70,70,70,70	0
54	MG	CA	1606	1/1	0.97	0.12	-	68,68,68,68	0
54	MG	BA	3080	1/1	0.89	0.14	-	73,73,73,73	0
54	MG	DA	2947	1/1	0.96	0.24	-	40,40,40,40	0
54	MG	BA	3139	1/1	0.75	0.31	-	78,78,78,78	0
54	MG	DA	3051	1/1	0.94	0.15	-	89,89,89,89	0
54	MG	DA	3041	1/1	0.88	0.17	-	51,51,51,51	0
54	MG	BA	3193	1/1	0.93	0.38	-	53,53,53,53	0
54	MG	BA	3191	1/1	0.72	0.37	-	76,76,76,76	0
54	MG	CV	6301	1/1	0.65	0.22	-	98,98,98,98	0
54	MG	AA	1738	1/1	0.83	0.28	-	70,70,70,70	0
54	MG	DA	2931	1/1	0.99	0.25	-	23,23,23,23	0
54	MG	BA	3163	1/1	0.54	0.49	-	72,72,72,72	0
54	MG	DA	3005	1/1	0.91	0.32	-	33,33,33,33	0
54	MG	BA	3203	1/1	0.98	0.19	-	41,41,41,41	0
54	MG	AA	1605	1/1	0.88	0.57	-	42,42,42,42	0
54	MG	BA	3003	1/1	0.93	0.28	-	48,48,48,48	0
54	MG	AA	1658	1/1	0.86	0.09	-	94,94,94,94	0
54	MG	DA	3059	1/1	0.83	0.21	-	67,67,67,67	0
54	MG	DA	3286	1/1	0.88	0.34	-	98,98,98,98	0
54	MG	DA	3112	1/1	0.91	0.20	-	60,60,60,60	0
54	MG	BA	3081	1/1	0.93	0.14	-	65,65,65,65	0
54	MG	CA	1619	1/1	0.97	0.34	-	61,61,61,61	0
54	MG	CA	1734	1/1	0.98	0.15	-	117,117,117,117	0
54	MG	BA	2957	1/1	0.95	0.57	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1671	1/1	0.96	0.14	-	114,114,114,114	0
54	MG	DA	3290	1/1	0.58	0.17	-	85,85,85,85	0
54	MG	DA	3212	1/1	0.83	0.49	-	78,78,78,78	0
54	MG	CA	1646	1/1	0.87	0.15	-	78,78,78,78	0
54	MG	BB	204	1/1	0.98	0.12	-	87,87,87,87	0
54	MG	DA	2912	1/1	0.98	0.45	-	18,18,18,18	0
54	MG	CA	1731	1/1	0.88	0.13	-	90,90,90,90	0
54	MG	DA	3211	1/1	0.96	0.18	-	38,38,38,38	0
54	MG	DA	3088	1/1	0.83	0.10	-	70,70,70,70	0
54	MG	AA	1749	1/1	0.90	0.25	-	90,90,90,90	0
54	MG	DA	3275	1/1	0.93	0.17	-	78,78,78,78	0
54	MG	DA	3136	1/1	0.79	0.37	-	68,68,68,68	0
54	MG	BA	3111	1/1	0.87	0.54	-	46,46,46,46	0
54	MG	AA	1698	1/1	0.64	0.47	-	88,88,88,88	0
54	MG	AV	6301	1/1	0.85	0.10	-	72,72,72,72	0
54	MG	BA	3238	1/1	0.90	0.14	-	91,91,91,91	0
54	MG	BA	3161	1/1	0.97	0.26	-	62,62,62,62	0
54	MG	DA	2903	1/1	0.98	0.33	-	7,7,7,7	0
54	MG	BA	3260	1/1	0.97	0.13	-	62,62,62,62	0
54	MG	DA	3247	1/1	0.93	0.21	-	40,40,40,40	0
54	MG	DA	2923	1/1	0.98	0.23	-	17,17,17,17	0
54	MG	CA	1659	1/1	0.98	0.38	-	71,71,71,71	0
54	MG	BA	3095	1/1	0.77	0.14	-	83,83,83,83	0
54	MG	DA	3157	1/1	0.91	0.14	-	71,71,71,71	0
54	MG	AA	1717	1/1	0.86	0.35	-	81,81,81,81	0
54	MG	DA	3075	1/1	0.98	0.23	-	64,64,64,64	0
54	MG	BA	3012	1/1	0.86	0.16	-	91,91,91,91	0
54	MG	AA	1726	1/1	0.93	0.08	-	108,108,108,108	0
54	MG	DA	3014	1/1	0.60	0.40	-	69,69,69,69	0
54	MG	BA	3155	1/1	0.79	0.38	-	85,85,85,85	0
54	MG	BA	3034	1/1	0.84	0.87	-	102,102,102,102	0
54	MG	DA	2996	1/1	0.95	0.40	-	43,43,43,43	0
54	MG	BA	3289	1/1	0.88	0.25	-	65,65,65,65	0
54	MG	CA	1732	1/1	0.93	0.23	-	73,73,73,73	0
54	MG	DA	3245	1/1	0.91	0.55	-	54,54,54,54	0
54	MG	BA	3129	1/1	0.89	0.13	-	75,75,75,75	0
54	MG	BA	3294	1/1	0.92	0.17	-	64,64,64,64	0
54	MG	DA	3155	1/1	0.90	0.07	-	124,124,124,124	0
54	MG	DA	3278	1/1	0.49	0.34	-	75,75,75,75	0
54	MG	DA	3089	1/1	0.88	0.26	-	76,76,76,76	0
54	MG	BA	3024	1/1	0.96	0.53	-	67,67,67,67	0
54	MG	DB	206	1/1	0.78	0.29	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3318	1/1	0.74	0.36	-	101,101,101,101	0
54	MG	DA	3288	1/1	0.87	0.43	-	78,78,78,78	0
54	MG	CA	1716	1/1	0.95	0.22	-	77,77,77,77	0
54	MG	DA	3303	1/1	0.89	0.15	-	66,66,66,66	0
54	MG	DA	3038	1/1	0.89	0.26	-	71,71,71,71	0
