



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:02 PM GMT

PDB ID : 4V5C
Title : Structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, paromomycin, acylated A-site tRNA, deacylated P-site tRNA, and E-site tRNA.
Authors : Voorhees, R.M.; Weixlbaumer, A.; Loakes, D.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-03-24
Resolution : 3.30 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

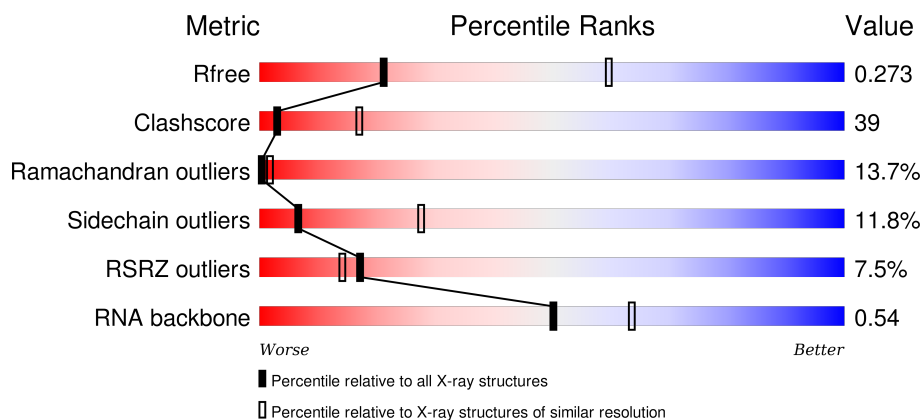
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



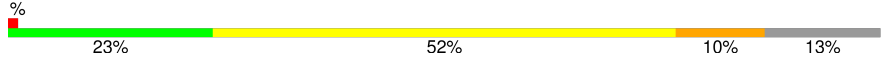
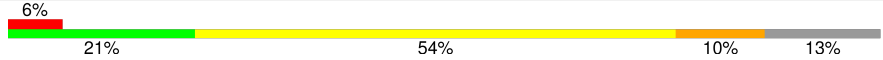

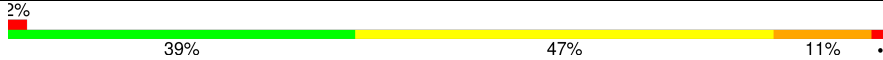
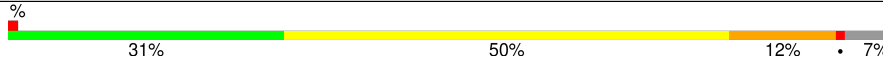
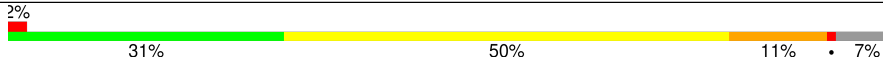
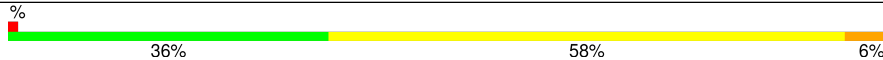
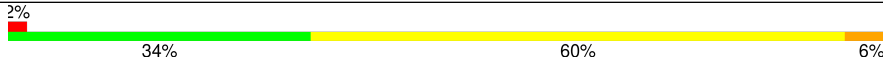
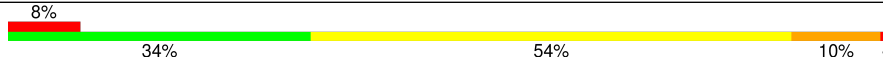
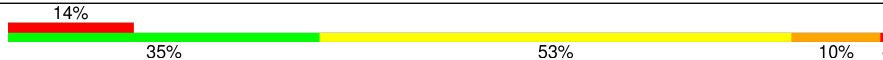
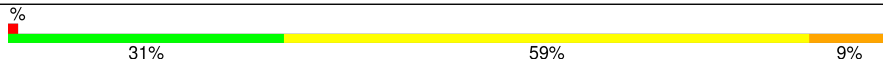
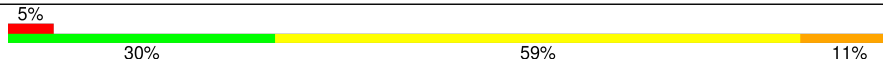
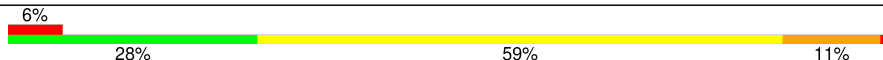
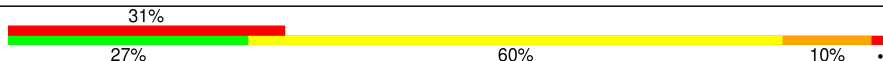
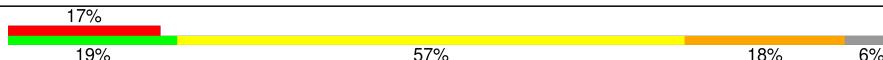
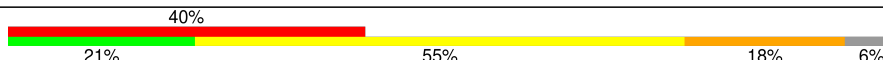
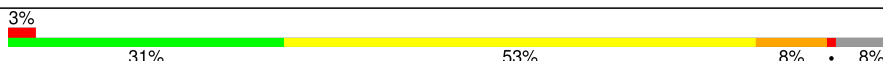
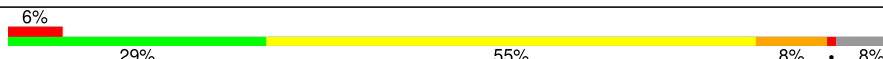
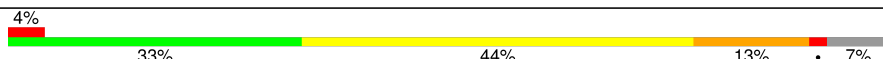
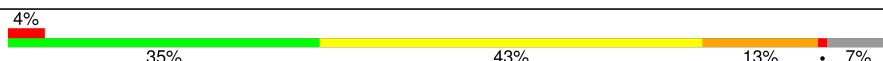
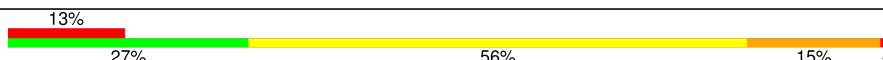
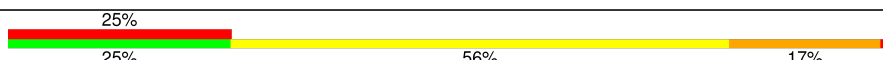
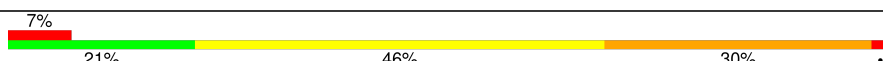
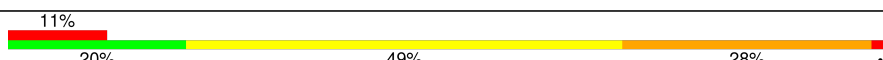
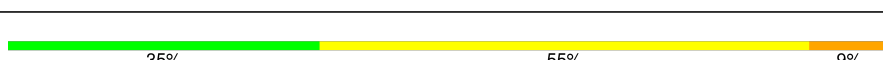
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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	1522	<div> <div>2%</div> <div>27%</div> <div>61%</div> <div>10%</div> <div>..</div> </div>
1	CA	1522	<div> <div>2%</div> <div>26%</div> <div>61%</div> <div>10%</div> <div>..</div> </div>
2	AB	256	<div> <div>6%</div> <div>20%</div> <div>56%</div> <div>14%</div> <div>8%</div> </div>
2	CB	256	<div> <div>11%</div> <div>18%</div> <div>59%</div> <div>14%</div> <div>8%</div> </div>



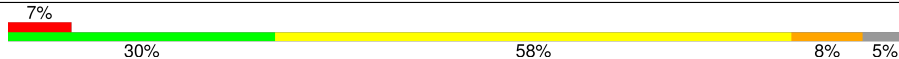
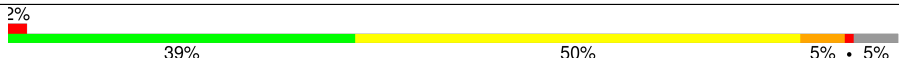
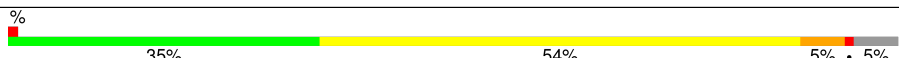
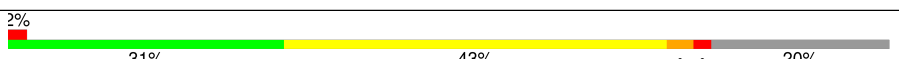
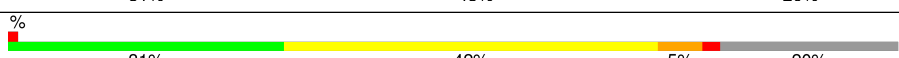
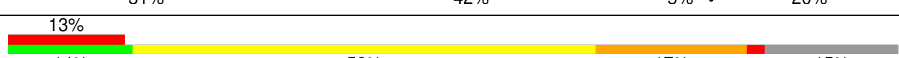
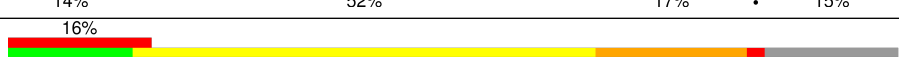
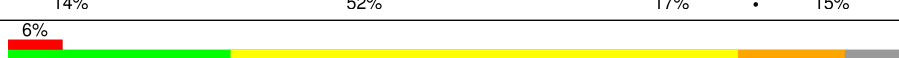
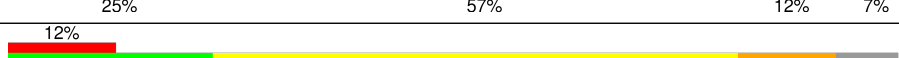
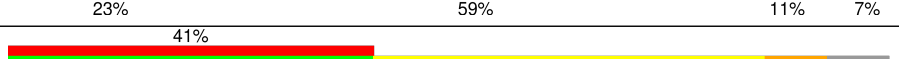



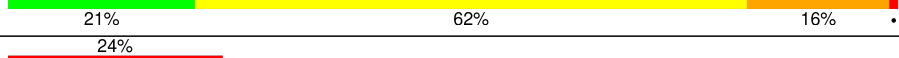
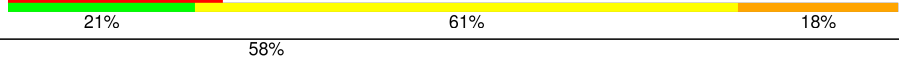

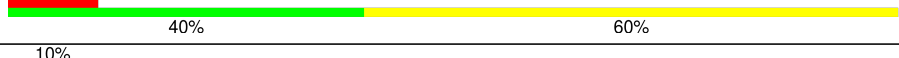
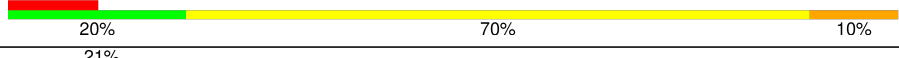
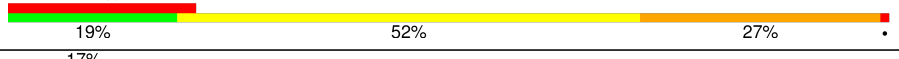
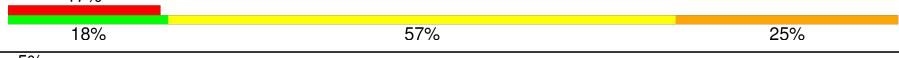
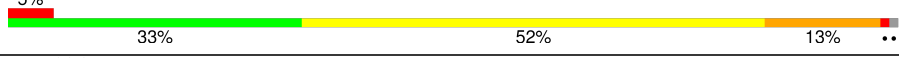

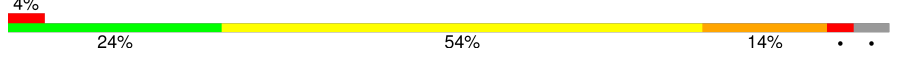
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126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

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	CV	77	
23	AW	76	
23	CW	76	
24	AX	10	
24	CX	10	
25	AY	77	
25	CY	77	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	

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Mol	Chain	Length	Quality of chain
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2822	
36	DA	2822	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	
39	DD	276	
40	BE	206	

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Mol	Chain	Length	Quality of chain
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BI	148	
44	DI	148	
45	BN	140	
45	DN	140	
46	BO	122	
46	DO	122	
47	BP	150	
47	DP	150	
48	BQ	141	
48	DQ	141	
49	BR	118	
49	DR	118	
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	
52	DU	118	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	1604	-	-	-	X
58	MG	AA	1613	-	-	-	X
58	MG	AA	1616	-	-	-	X
58	MG	AA	1627	-	-	-	X
58	MG	AA	1628	-	-	-	X
58	MG	AA	1638	-	-	-	X
58	MG	AA	1640	-	-	-	X
58	MG	AA	1663	-	-	-	X
58	MG	AA	1670	-	-	-	X
58	MG	AA	1683	-	-	-	X
58	MG	AA	1686	-	-	-	X
58	MG	AA	1695	-	-	-	X
58	MG	AA	1698	-	-	-	X
58	MG	AA	1701	-	-	-	X
58	MG	AA	1712	-	-	-	X
58	MG	AA	1717	-	-	-	X
58	MG	AA	1728	-	-	-	X
58	MG	AA	1741	-	-	-	X
58	MG	AA	1743	-	-	-	X
58	MG	AA	1783	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	1785	-	-	-	X
58	MG	AA	1786	-	-	-	X
58	MG	AA	1810	-	-	-	X
58	MG	AG	201	-	-	-	X
58	MG	AW	116	-	-	-	X
58	MG	B2	602	-	-	-	X
58	MG	B7	101	-	-	-	X
58	MG	BA	3003	-	-	-	X
58	MG	BA	3007	-	-	-	X
58	MG	BA	3008	-	-	-	X
58	MG	BA	3020	-	-	-	X
58	MG	BA	3024	-	-	-	X
58	MG	BA	3026	-	-	-	X
58	MG	BA	3028	-	-	-	X
58	MG	BA	3029	-	-	-	X
58	MG	BA	3031	-	-	-	X
58	MG	BA	3038	-	-	-	X
58	MG	BA	3048	-	-	-	X
58	MG	BA	3049	-	-	-	X
58	MG	BA	3051	-	-	-	X
58	MG	BA	3054	-	-	-	X
58	MG	BA	3058	-	-	-	X
58	MG	BA	3060	-	-	-	X
58	MG	BA	3063	-	-	-	X
58	MG	BA	3065	-	-	-	X
58	MG	BA	3067	-	-	-	X
58	MG	BA	3068	-	-	-	X
58	MG	BA	3071	-	-	-	X
58	MG	BA	3072	-	-	-	X
58	MG	BA	3073	-	-	-	X
58	MG	BA	3076	-	-	-	X
58	MG	BA	3077	-	-	-	X
58	MG	BA	3082	-	-	-	X
58	MG	BA	3090	-	-	-	X
58	MG	BA	3094	-	-	-	X
58	MG	BA	3095	-	-	-	X
58	MG	BA	3100	-	-	-	X
58	MG	BA	3113	-	-	-	X
58	MG	BA	3115	-	-	-	X
58	MG	BA	3117	-	-	-	X
58	MG	BA	3120	-	-	-	X
58	MG	BA	3121	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	BA	3123	-	-	-	X
58	MG	BA	3126	-	-	-	X
58	MG	BA	3132	-	-	-	X
58	MG	BA	3134	-	-	-	X
58	MG	BA	3144	-	-	-	X
58	MG	BA	3150	-	-	-	X
58	MG	BA	3156	-	-	-	X
58	MG	BA	3167	-	-	-	X
58	MG	BA	3169	-	-	-	X
58	MG	BA	3172	-	-	-	X
58	MG	BA	3178	-	-	-	X
58	MG	BA	3182	-	-	-	X
58	MG	BA	3196	-	-	-	X
58	MG	BA	3198	-	-	-	X
58	MG	BA	3199	-	-	-	X
58	MG	BA	3212	-	-	-	X
58	MG	BA	3221	-	-	-	X
58	MG	BA	3223	-	-	-	X
58	MG	BA	3226	-	-	-	X
58	MG	BA	3236	-	-	-	X
58	MG	BA	3240	-	-	-	X
58	MG	BA	3246	-	-	-	X
58	MG	BA	3249	-	-	-	X
58	MG	BA	3254	-	-	-	X
58	MG	BA	3255	-	-	-	X
58	MG	BA	3265	-	-	-	X
58	MG	BA	3281	-	-	-	X
58	MG	BA	3285	-	-	-	X
58	MG	BA	3290	-	-	-	X
58	MG	BA	3292	-	-	-	X
58	MG	BA	3303	-	-	-	X
58	MG	BA	3311	-	-	-	X
58	MG	BA	3312	-	-	-	X
58	MG	BA	3313	-	-	-	X
58	MG	BA	3342	-	-	-	X
58	MG	BA	3351	-	-	-	X
58	MG	BA	3366	-	-	-	X
58	MG	BA	3367	-	-	-	X
58	MG	BA	3373	-	-	-	X
58	MG	BA	3389	-	-	-	X
58	MG	BA	3396	-	-	-	X
58	MG	BA	3403	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	BA	3405	-	-	-	X
58	MG	BA	3427	-	-	-	X
58	MG	BA	3440	-	-	-	X
58	MG	BA	3447	-	-	-	X
58	MG	BB	204	-	-	-	X
58	MG	BB	205	-	-	-	X
58	MG	BB	216	-	-	-	X
58	MG	BN	201	-	-	-	X
58	MG	CA	1619	-	-	-	X
58	MG	CA	1624	-	-	-	X
58	MG	CA	1627	-	-	-	X
58	MG	CA	1628	-	-	-	X
58	MG	CA	1630	-	-	-	X
58	MG	CA	1638	-	-	-	X
58	MG	CA	1640	-	-	-	X
58	MG	CA	1642	-	-	-	X
58	MG	CA	1664	-	-	-	X
58	MG	CA	1671	-	-	-	X
58	MG	CA	1684	-	-	-	X
58	MG	CA	1696	-	-	-	X
58	MG	CA	1702	-	-	-	X
58	MG	CA	1713	-	-	-	X
58	MG	CA	1714	-	-	-	X
58	MG	CA	1721	-	-	-	X
58	MG	CA	1729	-	-	-	X
58	MG	CA	1742	-	-	-	X
58	MG	CA	1795	-	-	-	X
58	MG	CW	121	-	-	-	X
58	MG	D7	102	-	-	-	X
58	MG	DA	3006	-	-	-	X
58	MG	DA	3007	-	-	-	X
58	MG	DA	3009	-	-	-	X
58	MG	DA	3011	-	-	-	X
58	MG	DA	3013	-	-	-	X
58	MG	DA	3018	-	-	-	X
58	MG	DA	3019	-	-	-	X
58	MG	DA	3023	-	-	-	X
58	MG	DA	3027	-	-	-	X
58	MG	DA	3028	-	-	-	X
58	MG	DA	3030	-	-	-	X
58	MG	DA	3036	-	-	-	X
58	MG	DA	3047	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	DA	3048	-	-	-	X
58	MG	DA	3050	-	-	-	X
58	MG	DA	3057	-	-	-	X
58	MG	DA	3060	-	-	-	X
58	MG	DA	3062	-	-	-	X
58	MG	DA	3064	-	-	-	X
58	MG	DA	3072	-	-	-	X
58	MG	DA	3076	-	-	-	X
58	MG	DA	3079	-	-	-	X
58	MG	DA	3081	-	-	-	X
58	MG	DA	3089	-	-	-	X
58	MG	DA	3093	-	-	-	X
58	MG	DA	3094	-	-	-	X
58	MG	DA	3099	-	-	-	X
58	MG	DA	3107	-	-	-	X
58	MG	DA	3111	-	-	-	X
58	MG	DA	3112	-	-	-	X
58	MG	DA	3114	-	-	-	X
58	MG	DA	3116	-	-	-	X
58	MG	DA	3120	-	-	-	X
58	MG	DA	3125	-	-	-	X
58	MG	DA	3131	-	-	-	X
58	MG	DA	3137	-	-	-	X
58	MG	DA	3143	-	-	-	X
58	MG	DA	3146	-	-	-	X
58	MG	DA	3148	-	-	-	X
58	MG	DA	3154	-	-	-	X
58	MG	DA	3164	-	-	-	X
58	MG	DA	3172	-	-	-	X
58	MG	DA	3175	-	-	-	X
58	MG	DA	3182	-	-	-	X
58	MG	DA	3190	-	-	-	X
58	MG	DA	3194	-	-	-	X
58	MG	DA	3195	-	-	-	X
58	MG	DA	3199	-	-	-	X
58	MG	DA	3201	-	-	-	X
58	MG	DA	3209	-	-	-	X
58	MG	DA	3217	-	-	-	X
58	MG	DA	3222	-	-	-	X
58	MG	DA	3236	-	-	-	X
58	MG	DA	3239	-	-	-	X
58	MG	DA	3242	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	DA	3245	-	-	-	X
58	MG	DA	3261	-	-	-	X
58	MG	DA	3269	-	-	-	X
58	MG	DA	3275	-	-	-	X
58	MG	DA	3281	-	-	-	X
58	MG	DA	3305	-	-	-	X
58	MG	DA	3307	-	-	-	X
58	MG	DA	3308	-	-	-	X
58	MG	DA	3316	-	-	-	X
58	MG	DA	3353	-	-	-	X
58	MG	DA	3390	-	-	-	X
58	MG	DA	3401	-	-	-	X
58	MG	DA	3403	-	-	-	X
58	MG	DA	3417	-	-	-	X
58	MG	DA	3430	-	-	-	X
58	MG	DA	3431	-	-	-	X
58	MG	DA	3438	-	-	-	X
58	MG	DA	3443	-	-	-	X
58	MG	DE	302	-	-	-	X
58	MG	DN	201	-	-	-	X
59	PAR	AA	1814	-	-	-	X
59	PAR	CA	1817	-	-	-	X
60	ZN	B9	101	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 296168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

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

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is a RNA chain called P-SITE TRNA FMET.

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

- Molecule 23 is a RNA chain called E-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			
24	CX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 25 is a RNA chain called A-SITE PHE-TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
25	CY	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
30	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
35	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			
36	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	191	Total	C	N	O		0	0	1
			1142	691	221	230				
38	DC	191	Total	C	N	O		0	0	1
			1142	691	221	230				

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
48	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
51	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BA	453	Total	Mg	0	0
			453	453		

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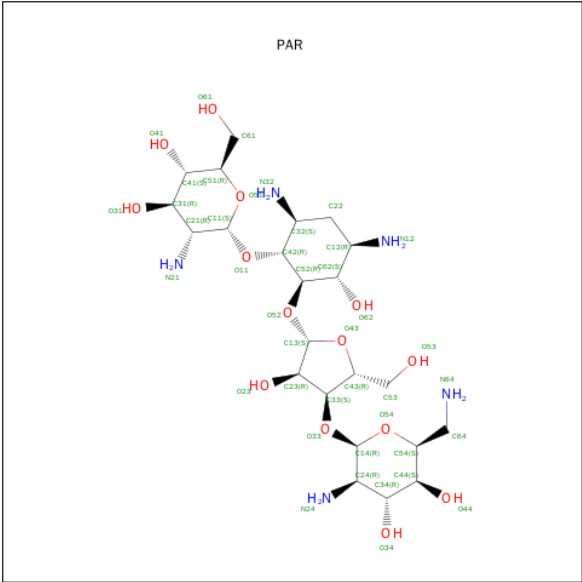
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CA	216	Total 216	Mg 216	0	0
58	DF	1	Total 1	Mg 1	0	0
58	CV	8	Total 8	Mg 8	0	0
58	D2	3	Total 3	Mg 3	0	0
58	BE	1	Total 1	Mg 1	0	0
58	AW	20	Total 20	Mg 20	0	0
58	B1	1	Total 1	Mg 1	0	0
58	BP	2	Total 2	Mg 2	0	0
58	AX	4	Total 4	Mg 4	0	0
58	DN	3	Total 3	Mg 3	0	0
58	DD	2	Total 2	Mg 2	0	0
58	B5	2	Total 2	Mg 2	0	0
58	BB	19	Total 19	Mg 19	0	0
58	AE	1	Total 1	Mg 1	0	0
58	BF	2	Total 2	Mg 2	0	0
58	AV	8	Total 8	Mg 8	0	0
58	BX	2	Total 2	Mg 2	0	0
58	B2	2	Total 2	Mg 2	0	0
58	AA	213	Total 213	Mg 213	0	0
58	D7	2	Total 2	Mg 2	0	0
58	CX	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DV	2	Total 2	Mg 2	0	0
58	AD	1	Total 1	Mg 1	0	0
58	BN	2	Total 2	Mg 2	0	0
58	DE	2	Total 2	Mg 2	0	0
58	DX	3	Total 3	Mg 3	0	0
58	DA	451	Total 451	Mg 451	0	0
58	AU	1	Total 1	Mg 1	0	0
58	B7	1	Total 1	Mg 1	0	0
58	BV	2	Total 2	Mg 2	0	0
58	AG	1	Total 1	Mg 1	0	0
58	BO	1	Total 1	Mg 1	0	0
58	D1	2	Total 2	Mg 2	0	0
58	CW	21	Total 21	Mg 21	0	0
58	D5	1	Total 1	Mg 1	0	0
58	BD	1	Total 1	Mg 1	0	0
58	CE	1	Total 1	Mg 1	0	0
58	BW	1	Total 1	Mg 1	0	0
58	CK	1	Total 1	Mg 1	0	0
58	CL	1	Total 1	Mg 1	0	0
58	DB	18	Total 18	Mg 18	0	0

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total	C	N	O	0	0
			42	23	5	14		
59	CA	1	Total	C	N	O	0	0
			42	23	5	14		

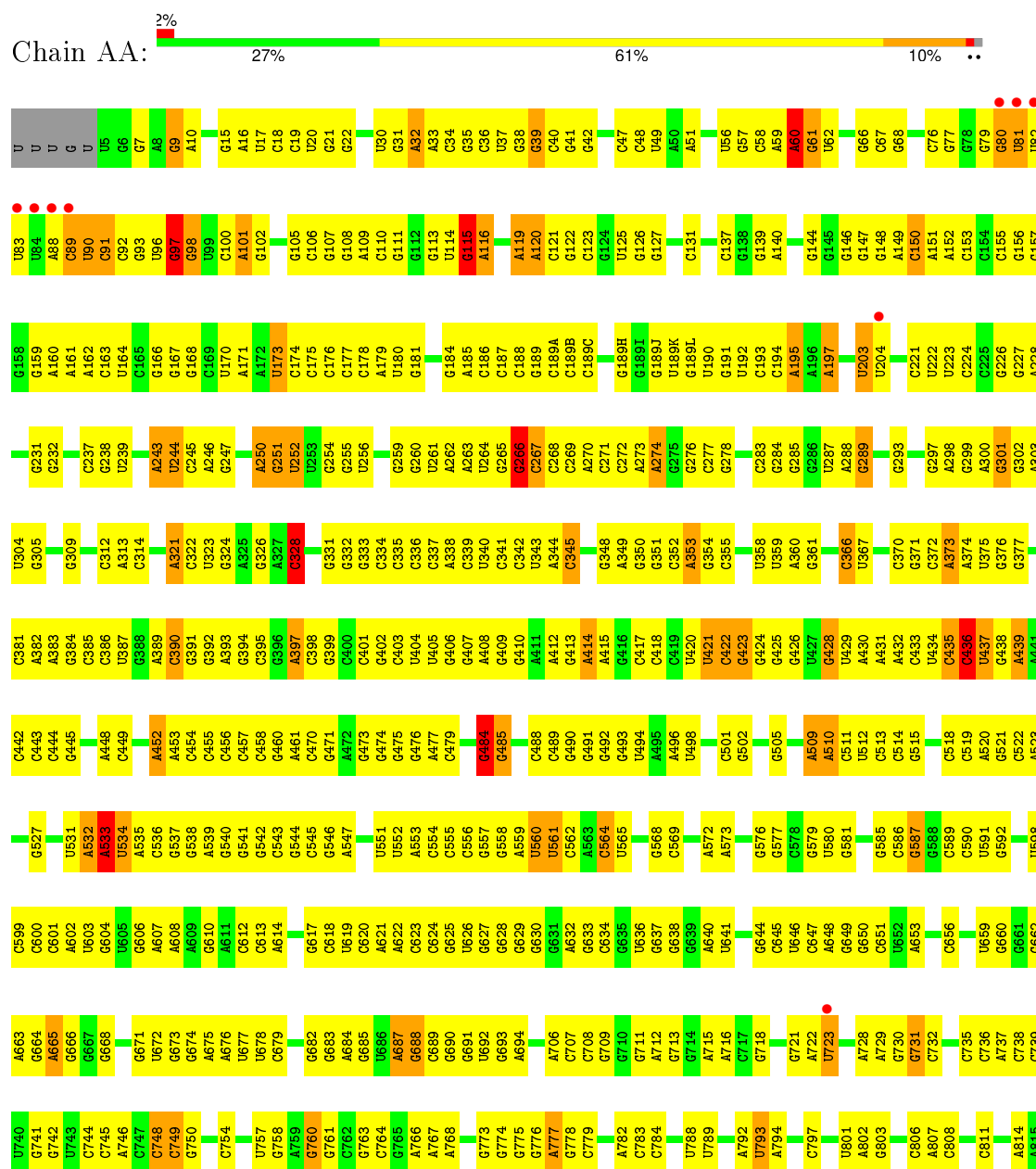
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

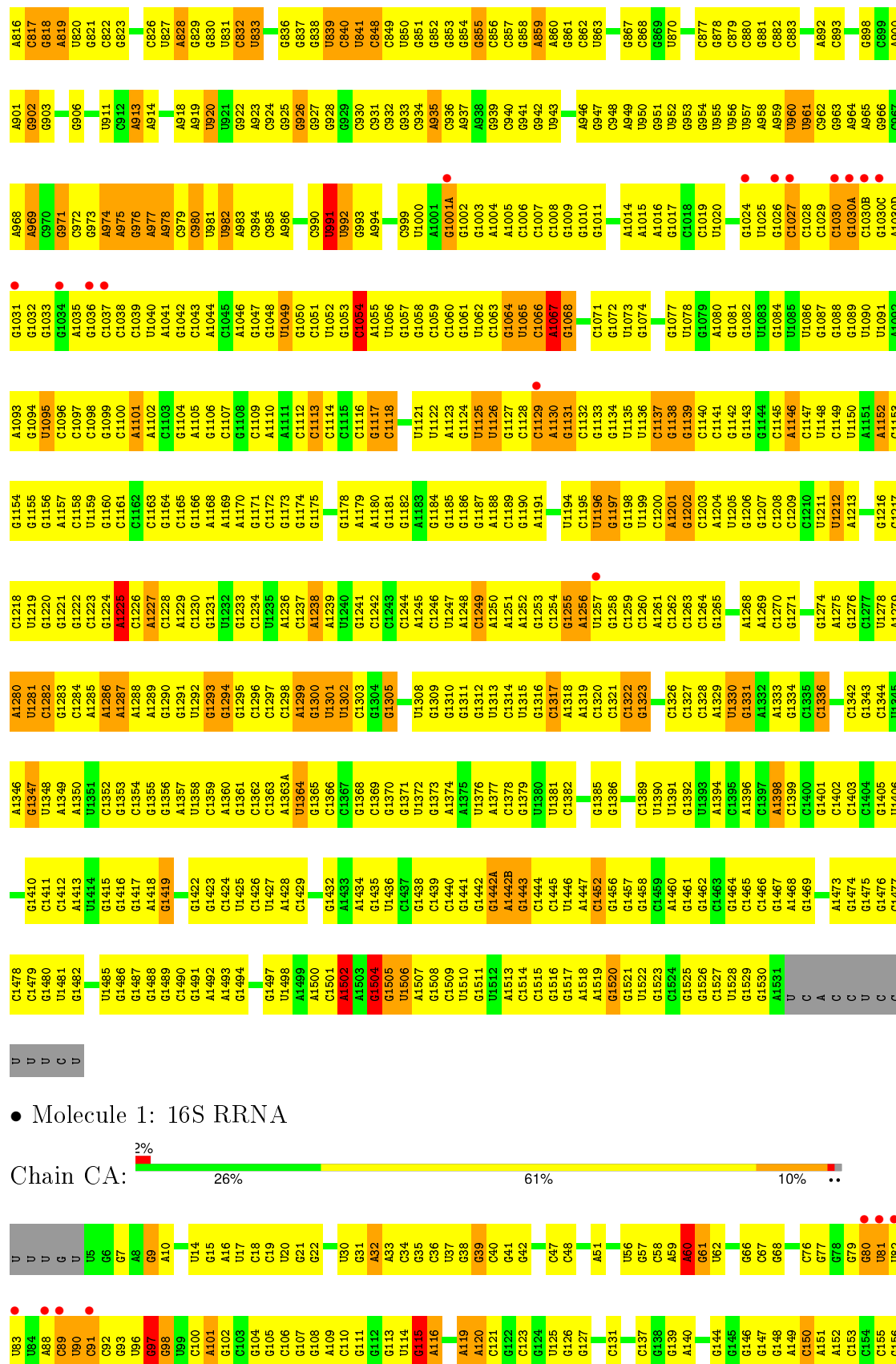
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CN	1	Total	Zn	0	0
			1	1		
60	AN	1	Total	Zn	0	0
			1	1		
60	B9	1	Total	Zn	0	0
			1	1		
60	D9	1	Total	Zn	0	0
			1	1		
60	CD	1	Total	Zn	0	0
			1	1		
60	AD	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

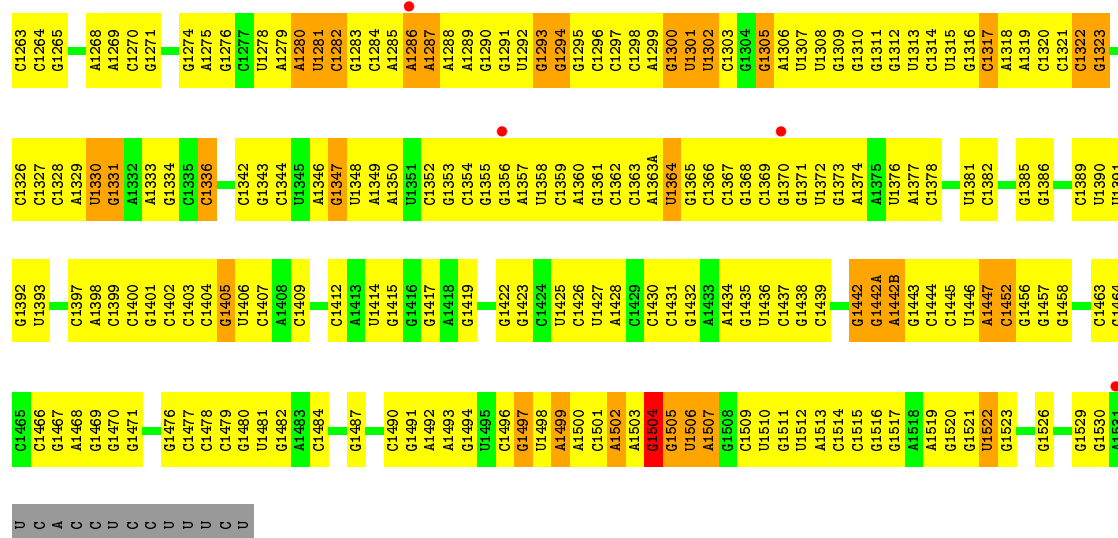
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

