



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:57 PM GMT

PDB ID : 4V5D
Title : Structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, paromomycin, acylated A- and P-site tRNAs, and E-site tRNA.
Authors : Voorhees, R.M.; Weixlbaumer, A.; Loakes, D.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-03-24
Resolution : 3.50 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

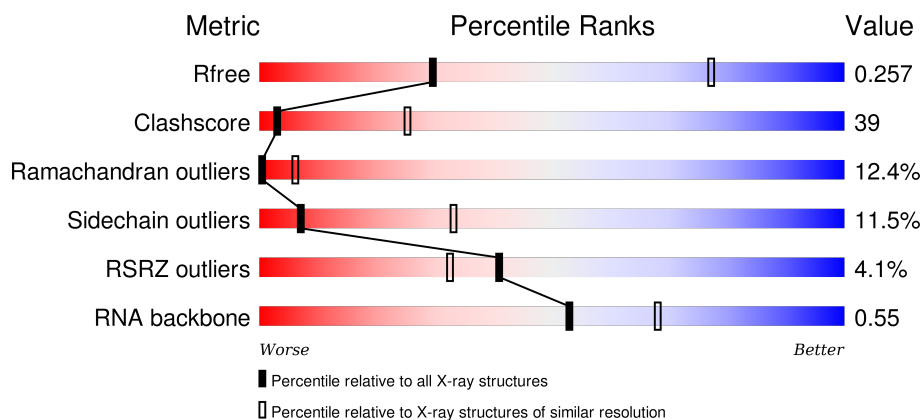
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



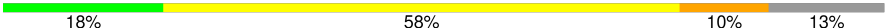
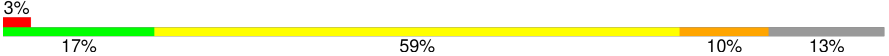
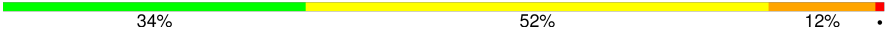
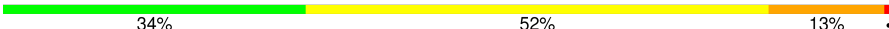
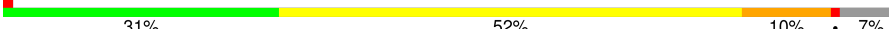
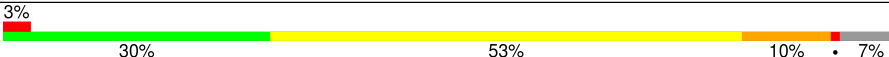


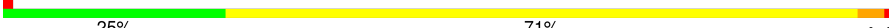
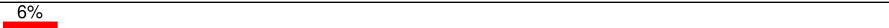

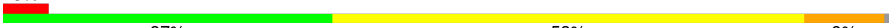
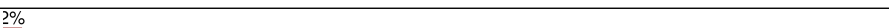



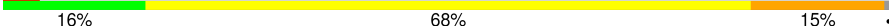

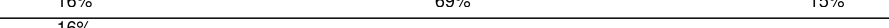
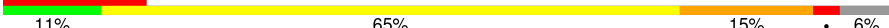


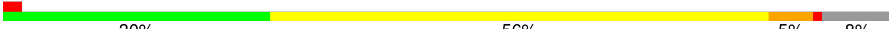


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>60%</div> <div>11%</div> <div>..</div> </div>
1	CA	1522	<div> <div>2%</div> <div>26%</div> <div>61%</div> <div>11%</div> <div>..</div> </div>
2	AB	256	<div> <div>3%</div> <div>17%</div> <div>58%</div> <div>14%</div> <div>• 8%</div> </div>
2	CB	256	<div> <div>2%</div> <div>17%</div> <div>58%</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	


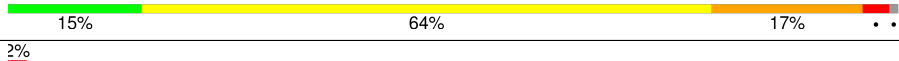


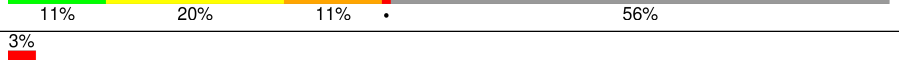
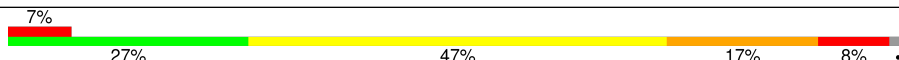
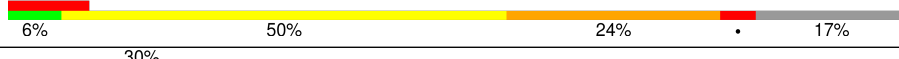


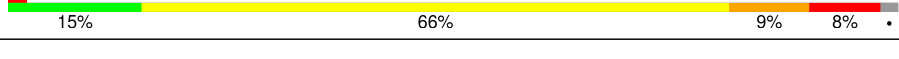
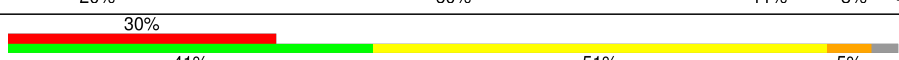


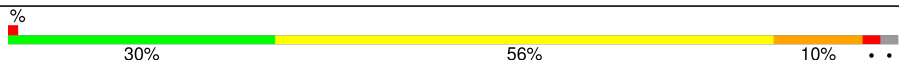
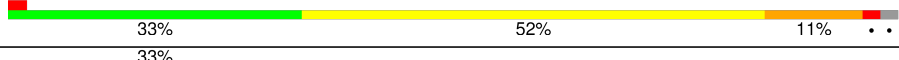
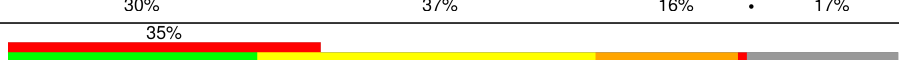

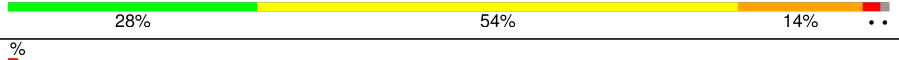
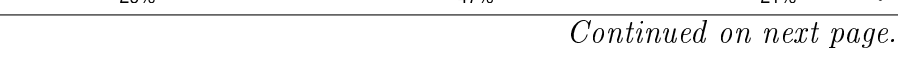


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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AY	77	
22	CV	77	
22	CY	77	
23	AW	76	
23	CW	76	
24	AX	11	
24	CX	11	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	