54	MG	BA	3013	1/1	0.73	0.10	-	90,90,90,90	0
54	MG	DA	3297	1/1	0.83	0.38	-	49,49,49,49	0
54	MG	BA	3136	1/1	0.72	0.22	-	87,87,87,87	0
54	MG	CA	1637	1/1	0.72	0.17	-	112,112,112,112	0
54	MG	BA	3098	1/1	0.84	0.19	-	78,78,78,78	0
54	MG	BA	2905	1/1	0.94	0.54	-	12,12,12,12	0
54	MG	AA	1617	1/1	0.98	0.19	-	77,77,77,77	0
54	MG	BA	2928	1/1	0.97	0.36	-	42,42,42,42	0
54	MG	AA	1625	1/1	0.88	1.01	-	88,88,88,88	0
54	MG	DA	3172	1/1	0.85	0.35	-	81,81,81,81	0
54	MG	BA	2947	1/1	0.98	0.30	-	14,14,14,14	0
54	MG	AA	1744	1/1	0.96	0.25	-	82,82,82,82	0
54	MG	CA	1677	1/1	0.92	0.28	-	85,85,85,85	0
54	MG	BA	2959	1/1	0.97	0.39	-	55,55,55,55	0
54	MG	CA	1711	1/1	0.78	0.36	-	87,87,87,87	0
54	MG	DA	3325	1/1	0.55	0.71	-	92,92,92,92	0
54	MG	DA	3133	1/1	0.91	0.13	-	89,89,89,89	0
54	MG	BA	3183	1/1	0.96	0.37	-	27,27,27,27	0
54	MG	BA	3281	1/1	0.76	0.33	-	84,84,84,84	0
54	MG	BA	3104	1/1	0.85	0.34	-	63,63,63,63	0
54	MG	BA	2906	1/1	1.00	0.22	-	5,5,5,5	0
54	MG	DA	3178	1/1	0.84	0.27	-	83,83,83,83	0
54	MG	DA	3147	1/1	0.92	0.14	-	78,78,78,78	0
54	MG	DA	3077	1/1	0.87	0.61	-	67,67,67,67	0
54	MG	AA	1653	1/1	0.84	0.32	-	89,89,89,89	0
54	MG	AA	1710	1/1	0.97	0.26	-	65,65,65,65	0
54	MG	DA	3182	1/1	0.95	0.59	-	86,86,86,86	0
54	MG	DB	215	1/1	0.48	0.44	-	103,103,103,103	0
54	MG	BA	2934	1/1	0.98	0.44	-	28,28,28,28	0
54	MG	BA	3082	1/1	0.92	0.18	-	61,61,61,61	0
54	MG	BA	3265	1/1	0.87	0.33	-	80,80,80,80	0
54	MG	DA	3069	1/1	0.88	0.17	-	81,81,81,81	0
54	MG	BA	3140	1/1	0.86	0.43	-	76,76,76,76	0
54	MG	CA	1674	1/1	0.84	0.15	-	74,74,74,74	0
54	MG	AA	1645	1/1	0.76	0.59	-	79,79,79,79	0
54	MG	DA	3204	1/1	0.99	0.14	-	54,54,54,54	0
54	MG	DA	3321	1/1	0.95	0.51	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3328	1/1	0.98	0.10	-	45,45,45,45	0
54	MG	BA	3202	1/1	0.93	0.60	-	63,63,63,63	0
54	MG	DA	3035	1/1	0.90	0.42	-	77,77,77,77	0
54	MG	CA	1652	1/1	0.96	0.43	-	85,85,85,85	0
54	MG	DA	3087	1/1	0.70	0.29	-	67,67,67,67	0
54	MG	CA	1687	1/1	0.81	0.27	-	64,64,64,64	0
54	MG	AA	1760	1/1	0.91	0.16	-	84,84,84,84	0
54	MG	DA	3210	1/1	0.91	0.10	-	59,59,59,59	0
54	MG	AA	1750	1/1	0.94	0.46	-	109,109,109,109	0
54	MG	DA	3092	1/1	0.83	0.09	-	98,98,98,98	0
54	MG	BA	3032	1/1	0.91	0.26	-	59,59,59,59	0
54	MG	BA	3000	1/1	0.86	0.17	-	65,65,65,65	0
54	MG	BA	3120	1/1	0.96	0.30	-	57,57,57,57	0
54	MG	DA	3130	1/1	0.79	0.32	-	82,82,82,82	0
54	MG	DA	2910	1/1	0.98	0.30	-	6,6,6,6	0
54	MG	DA	2988	1/1	0.90	0.52	-	41,41,41,41	0
54	MG	BA	2919	1/1	0.97	0.41	-	24,24,24,24	0
54	MG	DA	3100	1/1	0.71	0.45	-	59,59,59,59	0
54	MG	AA	1745	1/1	0.64	0.27	-	97,97,97,97	0
54	MG	BA	3177	1/1	0.90	0.23	-	93,93,93,93	0
54	MG	BA	3047	1/1	0.92	0.39	-	65,65,65,65	0
54	MG	BA	3067	1/1	0.91	0.08	-	86,86,86,86	0
54	MG	DA	3319	1/1	0.91	0.63	-	83,83,83,83	0
54	MG	DA	2960	1/1	0.91	0.29	-	42,42,42,42	0
54	MG	DA	2972	1/1	0.69	0.48	-	47,47,47,47	0
54	MG	AA	1747	1/1	0.72	0.81	-	75,75,75,75	0
54	MG	DA	2962	1/1	0.98	0.38	-	37,37,37,37	0
54	MG	CA	1660	1/1	0.96	0.16	-	100,100,100,100	0
54	MG	DA	2948	1/1	0.92	0.33	-	52,52,52,52	0
54	MG	DA	3121	1/1	0.87	0.21	-	69,69,69,69	0
54	MG	BA	3059	1/1	0.94	0.21	-	60,60,60,60	0
54	MG	DA	3280	1/1	0.92	0.30	-	84,84,84,84	0
54	MG	DA	3187	1/1	0.86	0.22	-	90,90,90,90	0
54	MG	DA	3137	1/1	0.89	0.18	-	68,68,68,68	0