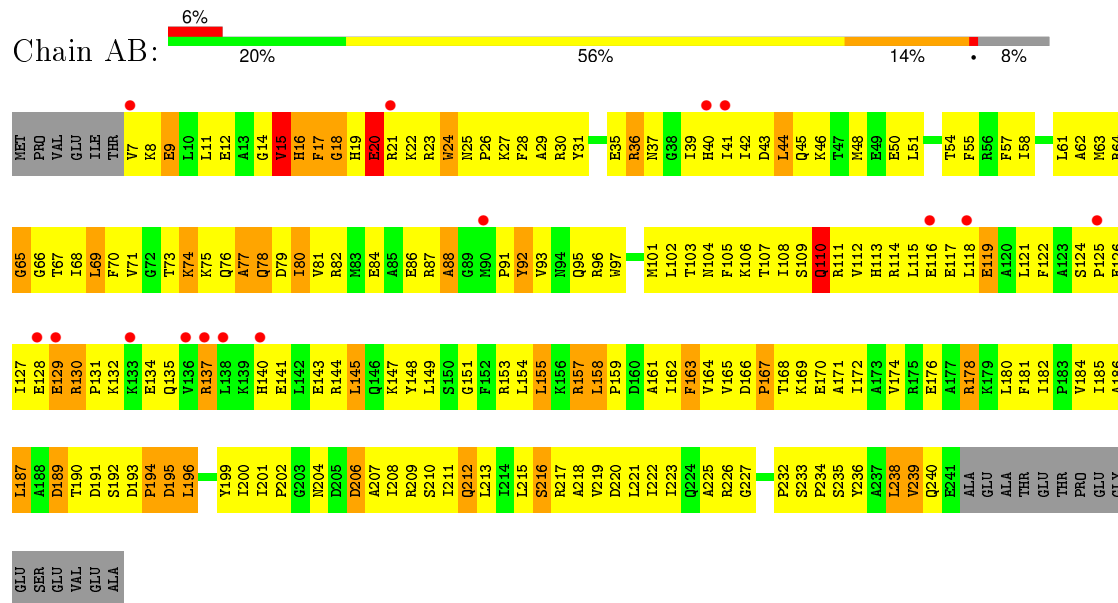




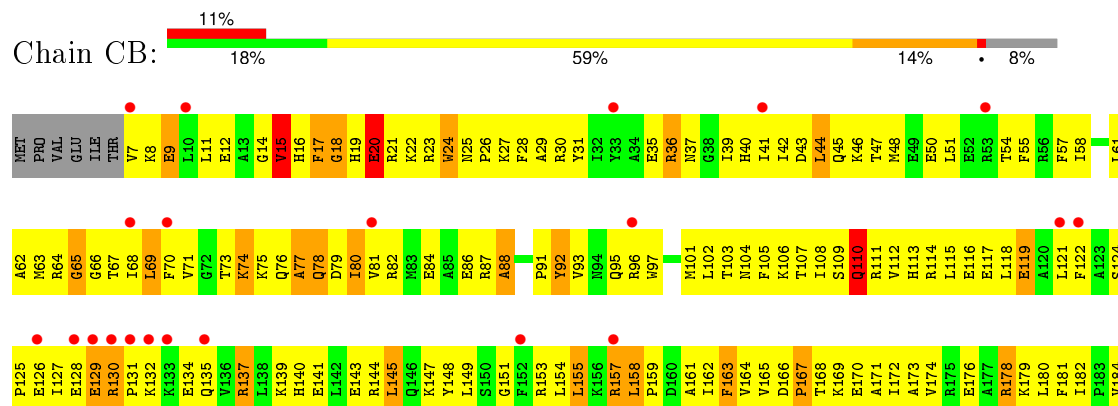
A1201	G1139	U1078	U1020	U955	G878	C808	C738	A665	U598	A532	A448	C385	A303	G226	G157
G1202	C1140	G1079	G1024	U956	C879	C811	C739	G666	C599	A533	A449	C386	A303	G227	G158
G1203	C1141	A1080	U1025	U957	C880		U740	G667	C600	A534	C452	U387	C312	A228	G159
A1204	G1142	G1081	U1026	A958	G881	A814	G741	G668	C601	A535		C388	G319	G231	A160
G1205	G1143	U1082	G1027	A959	C882	A815	G742		A602	C536	A453	C390	G320	G232	A161
U1206	G1144	U1083	G1028	U960	C883	A816	U743		U603	C537	A454	C391	A321	C163	A162
G1207	C1145	U1084	C1029	U961	U884	C817	C744		G604	C538	C455	G392	C322		C164
C1208	A1146	U1085	G1030	G962	G885	A818	C745		U605	A539	C456	G393	C323	C237	C165
C1209	C1147	U1086	G1030A	G963	G890	G818	A746		G606	A540	C457	G394	C324	G238	U164
G1210	U1148	G1087	U1030B	A964	G891	A819	C747		A607	C541	C458	G395	C325	U239	C166
C1211	C1149	U1088	U1030C	A965	G892	U820	C748			C542	C459	G396	A325	G167	C167
U1212	U1150	G1089	G1030D	G966	A892	G821	C749		C612	C543	G460	G397	G326	A243	C168
A1213	A1151	U1090	A1030D	G967	C893	C822	G750		C613	C544	A461	A397	A327	U244	G169
	A1152	U1091	G1031	A968		G823				C545	C470		C338	C245	U170
G1216	C1163	A1092	G1032	A969	G889	C824	C754		G617	C546	A471	C398	G331	A246	A171
C1217	G1154	U1093	G1033	G970	C889	G825			C618	A547	A472	G399	G332	G247	
G1218	U1094	G1034	G1034	G971	A900	C826	U757		U619	U551	G473	C401	G333	A250	U173
U1219	U1095	A1035	A1035	G972	A901	U827	G758		C620	U552	G474	G402	G334	G251	C175
G1220	C1096	G1036	G1036	G973	G902	A828	A759		A621	U553	G475	C403	C335	U252	C176
G1221	C1097	C1037	C1037	A974	G903	G829	G760		A622	A554	G476	U404	C336	C177	C177
G1222	C1098	C1038	C1038	A975		G830	G761		C623	C555	A477	G405	C337	G254	C178
C1223	G1099	C1039	C1039	G976	U911	U831	C762		C624	C556	C478	G406	A338	G255	A179
G1224	C1100	A977	C912	A977	C912	C832	G763		G625	C557		G407	A339		C179
	A1101	A978	A913	A978	A913	U833	G764		U626	C558	C484	A408	C339	U256	U180
C1225	A1102	G1041	A914	C979	A914	U834	G765		G627	G559	G485	G409	U340		G181
A1227	C1164	C1043	C980	C980		G836	A766		G628	A559		G410	C341	G259	
C1228	C1165	A1044	U981		A918	G837	A767		G629	U560	C488	A411	C342	G260	G184
A1229	G1166	C1045	U982	U982	A919	G838	A768		G630	U561	C489	A412	U343	U261	A185
C1230	A1168	A1046	A983	A983	U920	U839	G769		G631	C562	G490	A413	A344	A262	C186
	A1169	G1047	C984	C984		C840	C770		A632	A563	G491	A414	C345	A263	C187
G1233	A1170	U1048	C985	C985	G924	U841	G771		G633	C564	G492	A415	G346	U264	C188
C1234	G1171	U1049	A986	A986	G925	C848	U772		C634	U565	G493	G416	G347	G265	C189
U1235	C1172	G1050	C990	C990	G926	C849	G773		G635		U494	C417	G348	G266	C189A
A1236	G1173	C1051	U991	U991	G927	U850	G774		U636	G568	A495	C418	A349	C267	C189B
C1237	C1112	U1052	U992	U992	G928	G851	G775		G637	C569	A496	U420	G350	C268	C189C
A1238	G1113	G1053	G929	G929	G928	G852	G776		G638	U572	U498	U421	G351	C269	C189D
C1239	C1114	G1054	G930	G930	G930	G853	A777		G639	A573		C422	C352	A270	U189E
U1240	G1115	A1055	C931	A994	C931	C854	G778		A640		C501	C423	A353	C271	
G1241	C1116	U1056	C932		C932	G855	G779		U641	G576	G502	G424	C354	C272	G189H
C1242	G1117	G1057	G933	C999	C933	C856	A780		G644	G577	G503	G425	C355	A273	G189I
G1243	C1118	U1058	C934	U1000	C934	C857	G781		C645	C578	G504	G426	U359	G275	U189J
C1244	G1182	C1059	A1001	A1001	A935	G858	A782		U646	G579	A509	U427	A360	G276	U189K
A1245	A1183	G1060	G936	G936	C936	A860	C783		C720	G580	A510	G428	G370	C277	U189L
G1246	G1184	U1061	A937	A937	A937	G861	G784		G721	G581	C511	U429	U367	U190	
U1247	G1185	C1062	G938	G938	G938	C862			G722	U582	U512	G430	C371	G278	G191
C1248	G1186	G1063	G939	A1004	C940	U863	U789		G649	A583	C513	A431	C372	C283	C193
G1249	U1125	G1064	C941	A1005	C941	A864	U789		C650	C584	C514	A432	G373	G284	A195
A1250	A1188	U1065	G942	C1006	G942	G865	G724		C651	G585	C515	A433	A374	G285	C194
A1251	C1189	C1066	G942	G1007	G942	C866	G725		U652	C586	C516	U434	A375	G286	A196
A1252	G1190	A1067	U943	C1008	U943	G867			A653	G587	A520	C435	A376	G287	A197
G1253	A1191	G1068		G1009		C868	C795		C656	G588	G521	C436	A377	G288	
C1254	C1192	C1069	A946	G1010	A946	G869	C796		G657	C589	C522	C437	U375	U203	U204
G1255	G1193	U1070	G947	G1011	G947	U870	C797		G658	C590	A523	G438	G376	G289	
A1256	U1194	C1071	C948		C948	G871			G659	U591		A439	G377		C221
U1257	C1195	G1072	A949	A1014	A949	A872	U801		U659	G592	G527	A441		A298	
G1258	G1134	U1073	U950	A1015	U950	A873	A802		G660	G593	C528	C442	C381	G299	U222
C1259	U1135	G1074	G951	A1016	G951	A874	G803		G661	G594	G529	C443	A382	C300	U223
G1260	G1198	C1075	U952	G1017	U952	G874			G662	G595	G531	C444	A383	G301	C224
A1261	U1199	C1137	G953	G1018	G953	C877	C806		A663		U531	G445	G384	G302	C225

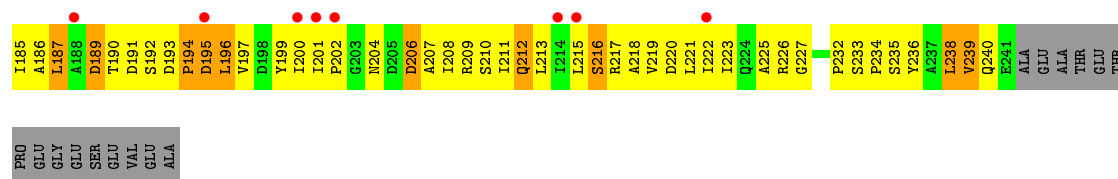


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

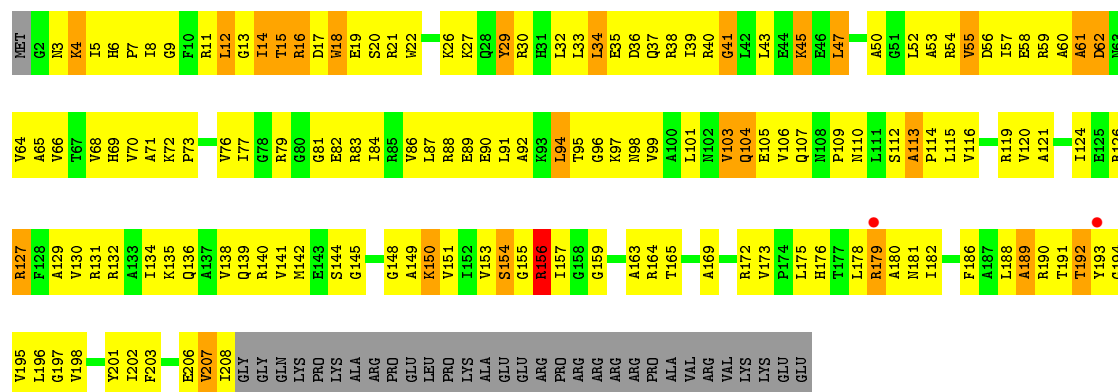


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

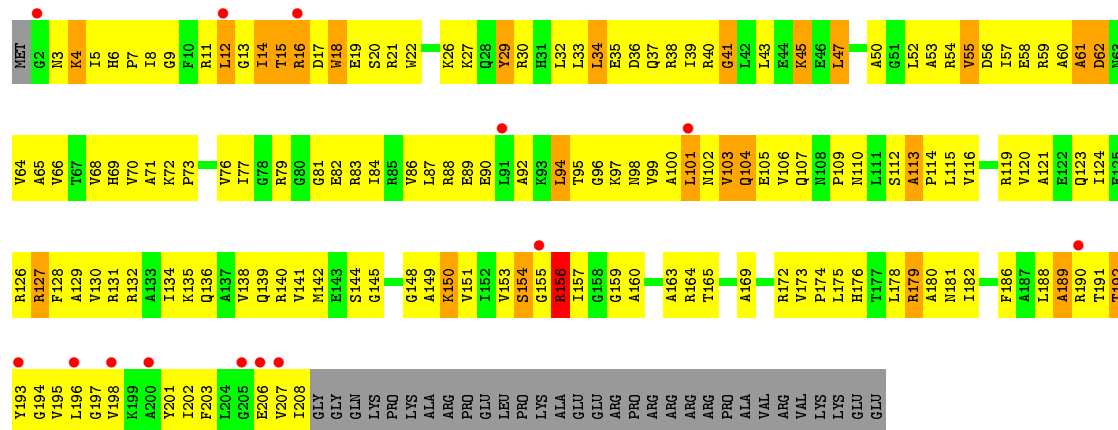




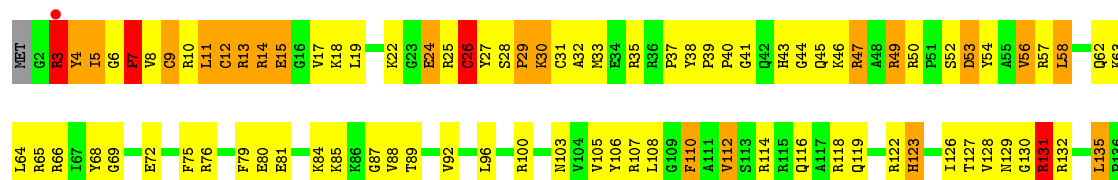
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

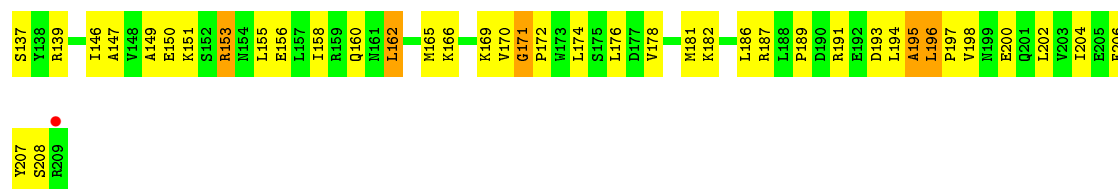


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

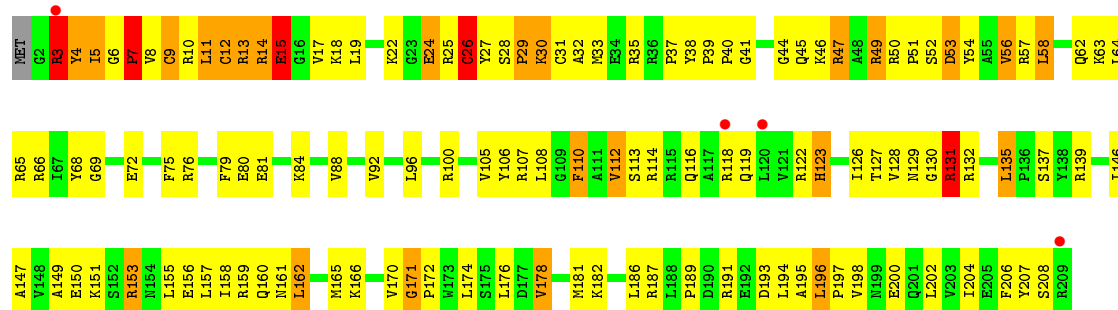


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

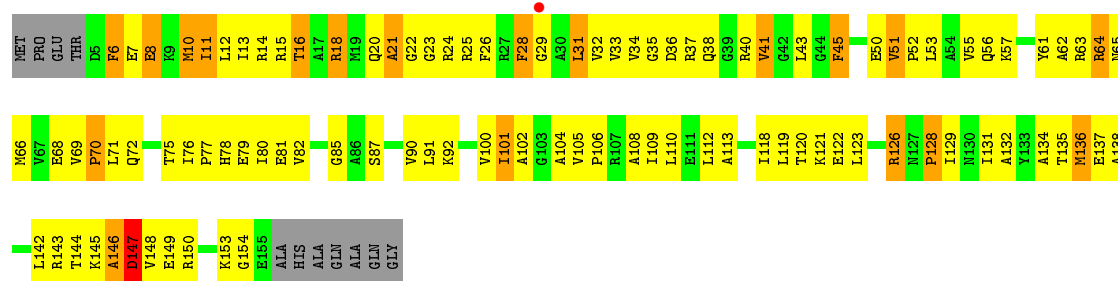




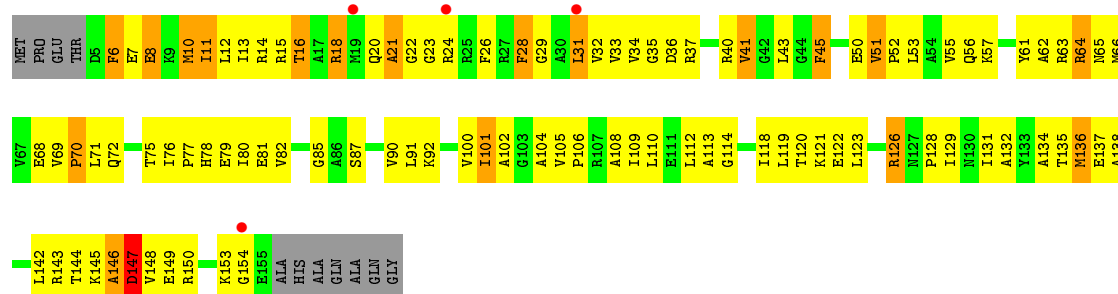
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 5: 30S RIBOSOMAL PROTEIN S5



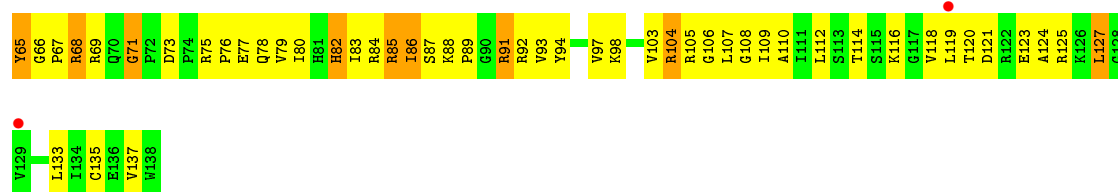
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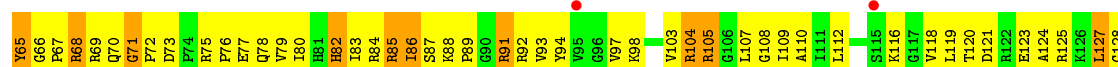
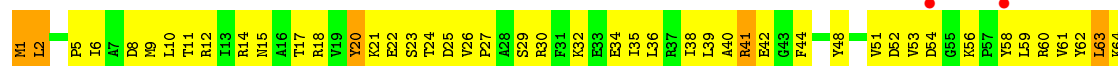
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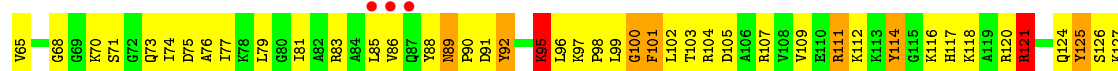




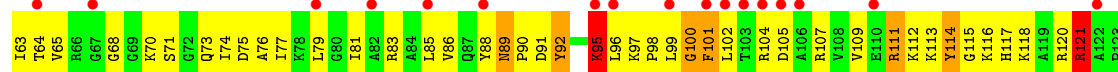
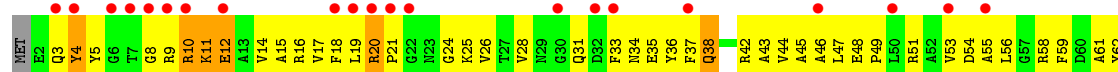
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

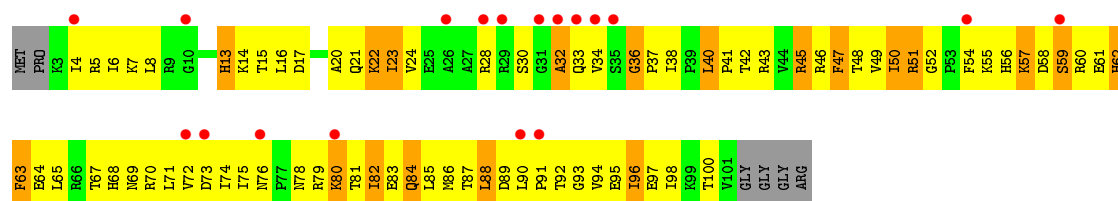


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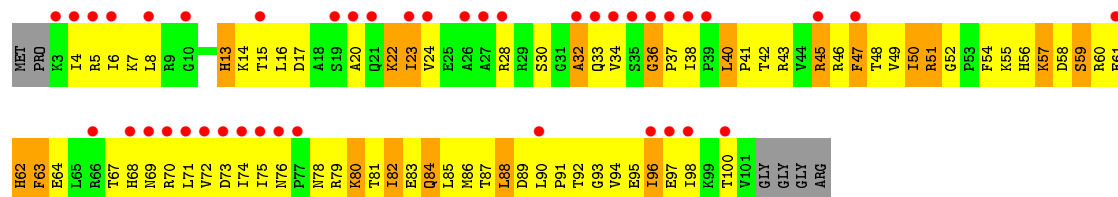


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

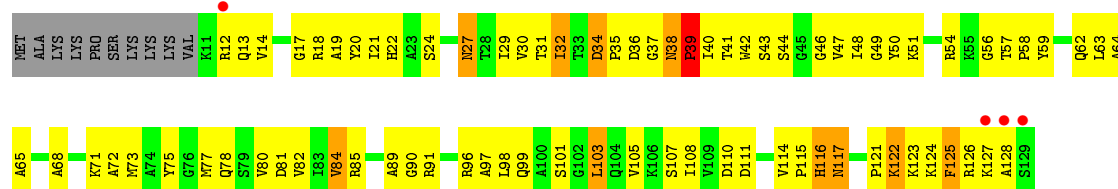




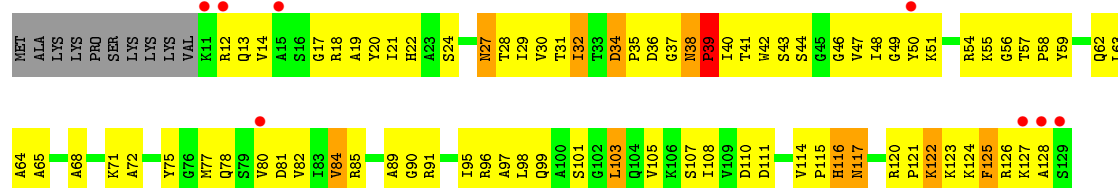
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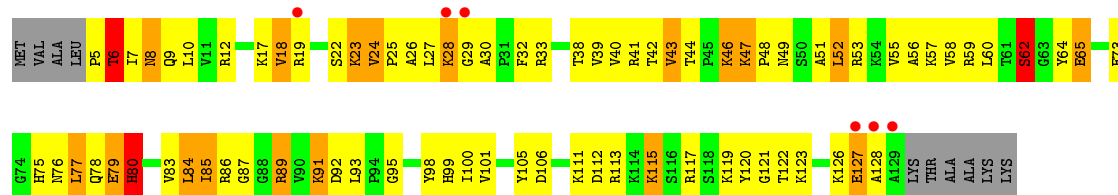
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



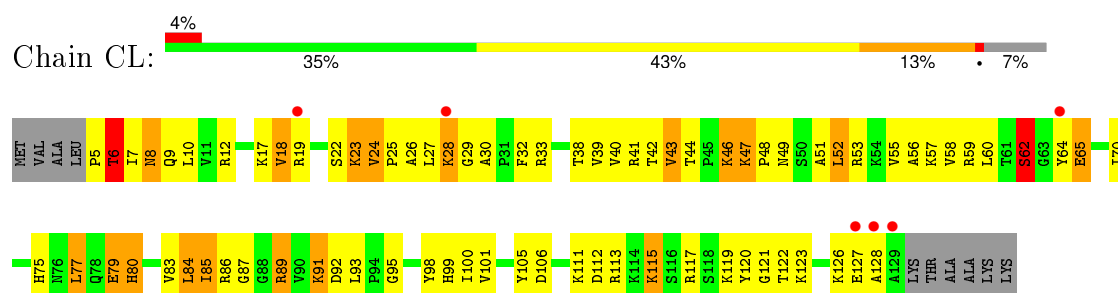
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



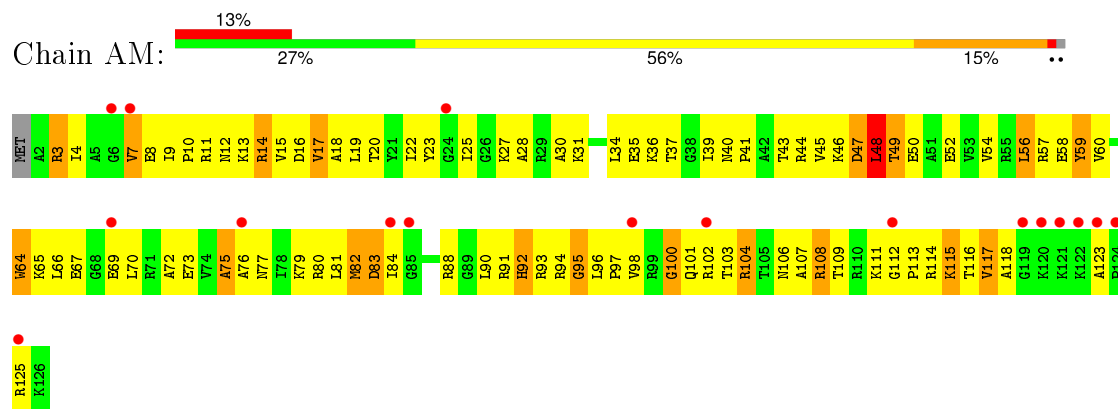
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



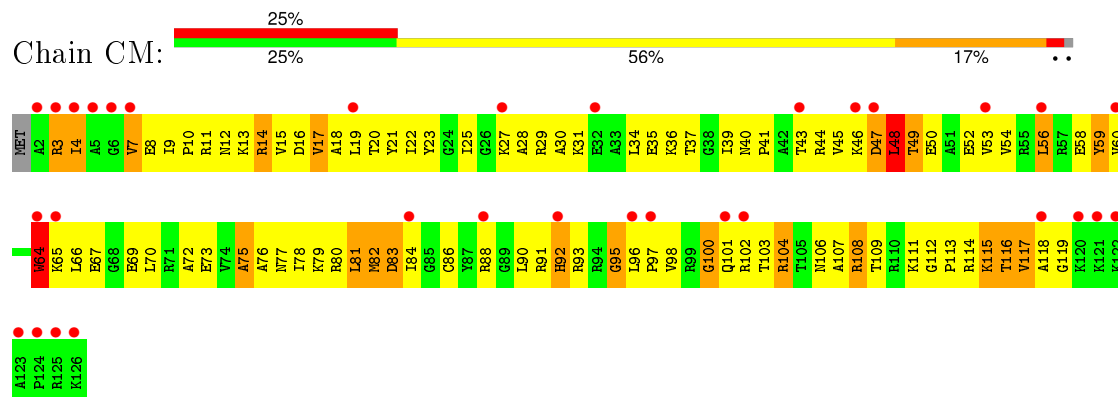
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



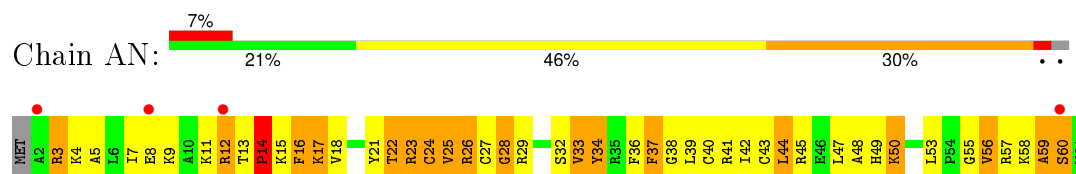
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



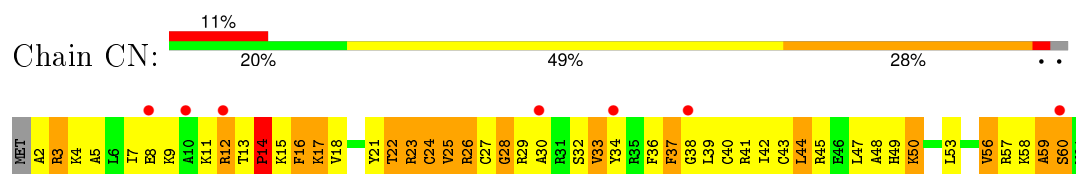
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



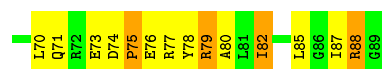
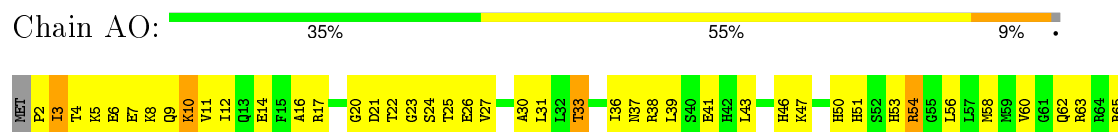
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



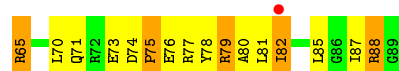
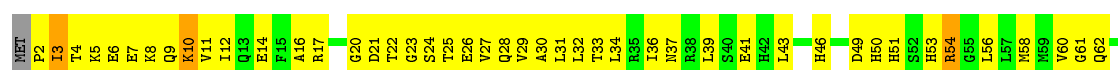
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



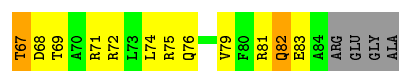
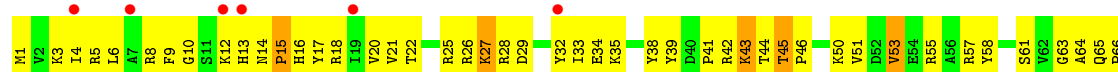
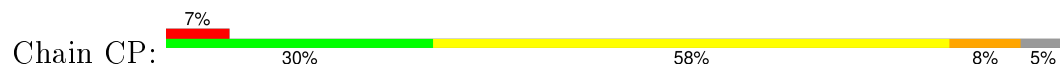
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



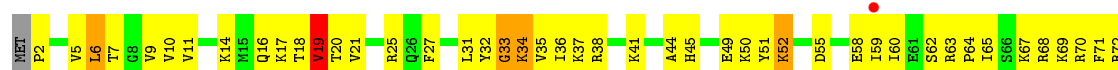
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



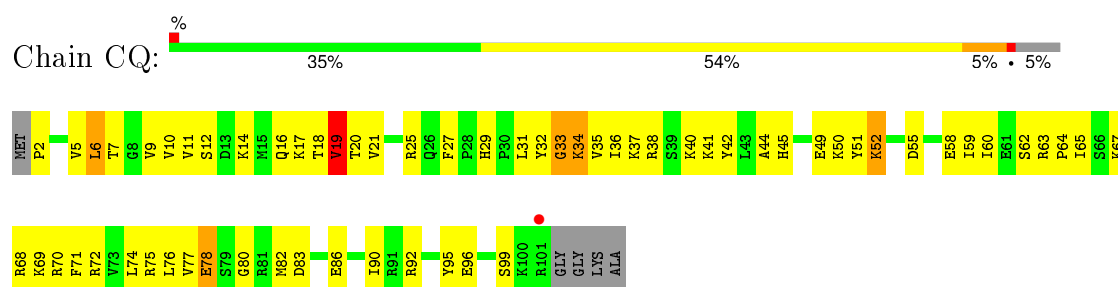
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



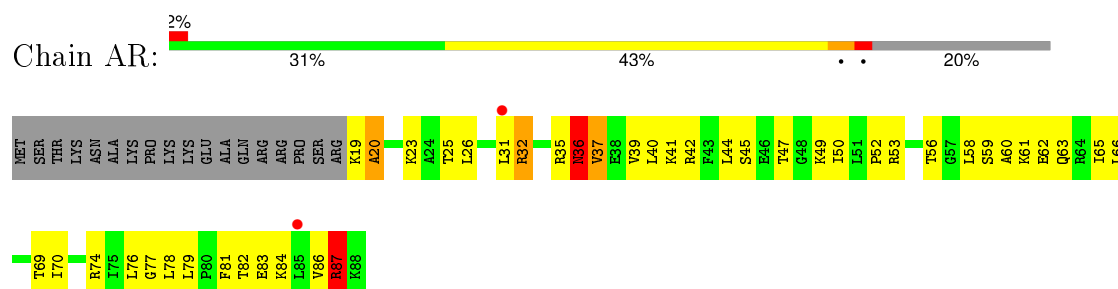
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



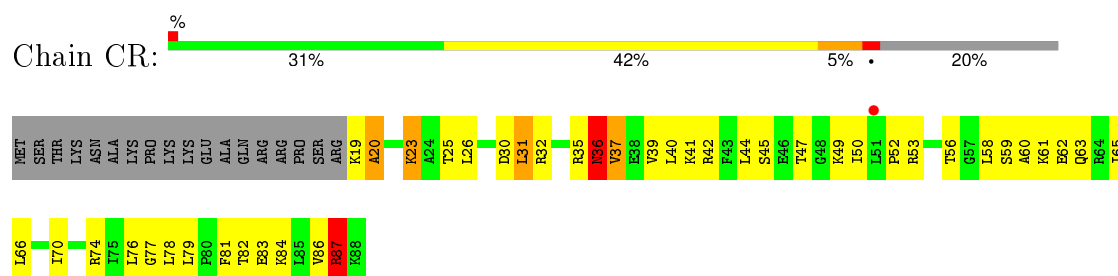
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



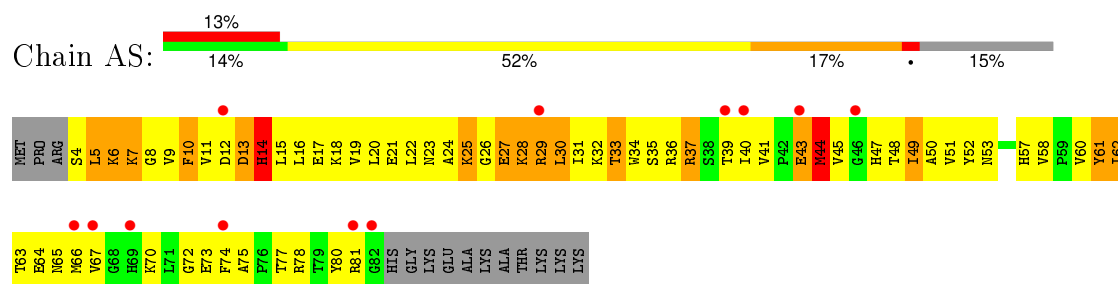
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



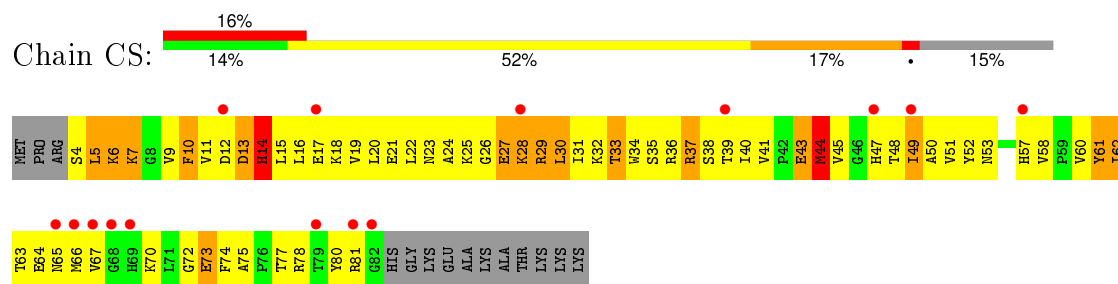
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



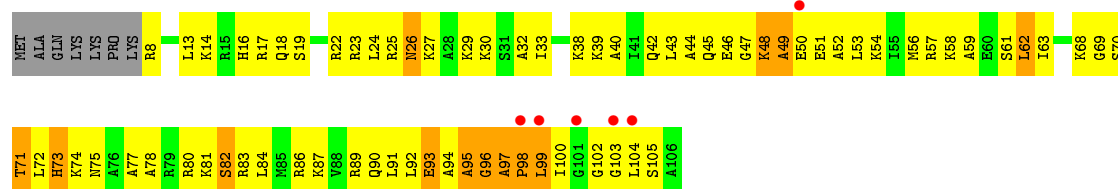
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



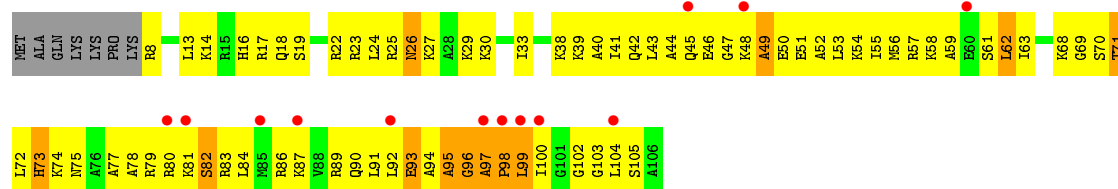
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



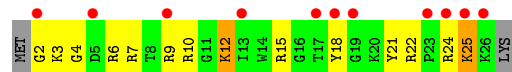
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



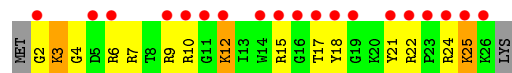
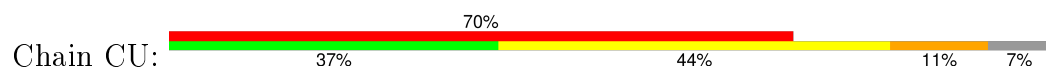
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



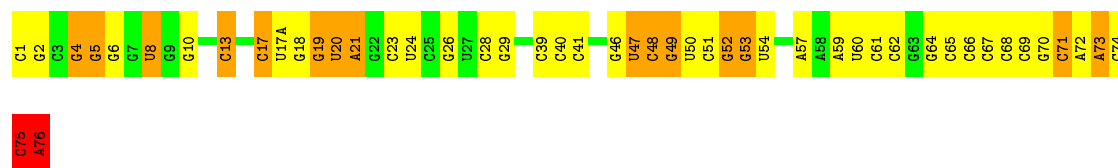
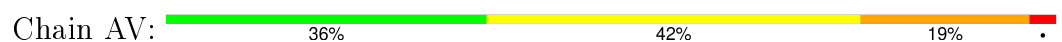
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



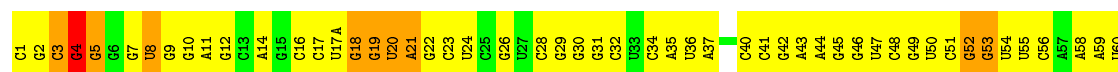
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: P-SITE TRNA FMET

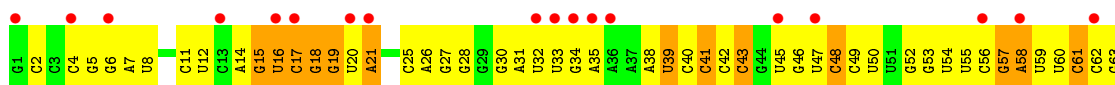


• Molecule 22: P-SITE TRNA FMET

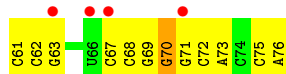
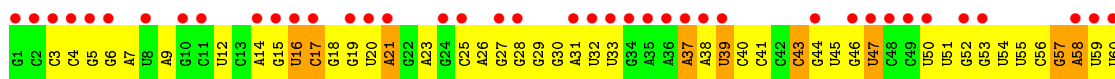




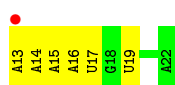
● Molecule 23: E-SITE TRNA PHE



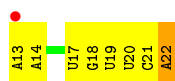
● Molecule 23: E-SITE TRNA PHE



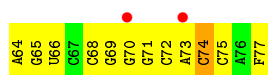
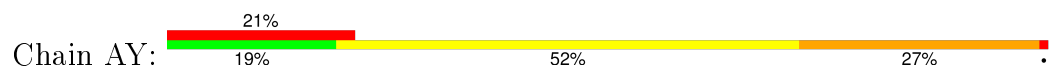
● Molecule 24: MRNA



● Molecule 24: MRNA

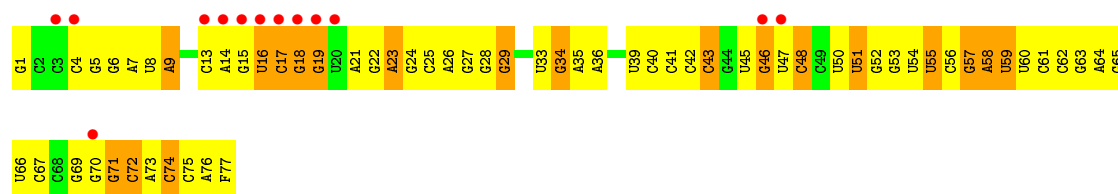


● Molecule 25: A-SITE PHE-TRNA PHE

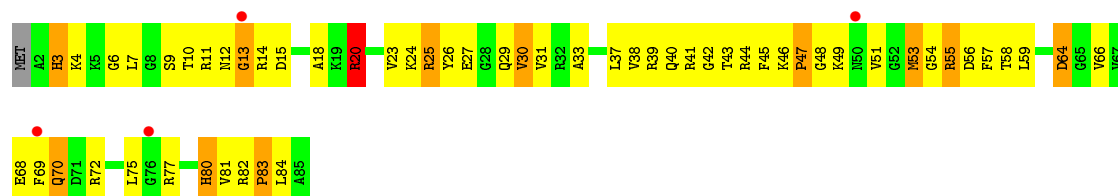


● Molecule 25: A-SITE PHE-TRNA PHE

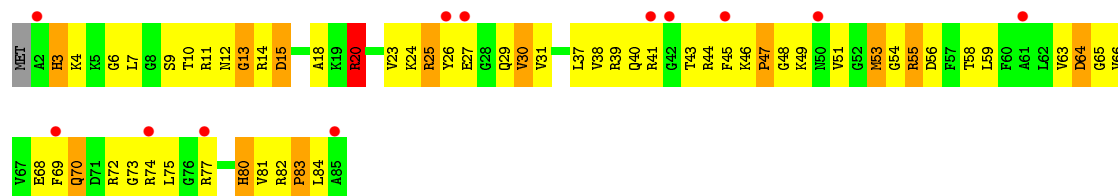




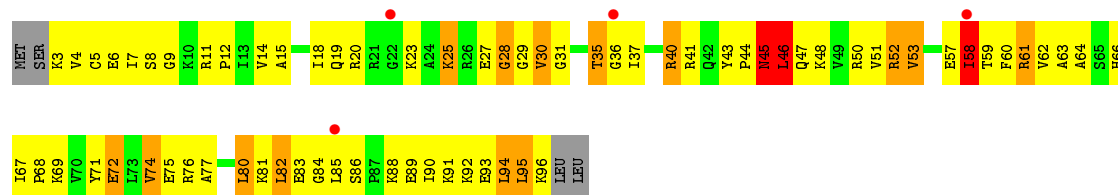
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



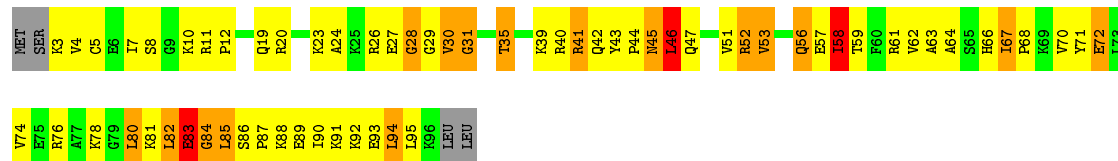
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