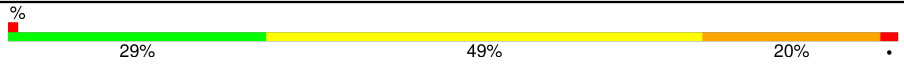

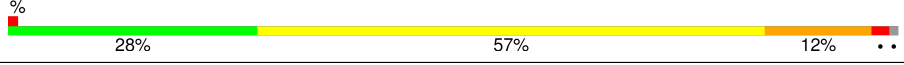
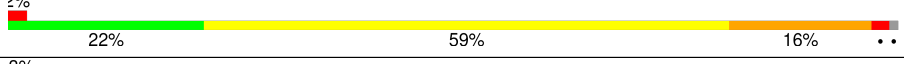
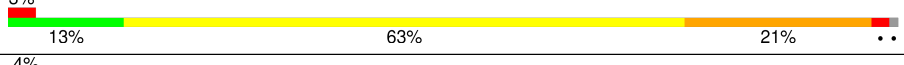
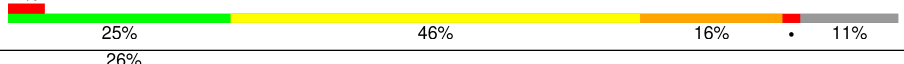
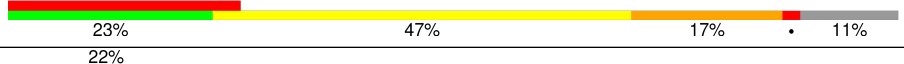
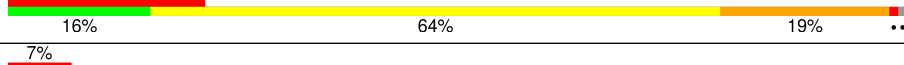
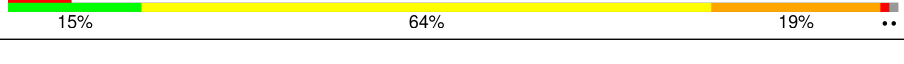
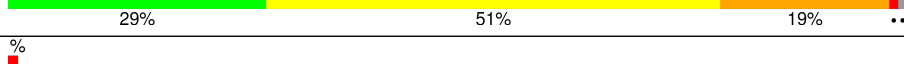

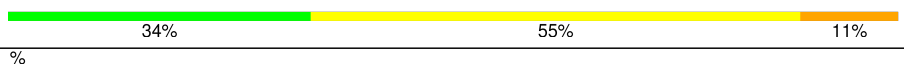
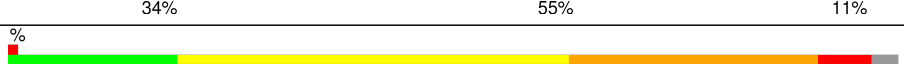
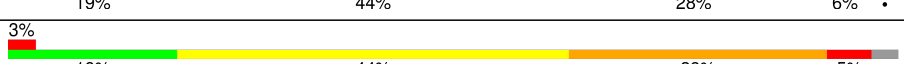
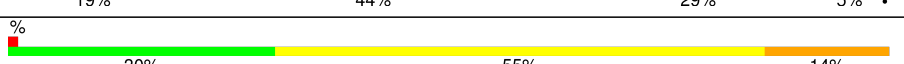
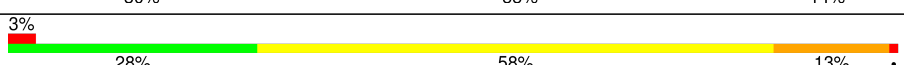
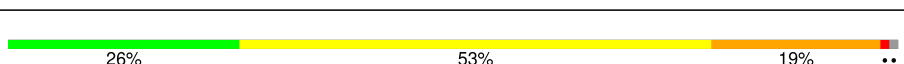
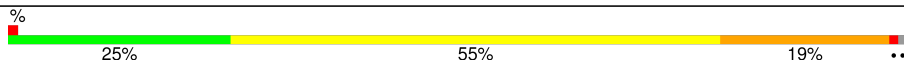
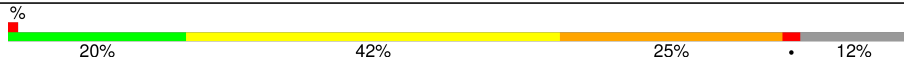


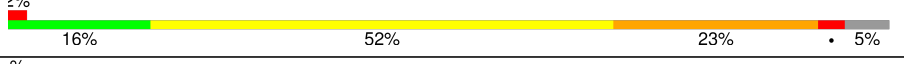

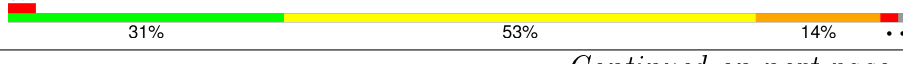

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Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2822	
35	DA	2822	
36	BB	122	
36	DB	122	
37	BC	229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