54	MG	BA	3305	1/1	0.40	0.58	-	103,103,103,103	0
54	MG	BA	3198	1/1	0.98	0.21	-	81,81,81,81	0
54	MG	BA	2977	1/1	0.98	0.28	-	52,52,52,52	0
54	MG	BA	2926	1/1	0.95	0.55	-	31,31,31,31	0
54	MG	DA	3119	1/1	0.66	0.65	-	88,88,88,88	0
54	MG	DA	3220	1/1	0.84	0.27	-	70,70,70,70	0
54	MG	BA	3212	1/1	0.79	0.40	-	69,69,69,69	0
54	MG	BB	203	1/1	0.91	0.14	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3256	1/1	0.85	0.21	-	82,82,82,82	0
54	MG	BA	3211	1/1	0.98	0.37	-	59,59,59,59	0
54	MG	DA	2920	1/1	0.91	0.44	-	30,30,30,30	0
54	MG	AA	1757	1/1	0.54	0.53	-	89,89,89,89	0
54	MG	DA	3253	1/1	0.92	0.17	-	92,92,92,92	0
54	MG	DA	3010	1/1	0.84	0.65	-	51,51,51,51	0
54	MG	DA	2925	1/1	0.93	0.45	-	24,24,24,24	0
54	MG	DA	3008	1/1	0.90	0.47	-	59,59,59,59	0
54	MG	AA	1737	1/1	0.83	0.25	-	86,86,86,86	0
54	MG	DA	3295	1/1	0.82	0.26	-	63,63,63,63	0
54	MG	AA	1689	1/1	0.76	0.26	-	68,68,68,68	0
54	MG	DB	214	1/1	0.87	0.20	-	90,90,90,90	0
54	MG	BA	2981	1/1	0.96	0.15	-	48,48,48,48	0
54	MG	BA	3048	1/1	0.87	0.33	-	67,67,67,67	0
54	MG	BA	3035	1/1	0.90	0.38	-	44,44,44,44	0
54	MG	BA	3101	1/1	0.81	0.45	-	75,75,75,75	0
54	MG	CA	1722	1/1	0.94	0.38	-	108,108,108,108	0
54	MG	DA	2922	1/1	0.95	0.31	-	7,7,7,7	0
54	MG	BA	2937	1/1	0.95	0.33	-	36,36,36,36	0
54	MG	CA	1642	1/1	0.94	0.17	-	71,71,71,71	0
54	MG	BA	3122	1/1	0.92	0.30	-	101,101,101,101	0
54	MG	AA	1638	1/1	0.94	0.48	-	63,63,63,63	0
54	MG	DA	3240	1/1	0.92	0.38	-	60,60,60,60	0
54	MG	BA	3239	1/1	0.92	0.57	-	82,82,82,82	0
54	MG	DA	2981	1/1	0.90	0.30	-	55,55,55,55	0
54	MG	DA	2929	1/1	0.96	0.35	-	39,39,39,39	0
54	MG	BA	2974	1/1	0.98	0.20	-	45,45,45,45	0
54	MG	D4	101	1/1	0.79	0.55	-	55,55,55,55	0
54	MG	DA	3167	1/1	0.99	0.17	-	68,68,68,68	0
54	MG	CA	1708	1/1	0.84	0.14	-	143,143,143,143	0
54	MG	DA	3184	1/1	0.88	0.28	-	117,117,117,117	0
54	MG	DA	3269	1/1	0.84	0.51	-	91,91,91,91	0
54	MG	BA	3075	1/1	0.72	0.21	-	67,67,67,67	0
54	MG	BA	3005	1/1	0.85	0.52	-	69,69,69,69	0
54	MG	AA	1641	1/1	0.75	0.35	-	85,85,85,85	0
54	MG	CA	1689	1/1	0.91	0.29	-	83,83,83,83	0
54	MG	DA	3093	1/1	0.91	0.39	-	69,69,69,69	0
54	MG	BB	209	1/1	0.88	0.24	-	83,83,83,83	0
54	MG	DA	3125	1/1	0.92	0.28	-	81,81,81,81	0
54	MG	AA	1727	1/1	0.93	0.13	-	100,100,100,100	0
54	MG	BA	3250	1/1	0.92	0.13	-	95,95,95,95	0
54	MG	DA	3049	1/1	0.78	0.21	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1733	1/1	0.84	0.12	-	72,72,72,72	0
54	MG	AA	1673	1/1	0.62	0.53	-	61,61,61,61	0
54	MG	DB	207	1/1	0.88	0.28	-	72,72,72,72	0
54	MG	AV	6303	1/1	0.86	0.13	-	67,67,67,67	0
54	MG	BA	3149	1/1	0.68	0.73	-	82,82,82,82	0
54	MG	BA	2932	1/1	0.98	0.26	-	41,41,41,41	0
54	MG	DA	2954	1/1	0.95	0.31	-	28,28,28,28	0
54	MG	DA	3207	1/1	0.74	0.37	-	42,42,42,42	0
54	MG	AA	1642	1/1	0.69	0.50	-	97,97,97,97	0
54	MG	DA	3042	1/1	0.96	0.56	-	79,79,79,79	0
54	MG	DA	3097	1/1	0.80	0.29	-	94,94,94,94	0
54	MG	CA	1726	1/1	0.92	0.34	-	87,87,87,87	0
54	MG	DA	3061	1/1	0.77	0.27	-	75,75,75,75	0
54	MG	AA	1659	1/1	0.96	0.42	-	51,51,51,51	0
54	MG	BA	3194	1/1	0.93	0.53	-	45,45,45,45	0
54	MG	BA	2944	1/1	0.92	0.15	-	17,17,17,17	0
54	MG	DA	3027	1/1	0.86	0.50	-	53,53,53,53	0
54	MG	CA	1682	1/1	0.94	0.21	-	97,97,97,97	0
54	MG	DA	3115	1/1	0.56	0.49	-	65,65,65,65	0
54	MG	DA	3261	1/1	0.93	0.27	-	73,73,73,73	0
54	MG	BA	3195	1/1	0.97	0.16	-	53,53,53,53	0
54	MG	CA	1737	1/1	0.93	0.20	-	70,70,70,70	0