• Molecule 27: 50S RIBOSOMAL PROTEIN L28

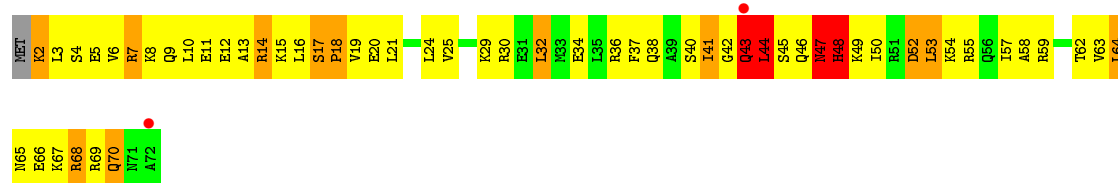


• Molecule 27: 50S RIBOSOMAL PROTEIN L28

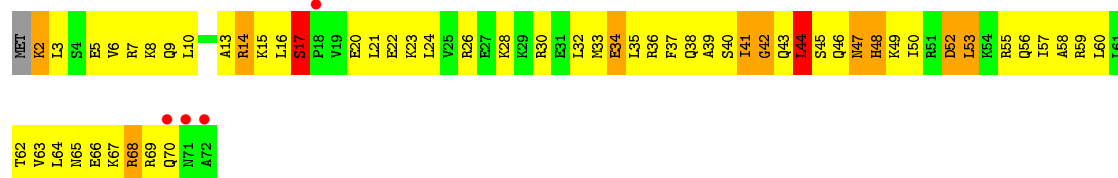


• Molecule 28: 50S RIBOSOMAL PROTEIN L29

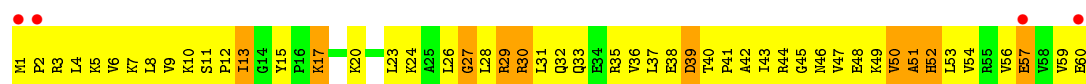




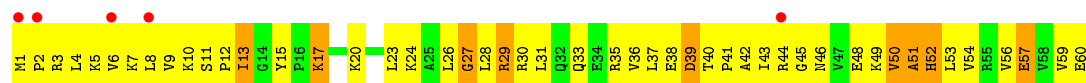
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



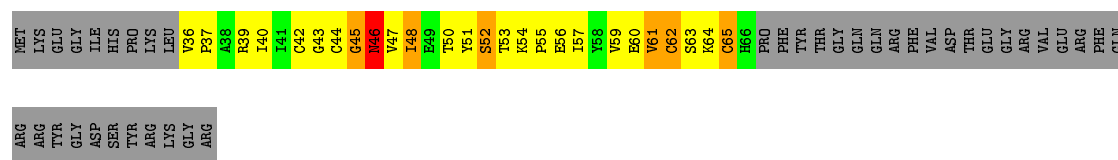
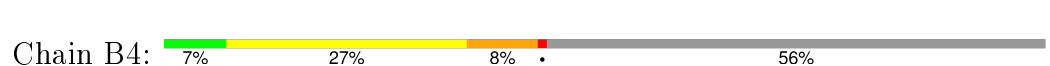
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



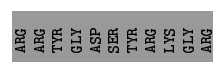
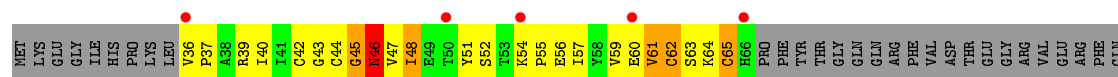
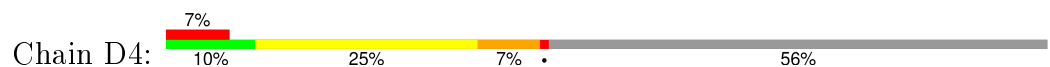
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



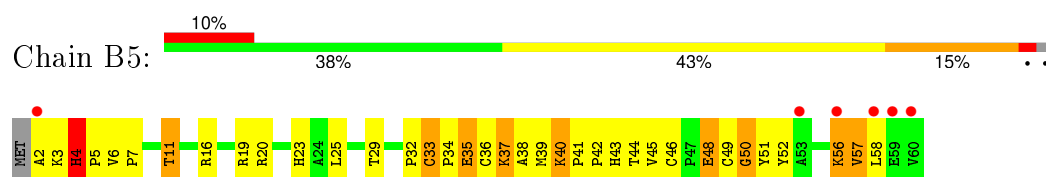
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



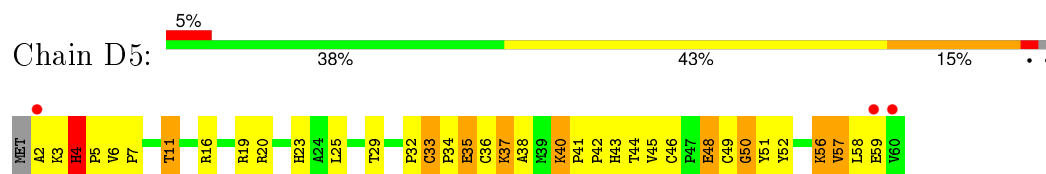
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



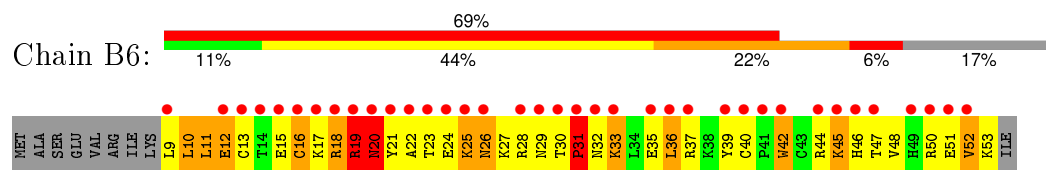
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



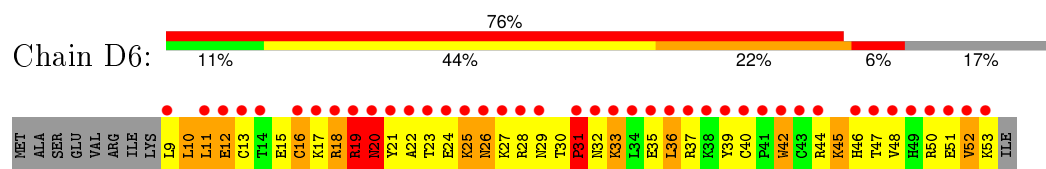
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



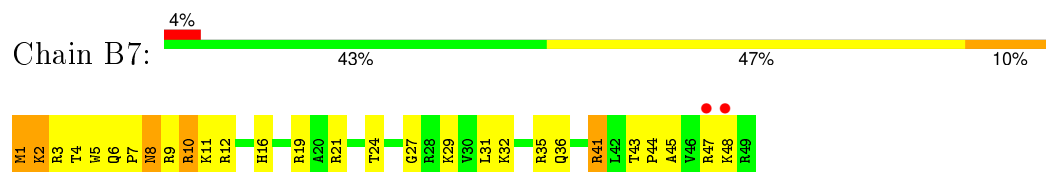
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



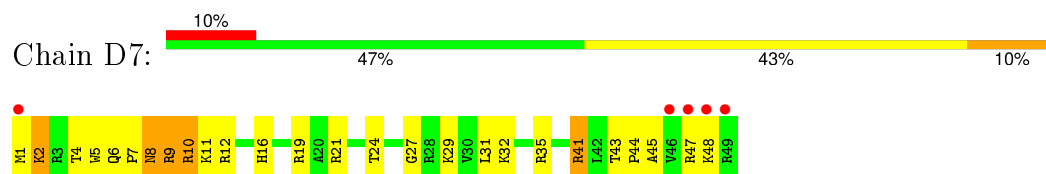
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



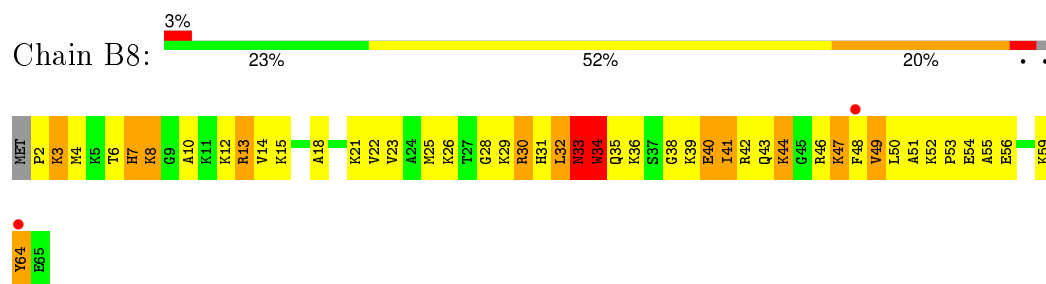
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



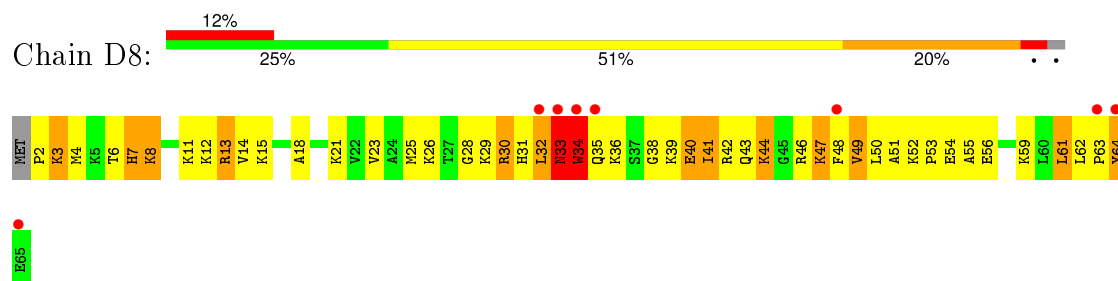
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



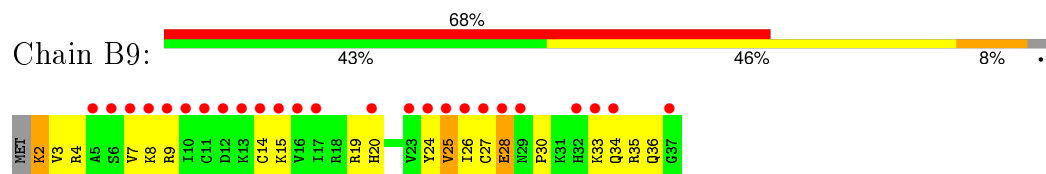
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



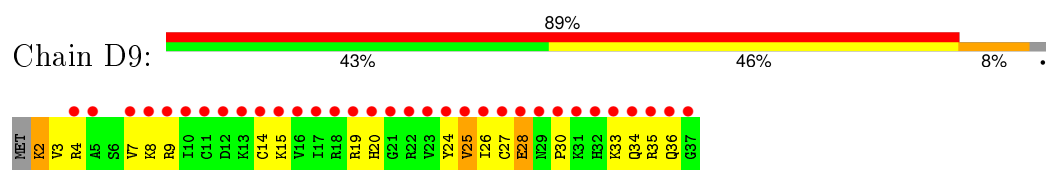
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



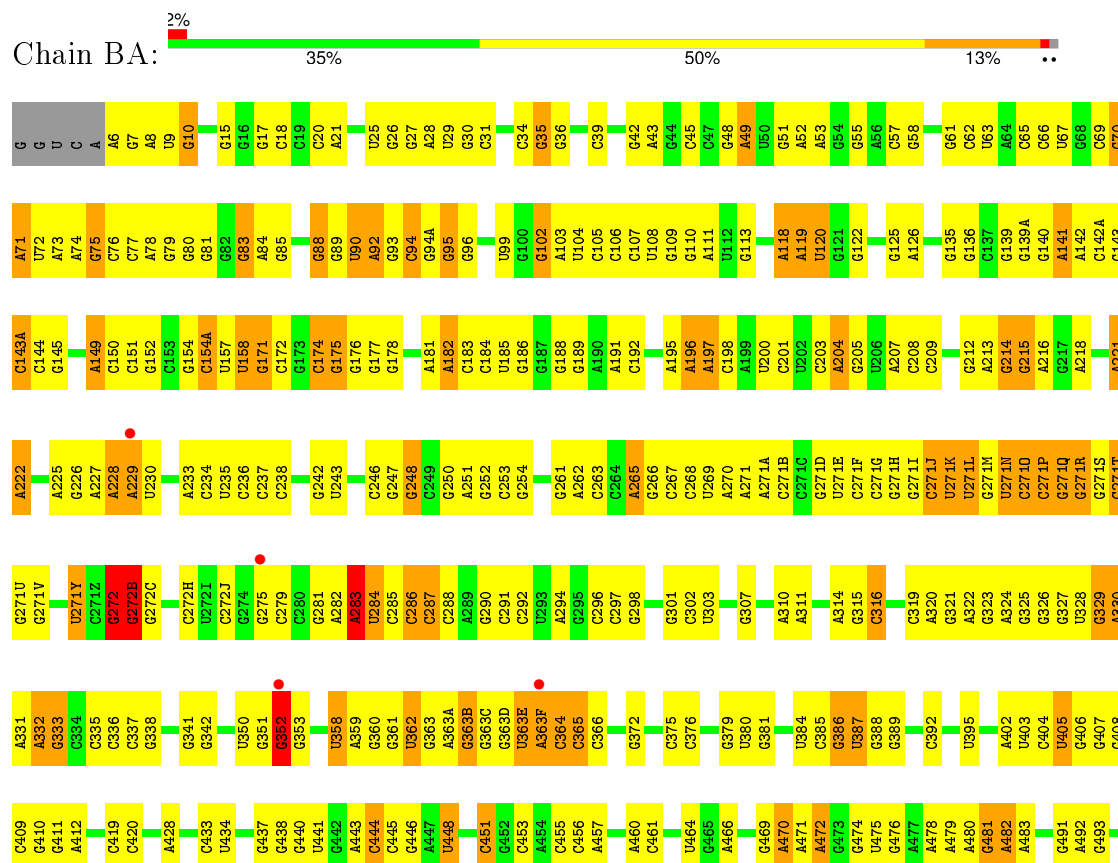
- Molecule 35: 50S RIBOSOMAL PROTEIN L36



- Molecule 35: 50S RIBOSOMAL PROTEIN L36

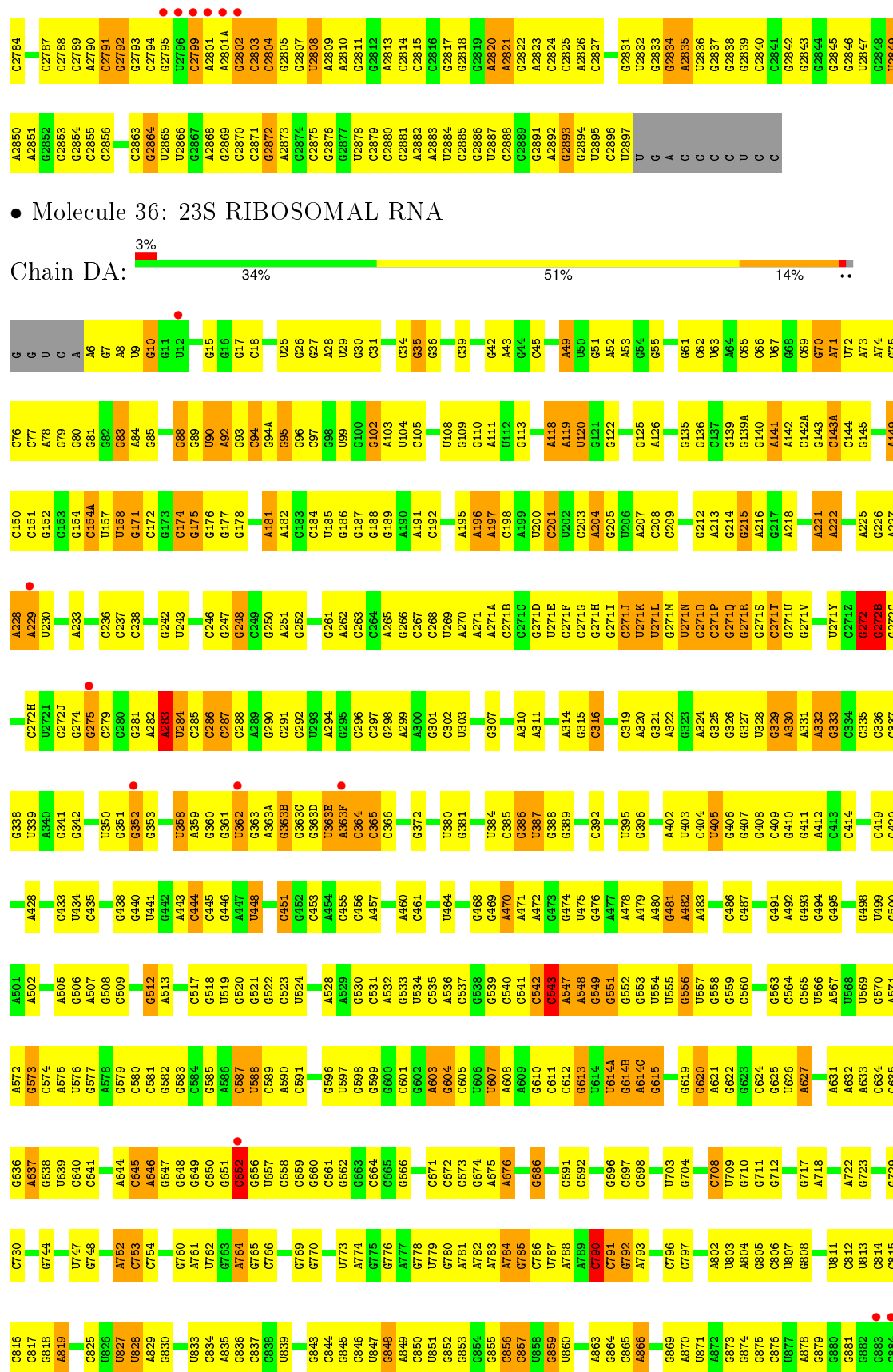


- Molecule 36: 23S RIBOSOMAL RNA

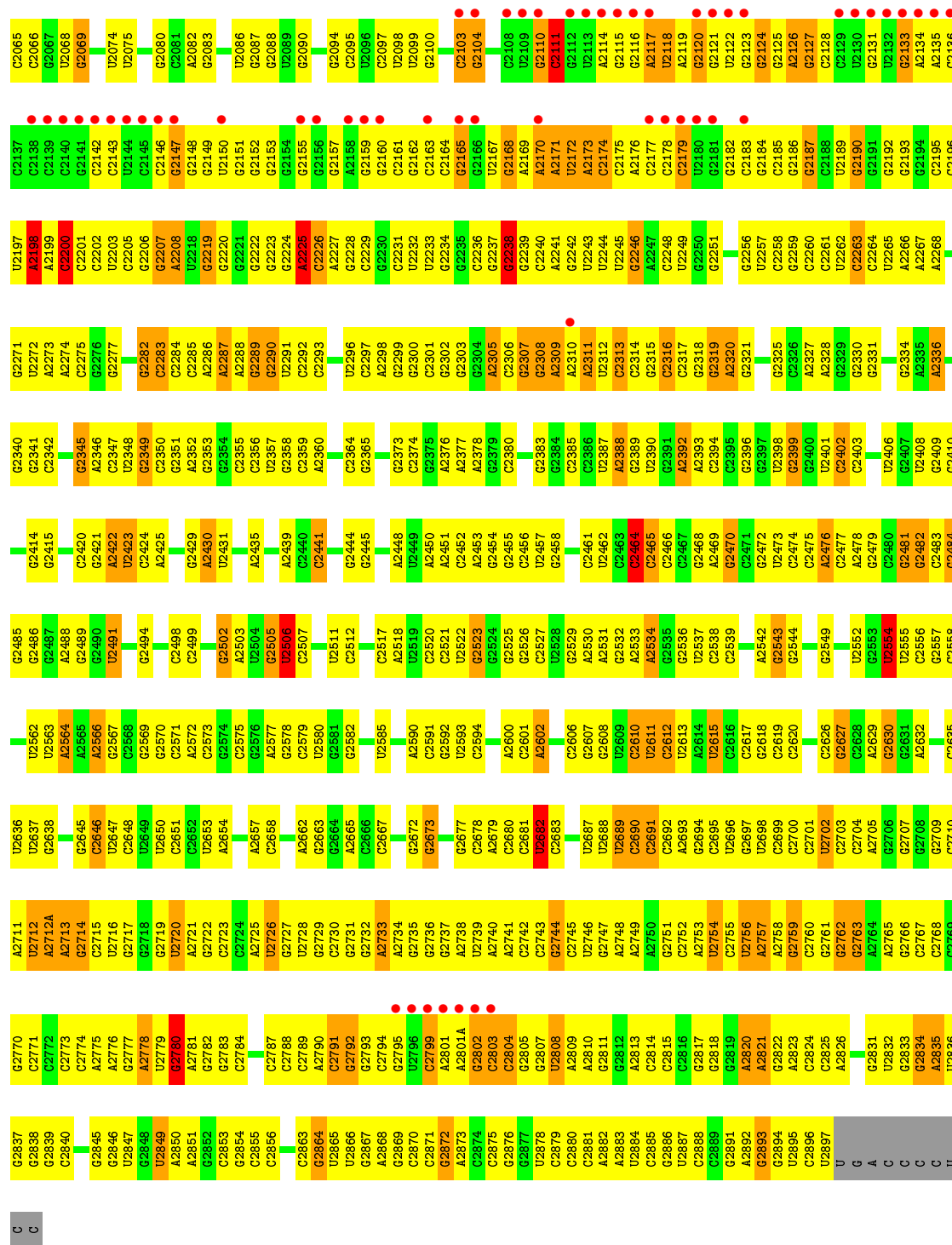


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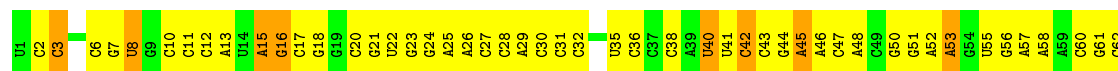


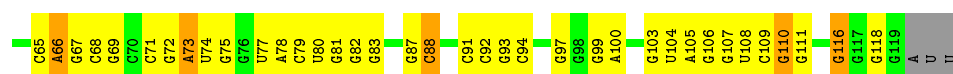




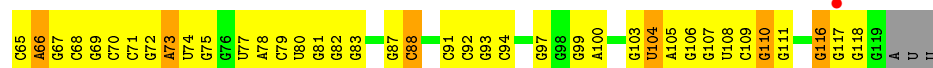
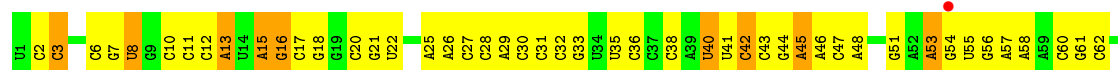
• Molecule 37: 5S RIBOSOMAL RNA

Chain BB: •

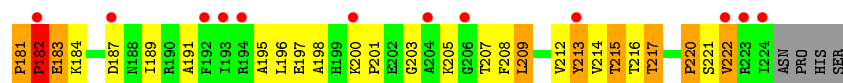
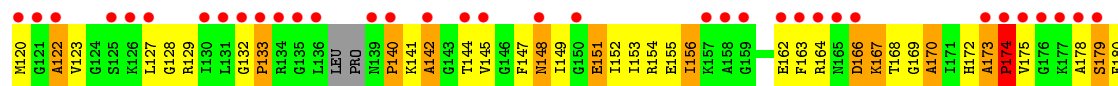
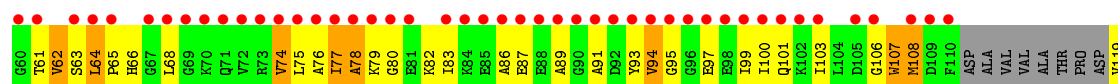




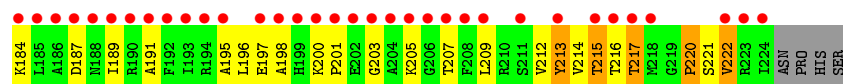
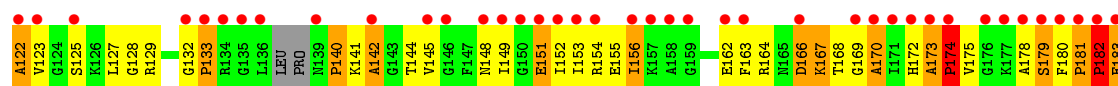
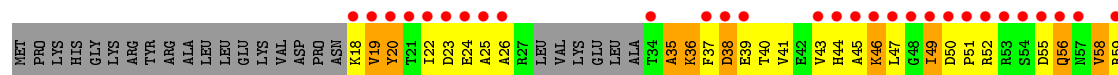
• Molecule 37: 5S RIBOSOMAL RNA



• Molecule 38: 50S RIBOSOMAL PROTEIN L1

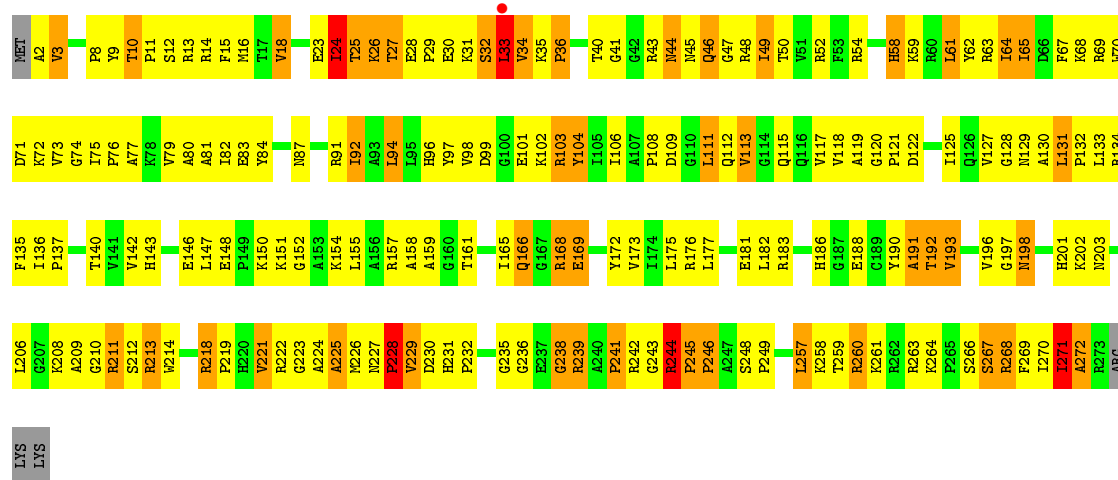


• Molecule 38: 50S RIBOSOMAL PROTEIN L1



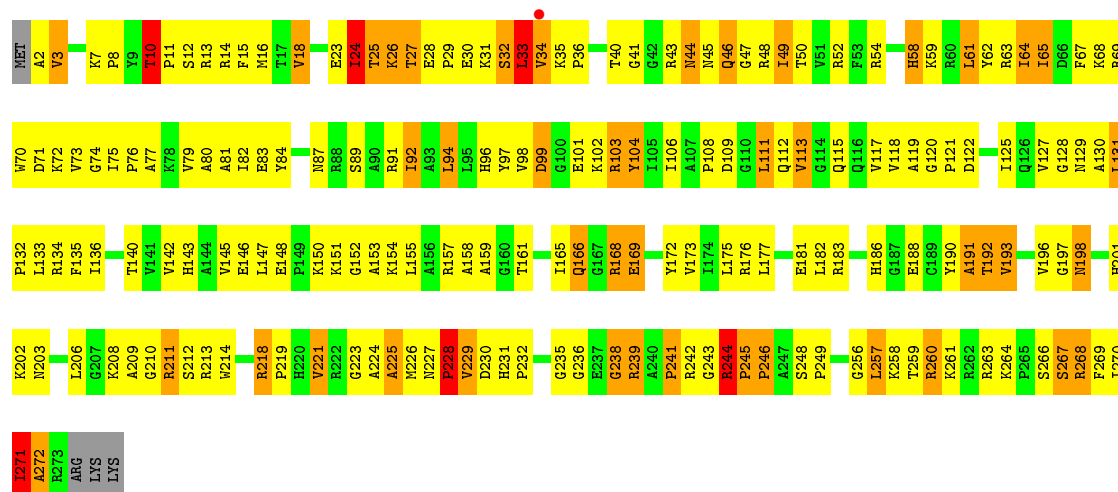
• Molecule 39: 50S RIBOSOMAL PROTEIN L2





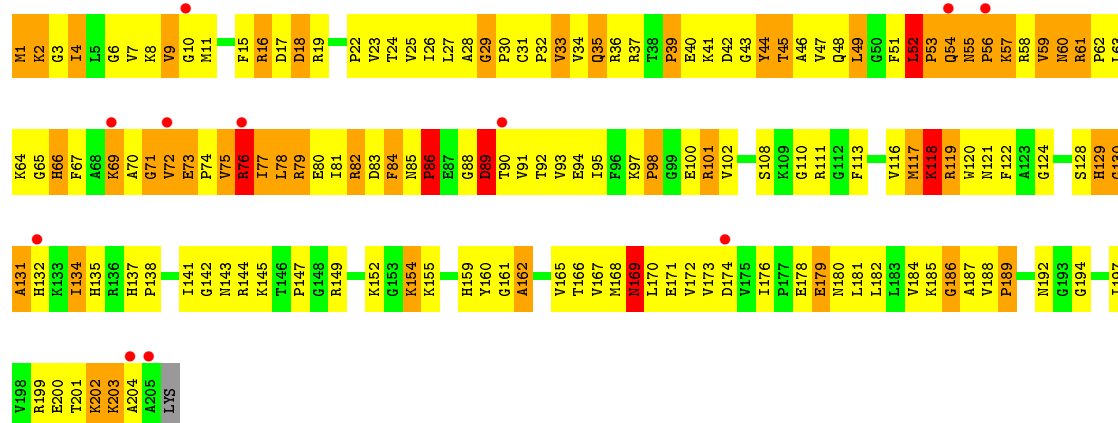
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD: 30% 50% 16%

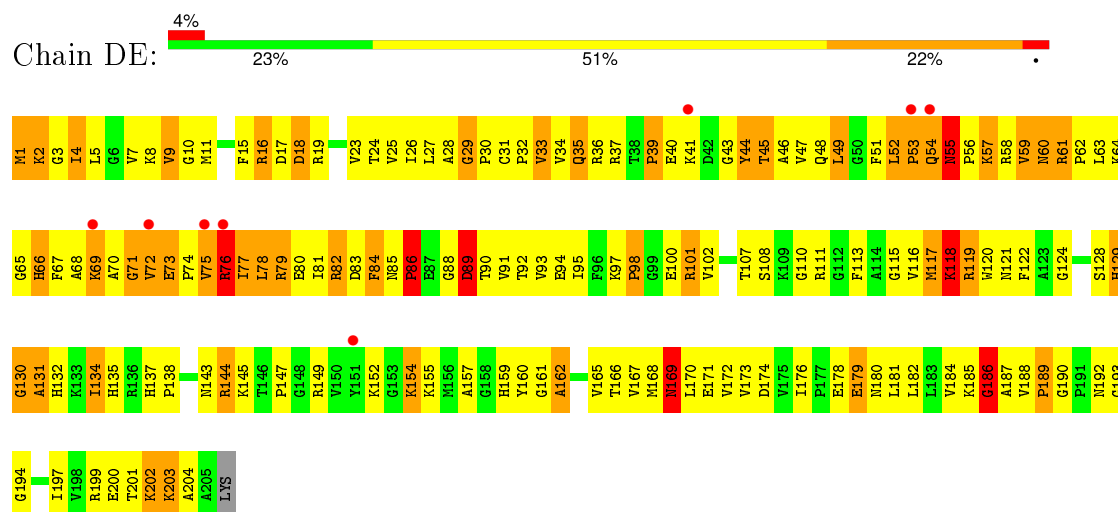


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

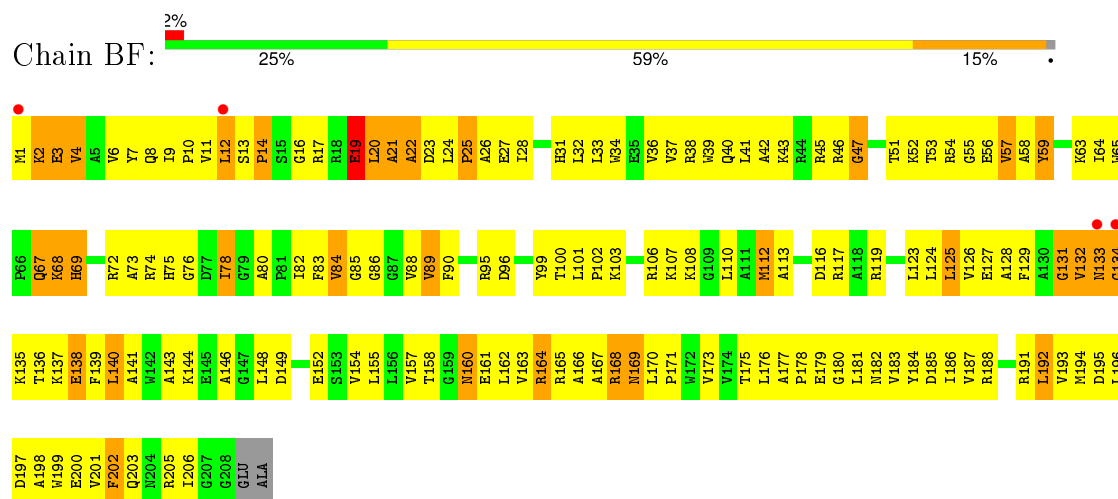
Chain BE: 24% 50% 23%



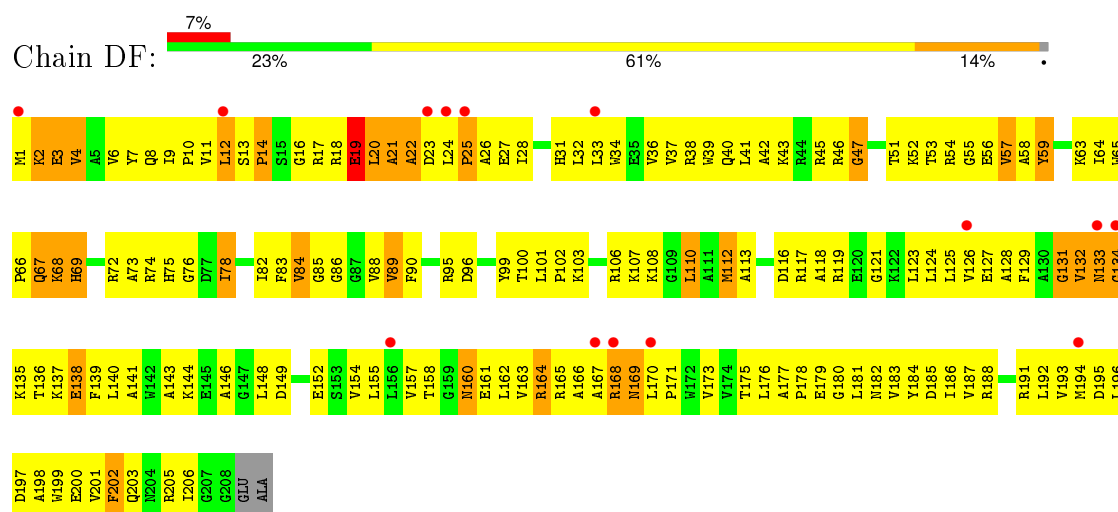
• Molecule 40: 50S RIBOSOMAL PROTEIN L3



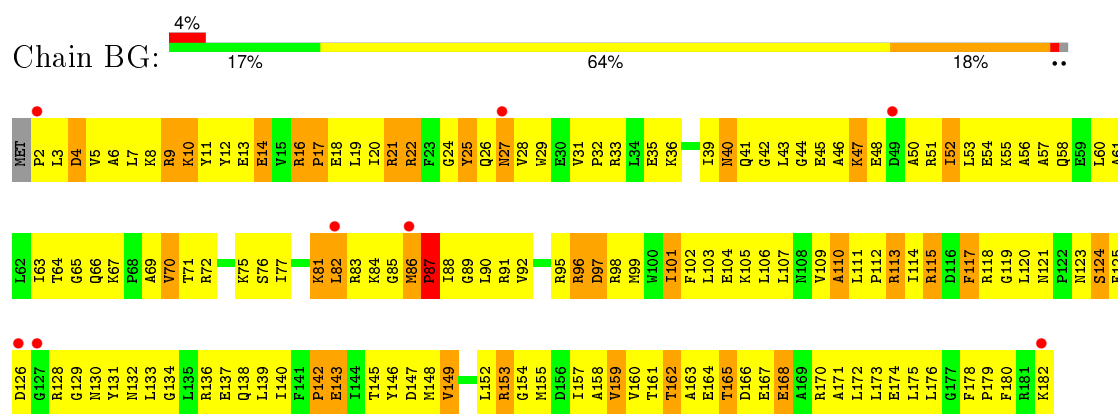
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



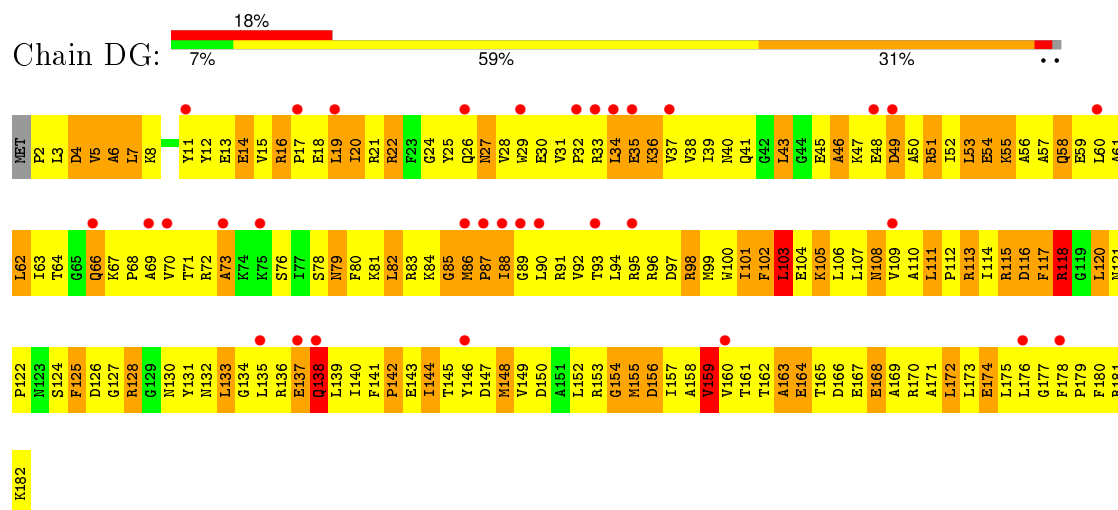
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



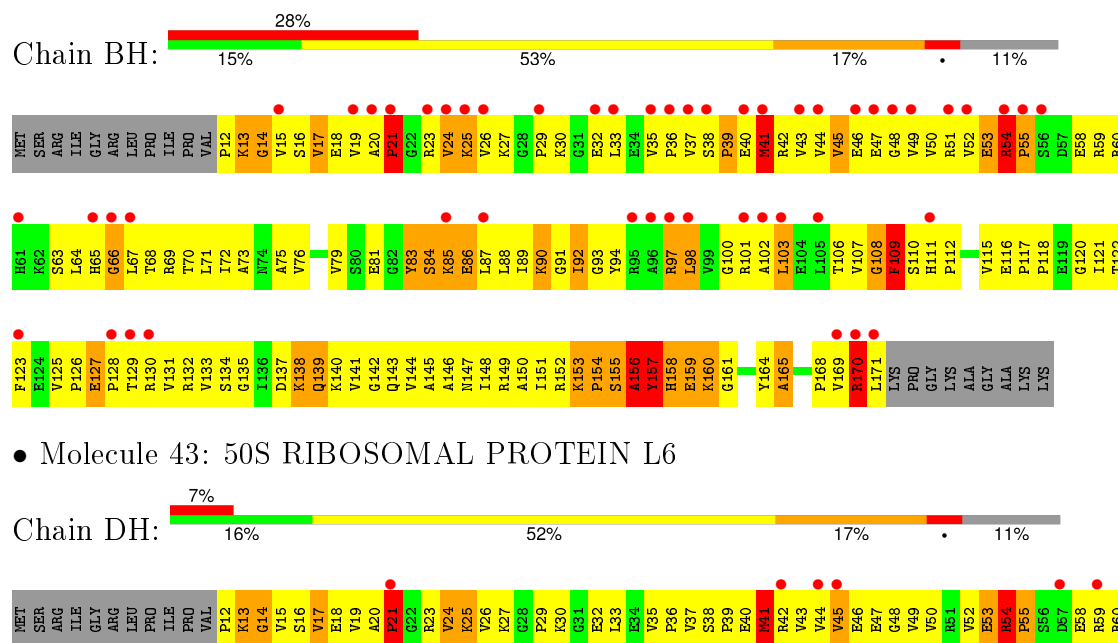
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



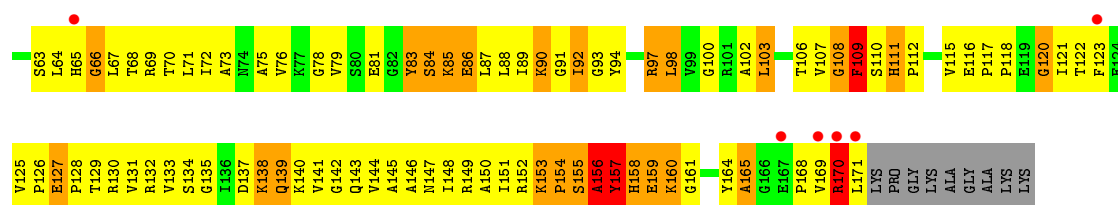
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