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

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Mol	Chain	Length	Quality of chain
52	BV	101	
52	DV	101	
53	BW	113	
53	DW	113	
54	BX	96	
54	DX	96	
55	BY	110	
55	DY	110	
56	BZ	206	
56	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
57	MG	AA	1610	-	-	-	X
57	MG	AA	1623	-	-	-	X
57	MG	AA	1630	-	-	-	X
57	MG	AA	1634	-	-	-	X
57	MG	AA	1636	-	-	-	X
57	MG	AA	1664	-	-	-	X
57	MG	AA	1666	-	-	-	X
57	MG	AA	1682	-	-	-	X
57	MG	AA	1688	-	-	-	X
57	MG	AA	1694	-	-	-	X
57	MG	AA	1705	-	-	-	X
57	MG	AA	1706	-	-	-	X
57	MG	AA	1712	-	-	-	X
57	MG	AA	1715	-	-	-	X
57	MG	AA	1719	-	-	-	X
57	MG	AA	1721	-	-	-	X
57	MG	AA	1739	-	-	-	X
57	MG	AA	1773	-	-	-	X
57	MG	AA	1774	-	-	-	X
57	MG	AA	1781	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1786	-	-	-	X
57	MG	AA	1788	-	-	-	X
57	MG	B0	101	-	-	-	X
57	MG	B2	602	-	-	-	X
57	MG	B7	101	-	-	-	X
57	MG	BA	3001	-	-	-	X
57	MG	BA	3004	-	-	-	X
57	MG	BA	3005	-	-	-	X
57	MG	BA	3007	-	-	-	X
57	MG	BA	3009	-	-	-	X
57	MG	BA	3011	-	-	-	X
57	MG	BA	3012	-	-	-	X
57	MG	BA	3021	-	-	-	X
57	MG	BA	3022	-	-	-	X
57	MG	BA	3023	-	-	-	X
57	MG	BA	3025	-	-	-	X
57	MG	BA	3026	-	-	-	X
57	MG	BA	3028	-	-	-	X
57	MG	BA	3035	-	-	-	X
57	MG	BA	3039	-	-	-	X
57	MG	BA	3045	-	-	-	X
57	MG	BA	3046	-	-	-	X
57	MG	BA	3047	-	-	-	X
57	MG	BA	3048	-	-	-	X
57	MG	BA	3053	-	-	-	X
57	MG	BA	3055	-	-	-	X
57	MG	BA	3058	-	-	-	X
57	MG	BA	3060	-	-	-	X
57	MG	BA	3062	-	-	-	X
57	MG	BA	3064	-	-	-	X
57	MG	BA	3065	-	-	-	X
57	MG	BA	3067	-	-	-	X
57	MG	BA	3069	-	-	-	X
57	MG	BA	3070	-	-	-	X
57	MG	BA	3082	-	-	-	X
57	MG	BA	3086	-	-	-	X
57	MG	BA	3091	-	-	-	X
57	MG	BA	3092	-	-	-	X
57	MG	BA	3097	-	-	-	X
57	MG	BA	3105	-	-	-	X
57	MG	BA	3110	-	-	-	X
57	MG	BA	3112	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3113	-	-	-	X
57	MG	BA	3114	-	-	-	X
57	MG	BA	3117	-	-	-	X
57	MG	BA	3118	-	-	-	X
57	MG	BA	3120	-	-	-	X
57	MG	BA	3123	-	-	-	X
57	MG	BA	3129	-	-	-	X
57	MG	BA	3143	-	-	-	X
57	MG	BA	3150	-	-	-	X
57	MG	BA	3161	-	-	-	X
57	MG	BA	3169	-	-	-	X
57	MG	BA	3170	-	-	-	X
57	MG	BA	3178	-	-	-	X
57	MG	BA	3180	-	-	-	X
57	MG	BA	3190	-	-	-	X
57	MG	BA	3194	-	-	-	X
57	MG	BA	3200	-	-	-	X
57	MG	BA	3215	-	-	-	X
57	MG	BA	3216	-	-	-	X
57	MG	BA	3229	-	-	-	X
57	MG	BA	3233	-	-	-	X
57	MG	BA	3237	-	-	-	X
57	MG	BA	3239	-	-	-	X
57	MG	BA	3241	-	-	-	X
57	MG	BA	3255	-	-	-	X
57	MG	BA	3256	-	-	-	X
57	MG	BA	3266	-	-	-	X
57	MG	BA	3268	-	-	-	X
57	MG	BA	3271	-	-	-	X
57	MG	BA	3272	-	-	-	X
57	MG	BA	3275	-	-	-	X
57	MG	BA	3279	-	-	-	X
57	MG	BA	3291	-	-	-	X
57	MG	BA	3295	-	-	-	X
57	MG	BA	3299	-	-	-	X
57	MG	BA	3300	-	-	-	X
57	MG	BA	3301	-	-	-	X
57	MG	BA	3307	-	-	-	X
57	MG	BA	3340	-	-	-	X
57	MG	BA	3366	-	-	-	X
57	MG	BA	3375	-	-	-	X
57	MG	BA	3376	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3379	-	-	-	X
57	MG	BA	3381	-	-	-	X
57	MG	BA	3382	-	-	-	X
57	MG	BA	3398	-	-	-	X
57	MG	BA	3403	-	-	-	X
57	MG	BA	3409	-	-	-	X
57	MG	BA	3410	-	-	-	X
57	MG	BB	203	-	-	-	X
57	MG	BB	204	-	-	-	X
57	MG	BB	205	-	-	-	X
57	MG	BB	212	-	-	-	X
57	MG	BN	201	-	-	-	X
57	MG	BO	201	-	-	-	X
57	MG	BX	102	-	-	-	X
57	MG	CA	1609	-	-	-	X
57	MG	CA	1623	-	-	-	X
57	MG	CA	1625	-	-	-	X
57	MG	CA	1634	-	-	-	X
57	MG	CA	1636	-	-	-	X
57	MG	CA	1638	-	-	-	X
57	MG	CA	1652	-	-	-	X
57	MG	CA	1678	-	-	-	X
57	MG	CA	1686	-	-	-	X
57	MG	CA	1690	-	-	-	X
57	MG	CA	1695	-	-	-	X
57	MG	CA	1707	-	-	-	X
57	MG	CA	1709	-	-	-	X
57	MG	CA	1716	-	-	-	X
57	MG	CA	1719	-	-	-	X
57	MG	CA	1721	-	-	-	X
57	MG	CA	1739	-	-	-	X
57	MG	CA	1783	-	-	-	X
57	MG	CA	1785	-	-	-	X
57	MG	CA	1789	-	-	-	X
57	MG	D2	601	-	-	-	X
57	MG	D7	101	-	-	-	X
57	MG	D7	102	-	-	-	X
57	MG	DA	3005	-	-	-	X
57	MG	DA	3006	-	-	-	X
57	MG	DA	3010	-	-	-	X
57	MG	DA	3012	-	-	-	X
57	MG	DA	3013	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3018	-	-	-	X
57	MG	DA	3022	-	-	-	X
57	MG	DA	3023	-	-	-	X
57	MG	DA	3024	-	-	-	X
57	MG	DA	3027	-	-	-	X
57	MG	DA	3029	-	-	-	X
57	MG	DA	3036	-	-	-	X
57	MG	DA	3046	-	-	-	X
57	MG	DA	3047	-	-	-	X
57	MG	DA	3048	-	-	-	X
57	MG	DA	3049	-	-	-	X
57	MG	DA	3054	-	-	-	X
57	MG	DA	3056	-	-	-	X
57	MG	DA	3061	-	-	-	X
57	MG	DA	3063	-	-	-	X
57	MG	DA	3066	-	-	-	X
57	MG	DA	3070	-	-	-	X
57	MG	DA	3071	-	-	-	X
57	MG	DA	3074	-	-	-	X
57	MG	DA	3083	-	-	-	X
57	MG	DA	3088	-	-	-	X
57	MG	DA	3090	-	-	-	X
57	MG	DA	3092	-	-	-	X
57	MG	DA	3093	-	-	-	X
57	MG	DA	3098	-	-	-	X
57	MG	DA	3101	-	-	-	X
57	MG	DA	3106	-	-	-	X
57	MG	DA	3118	-	-	-	X
57	MG	DA	3119	-	-	-	X
57	MG	DA	3121	-	-	-	X
57	MG	DA	3124	-	-	-	X
57	MG	DA	3130	-	-	-	X
57	MG	DA	3144	-	-	-	X
57	MG	DA	3146	-	-	-	X
57	MG	DA	3148	-	-	-	X
57	MG	DA	3152	-	-	-	X
57	MG	DA	3158	-	-	-	X
57	MG	DA	3163	-	-	-	X
57	MG	DA	3165	-	-	-	X
57	MG	DA	3171	-	-	-	X
57	MG	DA	3172	-	-	-	X
57	MG	DA	3178	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3182	-	-	-	X
57	MG	DA	3184	-	-	-	X
57	MG	DA	3192	-	-	-	X
57	MG	DA	3196	-	-	-	X
57	MG	DA	3202	-	-	-	X
57	MG	DA	3217	-	-	-	X
57	MG	DA	3222	-	-	-	X
57	MG	DA	3231	-	-	-	X
57	MG	DA	3235	-	-	-	X
57	MG	DA	3239	-	-	-	X
57	MG	DA	3241	-	-	-	X
57	MG	DA	3258	-	-	-	X
57	MG	DA	3270	-	-	-	X
57	MG	DA	3274	-	-	-	X
57	MG	DA	3283	-	-	-	X
57	MG	DA	3293	-	-	-	X
57	MG	DA	3297	-	-	-	X
57	MG	DA	3341	-	-	-	X
57	MG	DA	3364	-	-	-	X
57	MG	DA	3378	-	-	-	X
57	MG	DA	3380	-	-	-	X
57	MG	DA	3395	-	-	-	X
57	MG	DA	3399	-	-	-	X
57	MG	DA	3409	-	-	-	X
57	MG	DB	212	-	-	-	X
57	MG	DD	301	-	-	-	X
57	MG	DF	302	-	-	-	X
57	MG	DN	201	-	-	-	X
57	MG	DO	201	-	-	-	X
58	PAR	AA	1799	-	-	-	X
58	PAR	CA	1800	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 296042 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 AND A-SITE PHE-TRNA PHE.