54	MG	BA	3217	1/1	0.47	0.34	-	111,111,111,111	0
54	MG	BA	2948	1/1	0.86	0.72	-	39,39,39,39	0
54	MG	CA	1616	1/1	0.78	0.47	-	75,75,75,75	0
54	MG	DA	3102	1/1	0.98	0.20	-	68,68,68,68	0
54	MG	AV	6304	1/1	0.33	0.43	-	118,118,118,118	0
54	MG	AA	1729	1/1	0.28	0.13	-	75,75,75,75	0
54	MG	BA	2989	1/1	0.95	0.35	-	53,53,53,53	0
54	MG	AA	1665	1/1	0.88	0.26	-	82,82,82,82	0
54	MG	BA	3224	1/1	0.98	0.22	-	45,45,45,45	0
54	MG	AA	1722	1/1	0.70	0.28	-	83,83,83,83	0
54	MG	DA	3307	1/1	0.78	0.38	-	73,73,73,73	0
54	MG	BA	3283	1/1	0.71	0.16	-	76,76,76,76	0
54	MG	DA	3244	1/1	0.75	0.27	-	87,87,87,87	0
54	MG	BA	3107	1/1	0.94	0.26	-	87,87,87,87	0
54	MG	BA	2907	1/1	0.96	0.26	-	7,7,7,7	0
54	MG	DA	3239	1/1	0.95	0.23	-	42,42,42,42	0
54	MG	BA	2936	1/1	0.98	0.18	-	43,43,43,43	0
54	MG	CA	1736	1/1	0.82	1.13	-	115,115,115,115	0
54	MG	BA	2978	1/1	0.93	0.35	-	59,59,59,59	0
54	MG	BA	2939	1/1	0.95	0.46	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1761	1/1	0.82	0.20	-	104,104,104,104	0
54	MG	BA	3286	1/1	0.97	0.38	-	67,67,67,67	0
54	MG	BA	2985	1/1	0.83	0.52	-	54,54,54,54	0
54	MG	CA	1611	1/1	0.88	0.19	-	76,76,76,76	0
54	MG	BA	3130	1/1	0.94	0.17	-	78,78,78,78	0
54	MG	DA	3258	1/1	0.74	0.48	-	72,72,72,72	0
54	MG	BA	3115	1/1	0.74	0.32	-	91,91,91,91	0
54	MG	AA	1656	1/1	0.97	0.31	-	72,72,72,72	0
54	MG	CA	1707	1/1	0.95	0.08	-	104,104,104,104	0
54	MG	CA	1640	1/1	0.95	0.38	-	69,69,69,69	0
54	MG	BA	3176	1/1	0.38	0.33	-	99,99,99,99	0
54	MG	CA	1704	1/1	0.41	0.52	-	108,108,108,108	0
54	MG	CA	1739	1/1	0.90	0.10	-	99,99,99,99	0
54	MG	DA	3152	1/1	0.88	0.21	-	77,77,77,77	0
54	MG	DA	3068	1/1	0.87	0.41	-	72,72,72,72	0
54	MG	AA	1651	1/1	0.83	0.51	-	97,97,97,97	0
54	MG	DA	3120	1/1	0.83	0.64	-	66,66,66,66	0
54	MG	DA	3334	1/1	0.82	0.25	-	72,72,72,72	0
54	MG	DA	3225	1/1	0.96	0.08	-	80,80,80,80	0
54	MG	DA	3246	1/1	0.70	0.60	-	67,67,67,67	0
54	MG	CA	1628	1/1	0.87	0.20	-	100,100,100,100	0
54	MG	DA	2924	1/1	0.98	0.48	-	41,41,41,41	0
54	MG	DA	3017	1/1	0.41	0.22	-	93,93,93,93	0
54	MG	BA	3056	1/1	0.89	0.49	-	62,62,62,62	0
54	MG	DA	3287	1/1	0.88	0.51	-	69,69,69,69	0
54	MG	CA	1601	1/1	0.83	0.45	-	53,53,53,53	0
54	MG	CA	1618	1/1	0.87	0.72	-	63,63,63,63	0
54	MG	DA	3175	1/1	0.83	0.18	-	81,81,81,81	0
54	MG	BA	3158	1/1	0.78	0.20	-	105,105,105,105	0
54	MG	CA	1693	1/1	0.92	0.34	-	65,65,65,65	0
54	MG	BA	3002	1/1	0.93	0.38	-	45,45,45,45	0
54	MG	CA	1602	1/1	0.99	0.09	-	64,64,64,64	0
54	MG	DA	3164	1/1	0.96	0.05	-	88,88,88,88	0
54	MG	DA	3103	1/1	0.84	0.41	-	79,79,79,79	0
54	MG	DA	3237	1/1	0.98	0.23	-	87,87,87,87	0
54	MG	BA	3215	1/1	0.97	0.36	-	68,68,68,68	0
54	MG	DA	3194	1/1	0.98	0.36	-	10,10,10,10	0
54	MG	BA	3274	1/1	0.97	0.06	-	78,78,78,78	0
54	MG	AA	1614	1/1	0.84	0.52	-	85,85,85,85	0
54	MG	DA	2956	1/1	0.95	0.28	-	45,45,45,45	0
54	MG	BA	3295	1/1	0.83	0.60	-	70,70,70,70	0
54	MG	CA	1653	1/1	0.97	0.20	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3267	1/1	0.79	0.25	-	76,76,76,76	0
54	MG	BA	2927	1/1	0.94	0.29	-	37,37,37,37	0
54	MG	BA	3279	1/1	0.95	0.27	-	77,77,77,77	0
54	MG	BA	3134	1/1	0.98	0.17	-	64,64,64,64	0
54	MG	DA	3016	1/1	0.96	0.21	-	74,74,74,74	0
54	MG	BA	3112	1/1	0.82	0.34	-	68,68,68,68	0
54	MG	DA	3181	1/1	0.61	0.18	-	106,106,106,106	0
54	MG	BA	2912	1/1	0.94	0.66	-	36,36,36,36	0