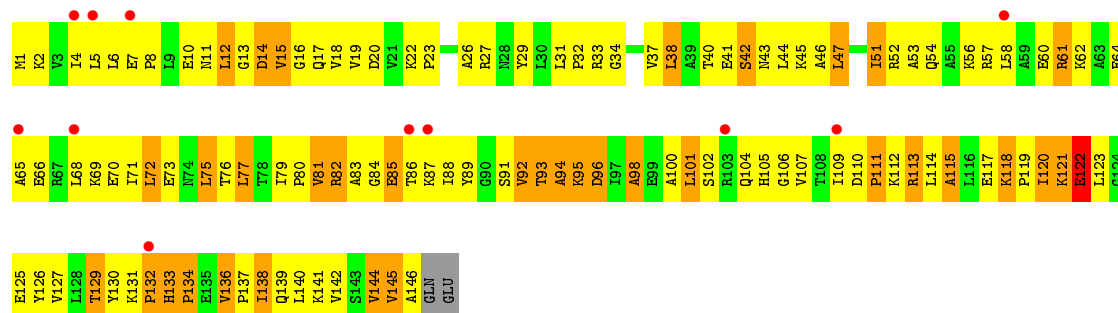
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



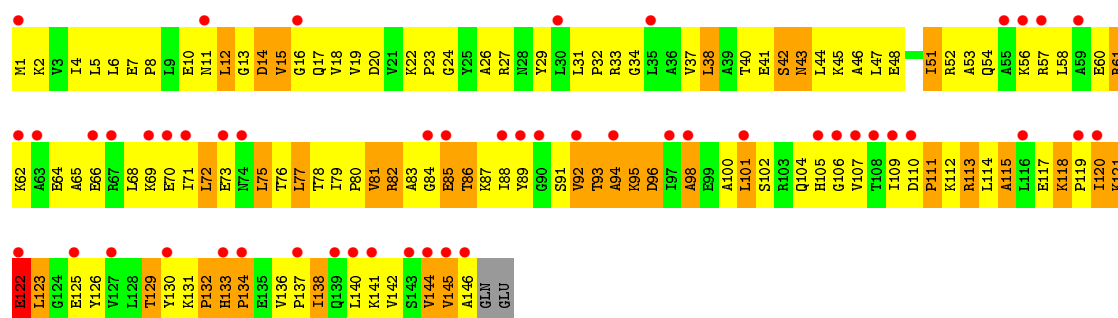
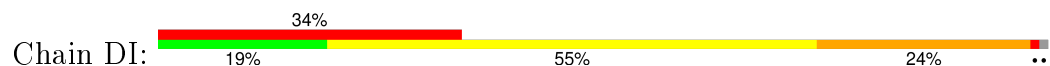
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



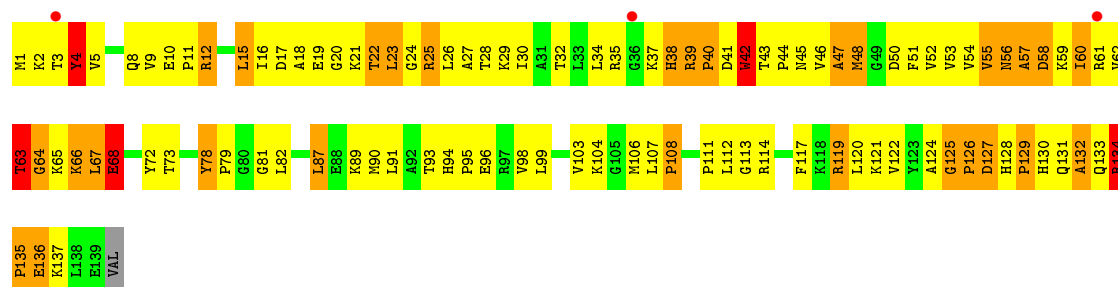
• Molecule 44: 50S RIBOSOMAL PROTEIN L9



• Molecule 44: 50S RIBOSOMAL PROTEIN L9

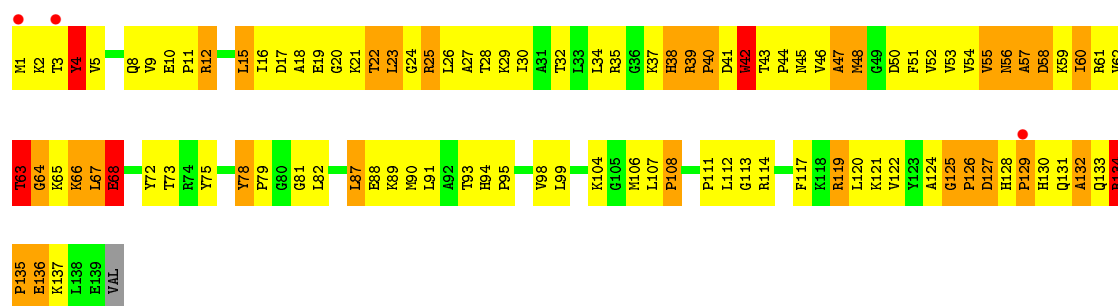


• Molecule 45: 50S RIBOSOMAL PROTEIN L13

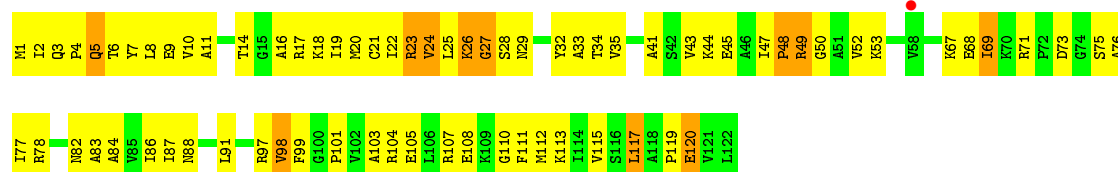


• Molecule 45: 50S RIBOSOMAL PROTEIN L13

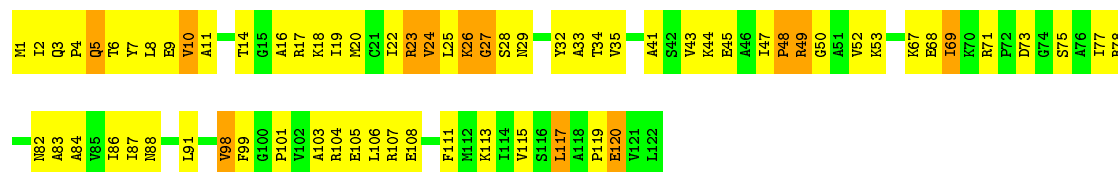




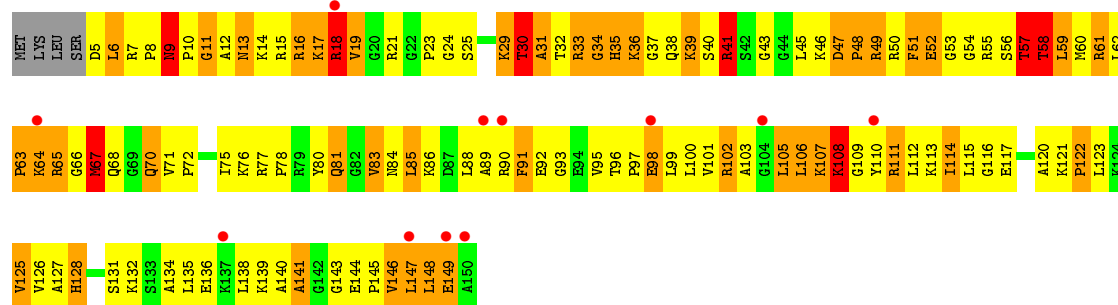
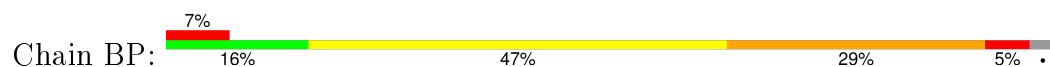
- Molecule 46: 50S RIBOSOMAL PROTEIN L14



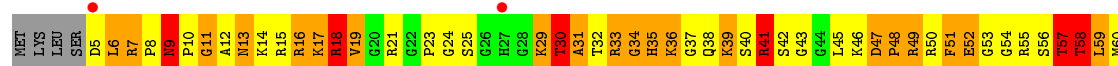
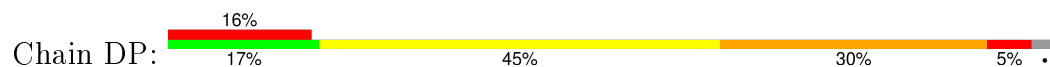
- Molecule 46: 50S RIBOSOMAL PROTEIN L14

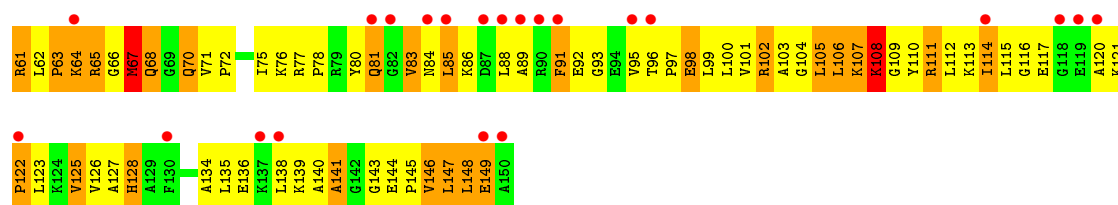


- Molecule 47: 50S RIBOSOMAL PROTEIN L15

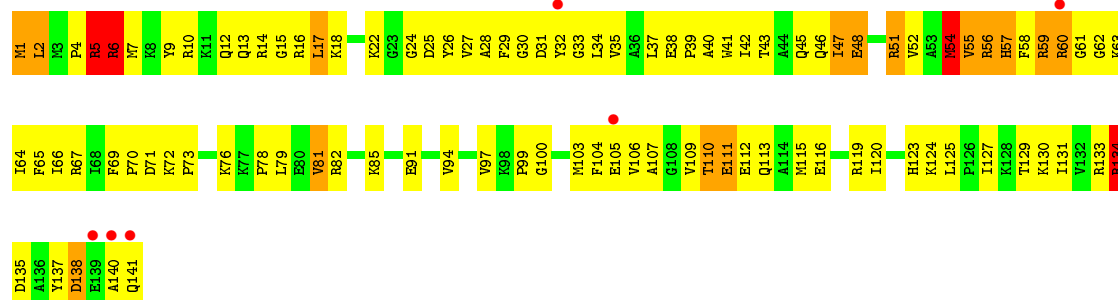


- Molecule 47: 50S RIBOSOMAL PROTEIN L15

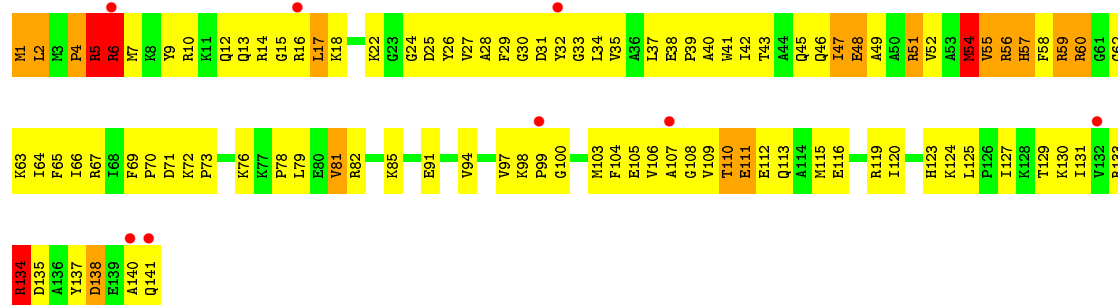




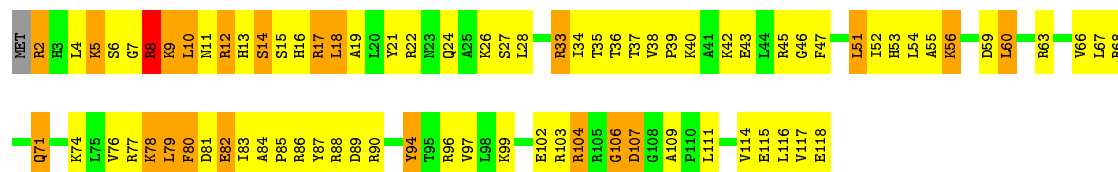
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



• Molecule 48: 50S RIBOSOMAL PROTEIN L16



• Molecule 49: 50S RIBOSOMAL PROTEIN L17

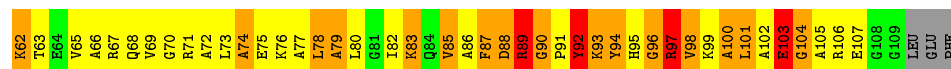
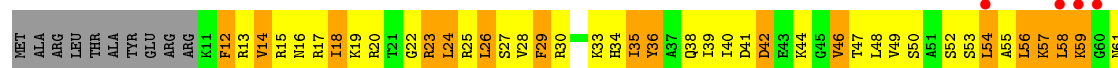


• Molecule 49: 50S RIBOSOMAL PROTEIN L17

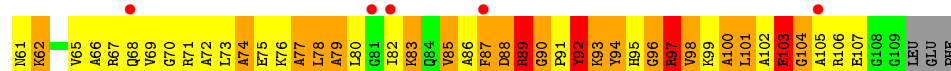
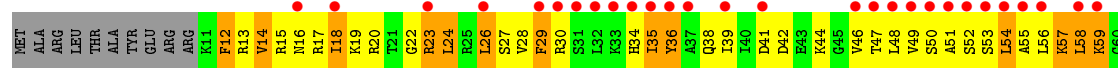
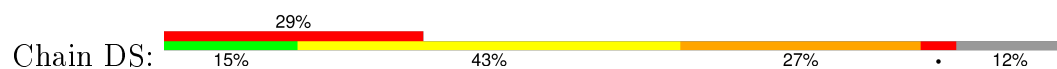




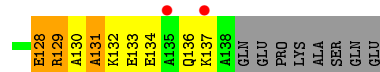
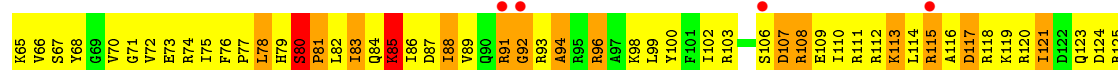
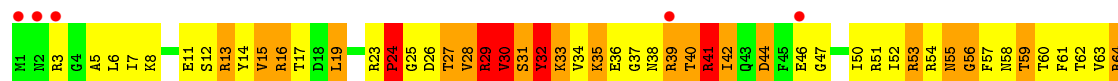
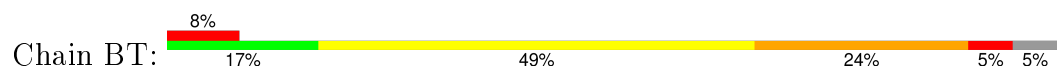
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



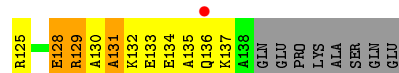
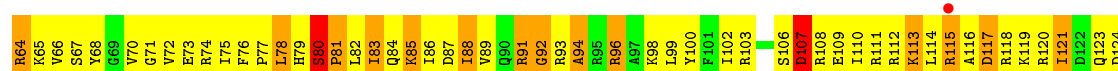
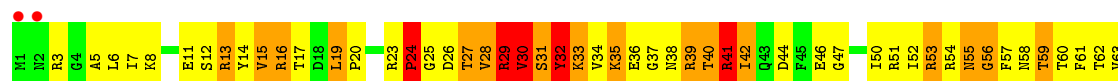
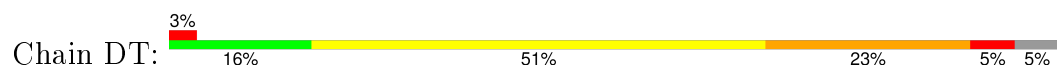
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



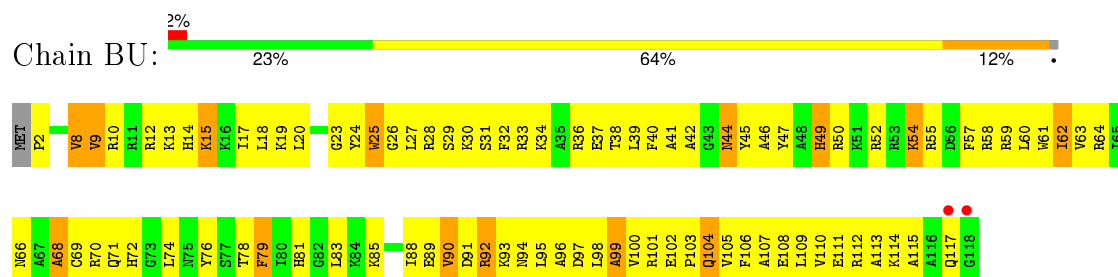
• Molecule 51: 50S RIBOSOMAL PROTEIN L19



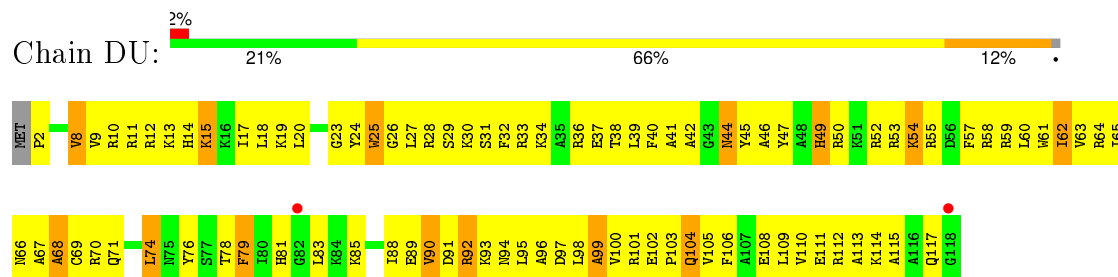
• Molecule 51: 50S RIBOSOMAL PROTEIN L19



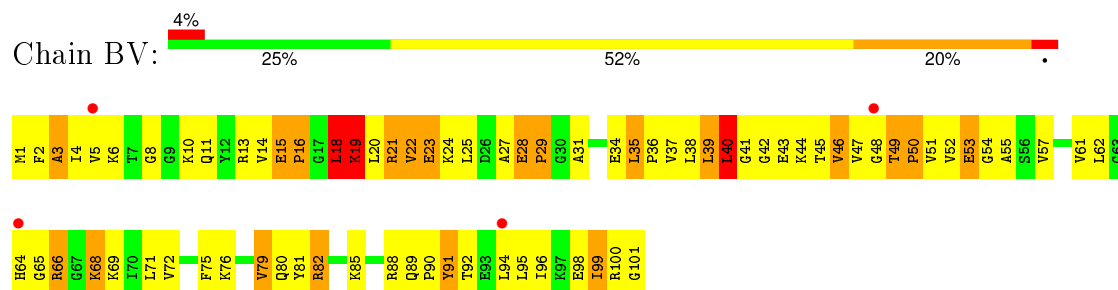
- Molecule 52: 50S RIBOSOMAL PROTEIN L20



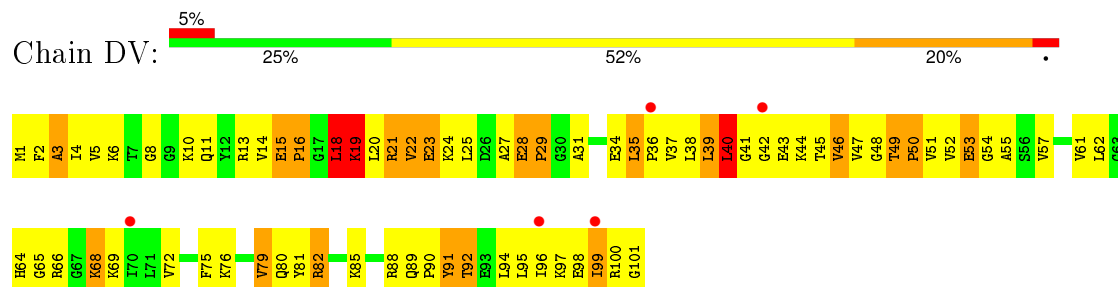
- Molecule 52: 50S RIBOSOMAL PROTEIN L20



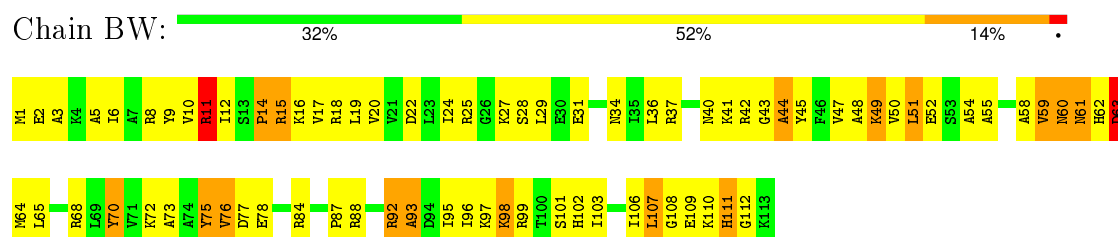
- Molecule 53: 50S RIBOSOMAL PROTEIN L21



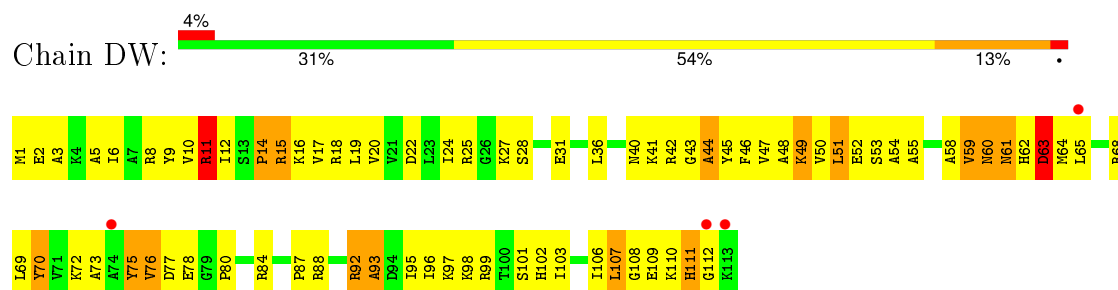
- Molecule 53: 50S RIBOSOMAL PROTEIN L21



- Molecule 54: 50S RIBOSOMAL PROTEIN L22



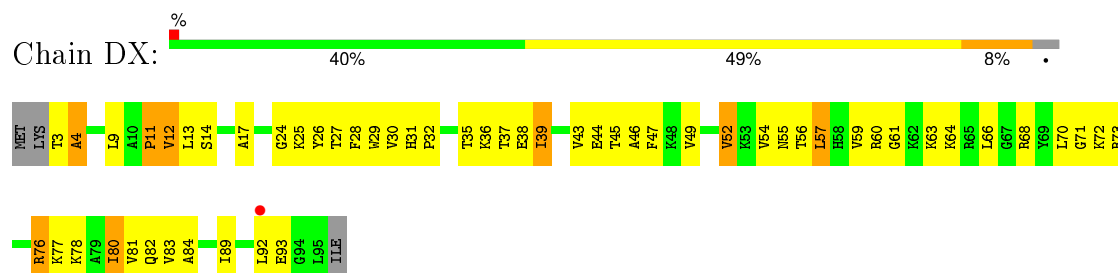
- Molecule 54: 50S RIBOSOMAL PROTEIN L22



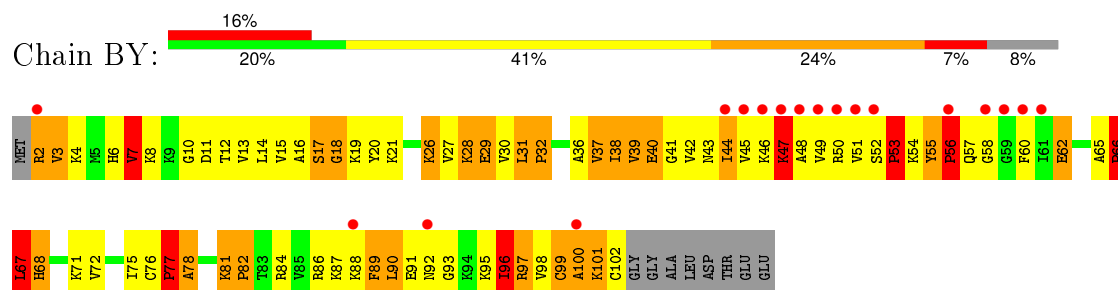
- Molecule 55: 50S RIBOSOMAL PROTEIN L23



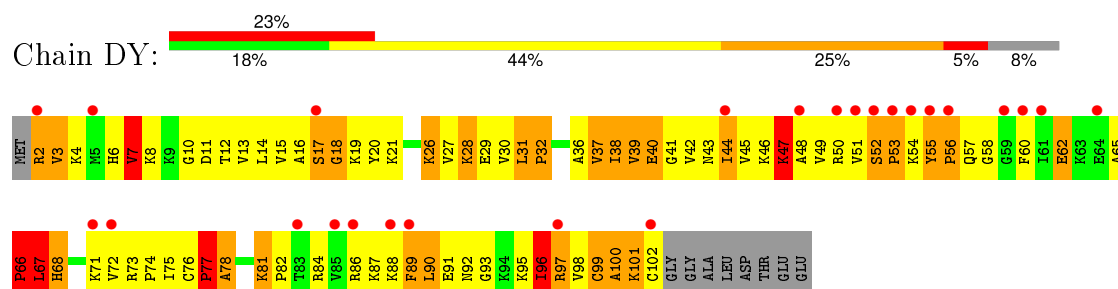
- Molecule 55: 50S RIBOSOMAL PROTEIN L23



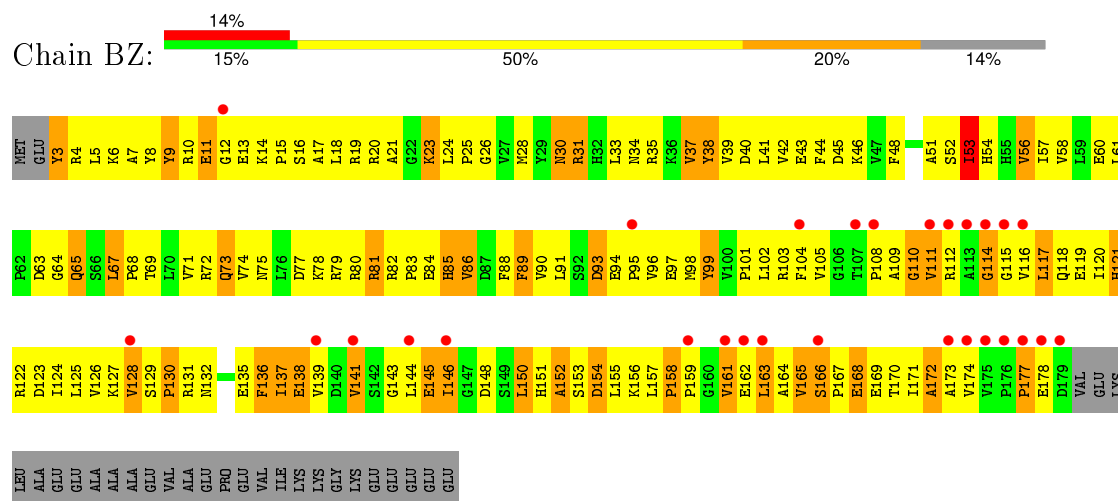
- Molecule 56: 50S RIBOSOMAL PROTEIN L24



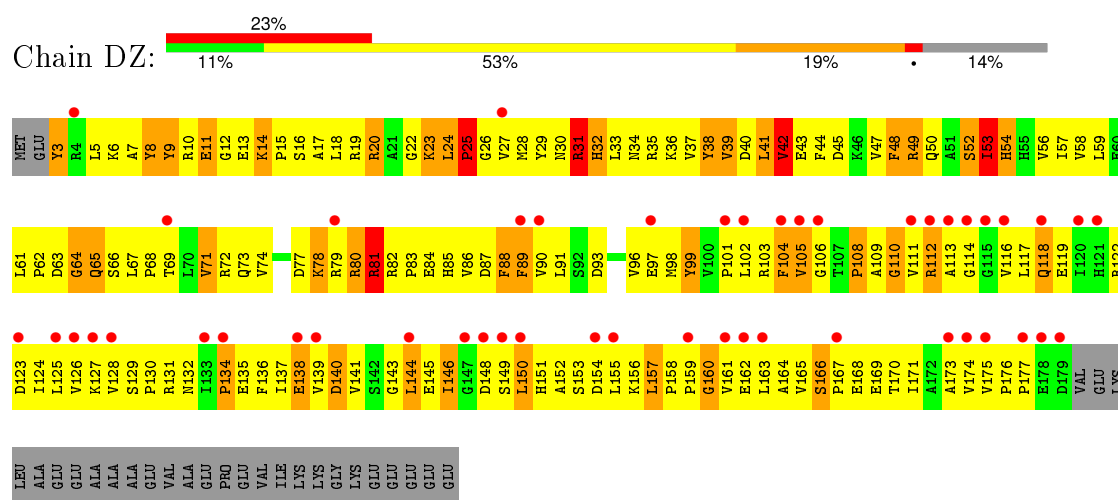
- Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.13Å 450.80Å 629.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.99 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.30) 98.2 (49.99-3.01)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.272 0.226 , 0.273	Depositor DCC
R_{free} test set	41366 reflections (4.87%)	DCC
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 111.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 1160000 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	296168	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% 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: 5MU, MG, ZN, PHA, PAR, 8AN

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	0.45	0/36190	0.70	18/56486 (0.0%)
1	CA	0.43	0/36190	0.70	14/56486 (0.0%)
2	AB	0.34	0/1936	0.62	0/2611
2	CB	0.34	0/1936	0.61	0/2611
3	AC	0.35	0/1637	0.60	0/2207
3	CC	0.34	0/1637	0.59	0/2207
4	AD	0.39	0/1733	0.66	0/2318
4	CD	0.37	0/1733	0.65	0/2318
5	AE	0.39	0/1163	0.66	0/1566
5	CE	0.38	0/1163	0.65	0/1566
6	AF	0.36	0/856	0.65	0/1154
6	CF	0.35	0/856	0.65	0/1154
7	AG	0.34	0/1276	0.57	0/1709
7	CG	0.33	0/1276	0.57	0/1709
8	AH	0.34	0/1136	0.64	0/1527
8	CH	0.34	0/1136	0.64	0/1527
9	AI	0.33	0/1027	0.60	0/1372
9	CI	0.34	0/1027	0.60	0/1372
10	AJ	0.38	0/808	0.64	0/1087
10	CJ	0.37	0/808	0.64	0/1087
11	AK	0.36	0/900	0.66	0/1213
11	CK	0.36	0/900	0.66	0/1213
12	AL	0.43	0/987	0.76	0/1322
12	CL	0.43	0/987	0.76	0/1322
13	AM	0.35	0/994	0.67	0/1322
13	CM	0.33	0/994	0.66	0/1322
14	AN	0.37	0/501	0.63	0/664
14	CN	0.37	0/501	0.63	0/664
15	AO	0.36	0/745	0.58	0/992
15	CO	0.35	0/745	0.58	0/992
16	AP	0.38	0/717	0.65	0/965
16	CP	0.38	0/717	0.63	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.38	0/837	0.64	0/1119
17	CQ	0.36	0/837	0.63	0/1119
18	AR	0.38	0/579	0.71	0/768
18	CR	0.39	0/579	0.70	0/768
19	AS	0.37	0/643	0.63	0/867
19	CS	0.38	0/643	0.63	0/867
20	AT	0.35	0/765	0.64	0/1007
20	CT	0.31	0/765	0.63	0/1007
21	AU	0.45	0/213	0.59	0/279
21	CU	0.45	0/213	0.59	0/279
22	AV	0.47	0/1810	0.73	2/2821 (0.1%)
22	CV	0.46	0/1810	0.72	0/2821
23	AW	0.48	0/1809	0.73	0/2819
23	CW	0.53	0/1809	0.71	0/2819
24	AX	0.54	0/235	0.78	0/364
24	CX	0.46	0/235	0.74	1/364 (0.3%)
25	AY	0.48	0/1784	0.75	0/2780
25	CY	0.46	0/1784	0.75	0/2780
26	B0	0.39	0/671	0.67	0/892
26	D0	0.39	0/671	0.67	0/892
27	B1	0.46	0/739	0.84	1/983 (0.1%)
27	D1	0.46	0/739	0.83	1/983 (0.1%)
28	B2	0.43	0/600	0.71	0/793
28	D2	0.38	0/600	0.63	0/793
29	B3	0.38	0/473	0.67	0/636
29	D3	0.38	0/473	0.66	0/636
30	B4	0.44	0/229	0.65	0/311
30	D4	0.44	0/229	0.65	0/311
31	B5	0.37	0/473	0.68	0/639
31	D5	0.38	0/473	0.70	0/639
32	B6	0.43	0/387	0.61	0/517
32	D6	0.42	0/387	0.60	0/517
33	B7	0.56	0/427	0.74	0/563
33	D7	0.58	0/427	0.74	0/563
34	B8	0.52	0/516	0.85	0/681
34	D8	0.49	0/516	0.85	0/681
35	B9	0.31	0/302	0.58	0/397
35	D9	0.33	0/302	0.58	0/397
36	BA	0.53	3/67716 (0.0%)	0.75	39/105718 (0.0%)
36	DA	0.55	3/67716 (0.0%)	0.75	42/105718 (0.0%)
37	BB	0.40	0/2853	0.71	1/4451 (0.0%)
37	DB	0.44	0/2853	0.71	1/4451 (0.0%)
38	BC	0.37	0/1145	0.67	7/1556 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DC	0.38	0/1145	0.67	7/1556 (0.4%)
39	BD	0.53	0/2155	0.84	1/2907 (0.0%)
39	DD	0.54	0/2155	0.84	1/2907 (0.0%)
40	BE	0.44	0/1597	0.76	1/2155 (0.0%)
40	DE	0.46	0/1597	0.77	1/2155 (0.0%)
41	BF	0.45	0/1659	0.73	0/2246
41	DF	0.44	0/1659	0.73	0/2246
42	BG	0.41	0/1498	0.74	1/2013 (0.0%)
42	DG	0.37	0/1498	0.78	2/2013 (0.1%)
43	BH	0.37	0/1246	0.70	2/1684 (0.1%)
43	DH	0.40	0/1246	0.72	2/1684 (0.1%)
44	BI	0.37	0/1147	0.70	0/1553
44	DI	0.44	0/1147	0.71	0/1553
45	BN	0.39	0/1132	0.75	1/1527 (0.1%)
45	DN	0.41	0/1132	0.75	1/1527 (0.1%)
46	BO	0.41	0/943	0.72	0/1269
46	DO	0.46	0/943	0.74	0/1269
47	BP	0.50	0/1131	0.98	7/1504 (0.5%)
47	DP	0.46	0/1131	0.96	6/1504 (0.4%)
48	BQ	0.40	0/1143	0.69	0/1527
48	DQ	0.41	0/1143	0.70	0/1527
49	BR	0.39	0/974	0.76	0/1302
49	DR	0.42	0/974	0.78	1/1302 (0.1%)
50	BS	0.41	0/779	0.72	0/1038
50	DS	0.39	0/779	0.71	0/1038
51	BT	0.46	0/1156	0.83	2/1544 (0.1%)
51	DT	0.46	0/1156	0.82	3/1544 (0.2%)
52	BU	0.40	0/975	0.71	0/1297
52	DU	0.42	0/975	0.72	0/1297
53	BV	0.39	0/790	0.72	0/1057
53	DV	0.38	0/790	0.73	0/1057
54	BW	0.41	0/907	0.70	0/1216
54	DW	0.40	0/907	0.70	0/1216
55	BX	0.49	0/740	0.72	0/995
55	DX	0.48	0/740	0.72	0/995
56	BY	0.50	0/789	0.81	0/1053
56	DY	0.48	0/789	0.80	0/1053
57	BZ	0.39	0/1436	0.67	0/1951
57	DZ	0.39	0/1436	0.68	0/1951
All	All	0.48	6/320018 (0.0%)	0.72	166/478628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	18
1	CA	0	19
22	AV	0	4
22	CV	0	3
25	AY	0	2
36	BA	3	51
36	DA	5	43
37	DB	0	1
39	BD	0	1
45	DN	0	1
All	All	8	143

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	DA	786	C	P-OP2	7.36	1.61	1.49
36	DA	652	C	C3'-O3'	6.63	1.51	1.42
36	BA	652	C	C3'-O3'	6.51	1.51	1.42
36	DA	652	C	O3'-P	5.39	1.67	1.61
36	BA	656	G	O5'-C5'	5.38	1.53	1.44

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BA	1992	G	C2'-C3'-O3'	11.05	133.81	109.50
36	DA	1992	G	C2'-C3'-O3'	10.94	133.58	109.50
36	BA	1799	G	C2'-C3'-O3'	9.57	130.56	109.50
36	BA	1786	A	N9-C1'-C2'	9.41	126.24	114.00
47	DP	52	GLU	N-CA-C	9.36	136.27	111.00

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	BA	283	A	C3'
36	BA	1799	G	C3'
36	BA	1992	G	C3'
36	DA	283	A	C3'
36	DA	1653	G	C3'

5 of 143 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	265	G	Sidechain
1	AA	436	C	Sidechain
1	AA	484	G	Sidechain
1	AA	56	U	Sidechain
1	AA	97	G	Sidechain