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

- 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	11	Total	C	N	O	P	0	0	0
			227	104	39	74	10			
24	CX	11	Total	C	N	O	P	0	0	0
			227	104	39	74	10			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

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

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O	0	0	1
			1140	689	221	230			
37	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	422	Total	Mg	0	0
			422	422		
57	CA	199	Total	Mg	0	0
			199	199		
57	DF	2	Total	Mg	0	0
			2	2		
57	CV	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D2	3	Total 3	Mg 3	0	0
57	BE	1	Total 1	Mg 1	0	0
57	AW	8	Total 8	Mg 8	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	1	Total 1	Mg 1	0	0
57	AX	2	Total 2	Mg 2	0	0
57	CN	1	Total 1	Mg 1	0	0
57	DN	1	Total 1	Mg 1	0	0
57	DC	1	Total 1	Mg 1	0	0
57	DD	2	Total 2	Mg 2	0	0
57	B5	2	Total 2	Mg 2	0	0
57	BB	14	Total 14	Mg 14	0	0
57	DO	1	Total 1	Mg 1	0	0
57	AE	1	Total 1	Mg 1	0	0
57	BF	1	Total 1	Mg 1	0	0
57	AV	5	Total 5	Mg 5	0	0
57	BX	2	Total 2	Mg 2	0	0
57	B2	2	Total 2	Mg 2	0	0
57	AA	198	Total 198	Mg 198	0	0
57	D7	2	Total 2	Mg 2	0	0
57	CX	3	Total 3	Mg 3	0	0

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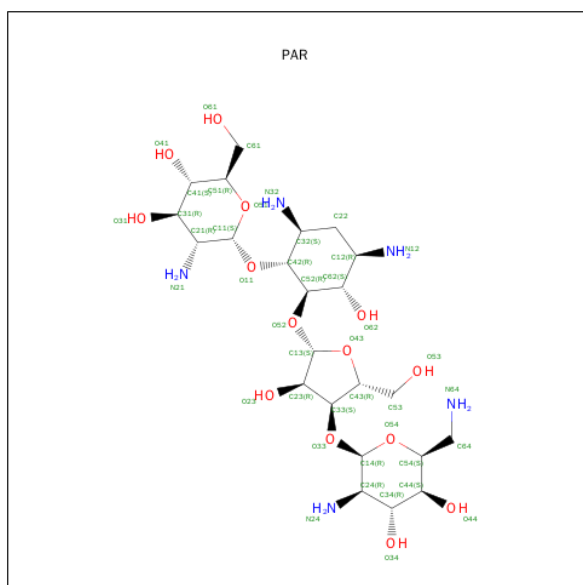
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DV	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	AD	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	AI	1	Total 1	Mg 1	0	0
57	DS	1	Total 1	Mg 1	0	0
57	DE	1	Total 1	Mg 1	0	0
57	DX	3	Total 3	Mg 3	0	0
57	DA	421	Total 421	Mg 421	0	0
57	B7	1	Total 1	Mg 1	0	0
57	AL	2	Total 2	Mg 2	0	0
57	BV	1	Total 1	Mg 1	0	0
57	AG	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	D1	1	Total 1	Mg 1	0	0
57	CI	1	Total 1	Mg 1	0	0
57	CW	7	Total 7	Mg 7	0	0
57	D5	2	Total 2	Mg 2	0	0
57	BD	2	Total 2	Mg 2	0	0
57	B0	1	Total 1	Mg 1	0	0
57	CE	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CL	1	Total	Mg	0	0
			1	1		
57	DB	13	Total	Mg	0	0
			13	13		

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

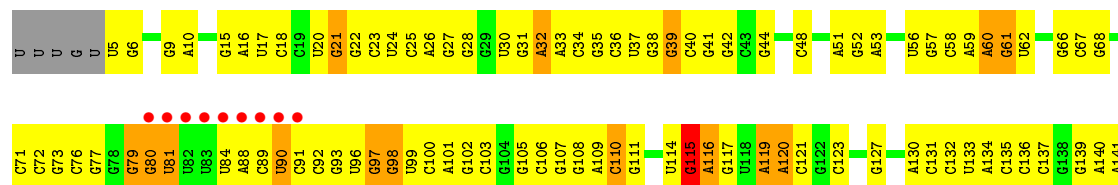
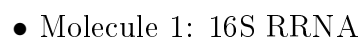
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