54	MG	BA	3160	1/1	0.89	0.54	-	106,106,106,106	0
54	MG	BA	2990	1/1	0.95	0.19	-	54,54,54,54	0
54	MG	CA	1631	1/1	0.91	0.13	-	68,68,68,68	0
54	MG	AA	1699	1/1	0.87	0.26	-	91,91,91,91	0
54	MG	DA	3335	1/1	0.92	0.29	-	90,90,90,90	0
54	MG	BA	3133	1/1	0.88	0.26	-	67,67,67,67	0
54	MG	BA	3074	1/1	0.89	0.34	-	61,61,61,61	0
54	MG	DA	3309	1/1	0.78	0.38	-	30,30,30,30	0
54	MG	DA	2986	1/1	0.93	0.22	-	55,55,55,55	0
54	MG	DA	3062	1/1	0.94	0.12	-	65,65,65,65	0
54	MG	DA	3242	1/1	0.80	0.31	-	96,96,96,96	0
54	MG	BA	3148	1/1	0.88	0.35	-	68,68,68,68	0
54	MG	AA	1678	1/1	0.85	0.24	-	115,115,115,115	0
54	MG	DA	3159	1/1	0.90	1.09	-	87,87,87,87	0
54	MG	DA	3122	1/1	0.95	0.22	-	87,87,87,87	0
54	MG	BA	3154	1/1	0.95	0.22	-	89,89,89,89	0
54	MG	BA	2996	1/1	0.87	0.29	-	54,54,54,54	0
54	MG	DA	3193	1/1	0.95	0.57	-	51,51,51,51	0
54	MG	BA	3060	1/1	0.67	0.69	-	74,74,74,74	0
54	MG	DA	3021	1/1	0.81	0.17	-	67,67,67,67	0
54	MG	DA	3110	1/1	0.52	0.31	-	86,86,86,86	0
54	MG	BA	3125	1/1	0.86	0.26	-	87,87,87,87	0
54	MG	DA	3271	1/1	0.71	0.18	-	97,97,97,97	0
54	MG	CA	1721	1/1	0.95	0.33	-	101,101,101,101	0
54	MG	AA	1730	1/1	0.99	0.09	-	49,49,49,49	0
54	MG	AA	1660	1/1	0.84	0.30	-	59,59,59,59	0
54	MG	DA	3140	1/1	0.95	0.14	-	67,67,67,67	0
54	MG	AA	1687	1/1	0.90	0.08	-	73,73,73,73	0
54	MG	DA	3257	1/1	0.90	0.16	-	94,94,94,94	0
54	MG	BB	215	1/1	0.95	0.19	-	131,131,131,131	0
54	MG	BA	3156	1/1	0.96	0.28	-	80,80,80,80	0
54	MG	AA	1666	1/1	0.97	0.10	-	100,100,100,100	0
54	MG	BA	3280	1/1	0.84	0.40	-	70,70,70,70	0
54	MG	DA	3158	1/1	0.88	0.18	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3218	1/1	0.91	0.49	-	48,48,48,48	0
54	MG	BA	3050	1/1	0.87	0.17	-	41,41,41,41	0
54	MG	AA	1694	1/1	0.89	0.23	-	129,129,129,129	0
54	MG	DA	3090	1/1	0.85	0.21	-	71,71,71,71	0
54	MG	BA	3045	1/1	0.90	0.20	-	80,80,80,80	0
54	MG	BA	2960	1/1	0.94	0.57	-	40,40,40,40	0
54	MG	DA	3073	1/1	0.96	0.10	-	80,80,80,80	0
54	MG	BA	3051	1/1	0.85	0.34	-	66,66,66,66	0
54	MG	BA	3071	1/1	0.93	0.17	-	72,72,72,72	0
54	MG	DA	3206	1/1	0.97	0.32	-	37,37,37,37	0
54	MG	DA	3160	1/1	0.96	0.16	-	71,71,71,71	0
54	MG	BA	3044	1/1	0.94	0.12	-	64,64,64,64	0
54	MG	AA	1680	1/1	0.64	0.14	-	90,90,90,90	0
54	MG	BB	206	1/1	0.80	0.23	-	70,70,70,70	0
54	MG	BA	3084	1/1	0.66	0.41	-	51,51,51,51	0
54	MG	CA	1668	1/1	0.72	1.09	-	116,116,116,116	0
54	MG	DA	2941	1/1	0.93	0.23	-	37,37,37,37	0
54	MG	DA	3279	1/1	0.86	0.09	-	88,88,88,88	0
54	MG	CA	1720	1/1	0.89	0.35	-	63,63,63,63	0
54	MG	CA	1667	1/1	0.94	0.10	-	67,67,67,67	0
54	MG	DA	3138	1/1	0.89	0.12	-	70,70,70,70	0
54	MG	BA	3016	1/1	0.90	0.31	-	60,60,60,60	0
54	MG	BA	3275	1/1	0.00	0.91	-	87,87,87,87	0
54	MG	DA	3143	1/1	0.70	0.25	-	77,77,77,77	0
54	MG	DA	3262	1/1	0.73	0.27	-	82,82,82,82	0
54	MG	BA	3015	1/1	0.97	0.42	-	58,58,58,58	0
54	MG	CA	1669	1/1	0.96	0.14	-	66,66,66,66	0
54	MG	CA	1690	1/1	0.99	0.52	-	61,61,61,61	0
54	MG	AA	1715	1/1	0.96	0.35	-	63,63,63,63	0
54	MG	AA	1648	1/1	0.96	0.40	-	76,76,76,76	0
54	MG	BA	3009	1/1	0.84	0.51	-	87,87,87,87	0
54	MG	DA	3330	1/1	0.88	0.39	-	69,69,69,69	0
54	MG	BA	3145	1/1	0.82	0.19	-	67,67,67,67	0
54	MG	DA	3296	1/1	0.79	0.15	-	104,104,104,104	0
54	MG	BA	3086	1/1	0.97	0.26	-	102,102,102,102	0
54	MG	BA	3246	1/1	0.95	0.24	-	73,73,73,73	0
54	MG	DA	3317	1/1	0.78	0.42	-	97,97,97,97	0