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	32329	0	16314	1195	0
1	CA	32329	0	16315	1202	0
2	AB	1901	0	1951	275	0
2	CB	1901	0	1951	287	0
3	AC	1613	0	1677	212	0
3	CC	1613	0	1677	206	0
4	AD	1703	0	1763	172	0
4	CD	1703	0	1763	167	0
5	AE	1147	0	1207	129	0
5	CE	1147	0	1207	128	0
6	AF	843	0	857	84	0
6	CF	843	0	857	87	0
7	AG	1257	0	1296	145	0
7	CG	1257	0	1296	145	0
8	AH	1116	0	1177	139	0
8	CH	1116	0	1177	150	0
9	AI	1011	0	1041	137	0
9	CI	1011	0	1041	141	0
10	AJ	795	0	840	152	0
10	CJ	795	0	840	148	0
11	AK	885	0	904	103	0
11	CK	885	0	904	115	0
12	AL	971	0	1057	110	0
12	CL	971	0	1057	109	0
13	AM	988	0	1055	130	0
13	CM	988	0	1055	132	0
14	AN	492	0	529	89	0
14	CN	492	0	529	92	0
15	AO	734	0	771	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	67	0
16	AP	701	0	720	61	0
16	CP	701	0	720	64	0
17	AQ	824	0	891	67	0
17	CQ	824	0	891	70	0
18	AR	574	0	644	60	0
18	CR	574	0	644	62	0
19	AS	630	0	652	110	0
19	CS	630	0	652	115	0
20	AT	763	0	861	100	0
20	CT	763	0	861	102	0
21	AU	209	0	221	16	0
21	CU	209	0	221	18	0
22	AV	1641	0	839	64	0
22	CV	1641	0	839	62	0
23	AW	1619	0	822	94	0
23	CW	1619	0	820	78	0
24	AX	210	0	108	10	0
24	CX	210	0	109	9	0
25	AY	1630	0	831	102	0
25	CY	1630	0	831	101	0
26	B0	662	0	688	74	0
26	D0	662	0	688	80	0
27	B1	732	0	808	96	0
27	D1	732	0	808	92	0
28	B2	598	0	653	72	0
28	D2	598	0	653	75	0
29	B3	468	0	523	67	0
29	D3	468	0	523	69	0
30	B4	226	0	229	34	0
30	D4	226	0	229	32	0
31	B5	459	0	480	51	0
31	D5	459	0	480	51	1
32	B6	381	0	390	63	0
32	D6	381	0	390	64	0
33	B7	419	0	467	46	0
33	D7	419	0	467	44	0
34	B8	508	0	576	100	0
34	D8	508	0	576	95	0
35	B9	299	0	326	22	0
35	D9	299	0	326	24	0
36	BA	60459	0	30476	2033	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DA	60459	0	30472	2076	0
37	BB	2551	0	1295	108	0
37	DB	2551	0	1295	125	0
38	BC	1142	0	865	105	0
38	DC	1142	0	865	100	0
39	BD	2105	0	2182	298	0
39	DD	2105	0	2182	297	0
40	BE	1564	0	1629	259	0
40	DE	1564	0	1629	258	0
41	BF	1624	0	1677	230	0
41	DF	1624	0	1677	229	0
42	BG	1474	0	1534	276	0
42	DG	1474	0	1534	430	0
43	BH	1223	0	1282	197	0
43	DH	1223	0	1282	206	0
44	BI	1132	0	1218	201	0
44	DI	1132	0	1218	209	0
45	BN	1105	0	1180	171	0
45	DN	1105	0	1180	171	0
46	BO	933	0	996	111	0
46	DO	933	0	996	105	0
47	BP	1114	0	1187	300	0
47	DP	1114	0	1187	298	0
48	BQ	1122	0	1179	142	0
48	DQ	1122	0	1179	146	0
49	BR	960	0	1021	145	0
49	DR	960	0	1021	154	0
50	BS	771	0	832	180	0
50	DS	771	0	832	177	0
51	BT	1142	0	1202	260	0
51	DT	1142	0	1202	261	0
52	BU	958	0	1015	179	0
52	DU	958	0	1014	177	0
53	BV	779	0	852	160	0
53	DV	779	0	852	157	1
54	BW	896	0	953	110	0
54	DW	896	0	953	107	0
55	BX	726	0	778	71	0
55	DX	726	0	778	72	0
56	BY	776	0	870	147	0
56	DY	776	0	870	144	0
57	BZ	1404	0	1432	228	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DZ	1404	0	1432	279	0
58	AA	213	0	0	0	0
58	AD	1	0	0	0	0
58	AE	1	0	0	0	0
58	AG	1	0	0	0	0
58	AU	1	0	0	0	0
58	AV	8	0	0	0	0
58	AW	20	0	0	0	0
58	AX	4	0	0	0	0
58	B1	1	0	0	0	0
58	B2	2	0	0	0	0
58	B5	2	0	0	0	0
58	B7	1	0	0	0	0
58	BA	453	0	0	0	0
58	BB	19	0	0	0	0
58	BD	1	0	0	0	0
58	BE	1	0	0	0	0
58	BF	2	0	0	0	0
58	BN	2	0	0	0	0
58	BO	1	0	0	0	0
58	BP	2	0	0	0	0
58	BV	2	0	0	0	0
58	BW	1	0	0	0	0
58	BX	2	0	0	0	0
58	CA	216	0	0	0	0
58	CE	1	0	0	0	0
58	CK	1	0	0	0	0
58	CL	1	0	0	0	0
58	CV	8	0	0	0	0
58	CW	21	0	0	0	0
58	CX	3	0	0	0	0
58	D1	2	0	0	0	0
58	D2	3	0	0	0	0
58	D5	1	0	0	0	0
58	D7	2	0	0	0	0
58	DA	451	0	0	0	0
58	DB	18	0	0	0	0
58	DD	2	0	0	0	0
58	DE	2	0	0	0	0
58	DF	1	0	0	0	0
58	DN	3	0	0	0	0
58	DV	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DX	3	0	0	0	0
59	AA	42	0	45	1	0
59	CA	42	0	45	3	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	0	0
60	CN	1	0	0	0	0
60	D9	1	0	0	0	0
All	All	296168	0	199731	19137	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 19137 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)
36:BA:1879:C:H2'	36:BA:1880:C:H5"	1.23	1.19
36:DA:1590:U:H2'	36:DA:1591:G:H5"	1.26	1.18
55:BX:27:THR:HG22	55:BX:80:ILE:HB	1.25	1.18
36:DA:271(S):G:H2'	36:DA:271(T):C:H5"	1.25	1.17
13:CM:112:GLY:HA2	13:CM:113:PRO:HD2	1.25	1.16

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)
31:D5:59:GLU:N	53:DV:51:VAL:N[4_545]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	148 (64%)	64 (28%)	21 (9%)	1	6
2	CB	233/256 (91%)	148 (64%)	64 (28%)	21 (9%)	1	6
3	AC	205/239 (86%)	137 (67%)	44 (22%)	24 (12%)	0	3
3	CC	205/239 (86%)	137 (67%)	43 (21%)	25 (12%)	0	2
4	AD	206/209 (99%)	145 (70%)	41 (20%)	20 (10%)	1	5
4	CD	206/209 (99%)	144 (70%)	40 (19%)	22 (11%)	0	4
5	AE	149/162 (92%)	112 (75%)	20 (13%)	17 (11%)	0	3
5	CE	149/162 (92%)	113 (76%)	19 (13%)	17 (11%)	0	3
6	AF	99/101 (98%)	82 (83%)	14 (14%)	3 (3%)	5	33
6	CF	99/101 (98%)	81 (82%)	15 (15%)	3 (3%)	5	33
7	AG	153/156 (98%)	107 (70%)	32 (21%)	14 (9%)	1	6
7	CG	153/156 (98%)	107 (70%)	32 (21%)	14 (9%)	1	6
8	AH	136/138 (99%)	101 (74%)	27 (20%)	8 (6%)	2	15
8	CH	136/138 (99%)	102 (75%)	26 (19%)	8 (6%)	2	15
9	AI	121/128 (94%)	86 (71%)	23 (19%)	12 (10%)	1	5
9	CI	121/128 (94%)	86 (71%)	23 (19%)	12 (10%)	1	5
10	AJ	97/105 (92%)	66 (68%)	22 (23%)	9 (9%)	1	6
10	CJ	97/105 (92%)	67 (69%)	21 (22%)	9 (9%)	1	6
11	AK	117/129 (91%)	93 (80%)	19 (16%)	5 (4%)	3	23
11	CK	117/129 (91%)	92 (79%)	20 (17%)	5 (4%)	3	23
12	AL	123/135 (91%)	83 (68%)	25 (20%)	15 (12%)	0	2
12	CL	123/135 (91%)	83 (68%)	26 (21%)	14 (11%)	0	3
13	AM	113/126 (90%)	67 (59%)	29 (26%)	17 (15%)	0	1
13	CM	113/126 (90%)	67 (59%)	28 (25%)	18 (16%)	0	1
14	AN	58/61 (95%)	37 (64%)	9 (16%)	12 (21%)	0	1
14	CN	58/61 (95%)	37 (64%)	9 (16%)	12 (21%)	0	1
15	AO	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	2	15
15	CO	86/89 (97%)	63 (73%)	18 (21%)	5 (6%)	2	15
16	AP	82/88 (93%)	57 (70%)	22 (27%)	3 (4%)	4	27
16	CP	82/88 (93%)	58 (71%)	21 (26%)	3 (4%)	4	27
17	AQ	98/105 (93%)	77 (79%)	14 (14%)	7 (7%)	1	11
17	CQ	98/105 (93%)	77 (79%)	14 (14%)	7 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	48 (71%)	15 (22%)	5 (7%)	1	10
18	CR	68/88 (77%)	45 (66%)	17 (25%)	6 (9%)	1	7
19	AS	77/93 (83%)	54 (70%)	11 (14%)	12 (16%)	0	1
19	CS	77/93 (83%)	53 (69%)	13 (17%)	11 (14%)	0	1
20	AT	97/106 (92%)	69 (71%)	17 (18%)	11 (11%)	0	3
20	CT	97/106 (92%)	69 (71%)	18 (19%)	10 (10%)	1	4
21	AU	23/27 (85%)	16 (70%)	4 (17%)	3 (13%)	0	2
21	CU	23/27 (85%)	16 (70%)	4 (17%)	3 (13%)	0	2
26	B0	82/85 (96%)	63 (77%)	12 (15%)	7 (8%)	1	7
26	D0	82/85 (96%)	63 (77%)	11 (13%)	8 (10%)	1	5
27	B1	92/98 (94%)	64 (70%)	19 (21%)	9 (10%)	1	5
27	D1	92/98 (94%)	67 (73%)	15 (16%)	10 (11%)	0	4
28	B2	69/72 (96%)	48 (70%)	12 (17%)	9 (13%)	0	2
28	D2	69/72 (96%)	52 (75%)	7 (10%)	10 (14%)	0	1
29	B3	58/60 (97%)	41 (71%)	7 (12%)	10 (17%)	0	1
29	D3	58/60 (97%)	41 (71%)	8 (14%)	9 (16%)	0	1
30	B4	29/71 (41%)	15 (52%)	7 (24%)	7 (24%)	0	0
30	D4	29/71 (41%)	15 (52%)	7 (24%)	7 (24%)	0	0
31	B5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	2
31	D5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	2
32	B6	41/54 (76%)	18 (44%)	12 (29%)	11 (27%)	0	0
32	D6	41/54 (76%)	18 (44%)	12 (29%)	11 (27%)	0	0
33	B7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	9	42
33	D7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	9	42
34	B8	62/65 (95%)	39 (63%)	14 (23%)	9 (14%)	0	1
34	D8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	1
35	B9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	6	34
35	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	6	34
38	BC	183/229 (80%)	84 (46%)	45 (25%)	54 (30%)	0	0
38	DC	183/229 (80%)	84 (46%)	43 (24%)	56 (31%)	0	0
39	BD	270/276 (98%)	205 (76%)	38 (14%)	27 (10%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	DD	270/276 (98%)	204 (76%)	40 (15%)	26 (10%)	1	5
40	BE	203/206 (98%)	128 (63%)	36 (18%)	39 (19%)	0	1
40	DE	203/206 (98%)	128 (63%)	34 (17%)	41 (20%)	0	1
41	BF	206/210 (98%)	128 (62%)	55 (27%)	23 (11%)	0	3
41	DF	206/210 (98%)	130 (63%)	53 (26%)	23 (11%)	0	3
42	BG	177/182 (97%)	111 (63%)	40 (23%)	26 (15%)	0	1
42	DG	177/182 (97%)	83 (47%)	53 (30%)	41 (23%)	0	0
43	BH	158/180 (88%)	93 (59%)	31 (20%)	34 (22%)	0	0
43	DH	158/180 (88%)	91 (58%)	34 (22%)	33 (21%)	0	1
44	BI	144/148 (97%)	88 (61%)	29 (20%)	27 (19%)	0	1
44	DI	144/148 (97%)	88 (61%)	28 (19%)	28 (19%)	0	1
45	BN	137/140 (98%)	84 (61%)	33 (24%)	20 (15%)	0	1
45	DN	137/140 (98%)	85 (62%)	32 (23%)	20 (15%)	0	1
46	BO	120/122 (98%)	99 (82%)	14 (12%)	7 (6%)	2	15
46	DO	120/122 (98%)	99 (82%)	14 (12%)	7 (6%)	2	15
47	BP	144/150 (96%)	78 (54%)	32 (22%)	34 (24%)	0	0
47	DP	144/150 (96%)	79 (55%)	31 (22%)	34 (24%)	0	0
48	BQ	139/141 (99%)	105 (76%)	18 (13%)	16 (12%)	0	3
48	DQ	139/141 (99%)	104 (75%)	18 (13%)	17 (12%)	0	2
49	BR	115/118 (98%)	83 (72%)	22 (19%)	10 (9%)	1	7
49	DR	115/118 (98%)	84 (73%)	21 (18%)	10 (9%)	1	7
50	BS	97/112 (87%)	38 (39%)	27 (28%)	32 (33%)	0	0
50	DS	97/112 (87%)	36 (37%)	30 (31%)	31 (32%)	0	0
51	BT	136/146 (93%)	75 (55%)	31 (23%)	30 (22%)	0	0
51	DT	136/146 (93%)	75 (55%)	31 (23%)	30 (22%)	0	0
52	BU	115/118 (98%)	70 (61%)	35 (30%)	10 (9%)	1	7
52	DU	115/118 (98%)	68 (59%)	37 (32%)	10 (9%)	1	7
53	BV	99/101 (98%)	61 (62%)	20 (20%)	18 (18%)	0	1
53	DV	99/101 (98%)	62 (63%)	19 (19%)	18 (18%)	0	1
54	BW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	0	4
54	DW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BX	91/96 (95%)	66 (72%)	20 (22%)	5 (6%)	2	16
55	DX	91/96 (95%)	65 (71%)	20 (22%)	6 (7%)	1	12
56	BY	99/110 (90%)	47 (48%)	19 (19%)	33 (33%)	0	0
56	DY	99/110 (90%)	47 (48%)	19 (19%)	33 (33%)	0	0
57	BZ	175/206 (85%)	101 (58%)	37 (21%)	37 (21%)	0	1
57	DZ	175/206 (85%)	91 (52%)	48 (27%)	36 (21%)	0	1
All	All	11662/12592 (93%)	7696 (66%)	2368 (20%)	1598 (14%)	0	2

5 of 1598 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	20	GLU
2	AB	88	ALA
2	AB	195	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	178 (88%)	24 (12%)	6	27
2	CB	202/220 (92%)	179 (89%)	23 (11%)	7	29
3	AC	160/188 (85%)	151 (94%)	9 (6%)	26	65
3	CC	160/188 (85%)	151 (94%)	9 (6%)	26	65
4	AD	180/181 (99%)	161 (89%)	19 (11%)	8	33
4	CD	180/181 (99%)	161 (89%)	19 (11%)	8	33
5	AE	115/123 (94%)	102 (89%)	13 (11%)	7	30
5	CE	115/123 (94%)	103 (90%)	12 (10%)	9	34
6	AF	90/90 (100%)	85 (94%)	5 (6%)	26	65
6	CF	90/90 (100%)	84 (93%)	6 (7%)	20	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/127 (99%)	116 (92%)	10 (8%)	15	49
7	CG	126/127 (99%)	116 (92%)	10 (8%)	15	49
8	AH	119/119 (100%)	111 (93%)	8 (7%)	20	58
8	CH	119/119 (100%)	110 (92%)	9 (8%)	16	51
9	AI	98/99 (99%)	87 (89%)	11 (11%)	7	30
9	CI	98/99 (99%)	87 (89%)	11 (11%)	7	30
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	6	24
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	6	24
11	AK	90/99 (91%)	81 (90%)	9 (10%)	9	36
11	CK	90/99 (91%)	81 (90%)	9 (10%)	9	36
12	AL	104/111 (94%)	93 (89%)	11 (11%)	8	33
12	CL	104/111 (94%)	93 (89%)	11 (11%)	8	33
13	AM	99/101 (98%)	88 (89%)	11 (11%)	8	31
13	CM	99/101 (98%)	88 (89%)	11 (11%)	8	31
14	AN	49/50 (98%)	41 (84%)	8 (16%)	3	14
14	CN	49/50 (98%)	42 (86%)	7 (14%)	4	19
15	AO	79/80 (99%)	72 (91%)	7 (9%)	12	43
15	CO	79/80 (99%)	72 (91%)	7 (9%)	12	43
16	AP	72/74 (97%)	63 (88%)	9 (12%)	6	24
16	CP	72/74 (97%)	65 (90%)	7 (10%)	10	38
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	17	52
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	17	52
18	AR	61/77 (79%)	57 (93%)	4 (7%)	21	59
18	CR	61/77 (79%)	57 (93%)	4 (7%)	21	59
19	AS	69/80 (86%)	58 (84%)	11 (16%)	3	14
19	CS	69/80 (86%)	58 (84%)	11 (16%)	3	14
20	AT	76/82 (93%)	72 (95%)	4 (5%)	28	66
20	CT	76/82 (93%)	72 (95%)	4 (5%)	28	66
21	AU	19/22 (86%)	18 (95%)	1 (5%)	28	66
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28	66
26	B0	66/67 (98%)	58 (88%)	8 (12%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	D0	66/67 (98%)	57 (86%)	9 (14%)	5	21
27	B1	78/83 (94%)	66 (85%)	12 (15%)	3	16
27	D1	78/83 (94%)	62 (80%)	16 (20%)	1	6
28	B2	66/67 (98%)	55 (83%)	11 (17%)	3	13
28	D2	66/67 (98%)	58 (88%)	8 (12%)	6	26
29	B3	51/52 (98%)	49 (96%)	2 (4%)	39	75
29	D3	51/52 (98%)	49 (96%)	2 (4%)	39	75
30	B4	27/63 (43%)	24 (89%)	3 (11%)	8	31
30	D4	27/63 (43%)	24 (89%)	3 (11%)	8	31
31	B5	51/52 (98%)	45 (88%)	6 (12%)	6	27
31	D5	51/52 (98%)	45 (88%)	6 (12%)	6	27
32	B6	43/52 (83%)	34 (79%)	9 (21%)	1	6
32	D6	43/52 (83%)	34 (79%)	9 (21%)	1	6
33	B7	41/42 (98%)	36 (88%)	5 (12%)	6	26
33	D7	41/42 (98%)	35 (85%)	6 (15%)	4	18
34	B8	53/55 (96%)	43 (81%)	10 (19%)	2	8
34	D8	53/55 (96%)	43 (81%)	10 (19%)	2	8
35	B9	33/34 (97%)	30 (91%)	3 (9%)	12	41
35	D9	33/34 (97%)	30 (91%)	3 (9%)	12	41
38	BC	61/181 (34%)	56 (92%)	5 (8%)	14	48
38	DC	61/181 (34%)	55 (90%)	6 (10%)	10	37
39	BD	213/218 (98%)	180 (84%)	33 (16%)	3	16
39	DD	213/218 (98%)	177 (83%)	36 (17%)	2	12
40	BE	165/166 (99%)	140 (85%)	25 (15%)	3	16
40	DE	165/166 (99%)	141 (86%)	24 (14%)	4	18
41	BF	165/166 (99%)	147 (89%)	18 (11%)	8	32
41	DF	165/166 (99%)	149 (90%)	16 (10%)	10	38
42	BG	155/156 (99%)	138 (89%)	17 (11%)	8	31
42	DG	155/156 (99%)	130 (84%)	25 (16%)	3	14
43	BH	132/148 (89%)	119 (90%)	13 (10%)	10	37
43	DH	132/148 (89%)	119 (90%)	13 (10%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BI	122/124 (98%)	107 (88%)	15 (12%)	6	25
44	DI	122/124 (98%)	108 (88%)	14 (12%)	7	29
45	BN	117/119 (98%)	96 (82%)	21 (18%)	2	10
45	DN	117/119 (98%)	96 (82%)	21 (18%)	2	10
46	BO	100/100 (100%)	94 (94%)	6 (6%)	24	62
46	DO	100/100 (100%)	93 (93%)	7 (7%)	19	56
47	BP	112/116 (97%)	86 (77%)	26 (23%)	1	4
47	DP	112/116 (97%)	85 (76%)	27 (24%)	1	3
48	BQ	111/111 (100%)	96 (86%)	15 (14%)	5	21
48	DQ	111/111 (100%)	96 (86%)	15 (14%)	5	21
49	BR	100/101 (99%)	86 (86%)	14 (14%)	4	20
49	DR	100/101 (99%)	86 (86%)	14 (14%)	4	20
50	BS	77/88 (88%)	67 (87%)	10 (13%)	5	22
50	DS	77/88 (88%)	68 (88%)	9 (12%)	7	28
51	BT	120/127 (94%)	98 (82%)	22 (18%)	2	9
51	DT	120/127 (94%)	100 (83%)	20 (17%)	3	13
52	BU	92/94 (98%)	85 (92%)	7 (8%)	16	51
52	DU	92/94 (98%)	85 (92%)	7 (8%)	16	51
53	BV	82/82 (100%)	72 (88%)	10 (12%)	6	26
53	DV	82/82 (100%)	71 (87%)	11 (13%)	5	21
54	BW	91/92 (99%)	82 (90%)	9 (10%)	10	37
54	DW	91/92 (99%)	82 (90%)	9 (10%)	10	37
55	BX	74/78 (95%)	67 (90%)	7 (10%)	11	38
55	DX	74/78 (95%)	67 (90%)	7 (10%)	11	38
56	BY	84/91 (92%)	69 (82%)	15 (18%)	2	10
56	DY	84/91 (92%)	70 (83%)	14 (17%)	3	13
57	BZ	155/179 (87%)	138 (89%)	17 (11%)	8	31
57	DZ	155/179 (87%)	136 (88%)	19 (12%)	6	25
All	All	9654/10432 (92%)	8513 (88%)	1141 (12%)	6	27

5 of 1141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	BV	91	TYR
7	CG	60	LYS
51	DT	13	ARG
55	BX	76	ARG
2	CB	137	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 323 such sidechains are listed below:

Mol	Chain	Res	Type
52	BU	94	ASN
6	CF	7	ASN
49	DR	24	GLN
54	BW	40	ASN
2	CB	146	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	206 (13%)	29 (1%)
1	CA	1503/1522 (98%)	207 (13%)	28 (1%)
22	AV	76/77 (98%)	16 (21%)	0
22	CV	76/77 (98%)	15 (19%)	1 (1%)
23	AW	75/76 (98%)	15 (20%)	0
23	CW	75/76 (98%)	15 (20%)	0
24	AX	9/10 (90%)	0	0
24	CX	9/10 (90%)	0	0
25	AY	74/77 (96%)	25 (33%)	1 (1%)
25	CY	74/77 (96%)	22 (29%)	0
36	BA	2806/2822 (99%)	523 (18%)	54 (1%)
36	DA	2806/2822 (99%)	523 (18%)	54 (1%)
37	BB	118/122 (96%)	16 (13%)	1 (0%)
37	DB	118/122 (96%)	16 (13%)	1 (0%)
All	All	9322/9412 (99%)	1599 (17%)	169 (1%)

5 of 1599 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	AA	47	C

5 of 169 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2481	G
1	CA	353	A
36	DA	2225	A
36	BA	2610	C
1	CA	30	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	5MU	AV	54	22	12,22,23	1.39	3 (25%)	14,32,35	4.44	3 (21%)
25	8AN	AY	76	25	15,24,25	1.30	1 (6%)	11,35,38	0.62	0
25	PHA	AY	77	25	10,11,11	0.59	0	10,13,13	0.55	0
22	5MU	CV	54	22	12,22,23	1.30	3 (25%)	14,32,35	4.51	3 (21%)
25	8AN	CY	76	25	15,24,25	1.28	1 (6%)	11,35,38	0.65	0
25	PHA	CY	77	25	10,11,11	0.53	0	10,13,13	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	AV	54	22	-	0/3/25/26	0/2/2/2
25	8AN	AY	76	25	-	0/3/25/26	0/3/3/3
25	PHA	AY	77	25	-	0/4/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	CV	54	22	-	0/3/25/26	0/2/2/2
25	8AN	CY	76	25	-	0/3/25/26	0/3/3/3
25	PHA	CY	77	25	-	0/4/6/6	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CY	76	8AN	C3'-N3'	-4.36	1.40	1.47
25	AY	76	8AN	C3'-N3'	-4.30	1.40	1.47
22	AV	54	5MU	C6-C5	-2.15	1.34	1.40
22	CV	54	5MU	C6-C5	-2.07	1.34	1.40
22	CV	54	5MU	C6-N1	2.31	1.38	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CV	54	5MU	C5-C4-N3	-8.97	115.15	125.14
22	AV	54	5MU	C5-C4-N3	-8.67	115.48	125.14
22	CV	54	5MU	C5M-C5-C6	2.09	122.83	118.62
22	AV	54	5MU	C5M-C5-C6	2.23	123.11	118.62
22	AV	54	5MU	C4-N3-C2	13.87	127.24	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	1	0
25	AY	77	PHA	1	0
22	CV	54	5MU	1	0
25	CY	76	8AN	2	0
25	CY	77	PHA	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1490 ligands modelled in this entry, 1488 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	PAR	AA	1814	-	45,45,45	1.43	9 (20%)	59,67,67	1.25	6 (10%)
59	PAR	CA	1817	-	45,45,45	1.70	11 (24%)	59,67,67	1.39	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PAR	AA	1814	-	-	0/18/94/94	0/4/4/4
59	PAR	CA	1817	-	-	0/18/94/94	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CA	1817	PAR	O52-C52	2.01	1.48	1.43
59	AA	1814	PAR	C31-C21	2.01	1.56	1.53
59	AA	1814	PAR	O54-C54	2.04	1.49	1.44
59	CA	1817	PAR	O51-C11	2.07	1.47	1.41
59	CA	1817	PAR	O11-C42	2.11	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	CA	1817	PAR	C11-O51-C51	2.45	118.50	113.75
59	AA	1814	PAR	C11-O51-C51	2.48	118.56	113.75
59	AA	1814	PAR	O11-C11-C21	3.06	113.63	107.96
59	AA	1814	PAR	O52-C13-C23	3.25	114.52	107.75
59	AA	1814	PAR	O33-C14-C24	3.32	114.11	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AA	1814	PAR	1	0
59	CA	1817	PAR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
42	DG	1
42	BG	1
32	D6	1
32	B6	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DG	112:PRO	C	113:ARG	N	6.74
1	D6	46:HIS	C	47:THR	N	5.22
1	B6	46:HIS	C	47:THR	N	5.21
1	AM	112:GLY	C	113:PRO	N	4.65
1	CM	112:GLY	C	113:PRO	N	4.62

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.19	23 (1%) 76 71	56, 99, 180, 200	0
1	CA	1504/1522 (98%)	-0.04	25 (1%) 73 67	55, 119, 194, 200	0
2	AB	235/256 (91%)	0.20	15 (6%) 23 19	65, 132, 188, 200	0
2	CB	235/256 (91%)	0.73	29 (12%) 5 4	83, 158, 197, 200	0
3	AC	207/239 (86%)	-0.06	2 (0%) 84 80	72, 120, 172, 200	0
3	CC	207/239 (86%)	0.40	14 (6%) 20 17	83, 147, 188, 200	0
4	AD	208/209 (99%)	-0.14	2 (0%) 84 80	59, 97, 139, 199	0
4	CD	208/209 (99%)	0.09	4 (1%) 70 63	70, 115, 158, 194	0
5	AE	151/162 (93%)	-0.18	1 (0%) 89 86	51, 99, 134, 164	0
5	CE	151/162 (93%)	0.26	4 (2%) 59 53	67, 116, 165, 199	0
6	AF	101/101 (100%)	-0.19	1 (0%) 84 80	69, 108, 147, 198	0
6	CF	101/101 (100%)	-0.03	2 (1%) 68 62	67, 107, 154, 167	0
7	AG	155/156 (99%)	0.37	13 (8%) 14 11	73, 120, 164, 188	0
7	CG	155/156 (99%)	0.74	22 (14%) 4 3	90, 155, 196, 200	0
8	AH	138/138 (100%)	0.01	2 (1%) 78 73	65, 102, 141, 173	0
8	CH	138/138 (100%)	0.25	7 (5%) 32 25	74, 121, 168, 200	0
9	AI	127/128 (99%)	0.45	8 (6%) 23 19	86, 139, 185, 198	0
9	CI	127/128 (99%)	1.70	40 (31%) 1 1	83, 170, 200, 200	0
10	AJ	99/105 (94%)	0.78	18 (18%) 2 1	81, 139, 195, 200	0
10	CJ	99/105 (94%)	2.05	42 (42%) 0 0	92, 170, 195, 200	0
11	AK	119/129 (92%)	0.15	4 (3%) 49 42	65, 100, 162, 200	0
11	CK	119/129 (92%)	0.46	8 (6%) 21 17	68, 118, 177, 200	0
12	AL	125/135 (92%)	0.17	6 (4%) 34 28	56, 93, 136, 200	0
12	CL	125/135 (92%)	0.18	6 (4%) 34 28	60, 90, 157, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.66	17 (13%) 4 3	86, 123, 177, 200	0
13	CM	125/126 (99%)	1.16	32 (25%) 1 1	100, 161, 200, 200	0
14	AN	60/61 (98%)	0.42	4 (6%) 21 17	72, 117, 161, 173	0
14	CN	60/61 (98%)	0.75	7 (11%) 6 5	84, 144, 185, 200	0
15	AO	88/89 (98%)	0.05	0 100 100	52, 92, 144, 159	0
15	CO	88/89 (98%)	0.13	1 (1%) 82 78	63, 107, 147, 155	0
16	AP	84/88 (95%)	0.14	1 (1%) 81 76	67, 87, 142, 154	0
16	CP	84/88 (95%)	0.48	6 (7%) 19 15	76, 113, 167, 192	0
17	AQ	100/105 (95%)	-0.00	2 (2%) 68 62	63, 95, 133, 147	0
17	CQ	100/105 (95%)	0.16	1 (1%) 84 80	73, 118, 154, 200	0
18	AR	70/88 (79%)	-0.02	2 (2%) 55 49	71, 104, 153, 170	0
18	CR	70/88 (79%)	0.16	1 (1%) 78 73	71, 110, 158, 170	0
19	AS	79/93 (84%)	0.86	12 (15%) 3 2	85, 136, 188, 200	0
19	CS	79/93 (84%)	1.10	15 (18%) 2 1	107, 160, 198, 200	0
20	AT	99/106 (93%)	0.39	6 (6%) 25 20	63, 105, 167, 199	0
20	CT	99/106 (93%)	0.82	13 (13%) 5 3	80, 128, 184, 200	0
21	AU	25/27 (92%)	1.78	11 (44%) 0 0	85, 125, 162, 187	0
21	CU	25/27 (92%)	4.12	19 (76%) 0 0	87, 142, 197, 200	0
22	AV	76/77 (98%)	-0.45	0 100 100	68, 102, 144, 189	0
22	CV	76/77 (98%)	-0.33	0 100 100	63, 116, 168, 182	0
23	AW	76/76 (100%)	1.41	18 (23%) 1 1	107, 196, 200, 200	0
23	CW	76/76 (100%)	2.63	44 (57%) 0 0	128, 199, 200, 200	0
24	AX	10/10 (100%)	0.18	1 (10%) 9 8	62, 94, 148, 162	0
24	CX	10/10 (100%)	0.71	1 (10%) 9 8	92, 111, 183, 192	0
25	AY	75/77 (97%)	1.21	16 (21%) 1 1	57, 187, 200, 200	0
25	CY	75/77 (97%)	1.26	13 (17%) 2 2	64, 189, 200, 200	0
26	B0	84/85 (98%)	0.54	4 (4%) 34 28	63, 94, 144, 189	0
26	D0	84/85 (98%)	0.71	12 (14%) 4 3	76, 127, 170, 191	0
27	B1	94/98 (95%)	0.14	4 (4%) 39 32	47, 77, 135, 155	0
27	D1	94/98 (95%)	0.09	0 100 100	49, 80, 138, 157	0
28	B2	71/72 (98%)	-0.06	2 (2%) 56 50	68, 99, 133, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D2	71/72 (98%)	0.34	4 (5%) 28 22	61, 105, 152, 190	0
29	B3	60/60 (100%)	0.46	4 (6%) 21 17	72, 108, 152, 188	0
29	D3	60/60 (100%)	0.93	5 (8%) 14 11	75, 134, 178, 200	0
30	B4	31/71 (43%)	-0.12	0 100 100	87, 126, 171, 176	0
30	D4	31/71 (43%)	0.99	5 (16%) 3 2	118, 175, 194, 200	0
31	B5	59/60 (98%)	0.39	6 (10%) 9 7	52, 100, 190, 200	0
31	D5	59/60 (98%)	0.12	3 (5%) 32 25	43, 99, 189, 200	0
32	B6	45/54 (83%)	4.79	37 (82%) 0 0	109, 171, 197, 200	0
32	D6	45/54 (83%)	5.16	41 (91%) 0 0	146, 183, 200, 200	0
33	B7	49/49 (100%)	0.16	2 (4%) 41 34	49, 65, 124, 185	0
33	D7	49/49 (100%)	0.33	5 (10%) 9 7	37, 62, 124, 198	0
34	B8	64/65 (98%)	0.32	2 (3%) 52 46	51, 87, 151, 173	0
34	D8	64/65 (98%)	0.88	8 (12%) 5 4	75, 110, 159, 200	0
35	B9	36/37 (97%)	3.11	25 (69%) 0 0	117, 148, 189, 200	0
35	D9	36/37 (97%)	4.21	33 (91%) 0 0	101, 145, 182, 197	0
36	BA	2807/2822 (99%)	-0.10	59 (2%) 67 60	48, 87, 188, 200	0
36	DA	2807/2822 (99%)	-0.03	81 (2%) 55 49	35, 94, 191, 200	0
37	BB	119/122 (97%)	-0.42	0 100 100	88, 121, 165, 179	0
37	DB	119/122 (97%)	0.20	2 (1%) 73 67	114, 168, 197, 200	0
38	BC	191/229 (83%)	2.88	119 (62%) 0 0	119, 183, 200, 200	0
38	DC	191/229 (83%)	3.93	143 (74%) 0 0	149, 184, 200, 200	0
39	BD	272/276 (98%)	-0.22	1 (0%) 93 92	39, 71, 116, 164	0
39	DD	272/276 (98%)	-0.16	1 (0%) 93 92	31, 69, 114, 173	0
40	BE	205/206 (99%)	0.26	11 (5%) 29 24	47, 96, 160, 200	0
40	DE	205/206 (99%)	0.07	8 (3%) 43 36	47, 90, 159, 199	0
41	BF	208/210 (99%)	-0.18	4 (1%) 70 63	43, 89, 164, 200	0
41	DF	208/210 (99%)	0.31	14 (6%) 21 17	44, 120, 179, 200	0
42	BG	181/182 (99%)	-0.01	8 (4%) 38 31	68, 118, 162, 194	0
42	DG	181/182 (99%)	0.93	33 (18%) 2 1	105, 163, 200, 200	0
43	BH	160/180 (88%)	1.37	50 (31%) 1 1	98, 160, 199, 200	0
43	DH	160/180 (88%)	0.55	12 (7%) 17 14	65, 135, 186, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BI	146/148 (98%)	0.44	11 (7%) 17 14	62, 122, 180, 199	0
44	DI	146/148 (98%)	2.02	51 (34%) 0 1	54, 152, 200, 200	0
45	BN	139/140 (99%)	0.22	3 (2%) 65 59	69, 110, 162, 198	0
45	DN	139/140 (99%)	0.10	3 (2%) 65 59	65, 107, 161, 190	0
46	BO	122/122 (100%)	-0.10	1 (0%) 87 84	53, 85, 116, 134	0
46	DO	122/122 (100%)	-0.19	0 100 100	48, 75, 110, 131	0
47	BP	146/150 (97%)	0.51	11 (7%) 17 14	46, 105, 171, 200	0
47	DP	146/150 (97%)	1.07	24 (16%) 2 2	60, 130, 184, 200	0
48	BQ	141/141 (100%)	0.26	6 (4%) 39 32	64, 103, 160, 200	0
48	DQ	141/141 (100%)	0.30	8 (5%) 27 22	55, 109, 156, 200	0
49	BR	117/118 (99%)	-0.06	0 100 100	53, 85, 130, 157	0
49	DR	117/118 (99%)	0.00	0 100 100	49, 91, 138, 150	0
50	BS	99/112 (88%)	0.35	4 (4%) 42 34	65, 115, 170, 200	0
50	DS	99/112 (88%)	1.52	33 (33%) 0 1	113, 164, 199, 200	0
51	BT	138/146 (94%)	0.09	11 (7%) 15 12	55, 102, 175, 200	0
51	DT	138/146 (94%)	-0.00	4 (2%) 55 49	62, 101, 178, 200	0
52	BU	117/118 (99%)	0.12	2 (1%) 73 67	52, 95, 146, 198	0
52	DU	117/118 (99%)	0.24	2 (1%) 73 67	59, 103, 156, 200	0
53	BV	101/101 (100%)	0.32	4 (3%) 42 34	66, 120, 158, 200	0
53	DV	101/101 (100%)	0.54	5 (4%) 32 26	57, 136, 175, 200	0
54	BW	113/113 (100%)	-0.10	0 100 100	48, 85, 143, 200	0
54	DW	113/113 (100%)	-0.01	4 (3%) 48 40	57, 93, 155, 200	0
55	BX	93/96 (96%)	-0.15	1 (1%) 82 78	56, 86, 120, 156	0
55	DX	93/96 (96%)	0.05	1 (1%) 82 78	57, 95, 135, 152	0
56	BY	101/110 (91%)	1.19	18 (17%) 2 1	67, 115, 183, 200	0
56	DY	101/110 (91%)	1.36	25 (24%) 1 1	62, 134, 192, 200	0
57	BZ	177/206 (85%)	0.86	28 (15%) 3 2	80, 150, 200, 200	0
57	DZ	177/206 (85%)	1.21	48 (27%) 1 1	94, 164, 200, 200	0
All	All	21244/22004 (96%)	0.29	1597 (7%) 17 14	31, 108, 192, 200	0