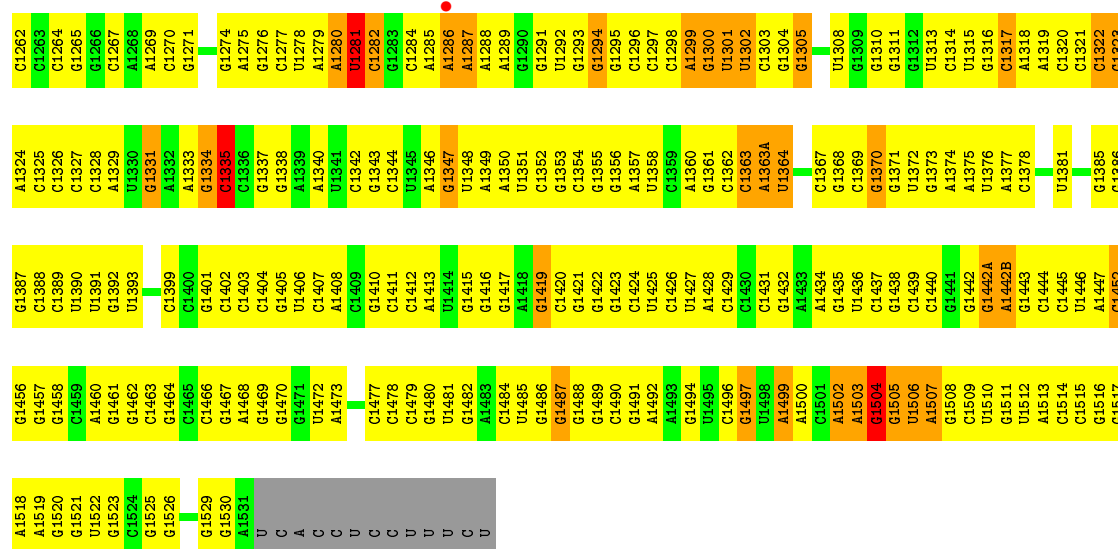
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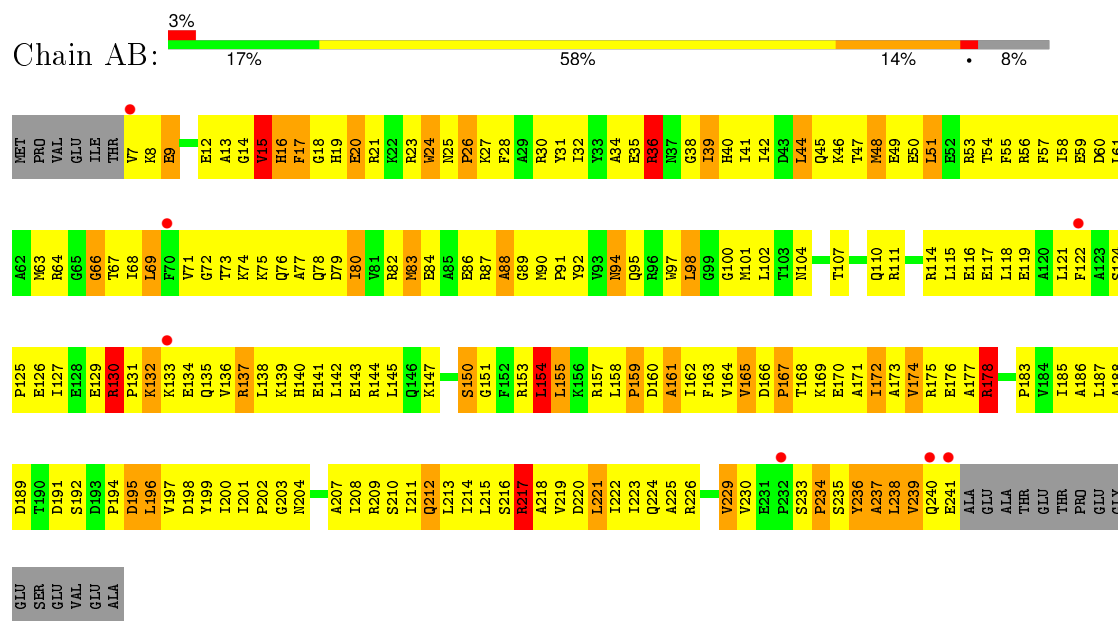
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		