54	MG	AA	1608	1/1	0.94	0.36	-	47,47,47,47	0
54	MG	DA	3135	1/1	0.95	0.22	-	65,65,65,65	0
54	MG	DA	3098	1/1	0.81	0.37	-	71,71,71,71	0
54	MG	DA	3081	1/1	0.98	0.10	-	71,71,71,71	0
54	MG	BA	3066	1/1	0.84	0.46	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3210	1/1	0.97	0.33	-	48,48,48,48	0
54	MG	CA	1636	1/1	0.72	0.33	-	93,93,93,93	0
54	MG	BA	3240	1/1	0.76	0.10	-	114,114,114,114	0
54	MG	BA	2935	1/1	0.94	0.56	-	34,34,34,34	0
54	MG	DA	3327	1/1	0.71	0.32	-	68,68,68,68	0
54	MG	DA	3127	1/1	0.81	0.37	-	90,90,90,90	0
54	MG	DA	3266	1/1	0.94	0.33	-	83,83,83,83	0
54	MG	DA	3243	1/1	0.60	0.35	-	72,72,72,72	0
54	MG	DA	3091	1/1	0.87	0.49	-	125,125,125,125	0
54	MG	DA	3116	1/1	0.79	0.25	-	115,115,115,115	0
54	MG	DA	3163	1/1	0.50	0.19	-	83,83,83,83	0
54	MG	BA	3029	1/1	0.92	0.58	-	63,63,63,63	0
54	MG	BA	3159	1/1	0.81	0.42	-	78,78,78,78	0
54	MG	AA	1675	1/1	0.86	0.15	-	77,77,77,77	0
54	MG	AA	1732	1/1	0.91	0.24	-	63,63,63,63	0
54	MG	BA	3165	1/1	0.84	0.26	-	71,71,71,71	0
54	MG	BA	3261	1/1	0.91	0.30	-	53,53,53,53	0
54	MG	AA	1746	1/1	0.92	0.27	-	100,100,100,100	0
54	MG	DA	3203	1/1	0.98	0.23	-	46,46,46,46	0
54	MG	DA	3032	1/1	0.88	0.10	-	49,49,49,49	0
54	MG	DA	2919	1/1	0.98	0.28	-	45,45,45,45	0
54	MG	BA	2984	1/1	0.95	0.22	-	41,41,41,41	0
54	MG	AA	1635	1/1	0.96	0.33	-	68,68,68,68	0
54	MG	DA	3196	1/1	0.73	1.09	-	39,39,39,39	0
54	MG	DA	3186	1/1	0.78	0.13	-	90,90,90,90	0
54	MG	BA	3064	1/1	0.95	0.31	-	40,40,40,40	0
54	MG	AA	1686	1/1	0.95	0.13	-	72,72,72,72	0
54	MG	BA	3076	1/1	0.96	0.25	-	68,68,68,68	0
54	MG	BA	2992	1/1	0.90	0.50	-	70,70,70,70	0
54	MG	AA	1683	1/1	0.93	0.17	-	102,102,102,102	0
54	MG	CA	1657	1/1	0.91	0.39	-	78,78,78,78	0
54	MG	BA	3062	1/1	0.76	0.36	-	76,76,76,76	0
54	MG	DA	2987	1/1	0.77	0.44	-	70,70,70,70	0
54	MG	BA	3099	1/1	0.85	0.15	-	78,78,78,78	0
54	MG	DA	3028	1/1	0.93	0.15	-	78,78,78,78	0
54	MG	CA	1727	1/1	0.82	0.26	-	75,75,75,75	0
54	MG	DA	3064	1/1	0.61	0.19	-	80,80,80,80	0
54	MG	CA	1627	1/1	0.94	0.18	-	67,67,67,67	0
54	MG	BA	3285	1/1	0.90	0.24	-	87,87,87,87	0
54	MG	BB	205	1/1	0.69	0.41	-	71,71,71,71	0
54	MG	DA	2957	1/1	0.96	0.09	-	63,63,63,63	0
54	MG	DA	3283	1/1	0.94	0.27	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3303	1/1	0.71	0.20	-	98,98,98,98	0
54	MG	CA	1697	1/1	0.50	0.47	-	74,74,74,74	0
54	MG	BA	3190	1/1	0.69	0.26	-	115,115,115,115	0
54	MG	BA	3178	1/1	0.68	0.50	-	72,72,72,72	0
55	ZN	AN	101	1/1	0.98	0.14	-	120,120,120,120	0
54	MG	AA	1602	1/1	0.91	0.58	-	49,49,49,49	0
54	MG	DA	2977	1/1	0.88	0.17	-	47,47,47,47	0
54	MG	BA	3300	1/1	0.88	0.45	-	83,83,83,83	0
54	MG	CA	1709	1/1	0.92	0.39	-	81,81,81,81	0
54	MG	CA	1724	1/1	0.68	0.32	-	74,74,74,74	0
54	MG	BA	3225	1/1	0.60	0.48	-	74,74,74,74	0
54	MG	DB	217	1/1	0.94	0.14	-	74,74,74,74	0
54	MG	AA	1709	1/1	0.71	0.37	-	83,83,83,83	0
54	MG	DA	3114	1/1	0.94	0.36	-	83,83,83,83	0
54	MG	BA	3094	1/1	0.89	0.68	-	70,70,70,70	0
54	MG	AA	1693	1/1	0.76	0.32	-	74,74,74,74	0
54	MG	DA	3170	1/1	0.88	0.20	-	80,80,80,80	0
54	MG	BA	3069	1/1	0.84	0.13	-	109,109,109,109	0
54	MG	DA	2979	1/1	0.89	0.23	-	69,69,69,69	0
54	MG	DA	3108	1/1	0.90	0.19	-	50,50,50,50	0
54	MG	DA	3291	1/1	0.74	0.48	-	78,78,78,78	0
54	MG	BA	3137	1/1	0.94	0.52	-	54,54,54,54	0
54	MG	DA	3336	1/1	0.92	0.07	-	89,89,89,89	0
54	MG	DA	3305	1/1	0.89	0.12	-	110,110,110,110	0