The worst 5 of 1597 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	BQ	140	ALA	21.0
25	CY	17	C	19.9
38	DC	172	HIS	18.7
13	AM	123	ALA	18.2
29	D3	1	MET	15.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
22	5MU	AV	54	21/22	0.91	0.14	-	104,135,151,151	0
25	PHA	CY	77	11/11	0.94	0.46	-	60,62,65,66	0
25	PHA	AY	77	11/11	0.94	0.34	-	60,62,65,66	0
25	8AN	CY	76	22/23	0.95	0.22	-	37,58,79,189	0
22	5MU	CV	54	21/22	0.82	0.27	-	173,181,194,194	0
25	8AN	AY	76	22/23	0.95	0.18	-	37,58,79,189	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
58	MG	BA	3351	1/1	0.66	1.07	57.46	125,125,125,125	0
58	MG	DA	3438	1/1	0.94	0.66	45.67	97,97,97,97	0
58	MG	BA	3367	1/1	0.86	0.59	45.50	107,107,107,107	0
58	MG	BA	3007	1/1	0.87	0.53	42.95	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	1743	1/1	0.58	0.73	42.07	86,86,86,86	0
58	MG	BA	3100	1/1	0.88	0.54	32.78	43,43,43,43	0
58	MG	BA	3373	1/1	0.85	0.68	30.69	56,56,56,56	1
58	MG	BA	3072	1/1	0.89	0.49	29.78	67,67,67,67	0
58	MG	DA	3143	1/1	0.93	0.72	29.64	63,63,63,63	0
58	MG	BA	3113	1/1	0.80	0.90	29.63	82,82,82,82	0
58	MG	DA	3201	1/1	0.81	0.65	27.32	55,55,55,55	0
58	MG	BA	3051	1/1	0.98	0.54	24.84	45,45,45,45	0
58	MG	DA	3114	1/1	0.99	0.46	24.30	33,33,33,33	0
58	MG	AA	1783	1/1	0.71	0.52	22.82	144,144,144,144	0
58	MG	BA	3003	1/1	0.94	0.38	22.45	68,68,68,68	0
58	MG	BB	205	1/1	0.85	1.13	22.27	45,45,45,45	1
58	MG	BA	3285	1/1	0.31	0.97	21.27	112,112,112,112	0
58	MG	BA	3156	1/1	0.90	0.69	20.53	89,89,89,89	0
58	MG	BA	3126	1/1	0.95	0.53	19.33	47,47,47,47	0
58	MG	BA	3226	1/1	0.90	0.34	19.16	33,33,33,33	0
58	MG	DA	3222	1/1	0.91	0.38	18.68	39,39,39,39	0
58	MG	DA	3060	1/1	0.94	0.48	18.53	35,35,35,35	0
58	MG	DA	3137	1/1	0.93	0.44	18.30	39,39,39,39	0
58	MG	DN	201	1/1	0.70	1.46	18.29	95,95,95,95	0
58	MG	CA	1627	1/1	0.53	0.87	18.10	97,97,97,97	0
58	MG	DA	3007	1/1	0.97	0.45	17.68	40,40,40,40	0
58	MG	BA	3167	1/1	0.93	0.44	17.39	55,55,55,55	0
58	MG	DA	3182	1/1	0.90	0.40	17.20	65,65,65,65	0
58	MG	DA	3209	1/1	0.56	0.64	17.14	105,105,105,105	0
58	MG	BA	3115	1/1	0.99	0.54	17.10	42,42,42,42	0
58	MG	DA	3164	1/1	0.89	0.35	16.83	63,63,63,63	0
58	MG	BA	3236	1/1	0.77	0.38	16.83	67,67,67,67	0
58	MG	BA	3221	1/1	0.55	0.47	16.46	72,72,72,72	0
58	MG	BA	3048	1/1	0.97	0.42	16.44	32,32,32,32	0
58	MG	BA	3249	1/1	0.59	0.36	16.24	57,57,57,57	0
58	MG	B7	101	1/1	0.95	1.06	15.68	73,73,73,73	1
58	MG	BA	3223	1/1	0.50	0.48	15.41	82,82,82,82	0
58	MG	DA	3018	1/1	0.83	0.53	15.35	51,51,51,51	0
58	MG	BA	3182	1/1	0.92	0.30	15.01	107,107,107,107	0
58	MG	AA	1627	1/1	0.93	0.57	14.54	74,74,74,74	0
58	MG	DA	3023	1/1	0.98	0.52	14.47	61,61,61,61	0
58	MG	DA	3093	1/1	0.83	0.37	14.12	50,50,50,50	0
58	MG	DA	3245	1/1	0.78	0.55	13.91	64,64,64,64	0
58	MG	AW	116	1/1	0.79	0.59	13.67	129,129,129,129	1
58	MG	DA	3050	1/1	0.92	0.57	13.64	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	1638	1/1	0.82	0.53	13.63	115,115,115,115	0
58	MG	BA	3094	1/1	0.93	0.41	13.58	63,63,63,63	0
58	MG	DA	3064	1/1	0.92	0.48	12.98	61,61,61,61	0
58	MG	CA	1684	1/1	0.86	0.26	12.88	67,67,67,67	0
58	MG	DA	3099	1/1	0.96	0.52	12.83	45,45,45,45	0
58	MG	BA	3071	1/1	0.80	0.34	12.58	70,70,70,70	0
58	MG	AA	1670	1/1	0.44	0.33	12.51	95,95,95,95	0
58	MG	CA	1742	1/1	0.76	0.61	12.45	94,94,94,94	0
58	MG	BA	3440	1/1	0.96	0.41	12.40	93,93,93,93	0
58	MG	BA	3303	1/1	0.96	0.32	12.35	89,89,89,89	0
58	MG	CA	1640	1/1	0.94	0.60	12.10	61,61,61,61	0
58	MG	AA	1683	1/1	0.78	0.35	12.09	72,72,72,72	0
58	MG	CA	1642	1/1	0.98	0.37	12.00	52,52,52,52	0
58	MG	BA	3447	1/1	0.72	0.39	11.88	104,104,104,104	0
58	MG	BA	3196	1/1	0.94	0.39	11.84	60,60,60,60	0
58	MG	DA	3242	1/1	0.98	0.30	11.71	22,22,22,22	0
58	MG	DA	3195	1/1	0.75	0.30	11.47	96,96,96,96	0
58	MG	CA	1638	1/1	0.76	0.46	11.14	82,82,82,82	0
58	MG	DA	3120	1/1	0.87	0.32	11.02	81,81,81,81	0
58	MG	BA	3144	1/1	0.88	0.44	10.88	68,68,68,68	0
58	MG	AA	1712	1/1	0.85	0.46	10.73	67,67,67,67	0
58	MG	BA	3150	1/1	0.78	0.44	10.71	73,73,73,73	0
58	MG	DA	3125	1/1	0.97	0.44	10.68	53,53,53,53	0
58	MG	BA	3290	1/1	0.78	0.28	10.53	51,51,51,51	0
58	MG	CA	1671	1/1	0.86	0.34	10.46	79,79,79,79	0
58	MG	CA	1619	1/1	0.75	0.78	10.18	119,119,119,119	0
58	MG	AA	1741	1/1	0.94	0.45	9.73	72,72,72,72	0
58	MG	DA	3217	1/1	0.91	0.47	9.51	109,109,109,109	0
58	MG	AA	1810	1/1	0.95	0.30	9.41	36,36,36,36	0
58	MG	DA	3199	1/1	0.85	0.31	9.21	68,68,68,68	0
58	MG	BA	3396	1/1	0.86	0.34	8.93	78,78,78,78	1
58	MG	BA	3008	1/1	0.98	0.37	8.87	31,31,31,31	0
58	MG	BN	201	1/1	0.81	0.94	8.78	79,79,79,79	0
58	MG	DA	3027	1/1	0.92	0.35	8.72	50,50,50,50	0
58	MG	BA	3029	1/1	0.90	0.40	8.69	63,63,63,63	0
58	MG	AA	1640	1/1	0.92	0.54	8.67	56,56,56,56	0
58	MG	DA	3401	1/1	0.82	0.34	8.52	68,68,68,68	0
58	MG	DA	3236	1/1	0.94	0.42	8.41	37,37,37,37	0
58	MG	DA	3107	1/1	0.73	0.32	8.41	95,95,95,95	0
58	MG	BA	3389	1/1	0.54	0.33	8.30	107,107,107,107	0
58	MG	BA	3246	1/1	0.98	0.29	8.11	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3120	1/1	0.93	0.29	7.90	87,87,87,87	0
58	MG	CA	1721	1/1	0.95	0.34	7.82	94,94,94,94	0
58	MG	BA	3068	1/1	0.99	0.33	7.78	40,40,40,40	0
58	MG	DA	3047	1/1	0.96	0.34	7.75	27,27,27,27	0
58	MG	AA	1686	1/1	0.80	0.33	7.74	75,75,75,75	0
58	MG	DA	3146	1/1	0.77	0.28	7.66	58,58,58,58	1
58	MG	DA	3175	1/1	0.69	0.33	7.59	87,87,87,87	0
58	MG	DA	3062	1/1	0.97	0.33	7.57	13,13,13,13	0
58	MG	DA	3072	1/1	0.95	0.40	7.49	31,31,31,31	0
58	MG	AA	1728	1/1	0.81	0.26	7.30	69,69,69,69	0
58	MG	BA	3117	1/1	0.99	0.34	7.15	38,38,38,38	0
58	MG	DA	3116	1/1	0.97	0.28	7.08	30,30,30,30	0
58	MG	CA	1624	1/1	0.96	0.33	7.06	99,99,99,99	0
58	MG	DA	3057	1/1	0.99	0.28	7.01	18,18,18,18	0
58	MG	BA	3134	1/1	0.90	0.28	6.99	70,70,70,70	0
58	MG	BA	3031	1/1	0.94	0.31	6.92	35,35,35,35	0
58	MG	DA	3006	1/1	0.88	0.27	6.90	87,87,87,87	0
58	MG	DA	3154	1/1	0.84	0.29	6.88	101,101,101,101	0
58	MG	DA	3048	1/1	0.86	0.35	6.82	44,44,44,44	0
58	MG	CA	1714	1/1	0.98	0.48	6.80	102,102,102,102	0
58	MG	BA	3073	1/1	0.97	0.42	6.76	36,36,36,36	0
58	MG	BA	3058	1/1	0.98	0.32	6.75	49,49,49,49	0
58	MG	BA	3060	1/1	0.83	0.27	6.73	72,72,72,72	0
58	MG	DA	3194	1/1	0.87	0.31	6.55	84,84,84,84	0
58	MG	BB	216	1/1	0.91	0.30	6.40	94,94,94,94	1
58	MG	BA	3342	1/1	0.95	0.33	6.37	92,92,92,92	0
58	MG	DA	3009	1/1	0.82	0.28	6.33	44,44,44,44	0
58	MG	CA	1702	1/1	0.94	0.32	6.28	88,88,88,88	0
58	MG	BA	3065	1/1	0.85	0.35	6.25	59,59,59,59	0
58	MG	DA	3190	1/1	0.98	0.44	6.13	49,49,49,49	0
58	MG	DA	3148	1/1	0.69	0.39	5.98	88,88,88,88	0
58	MG	DA	3417	1/1	0.90	0.31	5.98	71,71,71,71	0
58	MG	BA	3366	1/1	0.97	0.29	5.82	60,60,60,60	0
58	MG	DA	3275	1/1	0.86	0.29	5.68	57,57,57,57	0
58	MG	AA	1698	1/1	0.93	0.28	5.65	61,61,61,61	0
58	MG	DA	3011	1/1	0.98	0.32	5.60	27,27,27,27	0
58	MG	DA	3081	1/1	0.97	0.29	5.56	96,96,96,96	0
58	MG	BA	3172	1/1	0.90	0.25	5.55	78,78,78,78	0
58	MG	AA	1628	1/1	0.93	0.31	5.54	71,71,71,71	0
58	MG	BA	3403	1/1	0.71	0.39	5.54	58,58,58,58	0
58	MG	AA	1613	1/1	0.96	0.37	5.50	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3240	1/1	0.97	0.32	5.43	32,32,32,32	0
58	MG	AA	1695	1/1	0.73	0.26	5.42	62,62,62,62	0
58	MG	AA	1616	1/1	0.78	0.34	5.41	74,74,74,74	0
58	MG	DA	3403	1/1	0.91	0.50	5.29	72,72,72,72	0
58	MG	BA	3024	1/1	0.99	0.40	5.24	36,36,36,36	0
58	MG	DA	3443	1/1	0.00	0.22	5.08	111,111,111,111	0
58	MG	BA	3090	1/1	0.98	0.26	5.03	40,40,40,40	0
58	MG	BA	3076	1/1	0.97	0.29	4.93	40,40,40,40	0
58	MG	BA	3178	1/1	0.88	0.30	4.89	67,67,67,67	0
58	MG	DA	3094	1/1	0.98	0.27	4.87	43,43,43,43	0
58	MG	BA	3255	1/1	0.83	0.19	4.85	102,102,102,102	0
58	MG	BB	204	1/1	0.66	0.24	4.79	103,103,103,103	0
58	MG	BA	3199	1/1	0.70	0.23	4.74	73,73,73,73	0
58	MG	AA	1785	1/1	0.78	0.27	4.63	70,70,70,70	0
58	MG	BA	3049	1/1	0.96	0.31	4.62	35,35,35,35	0
58	MG	BA	3077	1/1	0.96	0.28	4.59	55,55,55,55	0
58	MG	DA	3281	1/1	0.98	0.28	4.58	65,65,65,65	0
58	MG	DA	3131	1/1	0.94	0.27	4.53	40,40,40,40	0
58	MG	BA	3095	1/1	0.96	0.26	4.52	40,40,40,40	0
58	MG	DA	3172	1/1	0.96	0.27	4.51	42,42,42,42	0
58	MG	AG	201	1/1	0.68	1.30	4.42	127,127,127,127	0
58	MG	CA	1795	1/1	0.89	0.21	4.38	55,55,55,55	0
58	MG	AA	1604	1/1	0.79	0.41	4.37	99,99,99,99	0
58	MG	AA	1663	1/1	0.96	0.20	4.36	31,31,31,31	0
58	MG	DA	3112	1/1	0.90	0.32	4.36	70,70,70,70	0
58	MG	BA	3405	1/1	0.95	0.36	4.35	53,53,53,53	0
58	MG	DA	3353	1/1	0.97	0.20	4.34	58,58,58,58	0
58	MG	DA	3261	1/1	0.95	0.37	4.33	32,32,32,32	0
58	MG	CA	1729	1/1	0.82	0.35	4.32	81,81,81,81	0
58	MG	DE	302	1/1	0.93	0.53	4.29	83,83,83,83	0
58	MG	BA	3311	1/1	0.98	0.33	4.27	71,71,71,71	1
58	MG	AA	1786	1/1	0.90	0.24	4.20	55,55,55,55	0
58	MG	AA	1701	1/1	0.93	0.33	4.19	61,61,61,61	0
58	MG	DA	3305	1/1	0.89	0.33	4.17	60,60,60,60	0
58	MG	BA	3198	1/1	0.87	0.23	4.16	61,61,61,61	0
58	MG	DA	3028	1/1	0.89	0.32	4.15	63,63,63,63	0
58	MG	DA	3089	1/1	0.99	0.26	4.11	45,45,45,45	0
58	MG	BA	3427	1/1	0.97	0.28	4.08	106,106,106,106	0
58	MG	BA	3020	1/1	0.95	0.34	3.99	41,41,41,41	0
58	MG	DA	3013	1/1	0.87	0.24	3.90	67,67,67,67	0
58	MG	CA	1628	1/1	0.96	0.34	3.82	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	D7	102	1/1	0.71	0.63	3.78	73,73,73,73	1
58	MG	BA	3132	1/1	0.89	0.27	3.71	36,36,36,36	0
58	MG	BA	3067	1/1	0.97	0.27	3.71	34,34,34,34	0
58	MG	BA	3063	1/1	0.94	0.25	3.65	20,20,20,20	0
58	MG	BA	3265	1/1	0.97	0.36	3.62	32,32,32,32	0
58	MG	BA	3281	1/1	0.97	0.27	3.55	54,54,54,54	0
58	MG	CA	1664	1/1	0.97	0.25	3.40	40,40,40,40	0
58	MG	DA	3239	1/1	0.89	0.23	3.38	63,63,63,63	0
58	MG	BA	3292	1/1	0.81	0.24	3.28	65,65,65,65	0
58	MG	DA	3030	1/1	0.95	0.21	3.14	24,24,24,24	0
58	MG	CA	1630	1/1	0.94	0.22	3.12	81,81,81,81	0
58	MG	BA	3026	1/1	0.97	0.20	3.12	52,52,52,52	0
58	MG	DA	3390	1/1	0.79	0.29	3.11	112,112,112,112	0
58	MG	BA	3312	1/1	0.98	0.34	3.08	32,32,32,32	0
58	MG	BA	3121	1/1	0.86	0.20	3.04	82,82,82,82	0
58	MG	DA	3307	1/1	0.97	0.29	3.03	30,30,30,30	0
58	MG	B2	602	1/1	0.89	0.31	3.02	112,112,112,112	0
58	MG	DA	3076	1/1	0.96	0.26	2.92	48,48,48,48	0
58	MG	BA	3169	1/1	0.94	0.17	2.85	83,83,83,83	0
58	MG	DA	3036	1/1	0.78	0.18	2.85	94,94,94,94	0
58	MG	DA	3308	1/1	0.89	0.26	2.83	48,48,48,48	0
58	MG	BA	3313	1/1	0.83	0.23	2.80	38,38,38,38	0
58	MG	DA	3431	1/1	0.86	0.22	2.78	137,137,137,137	0
58	MG	BA	3054	1/1	0.98	0.22	2.78	38,38,38,38	0
58	MG	DA	3430	1/1	0.82	0.21	2.67	106,106,106,106	0
59	PAR	AA	1814	42/42	0.93	0.22	2.66	80,85,103,108	0
58	MG	CA	1713	1/1	0.94	0.23	2.60	54,54,54,54	0
58	MG	BA	3038	1/1	0.98	0.23	2.59	35,35,35,35	0
58	MG	BA	3082	1/1	0.96	0.24	2.56	63,63,63,63	0
58	MG	DA	3316	1/1	0.99	0.28	2.47	41,41,41,41	0
58	MG	BA	3212	1/1	0.95	0.19	2.46	75,75,75,75	0
58	MG	BA	3254	1/1	0.90	0.18	2.45	74,74,74,74	0
58	MG	BA	3028	1/1	0.97	0.25	2.42	45,45,45,45	0
58	MG	AA	1717	1/1	0.95	0.32	2.42	48,48,48,48	0
58	MG	BA	3123	1/1	0.81	0.21	2.41	46,46,46,46	0
58	MG	DA	3111	1/1	0.95	0.21	2.39	44,44,44,44	0
58	MG	DA	3019	1/1	0.97	0.27	2.29	21,21,21,21	0
59	PAR	CA	1817	42/42	0.94	0.23	2.23	72,78,95,100	0
58	MG	DA	3079	1/1	0.97	0.24	2.14	22,22,22,22	0
58	MG	CA	1696	1/1	0.97	0.24	2.05	59,59,59,59	0
58	MG	DA	3269	1/1	0.82	0.18	2.03	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3176	1/1	0.77	0.22	2.00	62,62,62,62	0
58	MG	DD	302	1/1	0.83	0.37	1.99	64,64,64,64	0
58	MG	BA	3015	1/1	0.97	0.30	1.99	47,47,47,47	0
58	MG	DA	3298	1/1	0.72	0.27	1.93	50,50,50,50	0
58	MG	BA	3012	1/1	0.99	0.24	1.91	27,27,27,27	0
58	MG	BA	3322	1/1	0.99	0.25	1.90	42,42,42,42	0
58	MG	DA	3014	1/1	0.96	0.27	1.88	28,28,28,28	0
58	MG	BA	3195	1/1	0.94	0.27	1.85	48,48,48,48	0
58	MG	DA	3398	1/1	0.78	0.23	1.80	57,57,57,57	0
58	MG	CA	1712	1/1	0.87	0.16	1.75	128,128,128,128	0
58	MG	DA	3272	1/1	0.91	0.22	1.74	51,51,51,51	0
58	MG	DA	3067	1/1	0.98	0.22	1.69	31,31,31,31	0
58	MG	AA	1629	1/1	0.66	0.21	1.65	87,87,87,87	0
58	MG	BO	201	1/1	0.95	0.22	1.63	44,44,44,44	0
58	MG	BA	3057	1/1	0.99	0.22	1.54	35,35,35,35	0
58	MG	BA	3089	1/1	0.63	0.21	1.49	61,61,61,61	0
58	MG	BA	3200	1/1	0.69	0.20	1.45	52,52,52,52	0
58	MG	CA	1613	1/1	0.74	0.28	1.31	68,68,68,68	0
58	MG	BA	3383	1/1	0.95	0.19	1.25	89,89,89,89	0
58	MG	DD	301	1/1	0.97	0.26	1.25	27,27,27,27	0
58	MG	BA	3186	1/1	0.85	0.20	1.23	63,63,63,63	0
58	MG	DA	3404	1/1	0.84	0.21	1.22	51,51,51,51	0
58	MG	DA	3250	1/1	0.62	0.18	1.20	82,82,82,82	0
58	MG	CA	1805	1/1	0.84	0.19	1.15	59,59,59,59	1
58	MG	DA	3126	1/1	0.94	0.22	1.12	24,24,24,24	0
58	MG	DA	3122	1/1	0.90	0.20	1.11	49,49,49,49	0
58	MG	AA	1802	1/1	0.81	0.21	1.07	110,110,110,110	0
58	MG	CA	1610	1/1	0.98	0.20	1.02	46,46,46,46	0
58	MG	AV	101	1/1	0.98	0.24	0.95	34,34,34,34	0
58	MG	CA	1766	1/1	0.97	0.21	0.93	44,44,44,44	0
58	MG	DA	3078	1/1	0.96	0.19	0.88	24,24,24,24	0
58	MG	BA	3080	1/1	0.97	0.22	0.86	32,32,32,32	0
58	MG	BA	3037	1/1	0.93	0.14	0.84	61,61,61,61	0
58	MG	AA	1690	1/1	0.92	0.20	0.81	69,69,69,69	0
58	MG	BA	3147	1/1	0.99	0.23	0.75	20,20,20,20	0
58	MG	AA	1630	1/1	0.96	0.18	0.70	84,84,84,84	0
58	MG	BA	3368	1/1	0.96	0.18	0.68	74,74,74,74	0
58	MG	AA	1699	1/1	0.94	0.20	0.68	106,106,106,106	0
58	MG	CA	1718	1/1	0.97	0.24	0.64	71,71,71,71	0
58	MG	BA	3190	1/1	0.99	0.18	0.61	41,41,41,41	0
58	MG	DA	3386	1/1	0.97	0.21	0.56	49,49,49,49	0
58	MG	DA	3071	1/1	0.71	0.23	0.50	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	1705	1/1	0.67	0.21	0.50	76,76,76,76	0
58	MG	DA	3053	1/1	0.99	0.18	0.47	31,31,31,31	0
58	MG	DA	3191	1/1	0.60	0.25	0.39	75,75,75,75	0
60	ZN	CD	301	1/1	0.98	0.28	0.38	87,87,87,87	0
58	MG	DA	3066	1/1	0.98	0.19	0.29	22,22,22,22	0
58	MG	DA	3086	1/1	0.98	0.19	0.29	29,29,29,29	0
58	MG	CA	1706	1/1	0.93	0.17	0.22	56,56,56,56	0
58	MG	BA	3430	1/1	0.92	0.16	0.22	92,92,92,92	0
58	MG	DA	3025	1/1	0.98	0.18	0.13	42,42,42,42	0
58	MG	CV	101	1/1	0.99	0.20	0.10	25,25,25,25	0
58	MG	AA	1803	1/1	0.85	0.15	0.10	33,33,33,33	1
58	MG	AA	1642	1/1	0.93	0.19	0.09	34,34,34,34	0
60	ZN	AD	302	1/1	0.99	0.27	0.08	56,56,56,56	0
58	MG	BA	3102	1/1	0.99	0.22	0.08	49,49,49,49	0
58	MG	CA	1747	1/1	0.79	0.16	0.06	67,67,67,67	0
58	MG	DB	215	1/1	0.84	0.14	0.04	64,64,64,64	1
58	MG	BP	202	1/1	0.81	0.29	-0.05	14,14,14,14	1
58	MG	DA	3193	1/1	0.94	0.16	-0.05	62,62,62,62	0
58	MG	BF	302	1/1	0.97	0.19	-0.10	93,93,93,93	0
58	MG	AA	1610	1/1	0.99	0.17	-0.12	43,43,43,43	0
58	MG	AA	1713	1/1	0.93	0.21	-0.13	82,82,82,82	0
58	MG	DA	3276	1/1	0.97	0.21	-0.15	75,75,75,75	0
58	MG	BA	3325	1/1	0.85	0.38	-0.18	104,104,104,104	1
58	MG	CW	119	1/1	0.81	0.36	-0.18	108,108,108,108	0
58	MG	DA	3133	1/1	0.91	0.18	-0.22	52,52,52,52	0
58	MG	AA	1721	1/1	0.91	0.22	-0.22	55,55,55,55	0
58	MG	DA	3197	1/1	0.65	0.15	-0.23	89,89,89,89	1
58	MG	DA	3168	1/1	0.92	0.17	-0.23	62,62,62,62	0
58	MG	DA	3235	1/1	0.94	0.21	-0.26	44,44,44,44	0
58	MG	BA	3111	1/1	0.92	0.17	-0.31	38,38,38,38	0
58	MG	DA	3176	1/1	0.94	0.17	-0.37	49,49,49,49	0
58	MG	DA	3075	1/1	0.98	0.20	-0.41	33,33,33,33	0
58	MG	DA	3056	1/1	0.88	0.18	-0.47	48,48,48,48	0
58	MG	BA	3390	1/1	0.95	0.19	-0.50	57,57,57,57	0
58	MG	DA	3389	1/1	0.82	0.28	-0.51	42,42,42,42	1
58	MG	BF	301	1/1	0.85	0.19	-0.54	70,70,70,70	0
58	MG	BA	3075	1/1	0.95	0.17	-0.60	36,36,36,36	0
58	MG	DA	3424	1/1	0.89	0.22	-0.62	53,53,53,53	0
58	MG	DA	3428	1/1	0.77	0.13	-0.63	91,91,91,91	0
58	MG	CW	121	1/1	0.86	0.53	-0.66	125,125,125,125	0
58	MG	BA	3079	1/1	0.90	0.16	-0.69	28,28,28,28	0
58	MG	DA	3037	1/1	0.98	0.17	-0.74	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	ZN	AN	101	1/1	0.99	0.17	-0.77	106,106,106,106	0
58	MG	BA	3087	1/1	0.97	0.17	-0.79	47,47,47,47	0
58	MG	DA	3180	1/1	0.84	0.14	-0.87	79,79,79,79	0
60	ZN	B9	101	1/1	0.90	0.51	-0.91	199,199,199,199	0
58	MG	D2	103	1/1	0.97	0.17	-0.93	78,78,78,78	0
60	ZN	CN	101	1/1	0.98	0.16	-0.94	109,109,109,109	0
58	MG	BA	3239	1/1	0.99	0.14	-0.94	48,48,48,48	0
58	MG	DA	3080	1/1	0.96	0.17	-0.96	35,35,35,35	0
58	MG	DF	301	1/1	0.94	0.22	-0.98	90,90,90,90	0
58	MG	DA	3186	1/1	0.95	0.16	-1.10	49,49,49,49	0
58	MG	AA	1804	1/1	0.94	0.16	-1.12	49,49,49,49	0
58	MG	DA	3167	1/1	0.84	0.12	-1.12	79,79,79,79	0
58	MG	BA	3266	1/1	0.96	0.16	-1.14	64,64,64,64	0
58	MG	CA	1720	1/1	0.91	0.15	-1.18	79,79,79,79	0
58	MG	CA	1711	1/1	0.89	0.08	-1.18	95,95,95,95	0
58	MG	AA	1710	1/1	0.93	0.12	-1.19	82,82,82,82	0
58	MG	DA	3119	1/1	0.93	0.18	-1.23	50,50,50,50	0
58	MG	BA	3016	1/1	0.98	0.17	-1.28	50,50,50,50	0
58	MG	BA	3170	1/1	0.74	0.12	-1.29	65,65,65,65	0
58	MG	BA	3152	1/1	0.98	0.14	-1.34	30,30,30,30	0
58	MG	BA	3400	1/1	0.88	0.13	-1.35	67,67,67,67	0
58	MG	DA	3174	1/1	0.94	0.15	-1.42	77,77,77,77	0
58	MG	DA	3177	1/1	0.93	0.15	-1.42	103,103,103,103	0
58	MG	BA	3432	1/1	0.84	0.13	-1.44	57,57,57,57	0
58	MG	BA	3194	1/1	0.95	0.12	-1.47	43,43,43,43	0
58	MG	CA	1700	1/1	0.97	0.14	-1.50	102,102,102,102	0
58	MG	BA	3302	1/1	0.83	0.17	-1.52	56,56,56,56	0
58	MG	CA	1699	1/1	0.94	0.14	-1.53	44,44,44,44	0
58	MG	DA	3208	1/1	0.96	0.10	-1.54	76,76,76,76	0
58	MG	CA	1707	1/1	0.94	0.09	-1.56	82,82,82,82	0
58	MG	BA	3283	1/1	0.94	0.06	-1.58	100,100,100,100	0
58	MG	DA	3015	1/1	0.98	0.17	-1.59	45,45,45,45	0
58	MG	AA	1720	1/1	0.92	0.13	-1.61	56,56,56,56	0
58	MG	DA	3442	1/1	0.97	0.13	-1.63	71,71,71,71	0
58	MG	AA	1605	1/1	0.94	0.13	-1.68	53,53,53,53	0
58	MG	CA	1691	1/1	0.84	0.15	-1.77	67,67,67,67	0
58	MG	DA	3297	1/1	0.81	0.15	-1.79	84,84,84,84	0
58	MG	DA	3070	1/1	0.74	0.12	-1.81	54,54,54,54	0
58	MG	CA	1616	1/1	0.88	0.09	-1.82	75,75,75,75	0
58	MG	BA	3207	1/1	0.90	0.10	-1.83	59,59,59,59	0
58	MG	AW	119	1/1	0.79	0.15	-1.86	98,98,98,98	0
58	MG	CA	1790	1/1	0.94	0.10	-1.88	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	1804	1/1	0.85	0.13	-1.90	85,85,85,85	0
58	MG	DA	3243	1/1	0.96	0.16	-1.90	45,45,45,45	0
58	MG	BA	3247	1/1	0.94	0.16	-1.92	33,33,33,33	0
58	MG	AA	1624	1/1	0.77	0.12	-1.93	74,74,74,74	0
58	MG	BN	202	1/1	0.96	0.12	-1.97	97,97,97,97	1
58	MG	CA	1605	1/1	0.92	0.12	-1.97	72,72,72,72	0
58	MG	BA	3084	1/1	0.98	0.16	-1.99	39,39,39,39	0
58	MG	DA	3368	1/1	0.99	0.11	-2.08	57,57,57,57	1
58	MG	DA	3129	1/1	0.94	0.12	-2.26	58,58,58,58	1
58	MG	BA	3168	1/1	0.95	0.12	-2.26	72,72,72,72	0
58	MG	BA	3127	1/1	0.97	0.15	-2.45	35,35,35,35	0
58	MG	DA	3418	1/1	0.97	0.14	-2.46	60,60,60,60	0
58	MG	BA	3271	1/1	0.83	0.08	-2.50	114,114,114,114	0
58	MG	BA	3081	1/1	0.98	0.13	-2.60	46,46,46,46	0
58	MG	BA	3264	1/1	0.95	0.09	-2.60	27,27,27,27	0
58	MG	BA	3204	1/1	0.93	0.15	-2.66	51,51,51,51	0
60	ZN	D9	101	1/1	0.88	0.24	-2.68	196,196,196,196	0
58	MG	AA	1746	1/1	0.91	0.11	-2.69	57,57,57,57	0
58	MG	DB	207	1/1	0.90	0.07	-2.72	79,79,79,79	0
58	MG	BA	3014	1/1	0.92	0.11	-2.78	40,40,40,40	0
58	MG	AA	1716	1/1	0.96	0.07	-2.79	46,46,46,46	0
58	MG	AA	1641	1/1	0.89	0.08	-2.84	65,65,65,65	0
58	MG	BA	3179	1/1	0.97	0.10	-2.92	48,48,48,48	0
58	MG	BB	207	1/1	0.91	0.09	-2.93	81,81,81,81	0
58	MG	CA	1668	1/1	0.91	0.09	-2.96	80,80,80,80	0
58	MG	BA	3406	1/1	0.97	0.13	-2.99	38,38,38,38	0
58	MG	CA	1632	1/1	0.96	0.09	-3.11	73,73,73,73	0
58	MG	AA	1703	1/1	0.88	0.10	-3.11	45,45,45,45	0
58	MG	BA	3112	1/1	0.98	0.11	-3.27	35,35,35,35	0
58	MG	DA	3150	1/1	0.97	0.10	-3.29	46,46,46,46	0
58	MG	DA	3115	1/1	0.88	0.15	-3.30	36,36,36,36	0
58	MG	BA	3116	1/1	0.95	0.16	-3.39	38,38,38,38	0
58	MG	BA	3188	1/1	0.97	0.13	-3.43	47,47,47,47	0
58	MG	CA	1808	1/1	0.67	0.10	-3.52	107,107,107,107	0
58	MG	DA	3055	1/1	0.98	0.13	-3.79	44,44,44,44	0
58	MG	BA	3184	1/1	0.94	0.08	-3.90	52,52,52,52	0
58	MG	CA	1717	1/1	0.90	0.11	-4.39	67,67,67,67	0
58	MG	AA	1705	1/1	0.90	0.12	-4.39	35,35,35,35	0
58	MG	AA	1806	1/1	0.92	0.07	-4.44	68,68,68,68	0
58	MG	BA	3275	1/1	0.82	0.13	-4.47	61,61,61,61	0
58	MG	DA	3202	1/1	0.93	0.06	-4.48	38,38,38,38	0
58	MG	BA	3277	1/1	0.92	0.11	-4.59	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3285	1/1	0.97	0.07	-4.83	36,36,36,36	0
58	MG	DA	3315	1/1	0.97	0.06	-4.95	29,29,29,29	0
58	MG	DA	3347	1/1	0.89	0.09	-4.98	71,71,71,71	0
58	MG	DA	3271	1/1	0.94	0.08	-5.15	62,62,62,62	0
58	MG	DA	3270	1/1	0.89	0.12	-5.16	44,44,44,44	0
58	MG	BA	3248	1/1	0.97	0.08	-5.20	22,22,22,22	0
58	MG	CA	1641	1/1	0.96	0.12	-5.53	39,39,39,39	0
58	MG	BA	3056	1/1	0.96	0.13	-5.69	53,53,53,53	0
58	MG	DA	3244	1/1	0.98	0.12	-5.84	22,22,22,22	0
58	MG	BA	3280	1/1	0.89	0.07	-5.97	87,87,87,87	0
58	MG	BA	3274	1/1	0.89	0.12	-6.02	54,54,54,54	0
58	MG	DA	3074	1/1	0.91	0.12	-6.21	40,40,40,40	0
58	MG	DA	3118	1/1	0.90	0.10	-6.30	29,29,29,29	0
58	MG	BA	3320	1/1	0.93	0.07	-6.34	40,40,40,40	0
58	MG	BA	3386	1/1	0.83	0.09	-6.36	63,63,63,63	0
58	MG	BA	3119	1/1	0.96	0.06	-7.52	24,24,24,24	0
58	MG	CA	1787	1/1	0.88	0.09	-7.91	56,56,56,56	0
58	MG	BA	3444	1/1	0.95	0.09	-8.19	90,90,90,90	0
58	MG	BA	3161	1/1	0.86	0.42	-	68,68,68,68	0
58	MG	DA	3349	1/1	0.92	0.16	-	103,103,103,103	0
58	MG	DA	3184	1/1	0.94	0.26	-	56,56,56,56	0
58	MG	BA	3409	1/1	0.75	0.10	-	95,95,95,95	0
58	MG	AV	105	1/1	0.64	0.51	-	86,86,86,86	0
58	MG	BA	3291	1/1	0.56	0.16	-	90,90,90,90	0
58	MG	DA	3102	1/1	0.57	0.80	-	107,107,107,107	0
58	MG	CA	1728	1/1	0.95	0.10	-	86,86,86,86	0
58	MG	DA	3022	1/1	0.91	0.16	-	69,69,69,69	0
58	MG	AA	1753	1/1	0.78	0.37	-	81,81,81,81	0
58	MG	BA	3118	1/1	0.88	0.38	-	53,53,53,53	0
58	MG	BB	201	1/1	0.78	0.81	-	94,94,94,94	0
58	MG	CA	1604	1/1	0.98	0.13	-	107,107,107,107	0
58	MG	CA	1635	1/1	0.60	0.31	-	81,81,81,81	0
58	MG	BA	3315	1/1	0.97	0.40	-	100,100,100,100	1
58	MG	BA	3086	1/1	0.94	0.32	-	36,36,36,36	0
58	MG	AA	1688	1/1	-0.01	0.33	-	118,118,118,118	0
58	MG	CA	1803	1/1	0.91	0.07	-	70,70,70,70	0
58	MG	AA	1811	1/1	0.95	0.15	-	93,93,93,93	0
58	MG	B5	102	1/1	0.77	0.89	-	73,73,73,73	1
58	MG	CA	1611	1/1	0.95	0.23	-	61,61,61,61	0
58	MG	BA	3350	1/1	0.83	0.35	-	105,105,105,105	0
58	MG	CA	1654	1/1	0.96	0.27	-	76,76,76,76	1
58	MG	DA	3144	1/1	0.72	0.40	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3363	1/1	0.84	0.08	-	114,114,114,114	0
58	MG	BE	301	1/1	0.95	0.21	-	30,30,30,30	0
58	MG	DA	3051	1/1	0.95	0.11	-	110,110,110,110	1
58	MG	DA	3171	1/1	0.68	1.84	-	88,88,88,88	0
58	MG	BA	3093	1/1	0.97	0.28	-	37,37,37,37	0
58	MG	BA	3355	1/1	0.65	0.49	-	63,63,63,63	1
58	MG	AA	1725	1/1	0.32	0.31	-	77,77,77,77	0
58	MG	CA	1796	1/1	0.93	0.09	-	51,51,51,51	1
58	MG	DA	3357	1/1	0.36	0.24	-	111,111,111,111	0
58	MG	BD	301	1/1	0.95	0.16	-	44,44,44,44	0
58	MG	DA	3322	1/1	0.88	0.35	-	100,100,100,100	1
58	MG	AA	1634	1/1	0.92	0.15	-	106,106,106,106	0
58	MG	DA	3360	1/1	0.21	1.08	-	97,97,97,97	1
58	MG	DA	3215	1/1	0.97	0.10	-	82,82,82,82	0
58	MG	DA	3323	1/1	0.71	0.23	-	105,105,105,105	1
58	MG	DA	3310	1/1	0.97	0.26	-	110,110,110,110	1
58	MG	CA	1633	1/1	0.92	0.10	-	73,73,73,73	0
58	MG	BA	3371	1/1	0.86	0.27	-	81,81,81,81	0
58	MG	BA	3347	1/1	0.57	0.54	-	85,85,85,85	1
58	MG	BA	3001	1/1	0.78	0.32	-	71,71,71,71	0
58	MG	DA	3419	1/1	0.95	0.13	-	83,83,83,83	0
58	MG	DA	3437	1/1	0.91	0.36	-	52,52,52,52	0
58	MG	DA	3399	1/1	0.73	0.74	-	131,131,131,131	0
58	MG	BA	3449	1/1	0.93	0.47	-	107,107,107,107	1
58	MG	BA	3133	1/1	0.97	0.27	-	56,56,56,56	0
58	MG	BA	3078	1/1	0.96	0.15	-	23,23,23,23	0
58	MG	AA	1656	1/1	0.88	0.10	-	68,68,68,68	0
58	MG	AA	1615	1/1	0.88	0.15	-	63,63,63,63	0
58	MG	AA	1622	1/1	0.89	0.23	-	45,45,45,45	0
58	MG	DA	3341	1/1	0.84	0.47	-	78,78,78,78	1
58	MG	BA	3369	1/1	0.89	0.32	-	96,96,96,96	0
58	MG	AA	1678	1/1	0.88	0.32	-	93,93,93,93	1
58	MG	CA	1660	1/1	0.79	0.29	-	91,91,91,91	0
58	MG	DA	3149	1/1	0.94	0.48	-	73,73,73,73	0
58	MG	DA	3366	1/1	0.95	0.16	-	77,77,77,77	0
58	MG	BA	3166	1/1	0.86	0.27	-	71,71,71,71	0
58	MG	DA	3427	1/1	0.97	0.19	-	133,133,133,133	0
58	MG	BA	3232	1/1	0.73	0.67	-	101,101,101,101	0
58	MG	BA	3228	1/1	0.71	0.61	-	107,107,107,107	1
58	MG	AA	1748	1/1	0.87	0.12	-	76,76,76,76	0
58	MG	AA	1726	1/1	0.91	0.32	-	65,65,65,65	0
58	MG	CA	1810	1/1	0.46	0.76	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3291	1/1	0.62	0.22	-	105,105,105,105	0
58	MG	BA	3208	1/1	0.92	0.20	-	59,59,59,59	0
58	MG	DA	3187	1/1	0.87	0.28	-	71,71,71,71	0
58	MG	DA	3017	1/1	0.91	0.20	-	58,58,58,58	0
58	MG	DA	3351	1/1	0.55	0.52	-	79,79,79,79	1
58	MG	AA	1776	1/1	0.84	0.14	-	94,94,94,94	0
58	MG	DA	3138	1/1	0.99	0.14	-	25,25,25,25	0
58	MG	DA	3029	1/1	0.98	0.23	-	25,25,25,25	0
58	MG	CW	104	1/1	0.85	0.44	-	108,108,108,108	1
58	MG	AA	1669	1/1	0.87	0.42	-	82,82,82,82	0
58	MG	AA	1664	1/1	0.92	0.24	-	55,55,55,55	0