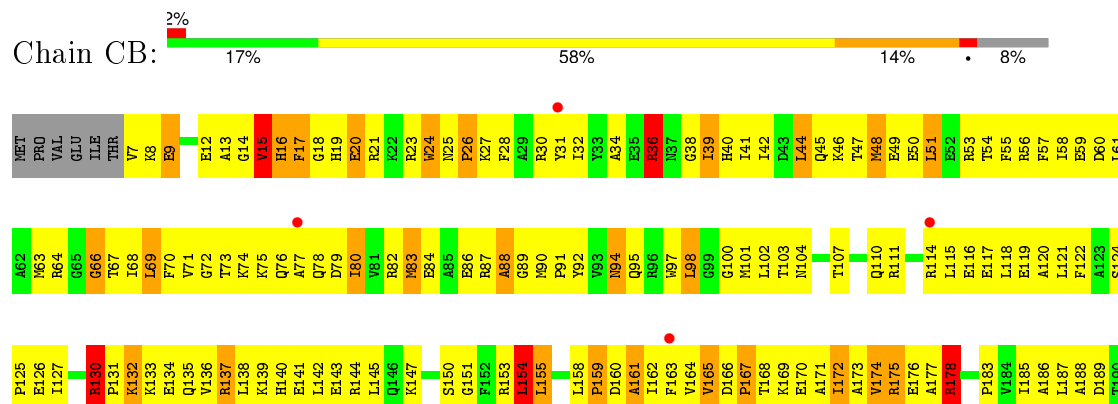
C1195	G1196	G1197	G1198	G1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	G1208	G1209	G1210	G1211	U1212	A1213	G1214	U1215	A1216	G1217	G1218	G1219	G1220	A1221	G1222	C1223	G1224	G1225	A1226	G1227	G1228	G1229	G1230	G1231	U1232	G1233	G1234	C1235	G1236	A1237	G1238	G1239	U1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	C1249	A1250	A1251	A1252	G1253	G1254	G1255	A1256	U1257	G1258	C1259	G1260																																																																																																																																																																																																																																																
A1130	G1131	G1132	G1133	G1134	U1135	G1136	G1137	G1138	G1139	C1140	G1141	G1142	G1143	G1144	G1145	A1146	C1147	G1148	G1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	G1157	C1158	G1159	A1160	G1161	A1162	C1163	U1164	G1165	G1166	G1167	G1168	C1169	U1170	A1171	G1172	G1173	G1174	C1175	C1176	C1177	A1178	U1179	U1180	G1181	U1182	G1183	G1184	A1185	C1186	C1187	C1188	G1189	C1189A	C1189B	C1189C	C1189D	G1189H	G1189I	G1189J	U1189K	G1189L	U1190	U1191	U1192	C1193	A1194	C1195	C1196																																																																																																																																																																																																																																						
U1062	C1063	G1064	U1065	C1066	A1067	G1068	G1069	C1070	G1071	U1072	U1073	G1074	G1075	G1076	A1077	G1078	G1079	A1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	U1088	U1089	U1090	U1091	A1092	A1093	G1094	U1095	C1096	C1097	G1098	G1099	C1100	A1101	A1102	G1103	G1104	A1105	G1106	G1107	G1108	G1109	A1110	G1111	C1112	U1113	G1114	C1115	G1116	G1117	C1118	C1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130																																																																																																																																																																																																																																													
U1000	A1001	G1001A	G1002	G1003	A1004	A1005	G1006	C1007	G1008	G1009	G1010	A1011	A1012	A1013	A1014	A1015	A1016	G1017	U1018	G1019	G1020	G1021	G1022	U1023	U1024	U1025	G1026	C1027	G1028	C1029	G1030	G1031	G1032	G1033	G1034	A1035	G1036	G1037	G1038	G1039	U1040	A1041	G1042	C1043	A1044	U1045	G1046	G1047	G1048	G1049	G1050	C1051	U1052	G1053	G1054	A1055	U1056	G1057	G1058	C1059	G1060	G1061																																																																																																																																																																																																																																																			
A935	C936	A937	A938	G939	C940	G941	G942	G943	G944	G945	A946	G947	C948	A949	U950	G951	U952	G953	G954	U955	U956	U957	A958	A959	U960	U961	C962	G963	A964	A965	G966	G967	G968	G969	G970	G971	G972	G973	A974	A975	G976	A977	A978	C979	G980	U981	G982	A983	A984	A985	A986	G987	G988	U989	U990	U991	U992	G993	A994	G995	G996	G997																																																																																																																																																																																																																																																			
A864	A865	C866	C867	C868	C869	G870	G871	G872	G873	C874	G875	C876	C877	G878	C879	C880	G881	C882	C883	C884	G885	U886	G887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	G901	U902	U903	U904	U905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	U920	U921	G922	A923	G924	G925	G926	G927	G928	G929	C930	G931	C932	G933	C934	C935	C936	C937	C938	C939	C940																																																																																																																																																																																																																																					
U706	C707	C708	G709	G710	G711	A712	G713	G714	G715	U723	U724	U725	C726	C727	C728	C729	U730	G731	C732	G733	C734	C735	C736	U737	C738	C739	U740	U741	U742	U743	U744	U745	U746	U747	U748	C749	G750	U751	C752	U753	U754	U755	C756	U757	U758	A759	U760	C761	C762	C763	C764	G765	A766	A767	A768	G769	C770	U771	U772	U773	G774	G775	G776	U777	C778	A779	U780	C781	C782	U783	U784	U785	U786	U787	U788	U789	U790																																																																																																																																																																																																																																				
C635	C636	C637	G638	G639	A640	C641	C642	C643	C644	C645	U646	C647	C648	G649	G650	C651	U652	A653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	A665	C666	C667	C668	G669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700																																																																																																																																																																																																																																																
G587	C588	C589	G590	U591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700																																																																																																																																																																																																
A412	A413	A414	A415	C416	C417	C418	C419	U420	C421	C422	C423	C424	C425	C426	G427	G428	A429	A430	U431	C432	C433	C434	C435	C436	U437	C438	A439	A440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	A461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500																																																																																																																																																																																																																									
G276	C277	C278	G279	C280	C281	C282	C283	C284	U285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301	C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500																																																																																	
A196	A197	C198	G199	G200	C201	G197	U202	C203	U204	C205	C206	C207	C208	C209	C210	C211	C212	C213	C214	C215	C216	C217	C218	C219	C220	C221	C222	C223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	C236	C237	C238	C239	C240	C241	C242	C243	C244	C245	C246	C247	C248	C249	C250	C251	C252	C253	C254	C255	C256	C257	C258	C259	C260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301	C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500
G142	A143	G144	G145	G146	G147	A148	U149	C150	C151	C152	C153	U154	C155	G156	A157	C158	A159	C160	C161	C162	C163	U164	C165	G166	G167	G168	C169	U170	A171	G172	U173	C174	C175	C176	C177	C178	A179	U180	G181	U182	G183	U184	C185	C186	C187	C188	G189	C189A	C189B	C189C	C189D	G189H	G189I	G189J	U189K	G189L	U190	U191	U192	C193	A194	C195	C196	C197	C198	C199	C200	C201	C202	C203	C204	C205	C206	C207	C208	C209	C210	C211	C212	C213	C214	C215	C216	C217	C218	C219	C220	C221	C222	C223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	C236	C237	C238	C239	C240	C241	C242	C243	C244	C245	C246	C247	C248	C249	C250	C251	C252	C253	C254	C255	C256	C257	C258	C259	C260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301	C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331																																																																																																											