54	MG	BA	2946	1/1	0.97	0.46	-	33,33,33,33	0
54	MG	DA	3213	1/1	0.96	0.20	-	66,66,66,66	0
54	MG	CA	1713	1/1	0.92	0.17	-	80,80,80,80	0
54	MG	AA	1701	1/1	0.81	0.35	-	83,83,83,83	0
54	MG	DA	3166	1/1	0.84	0.12	-	87,87,87,87	0
54	MG	BA	3117	1/1	0.61	0.11	-	77,77,77,77	0
54	MG	CA	1673	1/1	0.96	0.15	-	73,73,73,73	0
54	MG	BA	3164	1/1	0.46	0.63	-	88,88,88,88	0
54	MG	DA	3086	1/1	0.91	0.68	-	92,92,92,92	0
54	MG	BA	3108	1/1	0.88	0.42	-	99,99,99,99	0
54	MG	DA	3002	1/1	0.93	0.43	-	59,59,59,59	0
54	MG	BA	2983	1/1	0.95	0.45	-	62,62,62,62	0
54	MG	CA	1718	1/1	0.93	0.15	-	78,78,78,78	0
54	MG	DA	3095	1/1	0.90	0.17	-	67,67,67,67	0
54	MG	BA	2988	1/1	0.38	0.33	-	60,60,60,60	0
54	MG	BA	3162	1/1	0.96	0.08	-	94,94,94,94	0
54	MG	DA	3113	1/1	0.82	0.09	-	71,71,71,71	0
54	MG	DA	3219	1/1	0.98	0.29	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3272	1/1	0.61	0.45	-	119,119,119,119	0
54	MG	BA	3068	1/1	0.86	0.34	-	59,59,59,59	0
54	MG	CA	1714	1/1	0.94	0.29	-	74,74,74,74	0
54	MG	BA	3128	1/1	0.92	0.48	-	59,59,59,59	0
54	MG	DA	3044	1/1	0.98	0.08	-	59,59,59,59	0
54	MG	BA	3254	1/1	0.95	0.48	-	81,81,81,81	0
54	MG	CA	1654	1/1	0.93	0.13	-	111,111,111,111	0
54	MG	BA	2933	1/1	0.98	0.30	-	32,32,32,32	0
54	MG	BA	3150	1/1	0.88	0.38	-	79,79,79,79	0
54	MG	AA	1705	1/1	0.95	0.30	-	92,92,92,92	0
54	MG	DA	3117	1/1	0.94	0.20	-	87,87,87,87	0
54	MG	CA	1701	1/1	0.81	0.34	-	112,112,112,112	0
54	MG	BB	214	1/1	0.90	0.20	-	101,101,101,101	0
54	MG	AA	1734	1/1	0.67	0.37	-	103,103,103,103	0
54	MG	BA	3020	1/1	0.98	0.30	-	62,62,62,62	0
54	MG	BA	3072	1/1	0.78	0.43	-	67,67,67,67	0
54	MG	DA	3162	1/1	0.79	0.16	-	143,143,143,143	0
54	MG	BA	3146	1/1	0.84	0.28	-	83,83,83,83	0
54	MG	BA	2923	1/1	0.95	0.33	-	29,29,29,29	0
54	MG	AA	1691	1/1	0.77	0.42	-	78,78,78,78	0
54	MG	BA	3171	1/1	0.87	0.19	-	68,68,68,68	0
54	MG	BA	3042	1/1	0.94	0.15	-	90,90,90,90	0
54	MG	BA	3096	1/1	0.96	0.24	-	65,65,65,65	0
54	MG	DA	3126	1/1	0.90	0.08	-	77,77,77,77	0
54	MG	DA	3329	1/1	0.90	0.71	-	69,69,69,69	0
54	MG	AA	1696	1/1	0.61	0.24	-	132,132,132,132	0
54	MG	CA	1641	1/1	0.78	0.13	-	85,85,85,85	0
54	MG	BA	3038	1/1	0.81	0.17	-	65,65,65,65	0
54	MG	DA	3173	1/1	0.87	0.18	-	97,97,97,97	0
54	MG	BA	3207	1/1	0.92	0.36	-	94,94,94,94	0
54	MG	BA	3008	1/1	0.98	0.18	-	57,57,57,57	0
54	MG	DA	3045	1/1	0.95	0.30	-	48,48,48,48	0
54	MG	DA	3065	1/1	0.81	0.36	-	56,56,56,56	0
54	MG	DA	3063	1/1	0.97	0.26	-	79,79,79,79	0
54	MG	BA	2954	1/1	0.95	0.19	-	52,52,52,52	0
54	MG	BA	3023	1/1	0.82	0.51	-	64,64,64,64	0
54	MG	CA	1649	1/1	0.96	0.22	-	80,80,80,80	0
54	MG	DA	3300	1/1	0.76	0.21	-	68,68,68,68	0
54	MG	BA	3196	1/1	0.96	0.23	-	51,51,51,51	0
54	MG	DA	3270	1/1	0.95	0.29	-	81,81,81,81	0
54	MG	CA	1679	1/1	0.92	0.12	-	93,93,93,93	0
54	MG	BA	3147	1/1	0.91	0.32	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3221	1/1	0.85	0.34	-	48,48,48,48	0
54	MG	DA	3019	1/1	0.94	0.36	-	51,51,51,51	0
54	MG	BA	3031	1/1	0.82	0.83	-	87,87,87,87	0
54	MG	BA	3228	1/1	0.93	0.12	-	66,66,66,66	0
54	MG	BA	3116	1/1	0.86	0.39	-	85,85,85,85	0
54	MG	CA	1712	1/1	0.97	0.11	-	78,78,78,78	0
54	MG	DA	3265	1/1	0.65	0.32	-	120,120,120,120	0
54	MG	AA	1733	1/1	0.93	0.22	-	91,91,91,91	0
54	MG	DA	3058	1/1	0.95	0.11	-	54,54,54,54	0
54	MG	DA	2963	1/1	0.94	0.39	-	53,53,53,53	0
54	MG	BA	3025	1/1	0.57	0.30	-	65,65,65,65	0