58	MG	AA	1687	1/1	0.87	0.33	-	105,105,105,105	0
58	MG	CV	102	1/1	0.81	0.12	-	89,89,89,89	1
58	MG	CW	112	1/1	0.88	0.16	-	81,81,81,81	1
58	MG	BA	3027	1/1	0.98	0.33	-	25,25,25,25	0
58	MG	DA	3378	1/1	0.96	0.28	-	72,72,72,72	0
58	MG	BA	3032	1/1	0.97	0.17	-	68,68,68,68	0
58	MG	AA	1673	1/1	0.91	0.27	-	53,53,53,53	0
58	MG	DB	218	1/1	0.96	0.15	-	82,82,82,82	1
58	MG	BA	3069	1/1	0.98	0.42	-	31,31,31,31	0
58	MG	DA	3034	1/1	0.91	0.24	-	54,54,54,54	0
58	MG	BA	3334	1/1	0.93	0.11	-	137,137,137,137	0
58	MG	DA	3327	1/1	0.10	0.72	-	106,106,106,106	1
58	MG	BA	3289	1/1	0.80	0.21	-	93,93,93,93	0
58	MG	DA	3061	1/1	0.98	0.28	-	43,43,43,43	0
58	MG	BA	3267	1/1	0.80	0.23	-	66,66,66,66	0
58	MG	CA	1678	1/1	0.54	0.28	-	109,109,109,109	0
58	MG	BA	3377	1/1	0.75	0.55	-	94,94,94,94	0
58	MG	BA	3206	1/1	0.78	0.23	-	63,63,63,63	0
58	MG	AA	1702	1/1	0.89	0.24	-	57,57,57,57	0
58	MG	AA	1617	1/1	0.91	0.50	-	66,66,66,66	0
58	MG	CA	1665	1/1	0.72	0.32	-	64,64,64,64	0
58	MG	DA	3314	1/1	0.81	0.38	-	72,72,72,72	0
58	MG	BA	3210	1/1	0.96	0.23	-	43,43,43,43	0
58	MG	BA	3053	1/1	0.96	0.25	-	18,18,18,18	0
58	MG	DA	3218	1/1	0.87	0.19	-	75,75,75,75	0
58	MG	BA	3296	1/1	0.69	0.32	-	83,83,83,83	0
58	MG	DA	3420	1/1	0.53	0.38	-	66,66,66,66	0
58	MG	BA	3333	1/1	0.92	0.38	-	79,79,79,79	1
58	MG	DA	3395	1/1	0.52	0.34	-	73,73,73,73	1
58	MG	CA	1697	1/1	0.66	0.23	-	87,87,87,87	0
58	MG	DA	3290	1/1	0.88	0.59	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3165	1/1	0.88	0.08	-	100,100,100,100	0
58	MG	DA	3450	1/1	0.99	0.20	-	120,120,120,120	1
58	MG	DA	3238	1/1	0.92	0.53	-	135,135,135,135	0
58	MG	DA	3134	1/1	0.98	0.14	-	32,32,32,32	0
58	MG	D7	101	1/1	0.91	0.18	-	51,51,51,51	0
58	MG	AA	1665	1/1	0.94	0.48	-	55,55,55,55	0
58	MG	BA	3205	1/1	0.97	0.27	-	59,59,59,59	0
58	MG	DA	3211	1/1	0.96	0.31	-	61,61,61,61	0
58	MG	CW	117	1/1	0.82	0.74	-	125,125,125,125	0
58	MG	BA	3282	1/1	0.89	0.19	-	121,121,121,121	0
58	MG	BA	3279	1/1	0.73	0.36	-	105,105,105,105	0
58	MG	BA	3160	1/1	0.66	0.21	-	61,61,61,61	0
58	MG	AA	1764	1/1	0.78	0.08	-	94,94,94,94	0
58	MG	AA	1790	1/1	0.82	0.99	-	28,28,28,28	1
58	MG	DA	3033	1/1	0.84	0.30	-	91,91,91,91	0
58	MG	DB	213	1/1	0.52	0.60	-	102,102,102,102	0
58	MG	BA	3439	1/1	0.94	0.34	-	52,52,52,52	0
58	MG	AW	110	1/1	0.50	0.59	-	77,77,77,77	1
58	MG	DA	3396	1/1	0.98	0.06	-	83,83,83,83	0
58	MG	DA	3265	1/1	0.58	0.51	-	69,69,69,69	0
58	MG	BA	3376	1/1	0.95	0.21	-	68,68,68,68	1
58	MG	BA	3103	1/1	0.89	0.28	-	68,68,68,68	0
58	MG	AW	105	1/1	0.89	0.12	-	116,116,116,116	0
58	MG	DA	3142	1/1	0.89	0.93	-	125,125,125,125	0
58	MG	DA	3352	1/1	0.98	0.10	-	52,52,52,52	0
58	MG	AW	109	1/1	0.93	0.15	-	50,50,50,50	1
58	MG	AA	1689	1/1	0.77	0.21	-	106,106,106,106	0
58	MG	DA	3306	1/1	0.98	0.18	-	45,45,45,45	1
58	MG	DA	3140	1/1	0.85	0.26	-	64,64,64,64	0
58	MG	BA	3085	1/1	0.92	0.20	-	49,49,49,49	0
58	MG	DA	3136	1/1	0.96	0.29	-	44,44,44,44	0
58	MG	BA	3227	1/1	0.74	0.35	-	73,73,73,73	0
58	MG	BA	3192	1/1	0.78	0.36	-	124,124,124,124	0
58	MG	BA	3030	1/1	0.96	0.31	-	70,70,70,70	0
58	MG	BA	3356	1/1	0.94	0.30	-	67,67,67,67	0
58	MG	BA	3411	1/1	0.85	0.61	-	95,95,95,95	0
58	MG	BA	3297	1/1	0.93	0.57	-	51,51,51,51	0
58	MG	CA	1786	1/1	0.96	0.07	-	53,53,53,53	0
58	MG	CA	1812	1/1	0.97	0.22	-	39,39,39,39	0
58	MG	BA	3193	1/1	0.98	0.47	-	56,56,56,56	0
58	MG	AA	1606	1/1	0.67	0.24	-	76,76,76,76	0
58	MG	CA	1774	1/1	0.59	0.23	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3384	1/1	0.98	0.25	-	67,67,67,67	0
58	MG	CA	1724	1/1	0.46	0.67	-	91,91,91,91	1
58	MG	DX	101	1/1	0.95	0.23	-	51,51,51,51	0
58	MG	BA	3256	1/1	0.83	0.39	-	61,61,61,61	0
58	MG	BA	3153	1/1	0.85	0.62	-	118,118,118,118	0
58	MG	BA	3096	1/1	0.98	0.11	-	33,33,33,33	0
58	MG	BA	3231	1/1	0.77	0.30	-	114,114,114,114	0
58	MG	AA	1676	1/1	0.46	0.33	-	95,95,95,95	0
58	MG	DA	3362	1/1	0.84	0.17	-	111,111,111,111	0
58	MG	DA	3123	1/1	0.95	0.42	-	40,40,40,40	0
58	MG	DA	3132	1/1	0.95	0.17	-	34,34,34,34	0
58	MG	DA	3127	1/1	0.87	0.20	-	65,65,65,65	0
58	MG	DA	3213	1/1	0.19	0.49	-	124,124,124,124	0
58	MG	DA	3387	1/1	0.76	0.23	-	63,63,63,63	0
58	MG	BA	3317	1/1	0.86	0.25	-	117,117,117,117	0
58	MG	CA	1809	1/1	0.97	0.17	-	56,56,56,56	1
58	MG	DA	3012	1/1	0.92	0.60	-	70,70,70,70	0
58	MG	AA	1635	1/1	0.67	0.48	-	94,94,94,94	0
58	MG	CA	1760	1/1	0.94	0.19	-	85,85,85,85	1
58	MG	BA	3441	1/1	0.99	0.10	-	61,61,61,61	1
58	MG	BA	3424	1/1	0.16	0.55	-	107,107,107,107	0
58	MG	DA	3282	1/1	0.80	0.35	-	73,73,73,73	1
58	MG	CA	1778	1/1	0.99	0.48	-	68,68,68,68	0
58	MG	AA	1777	1/1	0.98	0.32	-	57,57,57,57	0
58	MG	BA	3189	1/1	0.90	0.33	-	54,54,54,54	0
58	MG	DA	3054	1/1	0.96	0.33	-	45,45,45,45	0
58	MG	DB	203	1/1	0.95	0.06	-	89,89,89,89	0
58	MG	BA	3293	1/1	0.86	0.30	-	75,75,75,75	0
58	MG	AA	1650	1/1	0.70	0.24	-	66,66,66,66	0
58	MG	DA	3284	1/1	0.91	0.24	-	70,70,70,70	0
58	MG	CA	1752	1/1	0.93	0.16	-	94,94,94,94	0
58	MG	DA	3449	1/1	0.67	0.10	-	92,92,92,92	0
58	MG	BA	3158	1/1	0.68	0.57	-	97,97,97,97	0
58	MG	DA	3337	1/1	0.98	0.12	-	82,82,82,82	0
58	MG	DA	3068	1/1	0.98	0.27	-	22,22,22,22	0
58	MG	DB	214	1/1	0.54	0.67	-	94,94,94,94	1
58	MG	DA	3346	1/1	0.46	1.09	-	109,109,109,109	0
58	MG	AW	111	1/1	0.92	0.10	-	24,24,24,24	1
58	MG	BA	3372	1/1	0.92	0.81	-	105,105,105,105	0
58	MG	AA	1760	1/1	0.73	0.44	-	66,66,66,66	0
58	MG	CA	1694	1/1	0.99	0.14	-	124,124,124,124	1
58	MG	BA	3370	1/1	0.97	0.34	-	110,110,110,110	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3224	1/1	0.55	0.98	-	99,99,99,99	1
58	MG	AA	1758	1/1	0.85	0.34	-	70,70,70,70	1
58	MG	DB	209	1/1	0.94	0.10	-	117,117,117,117	0
58	MG	DA	3226	1/1	0.88	0.33	-	121,121,121,121	0
58	MG	AA	1711	1/1	0.69	0.22	-	85,85,85,85	0
58	MG	BA	3099	1/1	0.97	0.11	-	59,59,59,59	0
58	MG	DA	3292	1/1	0.89	0.49	-	49,49,49,49	0
58	MG	BA	3422	1/1	0.58	0.28	-	67,67,67,67	0
58	MG	BA	3352	1/1	0.92	0.58	-	70,70,70,70	0
58	MG	CA	1781	1/1	0.92	0.35	-	82,82,82,82	0
58	MG	AA	1643	1/1	0.81	0.22	-	65,65,65,65	0
58	MG	DA	3241	1/1	0.76	0.57	-	60,60,60,60	0
58	MG	CA	1639	1/1	0.56	0.47	-	140,140,140,140	0
58	MG	CA	1625	1/1	0.96	0.20	-	40,40,40,40	0
58	MG	BA	3104	1/1	0.38	0.63	-	65,65,65,65	1
58	MG	DA	3216	1/1	0.82	0.15	-	78,78,78,78	1
58	MG	AW	120	1/1	0.87	0.22	-	92,92,92,92	1
58	MG	BA	3139	1/1	0.92	0.28	-	59,59,59,59	0
58	MG	AV	108	1/1	0.81	0.18	-	67,67,67,67	1
58	MG	CA	1601	1/1	0.81	0.29	-	49,49,49,49	0
58	MG	AA	1666	1/1	0.09	0.91	-	122,122,122,122	0
58	MG	BA	3359	1/1	0.99	0.13	-	92,92,92,92	0
58	MG	DA	3196	1/1	0.60	0.57	-	82,82,82,82	0
58	MG	BA	3381	1/1	0.78	0.10	-	108,108,108,108	0
58	MG	CA	1763	1/1	0.79	0.67	-	93,93,93,93	1
58	MG	AA	1757	1/1	0.95	0.13	-	71,71,71,71	0
58	MG	CA	1679	1/1	0.87	0.23	-	86,86,86,86	1
58	MG	CV	106	1/1	0.95	0.11	-	93,93,93,93	0
58	MG	DA	3313	1/1	0.77	0.62	-	73,73,73,73	0
58	MG	AA	1632	1/1	0.80	0.13	-	64,64,64,64	0
58	MG	DA	3203	1/1	0.87	0.30	-	50,50,50,50	0
58	MG	BA	3018	1/1	0.92	0.14	-	80,80,80,80	0
58	MG	BA	3337	1/1	0.86	0.08	-	116,116,116,116	0
58	MG	DA	3279	1/1	0.70	0.77	-	92,92,92,92	0
58	MG	AA	1649	1/1	0.97	0.32	-	53,53,53,53	0
58	MG	CA	1776	1/1	0.98	0.04	-	72,72,72,72	0
58	MG	CA	1614	1/1	0.85	0.31	-	71,71,71,71	0
58	MG	AA	1646	1/1	0.95	0.21	-	47,47,47,47	0
58	MG	DA	3321	1/1	0.86	0.28	-	100,100,100,100	0
58	MG	BA	3324	1/1	0.98	0.28	-	121,121,121,121	0
58	MG	AA	1618	1/1	0.72	0.69	-	106,106,106,106	0
58	MG	DB	205	1/1	0.84	0.32	-	58,58,58,58	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3183	1/1	0.60	0.29	-	68,68,68,68	0
58	MG	DA	3159	1/1	0.61	0.35	-	74,74,74,74	0
58	MG	DA	3192	1/1	0.97	0.21	-	65,65,65,65	0
58	MG	DA	3092	1/1	0.97	0.29	-	29,29,29,29	0
58	MG	DA	3441	1/1	0.92	0.44	-	74,74,74,74	0
58	MG	BA	3294	1/1	0.88	0.16	-	85,85,85,85	0
58	MG	DA	3426	1/1	0.63	0.52	-	88,88,88,88	0
58	MG	CA	1751	1/1	0.42	0.88	-	128,128,128,128	0
58	MG	BA	3107	1/1	0.94	0.30	-	46,46,46,46	0
58	MG	DA	3263	1/1	0.99	0.35	-	57,57,57,57	0
58	MG	AW	113	1/1	0.94	0.23	-	45,45,45,45	1
58	MG	AA	1700	1/1	0.52	0.53	-	90,90,90,90	0
58	MG	DA	3163	1/1	0.86	0.35	-	84,84,84,84	0
58	MG	DA	3249	1/1	0.75	0.33	-	83,83,83,83	0
58	MG	BA	3354	1/1	0.99	0.17	-	50,50,50,50	1
58	MG	BA	3404	1/1	0.68	0.50	-	97,97,97,97	0
58	MG	BA	3244	1/1	0.87	0.36	-	75,75,75,75	0
58	MG	AA	1723	1/1	0.79	0.39	-	85,85,85,85	1
58	MG	DA	3214	1/1	0.95	0.10	-	131,131,131,131	0
58	MG	CA	1725	1/1	0.80	0.49	-	131,131,131,131	0
58	MG	BA	3059	1/1	0.94	0.22	-	45,45,45,45	0
58	MG	CA	1784	1/1	0.78	0.35	-	78,78,78,78	0
58	MG	CA	1637	1/1	0.95	0.21	-	40,40,40,40	0
58	MG	BA	3262	1/1	0.77	0.17	-	81,81,81,81	0
58	MG	DA	3432	1/1	0.97	0.10	-	91,91,91,91	0
58	MG	AA	1619	1/1	0.87	0.48	-	78,78,78,78	0
58	MG	AA	1740	1/1	0.81	0.42	-	81,81,81,81	1
58	MG	AA	1652	1/1	0.50	0.43	-	107,107,107,107	0
58	MG	BA	3387	1/1	0.94	0.19	-	107,107,107,107	0
58	MG	BB	208	1/1	0.69	0.10	-	103,103,103,103	0
58	MG	CA	1744	1/1	0.86	0.72	-	75,75,75,75	0
58	MG	DA	3262	1/1	0.49	0.88	-	96,96,96,96	0
58	MG	BA	3417	1/1	0.91	0.28	-	49,49,49,49	0
58	MG	DA	3198	1/1	0.70	0.54	-	106,106,106,106	0
58	MG	BA	3429	1/1	0.75	0.67	-	87,87,87,87	0
58	MG	AA	1768	1/1	0.93	0.32	-	100,100,100,100	0
58	MG	AA	1633	1/1	0.87	0.14	-	75,75,75,75	0
58	MG	CA	1719	1/1	0.08	0.26	-	112,112,112,112	0
58	MG	CA	1692	1/1	0.96	0.12	-	92,92,92,92	0
58	MG	D1	102	1/1	0.94	0.09	-	54,54,54,54	1
58	MG	CL	201	1/1	0.93	0.54	-	51,51,51,51	0
58	MG	DA	3415	1/1	0.95	0.37	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3221	1/1	0.94	0.31	-	43,43,43,43	0
58	MG	BA	3327	1/1	0.79	0.14	-	123,123,123,123	0
58	MG	BA	3384	1/1	0.98	0.49	-	83,83,83,83	0
58	MG	DA	3317	1/1	0.64	0.23	-	88,88,88,88	1
58	MG	BA	3002	1/1	0.80	0.27	-	71,71,71,71	0
58	MG	AA	1789	1/1	0.33	0.56	-	152,152,152,152	0
58	MG	BA	3364	1/1	0.99	0.12	-	96,96,96,96	1
58	MG	BA	3004	1/1	0.78	0.47	-	109,109,109,109	0
58	MG	CA	1735	1/1	0.98	0.12	-	74,74,74,74	0
58	MG	BA	3340	1/1	0.48	0.39	-	97,97,97,97	1
58	MG	AA	1680	1/1	0.92	0.13	-	79,79,79,79	0
58	MG	BA	3399	1/1	0.93	0.21	-	70,70,70,70	1
58	MG	DA	3402	1/1	0.96	0.13	-	178,178,178,178	0
58	MG	BA	3154	1/1	0.88	0.36	-	106,106,106,106	1
58	MG	DA	3447	1/1	0.46	1.50	-	87,87,87,87	1
58	MG	CA	1675	1/1	0.73	0.68	-	116,116,116,116	0
58	MG	DA	3361	1/1	0.88	0.36	-	71,71,71,71	0
58	MG	BA	3318	1/1	0.94	0.36	-	110,110,110,110	0
58	MG	BA	3109	1/1	0.97	0.04	-	28,28,28,28	0
58	MG	AA	1769	1/1	0.69	0.45	-	74,74,74,74	0
58	MG	CA	1811	1/1	0.96	0.15	-	165,165,165,165	0
58	MG	AA	1614	1/1	0.89	0.19	-	76,76,76,76	0
58	MG	BA	3343	1/1	0.89	0.38	-	55,55,55,55	1
58	MG	DA	3328	1/1	0.99	0.15	-	103,103,103,103	0
58	MG	DA	3304	1/1	0.56	0.57	-	88,88,88,88	0
58	MG	BA	3088	1/1	0.92	0.29	-	69,69,69,69	0
58	MG	BA	3388	1/1	0.97	0.16	-	66,66,66,66	0
58	MG	AA	1626	1/1	0.78	0.31	-	99,99,99,99	0
58	MG	CA	1759	1/1	0.90	0.87	-	88,88,88,88	1
58	MG	BA	3452	1/1	0.95	0.35	-	114,114,114,114	1
58	MG	DA	3039	1/1	0.99	0.27	-	45,45,45,45	0
58	MG	DA	3388	1/1	0.77	0.37	-	94,94,94,94	0
58	MG	DA	3434	1/1	0.35	0.76	-	107,107,107,107	1
58	MG	BA	3143	1/1	0.96	0.17	-	90,90,90,90	0
58	MG	CA	1769	1/1	0.88	0.20	-	122,122,122,122	0
58	MG	CA	1708	1/1	0.85	0.52	-	81,81,81,81	0
58	MG	CA	1680	1/1	0.42	0.76	-	83,83,83,83	1
58	MG	BA	3091	1/1	0.99	0.39	-	34,34,34,34	0
58	MG	CA	1658	1/1	0.82	1.42	-	103,103,103,103	0
58	MG	DA	3109	1/1	0.91	0.22	-	43,43,43,43	0
58	MG	BA	3217	1/1	0.86	0.46	-	79,79,79,79	0
58	MG	BA	3321	1/1	0.77	0.43	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3225	1/1	0.96	0.35	-	38,38,38,38	0
58	MG	BA	3159	1/1	0.88	0.30	-	52,52,52,52	1
58	MG	DA	3391	1/1	0.76	0.66	-	86,86,86,86	1
58	MG	DA	3104	1/1	0.90	0.26	-	60,60,60,60	0
58	MG	CA	1623	1/1	0.97	0.10	-	74,74,74,74	0
58	MG	CA	1681	1/1	0.90	0.13	-	69,69,69,69	0
58	MG	AA	1697	1/1	0.78	0.18	-	92,92,92,92	0
58	MG	CA	1649	1/1	0.48	0.49	-	82,82,82,82	0
58	MG	AW	101	1/1	0.76	0.52	-	73,73,73,73	1
58	MG	DA	3301	1/1	0.60	0.77	-	91,91,91,91	0
58	MG	BA	3185	1/1	0.93	0.18	-	69,69,69,69	0
58	MG	CA	1645	1/1	0.84	0.41	-	78,78,78,78	0
58	MG	DA	3145	1/1	0.96	0.44	-	36,36,36,36	0
58	MG	AA	1745	1/1	0.56	1.50	-	121,121,121,121	0
58	MG	DA	3295	1/1	0.89	0.16	-	85,85,85,85	0
58	MG	B1	101	1/1	0.96	0.08	-	29,29,29,29	1
58	MG	DA	3283	1/1	0.76	0.48	-	66,66,66,66	1
58	MG	BA	3306	1/1	0.95	0.48	-	67,67,67,67	0
58	MG	BA	3235	1/1	0.76	0.52	-	82,82,82,82	0
58	MG	DA	3375	1/1	0.67	0.22	-	106,106,106,106	0
58	MG	BA	3083	1/1	0.97	0.34	-	47,47,47,47	0
58	MG	DA	3200	1/1	0.93	0.45	-	57,57,57,57	0
58	MG	BA	3233	1/1	0.71	0.11	-	98,98,98,98	0
58	MG	CA	1609	1/1	0.73	0.37	-	109,109,109,109	0
58	MG	AA	1706	1/1	0.96	0.06	-	63,63,63,63	0
58	MG	DA	3421	1/1	0.79	0.24	-	107,107,107,107	1
58	MG	AA	1799	1/1	0.69	0.47	-	117,117,117,117	0
58	MG	AA	1754	1/1	0.93	0.17	-	114,114,114,114	0
58	MG	BB	210	1/1	0.88	0.29	-	50,50,50,50	1
58	MG	DA	3091	1/1	0.91	0.53	-	84,84,84,84	0
58	MG	CA	1670	1/1	0.89	0.85	-	84,84,84,84	0
58	MG	CA	1748	1/1	0.89	0.24	-	88,88,88,88	1
58	MG	AW	112	1/1	0.58	0.18	-	107,107,107,107	1
58	MG	BA	3209	1/1	0.76	0.23	-	49,49,49,49	0
58	MG	BA	3416	1/1	0.89	1.92	-	95,95,95,95	0
58	MG	DA	3445	1/1	0.59	0.08	-	98,98,98,98	0
58	MG	BA	3251	1/1	0.99	0.10	-	58,58,58,58	1
58	MG	BA	3330	1/1	0.95	0.30	-	114,114,114,114	1
58	MG	BV	201	1/1	0.96	0.54	-	101,101,101,101	0
58	MG	DA	3052	1/1	0.98	0.21	-	9,9,9,9	0
58	MG	AA	1772	1/1	0.48	0.46	-	100,100,100,100	1
58	MG	DA	3429	1/1	0.94	0.13	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3338	1/1	0.93	0.19	-	123,123,123,123	0
58	MG	DA	3010	1/1	0.94	0.09	-	51,51,51,51	0
58	MG	AA	1655	1/1	0.61	0.86	-	89,89,89,89	0
58	MG	AW	108	1/1	0.88	0.16	-	143,143,143,143	0
58	MG	DA	3160	1/1	0.97	0.19	-	96,96,96,96	0
58	MG	CA	1750	1/1	0.81	0.28	-	109,109,109,109	0
58	MG	BA	3257	1/1	0.84	0.28	-	46,46,46,46	1
58	MG	AA	1631	1/1	0.71	0.49	-	109,109,109,109	0
58	MG	BA	3426	1/1	0.91	0.37	-	76,76,76,76	0
58	MG	DA	3416	1/1	0.95	0.28	-	114,114,114,114	0
58	MG	CA	1683	1/1	0.97	0.19	-	84,84,84,84	0
58	MG	CA	1800	1/1	0.94	0.23	-	108,108,108,108	0
58	MG	AA	1747	1/1	0.70	0.39	-	85,85,85,85	1
58	MG	DA	3147	1/1	0.92	0.25	-	105,105,105,105	0
58	MG	AA	1791	1/1	0.81	0.48	-	60,60,60,60	1
58	MG	BA	3042	1/1	0.90	0.14	-	35,35,35,35	0
58	MG	DA	3179	1/1	0.66	0.22	-	109,109,109,109	0
58	MG	CW	115	1/1	0.47	0.37	-	139,139,139,139	0
58	MG	AA	1778	1/1	0.83	0.23	-	84,84,84,84	0
58	MG	CW	109	1/1	0.86	0.16	-	57,57,57,57	1
58	MG	CA	1667	1/1	0.96	0.11	-	147,147,147,147	0
58	MG	AA	1709	1/1	0.85	1.06	-	119,119,119,119	0
58	MG	BA	3021	1/1	0.98	0.36	-	24,24,24,24	0
58	MG	AA	1752	1/1	0.80	0.48	-	104,104,104,104	0
58	MG	AA	1645	1/1	0.87	0.43	-	59,59,59,59	0
58	MG	CA	1634	1/1	0.86	0.14	-	97,97,97,97	0
58	MG	AA	1609	1/1	0.87	0.24	-	58,58,58,58	0
58	MG	BA	3218	1/1	0.90	0.21	-	87,87,87,87	0
58	MG	BA	3214	1/1	0.66	0.29	-	97,97,97,97	0
58	MG	CA	1768	1/1	0.94	0.29	-	65,65,65,65	1
58	MG	AA	1800	1/1	0.94	0.22	-	59,59,59,59	1
58	MG	CA	1606	1/1	0.83	0.35	-	66,66,66,66	0
58	MG	AA	1681	1/1	0.88	0.37	-	69,69,69,69	0
58	MG	BA	3299	1/1	0.86	0.26	-	68,68,68,68	0
58	MG	DA	3088	1/1	0.73	0.44	-	83,83,83,83	0
58	MG	BA	3243	1/1	0.94	0.30	-	45,45,45,45	0
58	MG	D5	101	1/1	0.96	0.16	-	51,51,51,51	0
58	MG	DA	3409	1/1	0.68	0.28	-	141,141,141,141	0
58	MG	BA	3055	1/1	0.84	0.16	-	33,33,33,33	0
58	MG	BA	3201	1/1	0.87	0.31	-	59,59,59,59	0
58	MG	AA	1651	1/1	0.99	0.27	-	95,95,95,95	0
58	MG	DN	202	1/1	0.53	0.76	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3097	1/1	0.99	0.16	-	46,46,46,46	0
58	MG	AA	1812	1/1	0.70	0.46	-	93,93,93,93	0
58	MG	CA	1662	1/1	0.91	0.12	-	114,114,114,114	0
58	MG	AV	104	1/1	0.93	0.36	-	98,98,98,98	1
58	MG	DA	3377	1/1	0.71	0.12	-	89,89,89,89	0
58	MG	BA	3034	1/1	0.64	0.47	-	73,73,73,73	0
58	MG	BA	3453	1/1	0.71	0.41	-	114,114,114,114	0
58	MG	BA	3316	1/1	0.69	0.49	-	81,81,81,81	0
58	MG	BB	219	1/1	0.65	0.26	-	89,89,89,89	1
58	MG	DX	102	1/1	0.86	0.73	-	68,68,68,68	0
58	MG	DA	3296	1/1	0.82	1.24	-	66,66,66,66	1
58	MG	CW	118	1/1	0.91	0.14	-	95,95,95,95	1
58	MG	CA	1656	1/1	0.81	0.63	-	74,74,74,74	0
58	MG	DA	3045	1/1	0.99	0.27	-	50,50,50,50	0
58	MG	DA	3334	1/1	0.64	0.48	-	107,107,107,107	1
58	MG	AA	1707	1/1	0.86	0.45	-	66,66,66,66	0
58	MG	DA	3158	1/1	0.90	0.39	-	51,51,51,51	0
58	MG	AW	107	1/1	0.94	0.09	-	74,74,74,74	1
58	MG	BA	3305	1/1	0.30	1.07	-	112,112,112,112	0
58	MG	BA	3300	1/1	0.84	0.11	-	80,80,80,80	0
58	MG	BA	3062	1/1	0.99	0.33	-	32,32,32,32	0
58	MG	BA	3374	1/1	0.98	0.20	-	95,95,95,95	0
58	MG	BA	3259	1/1	0.54	0.48	-	91,91,91,91	0
58	MG	BA	3175	1/1	0.98	0.29	-	70,70,70,70	0
58	MG	AA	1662	1/1	0.59	0.22	-	95,95,95,95	0
58	MG	AA	1773	1/1	0.47	0.22	-	71,71,71,71	0
58	MG	DA	3340	1/1	0.92	0.69	-	63,63,63,63	1
58	MG	DA	3444	1/1	0.96	0.07	-	70,70,70,70	0
58	MG	DV	201	1/1	0.91	0.33	-	95,95,95,95	0
58	MG	DA	3247	1/1	0.99	0.14	-	96,96,96,96	1
58	MG	CA	1659	1/1	0.82	0.39	-	64,64,64,64	1
58	MG	AA	1797	1/1	0.88	0.33	-	137,137,137,137	0
58	MG	BA	3050	1/1	0.31	0.76	-	84,84,84,84	0
58	MG	CA	1782	1/1	0.97	0.32	-	160,160,160,160	0
58	MG	DA	3359	1/1	0.99	0.17	-	84,84,84,84	1
58	MG	BA	3242	1/1	0.39	1.09	-	115,115,115,115	0
58	MG	DA	3408	1/1	0.84	1.01	-	106,106,106,106	0
58	MG	BA	3258	1/1	0.97	0.22	-	100,100,100,100	0
58	MG	DA	3436	1/1	0.91	0.23	-	60,60,60,60	0
58	MG	CA	1644	1/1	0.78	0.24	-	72,72,72,72	0
58	MG	CA	1643	1/1	0.61	0.40	-	95,95,95,95	0
58	MG	AW	115	1/1	0.94	0.15	-	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3149	1/1	0.83	0.42	-	116,116,116,116	0
58	MG	CA	1764	1/1	0.84	0.15	-	87,87,87,87	0
58	MG	DX	103	1/1	0.81	0.25	-	112,112,112,112	0
58	MG	BA	3006	1/1	0.84	0.37	-	104,104,104,104	0
58	MG	BA	3011	1/1	0.99	0.10	-	42,42,42,42	0
58	MG	DA	3287	1/1	0.76	0.36	-	77,77,77,77	0
58	MG	CW	114	1/1	-0.09	0.33	-	108,108,108,108	1
58	MG	BA	3241	1/1	0.98	0.25	-	31,31,31,31	0
58	MG	AA	1794	1/1	0.89	0.20	-	70,70,70,70	0
58	MG	AA	1677	1/1	0.88	0.44	-	96,96,96,96	0
58	MG	CA	1710	1/1	0.66	1.35	-	127,127,127,127	0
58	MG	AA	1654	1/1	0.98	0.21	-	129,129,129,129	0
58	MG	DB	216	1/1	0.71	0.60	-	108,108,108,108	0
58	MG	CA	1792	1/1	0.94	0.22	-	70,70,70,70	1
58	MG	DA	3252	1/1	0.72	0.27	-	65,65,65,65	0
58	MG	BA	3392	1/1	0.95	0.26	-	79,79,79,79	0
58	MG	DA	3422	1/1	0.93	0.28	-	69,69,69,69	0
58	MG	CA	1741	1/1	0.91	0.33	-	130,130,130,130	1
58	MG	BA	3213	1/1	0.36	0.56	-	109,109,109,109	0
58	MG	AE	201	1/1	0.77	0.13	-	110,110,110,110	0
58	MG	BA	3250	1/1	0.93	0.48	-	65,65,65,65	0
58	MG	AA	1782	1/1	0.89	0.59	-	71,71,71,71	0
58	MG	DA	3319	1/1	0.80	0.45	-	105,105,105,105	1
58	MG	BA	3401	1/1	0.71	0.64	-	119,119,119,119	0
58	MG	CV	103	1/1	0.92	0.09	-	89,89,89,89	0
58	MG	BA	3230	1/1	0.75	0.33	-	82,82,82,82	0
58	MG	CA	1676	1/1	0.97	0.27	-	88,88,88,88	0
58	MG	DA	3300	1/1	0.88	0.34	-	63,63,63,63	0
58	MG	CW	101	1/1	0.90	0.40	-	94,94,94,94	1
58	MG	BA	3220	1/1	0.67	0.13	-	80,80,80,80	1
58	MG	AA	1751	1/1	0.89	0.27	-	75,75,75,75	0
58	MG	AA	1647	1/1	0.72	0.14	-	94,94,94,94	0
58	MG	CA	1743	1/1	0.65	0.48	-	128,128,128,128	0
58	MG	BA	3309	1/1	0.53	0.31	-	94,94,94,94	0
58	MG	AX	101	1/1	0.96	0.17	-	85,85,85,85	0
58	MG	BA	3431	1/1	0.64	0.32	-	124,124,124,124	0
58	MG	DA	3040	1/1	0.84	0.13	-	78,78,78,78	0
58	MG	CA	1785	1/1	0.88	0.43	-	85,85,85,85	0
58	MG	AA	1636	1/1	0.91	0.16	-	44,44,44,44	1
58	MG	BA	3329	1/1	0.74	0.13	-	88,88,88,88	1
58	MG	CA	1669	1/1	0.98	0.30	-	118,118,118,118	0
58	MG	BA	3197	1/1	0.98	0.38	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3101	1/1	0.92	0.37	-	58,58,58,58	0
58	MG	BA	3039	1/1	0.97	0.22	-	45,45,45,45	0
58	MG	AA	1607	1/1	0.98	0.12	-	50,50,50,50	0
58	MG	BA	3106	1/1	0.96	0.42	-	52,52,52,52	0
58	MG	BA	3009	1/1	0.27	1.94	-	109,109,109,109	0
58	MG	BA	3203	1/1	0.94	0.49	-	86,86,86,86	0
58	MG	BA	3407	1/1	0.91	0.39	-	82,82,82,82	0
58	MG	DA	3267	1/1	0.94	0.37	-	79,79,79,79	0
58	MG	AA	1693	1/1	0.67	1.63	-	109,109,109,109	1
58	MG	AA	1787	1/1	0.91	0.23	-	58,58,58,58	0
58	MG	DA	3329	1/1	0.99	0.27	-	83,83,83,83	1
58	MG	AA	1691	1/1	0.80	0.31	-	54,54,54,54	0
58	MG	CA	1730	1/1	0.57	1.30	-	111,111,111,111	0
58	MG	BA	3052	1/1	0.94	0.60	-	134,134,134,134	1
58	MG	BA	3348	1/1	0.99	0.09	-	78,78,78,78	1
58	MG	DA	3325	1/1	0.65	0.21	-	90,90,90,90	0
58	MG	DA	3350	1/1	0.97	0.16	-	65,65,65,65	1
58	MG	CA	1814	1/1	0.89	0.69	-	115,115,115,115	1
58	MG	AA	1601	1/1	0.67	0.24	-	92,92,92,92	0
58	MG	B2	601	1/1	0.51	0.53	-	68,68,68,68	1
58	MG	CA	1618	1/1	0.72	1.09	-	109,109,109,109	0
58	MG	AA	1674	1/1	0.92	0.45	-	63,63,63,63	0
58	MG	AA	1661	1/1	0.55	0.18	-	83,83,83,83	0
58	MG	BA	3361	1/1	0.99	0.08	-	107,107,107,107	1
58	MG	BA	3215	1/1	0.97	0.37	-	51,51,51,51	0
58	MG	CA	1732	1/1	0.83	0.11	-	66,66,66,66	0
58	MG	DA	3229	1/1	0.94	0.12	-	101,101,101,101	0
58	MG	CA	1797	1/1	0.86	0.54	-	111,111,111,111	0
58	MG	AA	1625	1/1	0.93	0.20	-	39,39,39,39	0
58	MG	DA	3336	1/1	0.77	0.42	-	75,75,75,75	1
58	MG	AV	107	1/1	0.98	0.55	-	76,76,76,76	0
58	MG	CW	108	1/1	0.55	0.48	-	130,130,130,130	0
58	MG	BB	202	1/1	0.56	0.51	-	97,97,97,97	1
58	MG	BA	3145	1/1	0.94	0.45	-	61,61,61,61	0
58	MG	AA	1788	1/1	0.74	0.45	-	81,81,81,81	0
58	MG	CA	1617	1/1	0.75	0.70	-	73,73,73,73	0
58	MG	DA	3059	1/1	0.84	0.76	-	84,84,84,84	0
58	MG	CA	1608	1/1	0.96	0.21	-	80,80,80,80	0
58	MG	CA	1775	1/1	0.83	0.14	-	69,69,69,69	0
58	MG	CA	1740	1/1	0.97	0.25	-	132,132,132,132	0
58	MG	DA	3106	1/1	0.99	0.36	-	36,36,36,36	0
58	MG	BA	3308	1/1	0.76	0.85	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AV	103	1/1	0.76	0.17	-	102,102,102,102	0
58	MG	AA	1813	1/1	0.74	0.38	-	101,101,101,101	0
58	MG	CW	113	1/1	0.93	0.24	-	41,41,41,41	1
58	MG	BW	201	1/1	0.93	0.38	-	120,120,120,120	0
58	MG	BA	3022	1/1	0.97	0.40	-	64,64,64,64	0
58	MG	AA	1738	1/1	0.91	0.58	-	89,89,89,89	0
58	MG	BA	3448	1/1	0.94	0.05	-	67,67,67,67	0
58	MG	DA	3100	1/1	0.88	0.61	-	71,71,71,71	0
58	MG	DA	3207	1/1	0.96	0.09	-	60,60,60,60	0
58	MG	DA	3058	1/1	0.94	0.23	-	49,49,49,49	0
58	MG	CA	1723	1/1	0.93	0.08	-	47,47,47,47	0
58	MG	CA	1646	1/1	0.95	0.24	-	64,64,64,64	0
58	MG	DA	3433	1/1	0.96	0.09	-	94,94,94,94	1
58	MG	BA	3268	1/1	0.98	0.28	-	73,73,73,73	0
58	MG	DA	3026	1/1	0.94	0.47	-	49,49,49,49	0
58	MG	D2	101	1/1	0.87	0.27	-	73,73,73,73	0
58	MG	DA	3073	1/1	0.94	0.33	-	55,55,55,55	0
58	MG	DB	210	1/1	0.93	0.20	-	51,51,51,51	1
58	MG	BA	3245	1/1	0.89	0.55	-	81,81,81,81	0
58	MG	DA	3003	1/1	0.88	0.41	-	79,79,79,79	0
58	MG	BA	3402	1/1	0.94	0.42	-	59,59,59,59	0
58	MG	BA	3410	1/1	0.88	0.29	-	113,113,113,113	0
58	MG	DA	3178	1/1	0.59	0.55	-	125,125,125,125	0
58	MG	BA	3162	1/1	0.95	0.17	-	51,51,51,51	0
58	MG	DA	3153	1/1	0.97	0.16	-	45,45,45,45	1
58	MG	AA	1767	1/1	0.88	0.28	-	44,44,44,44	1
58	MG	DA	3407	1/1	0.93	0.29	-	140,140,140,140	0
58	MG	BA	3362	1/1	0.72	0.29	-	90,90,90,90	0
58	MG	CW	116	1/1	0.68	0.22	-	103,103,103,103	1
58	MG	DA	3256	1/1	0.95	0.28	-	82,82,82,82	1
58	MG	BA	3019	1/1	0.99	0.43	-	41,41,41,41	0
58	MG	DA	3414	1/1	0.71	0.78	-	130,130,130,130	0
58	MG	CA	1733	1/1	0.96	0.07	-	49,49,49,49	1
58	MG	BA	3260	1/1	0.59	0.58	-	102,102,102,102	1
58	MG	BA	3338	1/1	0.95	0.09	-	121,121,121,121	0
58	MG	CA	1777	1/1	0.94	0.30	-	99,99,99,99	0
58	MG	DA	3320	1/1	0.86	0.15	-	101,101,101,101	1
58	MG	BA	3451	1/1	0.81	0.10	-	85,85,85,85	0
58	MG	CW	111	1/1	0.93	0.73	-	89,89,89,89	1
58	MG	AA	1692	1/1	0.87	0.58	-	61,61,61,61	0
58	MG	AA	1808	1/1	0.67	0.50	-	101,101,101,101	0
58	MG	DA	3369	1/1	0.98	0.10	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3371	1/1	0.97	0.10	-	98,98,98,98	1
58	MG	AA	1749	1/1	0.96	0.41	-	117,117,117,117	0
58	MG	DA	3373	1/1	0.95	0.28	-	78,78,78,78	1
58	MG	BA	3425	1/1	0.99	0.16	-	108,108,108,108	0
58	MG	BA	3040	1/1	0.97	0.15	-	33,33,33,33	0
58	MG	AA	1798	1/1	0.97	0.17	-	135,135,135,135	0
58	MG	BA	3046	1/1	0.97	0.25	-	64,64,64,64	0
58	MG	DA	3385	1/1	0.96	0.23	-	138,138,138,138	0
58	MG	DA	3393	1/1	0.87	0.55	-	89,89,89,89	0
58	MG	BA	3108	1/1	0.80	0.24	-	87,87,87,87	0
58	MG	DA	3303	1/1	0.76	1.03	-	97,97,97,97	0
58	MG	BA	3146	1/1	0.99	0.39	-	31,31,31,31	0
58	MG	DV	202	1/1	0.86	0.40	-	63,63,63,63	1
58	MG	DB	206	1/1	0.93	0.19	-	78,78,78,78	0
58	MG	DA	3381	1/1	0.98	0.16	-	149,149,149,149	0
58	MG	CA	1648	1/1	0.89	0.23	-	108,108,108,108	0
58	MG	CA	1677	1/1	0.66	0.21	-	88,88,88,88	0