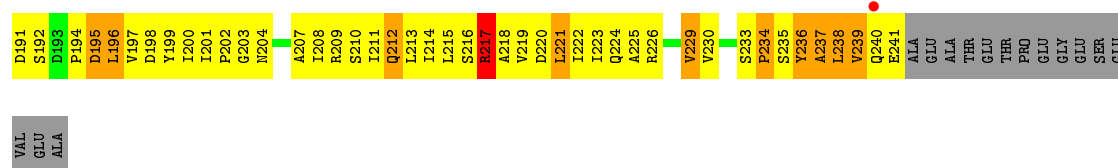


• Molecule 2: 30S RIBOSOMAL PROBLEM S2

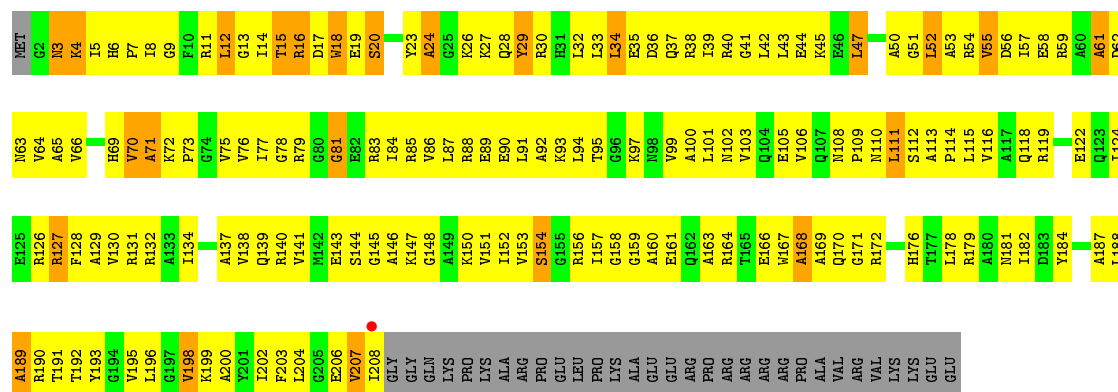


• Molecule 2: 30S RIBOSOMAL PROBLEM S2

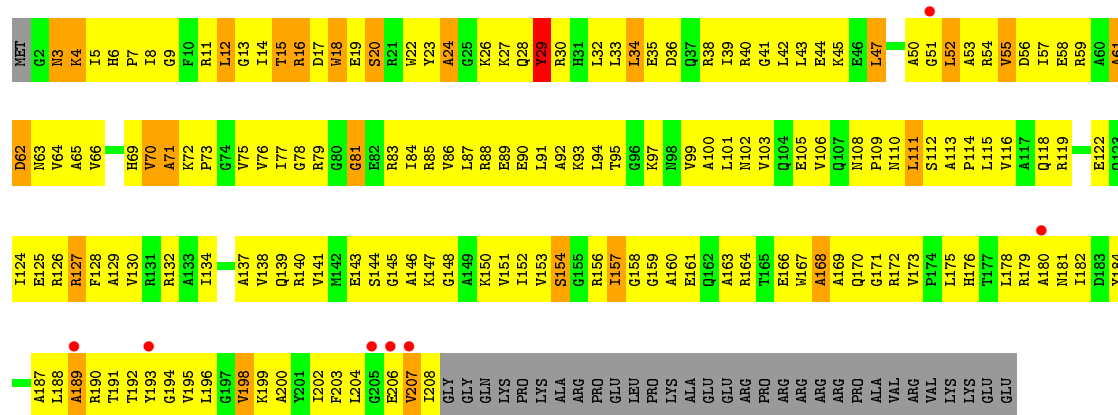




• Molecule 3: 30S RIBOSOMAL PROTEIN S3



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

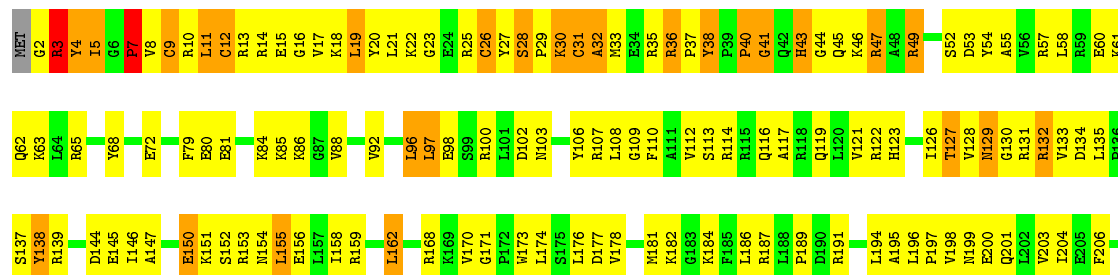


• Molecule 4: 30S RIBOSOMAL PROTEIN S4



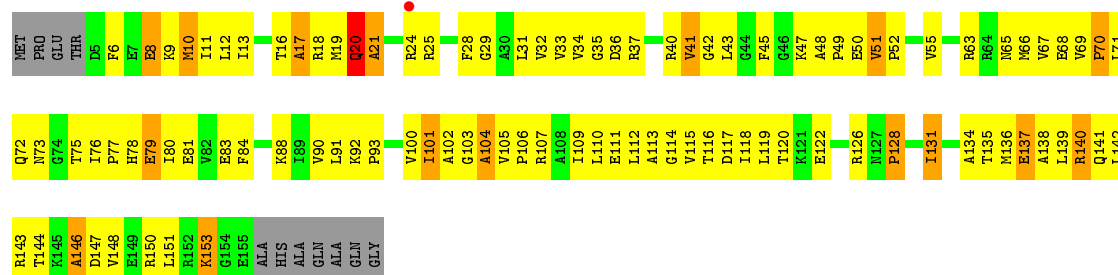
R209

- Molecule 4: 30S RIBOSOMAL PROTEIN S4

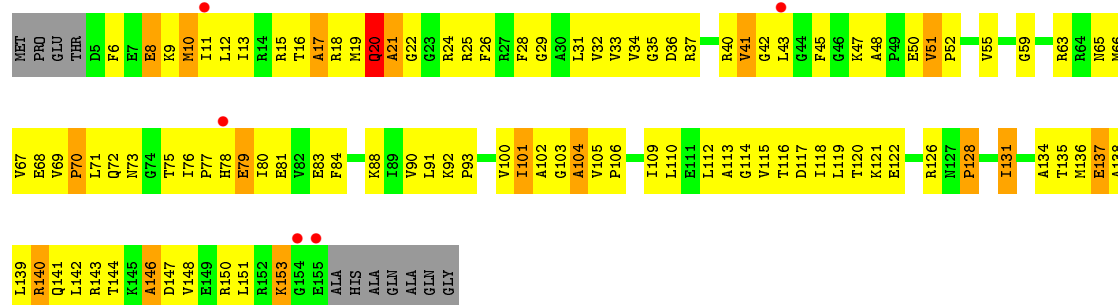
Chain CD:  34% 52% 13%

R209

- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:  31% 52% 10% 7%

- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:  3% 30% 53% 10% 7%

- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:  24% 70% 5%



• Molecule 6: 30S RIBOSOMAL PROTEIN S6



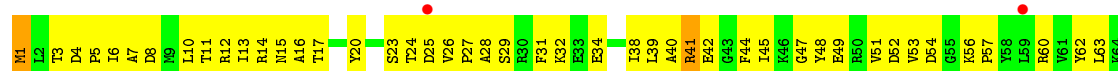
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

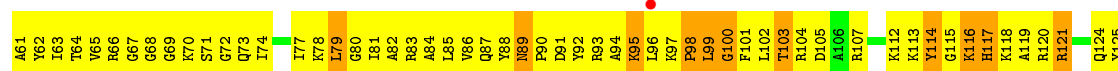
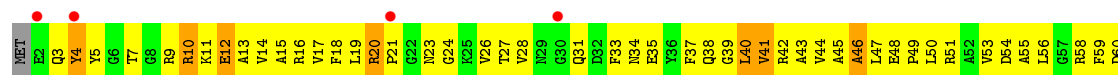




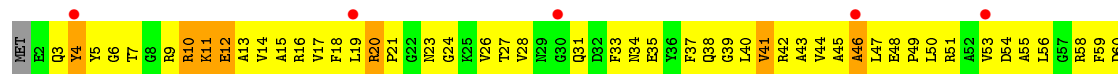
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



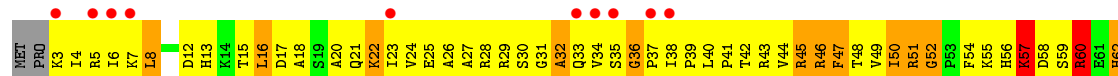
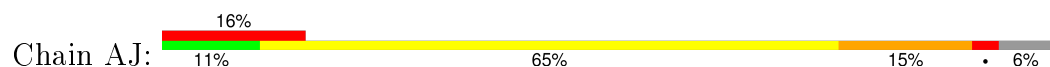
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

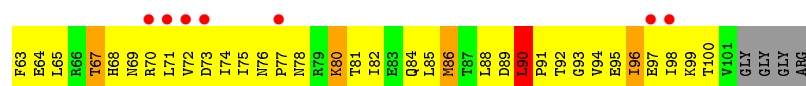


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

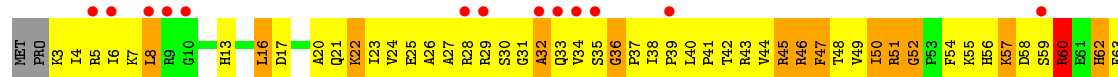
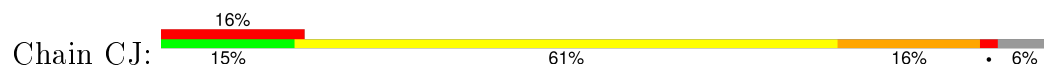