54	MG	CA	1639	1/1	0.51	0.63	-	66,66,66,66	0
54	MG	DA	2953	1/1	0.93	0.45	-	58,58,58,58	0
54	MG	DB	201	1/1	0.96	0.24	-	63,63,63,63	0
54	MG	BA	3092	1/1	0.93	0.17	-	63,63,63,63	0
54	MG	CA	1650	1/1	0.73	0.31	-	108,108,108,108	0
54	MG	AA	1606	1/1	0.98	0.36	-	53,53,53,53	0
54	MG	AA	1633	1/1	0.95	0.15	-	73,73,73,73	0
54	MG	DA	2997	1/1	0.98	0.17	-	35,35,35,35	0
54	MG	AA	1688	1/1	0.91	0.14	-	68,68,68,68	0
54	MG	DA	3107	1/1	0.92	0.27	-	67,67,67,67	0
54	MG	DA	3333	1/1	0.94	0.15	-	126,126,126,126	0
54	MG	DA	3229	1/1	0.73	0.42	-	64,64,64,64	0
54	MG	DA	3111	1/1	0.80	0.39	-	67,67,67,67	0
54	MG	CA	1656	1/1	0.92	0.14	-	79,79,79,79	0
54	MG	BA	3258	1/1	0.85	0.21	-	104,104,104,104	0
54	MG	DA	2952	1/1	0.93	0.30	-	50,50,50,50	0
54	MG	DA	3141	1/1	0.82	0.14	-	95,95,95,95	0
54	MG	AA	1706	1/1	0.72	0.38	-	103,103,103,103	0
54	MG	AA	1646	1/1	0.68	0.25	-	99,99,99,99	0
54	MG	DA	3308	1/1	0.67	0.37	-	91,91,91,91	0
54	MG	BA	3298	1/1	0.92	0.10	-	74,74,74,74	0
54	MG	BA	2963	1/1	0.87	0.19	-	54,54,54,54	0
54	MG	CA	1740	1/1	0.54	0.24	-	117,117,117,117	0
54	MG	AA	1623	1/1	0.63	0.39	-	93,93,93,93	0
54	MG	BA	3123	1/1	0.74	0.36	-	52,52,52,52	0
54	MG	BA	3132	1/1	0.94	0.20	-	79,79,79,79	0
54	MG	BA	2955	1/1	0.92	0.19	-	50,50,50,50	0
54	MG	CA	1675	1/1	0.94	0.28	-	107,107,107,107	0
54	MG	BA	3073	1/1	0.47	0.28	-	89,89,89,89	0
54	MG	BA	3109	1/1	0.71	0.83	-	90,90,90,90	0
54	MG	DA	2937	1/1	0.98	0.55	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3104	1/1	0.96	0.27	-	99,99,99,99	0
54	MG	DA	3169	1/1	0.80	0.12	-	112,112,112,112	0
54	MG	BA	3079	1/1	0.60	0.43	-	86,86,86,86	0
54	MG	DA	3326	1/1	0.94	0.18	-	85,85,85,85	0
54	MG	AA	1762	1/1	0.74	0.10	-	155,155,155,155	0
54	MG	AA	1610	1/1	0.70	0.28	-	78,78,78,78	0
54	MG	BA	2994	1/1	0.94	0.65	-	56,56,56,56	0
54	MG	DA	3177	1/1	0.84	0.32	-	62,62,62,62	0
54	MG	BA	3037	1/1	0.81	0.14	-	93,93,93,93	0
54	MG	DA	2940	1/1	0.75	0.71	-	51,51,51,51	0
54	MG	DA	3285	1/1	0.88	0.34	-	113,113,113,113	0
54	MG	BA	3141	1/1	0.43	0.17	-	78,78,78,78	0
54	MG	CA	1661	1/1	0.94	0.48	-	92,92,92,92	0
54	MG	DA	3031	1/1	0.94	0.07	-	62,62,62,62	0
54	MG	CA	1710	1/1	0.91	0.18	-	119,119,119,119	0
54	MG	AA	1712	1/1	0.84	0.50	-	75,75,75,75	0
54	MG	BA	3187	1/1	0.92	0.46	-	40,40,40,40	0
54	MG	AA	1616	1/1	0.94	0.19	-	63,63,63,63	0
54	MG	DA	3057	1/1	0.77	0.22	-	59,59,59,59	0
54	MG	DB	209	1/1	0.77	0.12	-	75,75,75,75	0
54	MG	DA	3332	1/1	0.74	0.45	-	60,60,60,60	0
54	MG	AA	1670	1/1	0.95	0.14	-	85,85,85,85	0
54	MG	BA	3121	1/1	0.93	0.26	-	77,77,77,77	0
54	MG	BA	2942	1/1	0.95	0.35	-	22,22,22,22	0
54	MG	BA	3119	1/1	0.82	0.28	-	64,64,64,64	0
54	MG	CA	1694	1/1	0.86	0.32	-	59,59,59,59	0
54	MG	CA	1678	1/1	0.94	0.11	-	107,107,107,107	0
54	MG	CA	1621	1/1	0.78	0.39	-	67,67,67,67	0
54	MG	BA	3026	1/1	0.81	0.39	-	82,82,82,82	0
54	MG	DA	3227	1/1	0.97	0.31	-	34,34,34,34	0
54	MG	CA	1729	1/1	0.97	0.17	-	98,98,98,98	0
54	MG	BA	2997	1/1	0.92	0.38	-	57,57,57,57	0
54	MG	BA	3247	1/1	0.99	0.15	-	52,52,52,52	0
54	MG	BA	3105	1/1	0.91	0.21	-	60,60,60,60	0
54	MG	CA	1665	1/1	0.94	0.25	-	89,89,89,89	0
54	MG	DA	2973	1/1	0.97	0.30	-	50,50,50,50	0
54	MG	DB	208	1/1	0.87	0.31	-	96,96,96,96	0
54	MG	DA	3080	1/1	0.72	0.41	-	69,69,69,69	0
54	MG	BA	3033	1/1	0.80	0.19	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.