58	MG	AX	102	1/1	0.98	0.14	-	85,85,85,85	0
58	MG	AA	1718	1/1	0.80	0.17	-	150,150,150,150	0
58	MG	CW	107	1/1	0.85	0.13	-	91,91,91,91	1
58	MG	BA	3219	1/1	0.98	0.10	-	106,106,106,106	0
58	MG	AA	1796	1/1	0.62	0.12	-	106,106,106,106	1
58	MG	D2	102	1/1	0.92	0.42	-	50,50,50,50	1
58	MG	AA	1659	1/1	0.90	0.84	-	88,88,88,88	0
58	MG	CA	1686	1/1	0.82	0.37	-	80,80,80,80	0
58	MG	CX	101	1/1	0.75	0.21	-	83,83,83,83	0
58	MG	AA	1731	1/1	0.78	0.12	-	64,64,64,64	0
58	MG	AA	1602	1/1	0.53	0.52	-	91,91,91,91	0
58	MG	BA	3098	1/1	0.94	0.33	-	45,45,45,45	0
58	MG	BA	3363	1/1	0.69	0.37	-	116,116,116,116	0
58	MG	BA	3428	1/1	0.62	0.80	-	90,90,90,90	0
58	MG	DA	3098	1/1	0.98	0.23	-	60,60,60,60	0
58	MG	DA	3280	1/1	0.92	0.54	-	107,107,107,107	0
58	MG	DA	3084	1/1	0.98	0.22	-	35,35,35,35	0
58	MG	DA	3253	1/1	0.78	0.41	-	72,72,72,72	1
58	MG	DA	3311	1/1	0.62	0.65	-	93,93,93,93	0
58	MG	AA	1805	1/1	0.86	0.58	-	88,88,88,88	1
58	MG	DA	3141	1/1	0.71	1.03	-	102,102,102,102	0
58	MG	DA	3254	1/1	0.84	0.28	-	123,123,123,123	0
58	MG	DA	3204	1/1	0.92	0.09	-	33,33,33,33	0
58	MG	AA	1612	1/1	0.81	0.33	-	80,80,80,80	0
58	MG	AA	1708	1/1	0.90	0.44	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3222	1/1	0.92	0.07	-	57,57,57,57	0
58	MG	AA	1679	1/1	0.88	0.15	-	49,49,49,49	1
58	MG	CA	1738	1/1	0.97	0.37	-	95,95,95,95	0
58	MG	DA	3005	1/1	0.60	1.00	-	138,138,138,138	0
58	MG	BA	3130	1/1	0.44	0.87	-	92,92,92,92	1
58	MG	DA	3326	1/1	0.89	0.32	-	134,134,134,134	0
58	MG	CA	1651	1/1	0.72	0.43	-	85,85,85,85	0
58	MG	DA	3205	1/1	0.76	0.58	-	81,81,81,81	0
58	MG	BA	3263	1/1	0.88	0.10	-	77,77,77,77	0
58	MG	BA	3446	1/1	0.46	0.19	-	92,92,92,92	0
58	MG	BA	3436	1/1	0.64	0.21	-	60,60,60,60	1
58	MG	AA	1657	1/1	0.93	0.37	-	73,73,73,73	0
58	MG	DA	3156	1/1	0.56	0.52	-	94,94,94,94	0
58	MG	CA	1755	1/1	0.80	0.23	-	105,105,105,105	0
58	MG	CX	102	1/1	0.87	0.09	-	95,95,95,95	0
58	MG	DA	3412	1/1	0.95	0.20	-	109,109,109,109	0
58	MG	DA	3302	1/1	0.87	0.10	-	86,86,86,86	0
58	MG	AA	1793	1/1	0.96	0.39	-	106,106,106,106	0
58	MG	DA	3004	1/1	0.90	0.34	-	54,54,54,54	0
58	MG	BA	3413	1/1	0.89	0.18	-	105,105,105,105	1
58	MG	DA	3257	1/1	0.90	0.17	-	99,99,99,99	0
58	MG	CA	1626	1/1	0.25	0.87	-	119,119,119,119	0
58	MG	DA	3356	1/1	0.89	0.69	-	78,78,78,78	1
58	MG	DA	3063	1/1	0.95	0.38	-	35,35,35,35	0
58	MG	CA	1631	1/1	0.89	0.32	-	88,88,88,88	0
58	MG	BA	3443	1/1	0.89	0.35	-	100,100,100,100	0
58	MG	DA	3082	1/1	0.95	0.26	-	37,37,37,37	0
58	MG	DA	3376	1/1	0.78	0.33	-	128,128,128,128	0
58	MG	AA	1739	1/1	0.97	0.24	-	102,102,102,102	0
58	MG	CA	1603	1/1	0.80	0.37	-	88,88,88,88	0
58	MG	CA	1722	1/1	0.33	0.16	-	106,106,106,106	0
58	MG	BA	3328	1/1	0.80	0.47	-	116,116,116,116	1
58	MG	DA	3411	1/1	0.47	0.30	-	115,115,115,115	1
58	MG	BA	3234	1/1	0.45	0.66	-	115,115,115,115	0
58	MG	BA	3394	1/1	0.61	1.27	-	105,105,105,105	0
58	MG	CA	1689	1/1	0.95	0.14	-	138,138,138,138	0
58	MG	DA	3095	1/1	0.96	0.13	-	33,33,33,33	0
58	MG	CA	1798	1/1	0.97	0.06	-	89,89,89,89	1
58	MG	BA	3438	1/1	0.97	0.33	-	71,71,71,71	0
58	MG	DB	212	1/1	0.99	0.05	-	30,30,30,30	1
58	MG	DA	3288	1/1	0.94	0.27	-	32,32,32,32	0
58	MG	BA	3035	1/1	0.93	0.18	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	1749	1/1	0.87	0.52	-	87,87,87,87	0
58	MG	BA	3397	1/1	0.98	0.19	-	112,112,112,112	1
58	MG	CA	1754	1/1	0.95	0.10	-	93,93,93,93	0
58	MG	DA	3157	1/1	0.89	0.25	-	47,47,47,47	1
58	MG	BA	3415	1/1	0.97	0.15	-	80,80,80,80	0
58	MG	CA	1789	1/1	0.86	0.31	-	61,61,61,61	0
58	MG	DA	3423	1/1	0.73	0.57	-	117,117,117,117	0
58	MG	CA	1739	1/1	0.41	0.72	-	109,109,109,109	0
58	MG	BA	3442	1/1	0.91	0.09	-	67,67,67,67	0
58	MG	BA	3202	1/1	0.72	0.28	-	80,80,80,80	1
58	MG	DA	3309	1/1	0.67	0.34	-	89,89,89,89	0
58	MG	BA	3141	1/1	0.71	0.22	-	60,60,60,60	0
58	MG	CA	1647	1/1	0.62	0.51	-	94,94,94,94	0
58	MG	BB	214	1/1	0.70	0.48	-	92,92,92,92	0
58	MG	CA	1615	1/1	0.84	0.17	-	81,81,81,81	0
58	MG	CA	1799	1/1	0.78	0.17	-	89,89,89,89	0
58	MG	AA	1774	1/1	0.84	0.15	-	70,70,70,70	0
58	MG	DA	3278	1/1	0.91	0.05	-	116,116,116,116	0
58	MG	AA	1653	1/1	0.91	0.54	-	82,82,82,82	1
58	MG	AA	1807	1/1	0.85	0.37	-	71,71,71,71	1
58	MG	DA	3173	1/1	0.95	0.15	-	46,46,46,46	0
58	MG	AA	1755	1/1	0.82	0.42	-	83,83,83,83	0
58	MG	BA	3163	1/1	0.61	1.03	-	132,132,132,132	0
58	MG	CA	1806	1/1	0.99	0.18	-	29,29,29,29	0
58	MG	DA	3274	1/1	0.92	0.23	-	141,141,141,141	0
58	MG	DA	3248	1/1	0.90	0.30	-	62,62,62,62	0
58	MG	BB	218	1/1	0.78	0.43	-	78,78,78,78	1
58	MG	BA	3180	1/1	0.92	0.26	-	93,93,93,93	0
58	MG	DA	3344	1/1	0.53	0.49	-	72,72,72,72	1
58	MG	BA	3278	1/1	0.62	0.49	-	119,119,119,119	0
58	MG	BA	3420	1/1	0.97	0.26	-	93,93,93,93	0
58	MG	BA	3211	1/1	0.99	0.20	-	55,55,55,55	0
58	MG	BA	3310	1/1	0.92	0.40	-	36,36,36,36	0
58	MG	BA	3005	1/1	0.85	0.48	-	85,85,85,85	0
58	MG	BA	3412	1/1	0.93	0.29	-	67,67,67,67	0
58	MG	BA	3326	1/1	0.91	0.60	-	111,111,111,111	1
58	MG	BA	3378	1/1	0.82	0.49	-	65,65,65,65	1
58	MG	AA	1781	1/1	0.94	0.20	-	89,89,89,89	0
58	MG	DA	3151	1/1	0.51	0.54	-	94,94,94,94	0
58	MG	DA	3002	1/1	0.94	0.10	-	63,63,63,63	0
58	MG	DA	3113	1/1	0.96	0.42	-	42,42,42,42	0
58	MG	BA	3043	1/1	0.99	0.27	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	1727	1/1	0.91	0.17	-	62,62,62,62	0
58	MG	CA	1794	1/1	0.94	0.78	-	77,77,77,77	0
58	MG	CA	1793	1/1	1.00	0.11	-	103,103,103,103	0
58	MG	AA	1671	1/1	0.94	0.41	-	61,61,61,61	0
58	MG	BA	3379	1/1	0.95	0.20	-	110,110,110,110	0
58	MG	BA	3124	1/1	0.94	0.40	-	40,40,40,40	0
58	MG	DA	3024	1/1	0.93	0.30	-	37,37,37,37	0
58	MG	CA	1703	1/1	0.92	0.36	-	71,71,71,71	0
58	MG	BA	3398	1/1	0.87	0.12	-	113,113,113,113	0
58	MG	AW	103	1/1	0.73	0.22	-	100,100,100,100	0
58	MG	AV	106	1/1	0.89	0.15	-	119,119,119,119	0
58	MG	DA	3251	1/1	0.67	0.18	-	95,95,95,95	0
58	MG	AA	1620	1/1	0.86	1.09	-	91,91,91,91	0
58	MG	BA	3273	1/1	0.83	0.32	-	76,76,76,76	0
58	MG	AA	1771	1/1	0.79	0.41	-	73,73,73,73	0
58	MG	DA	3370	1/1	0.76	1.78	-	74,74,74,74	1
58	MG	AA	1765	1/1	0.64	0.67	-	116,116,116,116	0
58	MG	AA	1639	1/1	0.90	0.20	-	57,57,57,57	0
58	MG	AA	1694	1/1	0.77	0.42	-	22,22,22,22	1
58	MG	AA	1732	1/1	0.94	0.19	-	64,64,64,64	1
58	MG	BA	3036	1/1	0.90	0.72	-	90,90,90,90	0
58	MG	BA	3092	1/1	0.95	0.57	-	100,100,100,100	0
58	MG	BB	206	1/1	0.97	0.30	-	130,130,130,130	0
58	MG	CA	1672	1/1	0.71	0.46	-	86,86,86,86	0
58	MG	DA	3333	1/1	0.80	0.21	-	130,130,130,130	0
58	MG	DA	3446	1/1	0.96	0.08	-	51,51,51,51	0
58	MG	DA	3294	1/1	0.95	0.57	-	63,63,63,63	0
58	MG	BA	3295	1/1	0.61	0.65	-	89,89,89,89	0
58	MG	DA	3038	1/1	0.98	0.24	-	53,53,53,53	0
58	MG	BA	3074	1/1	0.67	0.28	-	75,75,75,75	0
58	MG	AA	1742	1/1	0.70	0.25	-	96,96,96,96	0
58	MG	AU	101	1/1	0.89	0.53	-	117,117,117,117	0
58	MG	BA	3353	1/1	0.87	0.32	-	89,89,89,89	0
58	MG	DA	3266	1/1	0.90	0.09	-	87,87,87,87	0
58	MG	BA	3183	1/1	0.74	0.22	-	122,122,122,122	0
58	MG	DA	3405	1/1	0.93	0.66	-	129,129,129,129	0
58	MG	DA	3110	1/1	0.94	0.16	-	38,38,38,38	0
58	MG	BA	3142	1/1	0.81	0.41	-	77,77,77,77	0
58	MG	CV	107	1/1	0.88	0.20	-	66,66,66,66	0
58	MG	CA	1813	1/1	0.81	0.56	-	96,96,96,96	0
58	MG	AA	1763	1/1	0.32	1.06	-	114,114,114,114	1
58	MG	CE	201	1/1	0.35	0.28	-	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3046	1/1	0.98	0.25	-	30,30,30,30	0
58	MG	BB	217	1/1	0.76	0.43	-	121,121,121,121	0
58	MG	BA	3137	1/1	0.93	0.32	-	61,61,61,61	0
58	MG	DB	204	1/1	0.93	0.76	-	148,148,148,148	0
58	MG	CV	104	1/1	0.85	0.23	-	85,85,85,85	1
58	MG	BA	3252	1/1	0.94	0.12	-	46,46,46,46	0
58	MG	DA	3335	1/1	0.70	0.43	-	87,87,87,87	1
58	MG	DA	3043	1/1	0.67	0.41	-	111,111,111,111	0
58	MG	BA	3181	1/1	0.83	0.47	-	67,67,67,67	0
58	MG	BA	3298	1/1	0.62	0.35	-	91,91,91,91	0
58	MG	BX	102	1/1	0.61	0.46	-	97,97,97,97	0
58	MG	DA	3228	1/1	0.95	0.48	-	75,75,75,75	0
58	MG	DA	3124	1/1	0.88	0.20	-	63,63,63,63	0
58	MG	CA	1622	1/1	0.94	0.14	-	36,36,36,36	0
58	MG	BA	3129	1/1	0.94	0.46	-	63,63,63,63	0
58	MG	DA	3212	1/1	0.96	0.13	-	60,60,60,60	0
58	MG	DA	3367	1/1	0.97	0.50	-	127,127,127,127	0
58	MG	DA	3258	1/1	0.82	0.28	-	66,66,66,66	0
58	MG	CA	1602	1/1	0.84	0.15	-	64,64,64,64	0
58	MG	DA	3210	1/1	0.90	0.15	-	145,145,145,145	0
58	MG	DA	3225	1/1	0.98	0.13	-	115,115,115,115	0
58	MG	AA	1658	1/1	0.79	0.37	-	58,58,58,58	1
58	MG	AA	1715	1/1	0.91	0.26	-	63,63,63,63	0
58	MG	BA	3105	1/1	0.94	0.44	-	55,55,55,55	0
58	MG	DA	3139	1/1	0.98	0.16	-	106,106,106,106	0
58	MG	BA	3349	1/1	0.79	0.45	-	76,76,76,76	1
58	MG	AA	1696	1/1	0.50	0.83	-	103,103,103,103	0
58	MG	CK	201	1/1	0.74	0.62	-	95,95,95,95	1
58	MG	CV	105	1/1	0.56	0.80	-	110,110,110,110	0
58	MG	DN	203	1/1	0.93	0.12	-	109,109,109,109	1
58	MG	DA	3240	1/1	0.93	0.32	-	51,51,51,51	0
58	MG	AA	1809	1/1	0.93	0.19	-	88,88,88,88	0
58	MG	DA	3155	1/1	0.90	0.20	-	53,53,53,53	1
58	MG	BA	3419	1/1	0.81	0.77	-	93,93,93,93	0
58	MG	BA	3041	1/1	0.98	0.09	-	78,78,78,78	0
58	MG	AD	301	1/1	0.56	0.23	-	84,84,84,84	0
58	MG	BA	3288	1/1	-0.16	2.50	-	88,88,88,88	1
58	MG	BA	3345	1/1	0.55	0.60	-	93,93,93,93	1
58	MG	DA	3105	1/1	0.95	0.39	-	52,52,52,52	0
58	MG	BA	3171	1/1	0.94	0.14	-	59,59,59,59	0
58	MG	BA	3164	1/1	0.60	0.47	-	84,84,84,84	0
58	MG	DA	3237	1/1	0.98	0.35	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3173	1/1	0.88	0.32	-	72,72,72,72	1
58	MG	DA	3259	1/1	0.79	0.17	-	70,70,70,70	0
58	MG	BA	3061	1/1	0.84	0.28	-	38,38,38,38	0
58	MG	DA	3090	1/1	0.99	0.42	-	25,25,25,25	0
58	MG	BA	3331	1/1	0.72	0.20	-	119,119,119,119	0
58	MG	BA	3064	1/1	0.91	0.36	-	39,39,39,39	0
58	MG	BA	3365	1/1	0.81	0.61	-	76,76,76,76	1
58	MG	AA	1775	1/1	0.92	0.04	-	68,68,68,68	0
58	MG	CA	1762	1/1	0.63	0.53	-	60,60,60,60	1
58	MG	AA	1761	1/1	0.84	0.65	-	83,83,83,83	1
58	MG	AA	1675	1/1	0.85	0.29	-	69,69,69,69	0
58	MG	DA	3293	1/1	0.82	0.51	-	52,52,52,52	0
58	MG	CA	1695	1/1	0.95	0.37	-	49,49,49,49	1
58	MG	BA	3191	1/1	0.81	0.27	-	71,71,71,71	0
58	MG	BA	3319	1/1	0.86	0.39	-	75,75,75,75	0
58	MG	BA	3224	1/1	0.90	0.37	-	96,96,96,96	0
58	MG	DA	3268	1/1	0.88	0.21	-	79,79,79,79	0
58	MG	DA	3031	1/1	0.97	0.18	-	31,31,31,31	0
58	MG	BA	3395	1/1	0.97	0.34	-	70,70,70,70	0
58	MG	AA	1623	1/1	0.96	0.17	-	106,106,106,106	0
58	MG	AW	104	1/1	0.73	0.26	-	98,98,98,98	1
58	MG	CA	1753	1/1	0.85	0.13	-	74,74,74,74	0
58	MG	CA	1770	1/1	0.61	0.50	-	121,121,121,121	0
58	MG	DA	3277	1/1	0.69	0.16	-	104,104,104,104	0
58	MG	AA	1608	1/1	0.52	0.95	-	110,110,110,110	0
58	MG	DA	3121	1/1	0.95	0.29	-	44,44,44,44	0
58	MG	BA	3047	1/1	0.97	0.29	-	34,34,34,34	0
58	MG	CA	1716	1/1	0.54	0.73	-	83,83,83,83	0
58	MG	CA	1607	1/1	0.95	0.11	-	52,52,52,52	0
58	MG	AA	1719	1/1	0.81	0.26	-	91,91,91,91	0
58	MG	CA	1726	1/1	0.47	0.26	-	65,65,65,65	0
58	MG	DA	3233	1/1	0.92	0.22	-	50,50,50,50	0
58	MG	BA	3423	1/1	0.62	0.11	-	125,125,125,125	1
58	MG	DA	3380	1/1	0.67	0.44	-	85,85,85,85	1
58	MG	BA	3270	1/1	0.66	0.26	-	74,74,74,74	0
58	MG	BA	3148	1/1	0.70	0.23	-	59,59,59,59	1
58	MG	BA	3138	1/1	0.97	0.37	-	37,37,37,37	0
58	MG	DA	3087	1/1	0.95	0.25	-	45,45,45,45	0
58	MG	BA	3237	1/1	0.87	0.43	-	78,78,78,78	0
58	MG	AV	102	1/1	0.95	0.13	-	85,85,85,85	1
58	MG	AA	1685	1/1	0.59	0.49	-	101,101,101,101	0
58	MG	BB	212	1/1	0.94	0.12	-	59,59,59,59	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CW	106	1/1	0.72	0.24	-	106,106,106,106	0
58	MG	AA	1784	1/1	0.97	0.13	-	66,66,66,66	0
58	MG	DB	201	1/1	0.01	0.29	-	135,135,135,135	0
58	MG	DA	3227	1/1	0.46	0.40	-	91,91,91,91	0
58	MG	AA	1729	1/1	0.88	0.49	-	104,104,104,104	0
58	MG	CA	1653	1/1	0.81	0.52	-	110,110,110,110	0
58	MG	BA	3339	1/1	0.69	0.48	-	120,120,120,120	1
58	MG	DA	3439	1/1	0.98	0.15	-	65,65,65,65	1
58	MG	BA	3414	1/1	0.96	0.12	-	78,78,78,78	0
58	MG	BA	3136	1/1	0.88	0.17	-	64,64,64,64	0
58	MG	AW	114	1/1	0.84	0.67	-	91,91,91,91	1
58	MG	BA	3358	1/1	0.95	0.17	-	60,60,60,60	0
58	MG	DE	301	1/1	0.99	0.39	-	38,38,38,38	0
58	MG	DA	3312	1/1	0.97	0.18	-	101,101,101,101	0
58	MG	CA	1693	1/1	0.93	0.29	-	74,74,74,74	0
58	MG	BA	3045	1/1	0.98	0.16	-	69,69,69,69	0
58	MG	CA	1727	1/1	0.84	0.45	-	80,80,80,80	0
58	MG	DA	3234	1/1	0.59	1.45	-	91,91,91,91	0
58	MG	CA	1737	1/1	0.76	0.45	-	95,95,95,95	1
58	MG	CA	1620	1/1	0.92	0.61	-	65,65,65,65	0
58	MG	CW	102	1/1	0.89	1.02	-	98,98,98,98	1
58	MG	CA	1663	1/1	0.36	0.32	-	127,127,127,127	0
58	MG	CA	1629	1/1	0.70	0.22	-	89,89,89,89	0
58	MG	AW	118	1/1	0.85	0.43	-	103,103,103,103	1
58	MG	DA	3077	1/1	0.99	0.21	-	16,16,16,16	0
58	MG	BA	3382	1/1	0.94	0.31	-	86,86,86,86	0
58	MG	AA	1744	1/1	0.88	0.26	-	84,84,84,84	0
58	MG	BB	213	1/1	0.31	0.96	-	148,148,148,148	0
58	MG	DA	3035	1/1	0.72	0.50	-	78,78,78,78	0
58	MG	CA	1685	1/1	0.96	0.10	-	101,101,101,101	0
58	MG	DA	3339	1/1	0.98	0.41	-	85,85,85,85	1
58	MG	DA	3397	1/1	0.98	0.09	-	48,48,48,48	1
58	MG	AA	1770	1/1	0.93	0.20	-	55,55,55,55	0
58	MG	BA	3276	1/1	0.68	0.22	-	68,68,68,68	0
58	MG	BA	3174	1/1	0.85	1.33	-	77,77,77,77	0
58	MG	AA	1792	1/1	0.99	0.10	-	78,78,78,78	0
58	MG	DA	3331	1/1	0.72	0.98	-	116,116,116,116	1
58	MG	DA	3372	1/1	0.84	0.25	-	106,106,106,106	0
58	MG	DA	3440	1/1	0.63	0.10	-	77,77,77,77	0
58	MG	CA	1612	1/1	0.77	0.43	-	116,116,116,116	0
58	MG	AA	1704	1/1	0.65	0.14	-	87,87,87,87	0
58	MG	CA	1734	1/1	0.93	0.21	-	144,144,144,144	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	1636	1/1	0.42	0.19	-	103,103,103,103	1
58	MG	BB	209	1/1	0.75	0.23	-	114,114,114,114	0
58	MG	DA	3188	1/1	0.97	0.18	-	123,123,123,123	0
58	MG	BA	3380	1/1	0.88	0.07	-	66,66,66,66	0
58	MG	BA	3253	1/1	0.80	0.37	-	85,85,85,85	0
58	MG	DB	217	1/1	0.77	0.66	-	110,110,110,110	1
58	MG	DA	3286	1/1	0.88	0.19	-	53,53,53,53	0
58	MG	CA	1673	1/1	0.70	0.28	-	92,92,92,92	0
58	MG	BA	3044	1/1	0.90	0.50	-	115,115,115,115	0
58	MG	DA	3103	1/1	0.24	1.05	-	102,102,102,102	1
58	MG	AA	1762	1/1	0.38	1.01	-	76,76,76,76	1
58	MG	BA	3450	1/1	0.16	0.25	-	125,125,125,125	0
58	MG	CV	108	1/1	0.72	0.54	-	67,67,67,67	1
58	MG	CA	1674	1/1	0.93	0.55	-	89,89,89,89	0
58	MG	BA	3238	1/1	0.74	0.58	-	67,67,67,67	0
58	MG	DA	3185	1/1	0.95	0.20	-	40,40,40,40	0
58	MG	CA	1765	1/1	0.98	0.17	-	114,114,114,114	0
58	MG	CA	1746	1/1	0.93	0.20	-	87,87,87,87	0
58	MG	BA	3033	1/1	0.92	0.32	-	63,63,63,63	0
58	MG	BB	215	1/1	0.92	0.20	-	88,88,88,88	1
58	MG	BA	3314	1/1	0.84	0.32	-	74,74,74,74	0
58	MG	DA	3400	1/1	0.98	0.50	-	33,33,33,33	0
58	MG	DB	202	1/1	0.68	1.14	-	113,113,113,113	1
58	MG	DA	3189	1/1	0.82	0.39	-	77,77,77,77	0
58	MG	BA	3341	1/1	0.72	0.46	-	112,112,112,112	0
58	MG	AA	1750	1/1	0.95	0.74	-	97,97,97,97	0
58	MG	DA	3128	1/1	0.83	0.27	-	65,65,65,65	0
58	MG	DA	3364	1/1	0.65	0.45	-	95,95,95,95	0
58	MG	CA	1655	1/1	0.90	0.11	-	99,99,99,99	0
58	MG	BA	3434	1/1	0.96	0.15	-	90,90,90,90	0
58	MG	AA	1801	1/1	0.94	0.09	-	71,71,71,71	0
58	MG	DA	3394	1/1	0.99	0.20	-	48,48,48,48	1
58	MG	BA	3269	1/1	0.75	0.54	-	85,85,85,85	0
58	MG	DA	3181	1/1	0.81	0.61	-	74,74,74,74	0
58	MG	BA	3017	1/1	0.93	0.22	-	69,69,69,69	0
58	MG	CA	1652	1/1	0.91	0.18	-	113,113,113,113	0
58	MG	AA	1672	1/1	0.68	0.31	-	87,87,87,87	0
58	MG	CW	105	1/1	0.47	0.20	-	123,123,123,123	0
58	MG	BA	3216	1/1	0.99	0.20	-	90,90,90,90	0
58	MG	DA	3273	1/1	0.26	0.76	-	155,155,155,155	0
58	MG	BV	202	1/1	0.97	0.18	-	136,136,136,136	1
58	MG	AA	1795	1/1	0.98	0.08	-	91,91,91,91	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3108	1/1	0.97	0.12	-	32,32,32,32	0
58	MG	DA	3246	1/1	0.79	0.51	-	53,53,53,53	0
58	MG	BA	3165	1/1	0.92	0.15	-	63,63,63,63	0
58	MG	BA	3336	1/1	0.19	0.74	-	105,105,105,105	1
58	MG	DA	3374	1/1	0.60	0.21	-	72,72,72,72	0
58	MG	DA	3166	1/1	0.36	0.95	-	104,104,104,104	0
58	MG	DA	3096	1/1	0.99	0.19	-	43,43,43,43	0
58	MG	DA	3343	1/1	0.88	0.39	-	89,89,89,89	1
58	MG	CA	1657	1/1	0.95	0.15	-	78,78,78,78	0
58	MG	DA	3435	1/1	0.75	0.20	-	59,59,59,59	0
58	MG	BA	3332	1/1	0.90	0.15	-	138,138,138,138	0
58	MG	AX	103	1/1	0.95	0.21	-	98,98,98,98	0
58	MG	AA	1611	1/1	0.97	0.21	-	48,48,48,48	0
58	MG	BA	3357	1/1	0.98	0.08	-	56,56,56,56	0
58	MG	CA	1788	1/1	0.94	0.07	-	75,75,75,75	0
58	MG	AA	1660	1/1	0.86	0.49	-	90,90,90,90	0
58	MG	AA	1733	1/1	0.95	0.20	-	91,91,91,91	1
58	MG	DA	3382	1/1	0.96	0.14	-	59,59,59,59	0
58	MG	CA	1756	1/1	0.83	0.22	-	59,59,59,59	0
58	MG	DA	3348	1/1	0.68	0.52	-	94,94,94,94	0
58	MG	DA	3299	1/1	0.85	0.20	-	119,119,119,119	0
58	MG	AA	1779	1/1	0.73	0.34	-	72,72,72,72	1
58	MG	DB	208	1/1	0.86	0.15	-	87,87,87,87	0
58	MG	CA	1815	1/1	0.81	0.53	-	68,68,68,68	0
58	MG	AA	1766	1/1	0.88	0.33	-	74,74,74,74	0
58	MG	CA	1745	1/1	0.80	0.55	-	96,96,96,96	0
58	MG	BA	3307	1/1	0.77	0.19	-	104,104,104,104	0
58	MG	BA	3110	1/1	0.93	0.30	-	47,47,47,47	0
58	MG	BA	3070	1/1	0.67	0.86	-	116,116,116,116	0
58	MG	BA	3301	1/1	0.90	0.72	-	67,67,67,67	1
58	MG	DA	3044	1/1	0.97	0.37	-	66,66,66,66	0
58	MG	DA	3379	1/1	0.76	0.36	-	66,66,66,66	0
58	MG	AA	1737	1/1	0.94	0.30	-	78,78,78,78	0
58	MG	BA	3125	1/1	0.95	0.20	-	64,64,64,64	0
58	MG	BA	3229	1/1	0.96	0.12	-	117,117,117,117	0
58	MG	BA	3155	1/1	0.98	0.10	-	31,31,31,31	1
58	MG	DA	3219	1/1	0.49	0.43	-	102,102,102,102	0
58	MG	CA	1661	1/1	0.59	0.50	-	98,98,98,98	0
58	MG	AW	102	1/1	0.91	0.16	-	78,78,78,78	1
58	MG	BA	3375	1/1	0.77	0.76	-	58,58,58,58	1
58	MG	AA	1644	1/1	0.92	0.13	-	57,57,57,57	0
58	MG	DA	3152	1/1	0.97	0.16	-	65,65,65,65	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AX	104	1/1	0.82	0.65	-	71,71,71,71	1
58	MG	CA	1757	1/1	0.90	0.40	-	76,76,76,76	0
58	MG	DA	3392	1/1	0.95	0.32	-	74,74,74,74	0
58	MG	DA	3324	1/1	0.94	0.29	-	104,104,104,104	1
58	MG	BA	3128	1/1	0.85	0.24	-	37,37,37,37	0
58	MG	BA	3272	1/1	0.76	0.52	-	92,92,92,92	0
58	MG	DB	211	1/1	0.86	0.64	-	69,69,69,69	1
58	MG	B5	101	1/1	0.94	0.36	-	50,50,50,50	0
58	MG	DA	3358	1/1	0.38	0.36	-	102,102,102,102	0
58	MG	AA	1714	1/1	0.92	0.25	-	86,86,86,86	0
58	MG	AA	1734	1/1	0.64	0.42	-	92,92,92,92	0
58	MG	CA	1783	1/1	0.34	1.21	-	100,100,100,100	0
58	MG	CA	1688	1/1	0.39	1.02	-	115,115,115,115	0
58	MG	DA	3083	1/1	0.96	0.15	-	32,32,32,32	0
58	MG	BA	3435	1/1	0.99	0.08	-	80,80,80,80	1
58	MG	DA	3345	1/1	0.40	0.29	-	110,110,110,110	1
58	MG	AA	1724	1/1	0.97	0.17	-	109,109,109,109	0
58	MG	BB	211	1/1	0.87	0.99	-	75,75,75,75	1
58	MG	BA	3393	1/1	0.83	0.34	-	101,101,101,101	1
58	MG	CA	1650	1/1	0.78	0.41	-	98,98,98,98	0
58	MG	AA	1722	1/1	0.93	0.17	-	67,67,67,67	0
58	MG	DA	3117	1/1	0.81	0.63	-	69,69,69,69	0
58	MG	BA	3437	1/1	0.86	0.15	-	75,75,75,75	0
58	MG	BA	3287	1/1	0.69	0.75	-	92,92,92,92	1
58	MG	DA	3101	1/1	0.98	0.12	-	71,71,71,71	0
58	MG	DA	3223	1/1	0.53	0.38	-	82,82,82,82	0
58	MG	DA	3230	1/1	0.86	0.51	-	119,119,119,119	0
58	MG	DA	3169	1/1	0.94	0.05	-	52,52,52,52	0
58	MG	BA	3114	1/1	0.98	0.49	-	44,44,44,44	0
58	MG	BB	203	1/1	0.88	0.13	-	134,134,134,134	0
58	MG	AA	1735	1/1	0.91	0.25	-	58,58,58,58	0
58	MG	DA	3425	1/1	0.92	0.12	-	76,76,76,76	0
58	MG	AA	1637	1/1	0.98	0.20	-	44,44,44,44	0
58	MG	DA	3161	1/1	0.56	0.62	-	131,131,131,131	0
58	MG	CA	1698	1/1	0.97	0.10	-	106,106,106,106	0
58	MG	CA	1666	1/1	0.94	0.47	-	75,75,75,75	0
58	MG	CA	1621	1/1	0.70	0.20	-	91,91,91,91	0
58	MG	DA	3032	1/1	0.87	0.28	-	69,69,69,69	0
58	MG	DA	3289	1/1	0.83	0.19	-	73,73,73,73	0
58	MG	DA	3342	1/1	0.92	0.17	-	62,62,62,62	1
58	MG	DA	3130	1/1	0.94	0.13	-	80,80,80,80	0
58	MG	DA	3451	1/1	0.98	0.15	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	3323	1/1	0.85	0.16	-	83,83,83,83	1
58	MG	DA	3008	1/1	0.91	0.83	-	70,70,70,70	0
58	MG	CA	1736	1/1	0.90	0.28	-	73,73,73,73	0
58	MG	CA	1701	1/1	0.60	0.57	-	113,113,113,113	0
58	MG	CA	1780	1/1	0.78	0.86	-	81,81,81,81	1
58	MG	DA	3406	1/1	0.98	0.08	-	87,87,87,87	1
58	MG	DA	3042	1/1	0.88	0.56	-	76,76,76,76	0
58	MG	AA	1759	1/1	0.94	0.22	-	70,70,70,70	1
58	MG	AA	1736	1/1	0.98	0.36	-	60,60,60,60	1
58	MG	BA	3418	1/1	0.91	0.29	-	61,61,61,61	0
58	MG	AA	1648	1/1	0.96	0.15	-	95,95,95,95	0
58	MG	DA	3355	1/1	0.98	0.10	-	37,37,37,37	0
58	MG	CA	1791	1/1	0.88	0.87	-	27,27,27,27	1
58	MG	BA	3010	1/1	0.94	0.24	-	40,40,40,40	0
58	MG	BA	3140	1/1	0.98	0.15	-	75,75,75,75	0
58	MG	DA	3330	1/1	0.75	0.46	-	97,97,97,97	0
58	MG	DA	3020	1/1	0.95	0.33	-	15,15,15,15	0
58	MG	CW	110	1/1	0.88	0.31	-	85,85,85,85	1
58	MG	DA	3260	1/1	0.93	0.09	-	29,29,29,29	0
58	MG	BA	3187	1/1	0.51	0.15	-	98,98,98,98	0
58	MG	CA	1709	1/1	0.81	0.74	-	96,96,96,96	0
58	MG	DA	3135	1/1	0.84	0.36	-	52,52,52,52	0
58	MG	AA	1603	1/1	0.99	0.15	-	101,101,101,101	0
58	MG	BA	3151	1/1	0.87	0.38	-	64,64,64,64	0
58	MG	BA	3135	1/1	0.99	0.15	-	34,34,34,34	0
58	MG	BA	3013	1/1	0.66	0.60	-	80,80,80,80	0
58	MG	DA	3231	1/1	0.62	0.38	-	85,85,85,85	0
58	MG	BA	3346	1/1	0.77	0.23	-	76,76,76,76	1
58	MG	BA	3360	1/1	0.95	0.14	-	60,60,60,60	0
58	MG	DA	3413	1/1	0.94	0.27	-	96,96,96,96	0
58	MG	DA	3255	1/1	0.57	0.41	-	96,96,96,96	0
58	MG	DA	3448	1/1	0.33	0.12	-	97,97,97,97	0
58	MG	BA	3284	1/1	0.77	0.40	-	77,77,77,77	0
58	MG	CA	1816	1/1	0.61	1.29	-	102,102,102,102	0
58	MG	AA	1667	1/1	0.95	0.09	-	56,56,56,56	0
58	MG	BA	3445	1/1	0.79	0.25	-	84,84,84,84	0
58	MG	CW	120	1/1	0.90	0.29	-	117,117,117,117	1
58	MG	DA	3232	1/1	0.97	0.38	-	55,55,55,55	0
58	MG	CW	103	1/1	0.34	0.47	-	119,119,119,119	0
58	MG	BA	3066	1/1	0.99	0.14	-	39,39,39,39	0
58	MG	CA	1779	1/1	0.87	0.29	-	121,121,121,121	0
58	MG	DA	3085	1/1	0.95	0.56	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3383	1/1	0.98	0.11	-	76,76,76,76	0
58	MG	CA	1715	1/1	0.89	0.14	-	80,80,80,80	0
58	MG	DA	3016	1/1	0.91	0.18	-	74,74,74,74	0
58	MG	BA	3122	1/1	0.98	0.17	-	30,30,30,30	0
58	MG	BA	3177	1/1	0.81	0.13	-	55,55,55,55	0
58	MG	DA	3206	1/1	0.87	0.29	-	55,55,55,55	0
58	MG	AA	1780	1/1	0.62	0.52	-	84,84,84,84	0
58	MG	CA	1802	1/1	0.94	0.11	-	70,70,70,70	1
58	MG	DA	3049	1/1	0.82	0.88	-	83,83,83,83	0
58	MG	BX	101	1/1	0.93	0.30	-	69,69,69,69	0
58	MG	CA	1731	1/1	0.44	0.41	-	142,142,142,142	0
58	MG	BA	3157	1/1	0.83	0.45	-	78,78,78,78	1
58	MG	AA	1730	1/1	0.63	0.48	-	93,93,93,93	0
58	MG	BA	3023	1/1	0.86	0.26	-	71,71,71,71	0
58	MG	BP	201	1/1	0.96	0.14	-	66,66,66,66	0
58	MG	DA	3162	1/1	0.88	0.22	-	65,65,65,65	0
58	MG	DA	3365	1/1	0.95	0.19	-	135,135,135,135	1
58	MG	BA	3408	1/1	0.98	0.19	-	64,64,64,64	1
58	MG	CA	1771	1/1	0.96	0.12	-	47,47,47,47	0
58	MG	DA	3354	1/1	0.93	0.23	-	110,110,110,110	0
58	MG	BA	3344	1/1	0.87	0.21	-	46,46,46,46	1
58	MG	DA	3264	1/1	0.45	1.03	-	98,98,98,98	0
58	MG	AA	1756	1/1	0.98	0.49	-	64,64,64,64	0
58	MG	AA	1682	1/1	0.88	0.15	-	75,75,75,75	0
58	MG	BA	3385	1/1	0.99	0.12	-	88,88,88,88	1
58	MG	BA	3286	1/1	0.89	0.43	-	66,66,66,66	0
58	MG	BA	3421	1/1	0.90	0.24	-	110,110,110,110	0
58	MG	DA	3065	1/1	0.97	0.17	-	41,41,41,41	0
58	MG	CA	1772	1/1	0.44	0.67	-	101,101,101,101	0
58	MG	CA	1704	1/1	0.98	0.07	-	41,41,41,41	0
58	MG	CA	1773	1/1	0.67	0.47	-	82,82,82,82	1
58	MG	CA	1687	1/1	0.74	0.63	-	84,84,84,84	0
58	MG	DA	3318	1/1	0.82	0.34	-	122,122,122,122	0
58	MG	CA	1767	1/1	0.80	0.43	-	76,76,76,76	0
58	MG	CX	103	1/1	0.97	0.08	-	97,97,97,97	0
58	MG	AA	1668	1/1	0.74	0.34	-	66,66,66,66	0
58	MG	DA	3001	1/1	0.97	0.09	-	92,92,92,92	0
58	MG	DA	3041	1/1	0.95	0.30	-	56,56,56,56	0
58	MG	DA	3097	1/1	0.96	0.30	-	53,53,53,53	0
58	MG	CA	1807	1/1	0.87	0.49	-	62,62,62,62	1
58	MG	BA	3131	1/1	0.90	0.10	-	60,60,60,60	0
58	MG	D1	101	1/1	0.65	0.61	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3170	1/1	0.86	0.14	-	46,46,46,46	1
58	MG	CA	1690	1/1	0.81	0.12	-	122,122,122,122	0
58	MG	DA	3021	1/1	0.98	0.40	-	59,59,59,59	0
58	MG	BA	3335	1/1	0.99	0.10	-	89,89,89,89	1
58	MG	CA	1801	1/1	0.36	0.39	-	128,128,128,128	0
58	MG	AA	1621	1/1	0.91	0.13	-	55,55,55,55	0
58	MG	CA	1682	1/1	0.49	0.55	-	83,83,83,83	0
58	MG	AW	117	1/1	0.41	1.09	-	134,134,134,134	0
58	MG	DA	3410	1/1	0.68	0.97	-	99,99,99,99	0
58	MG	AW	106	1/1	0.91	0.27	-	103,103,103,103	0
58	MG	BA	3391	1/1	0.98	0.15	-	33,33,33,33	0
58	MG	BA	3304	1/1	0.84	0.34	-	95,95,95,95	0
58	MG	BA	3025	1/1	0.91	0.32	-	42,42,42,42	0
58	MG	AA	1684	1/1	0.97	0.16	-	97,97,97,97	0
58	MG	DA	3220	1/1	0.75	1.41	-	97,97,97,97	0
58	MG	DA	3069	1/1	0.86	0.20	-	79,79,79,79	0
58	MG	DA	3332	1/1	0.75	0.18	-	100,100,100,100	0
58	MG	CA	1761	1/1	0.89	0.63	-	94,94,94,94	0
58	MG	CA	1758	1/1	0.97	0.08	-	110,110,110,110	0
58	MG	BA	3433	1/1	0.89	0.14	-	121,121,121,121	0
58	MG	BA	3261	1/1	0.85	0.19	-	79,79,79,79	0

6.5 Other polymers

There are no such residues in this entry.