• Molecule 10: 30S RIBOSOMAL PROTEIN S10





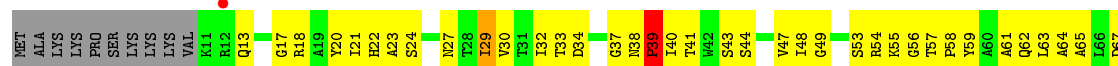
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



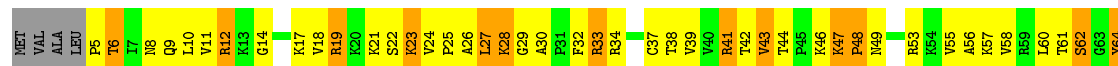
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



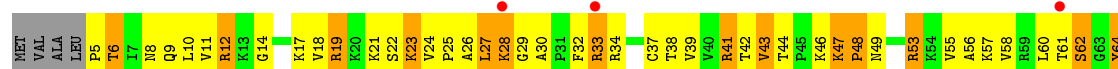
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

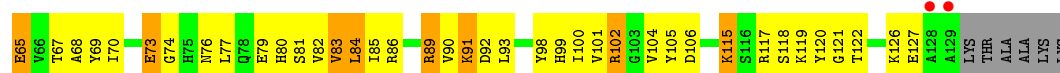


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

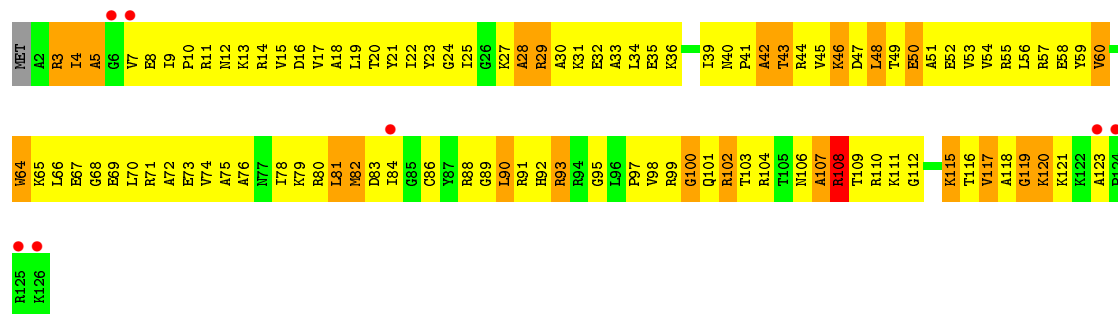


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

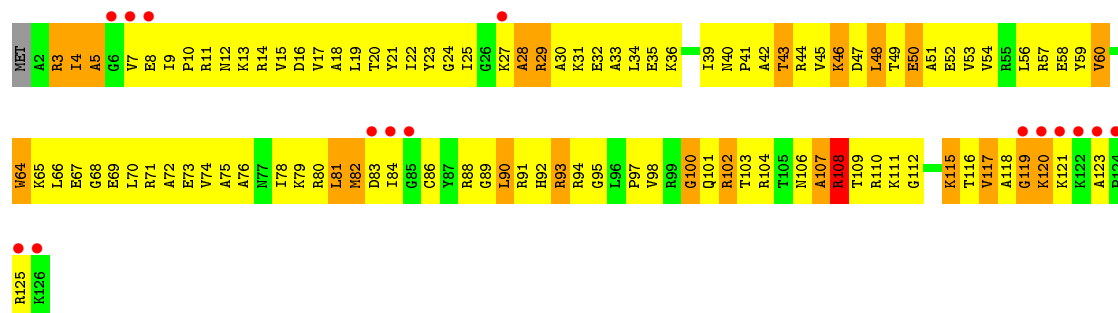




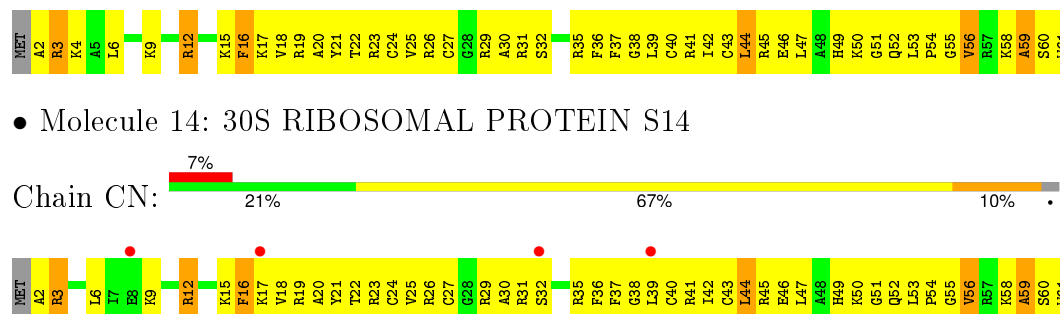
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



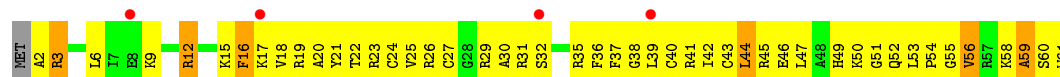
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



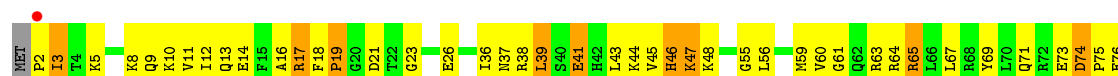
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

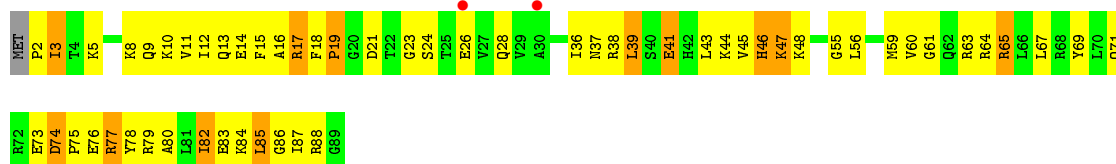


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

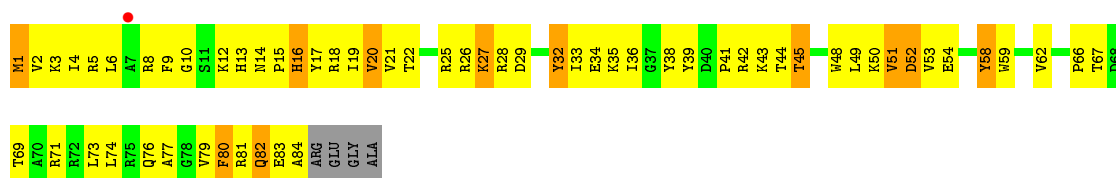




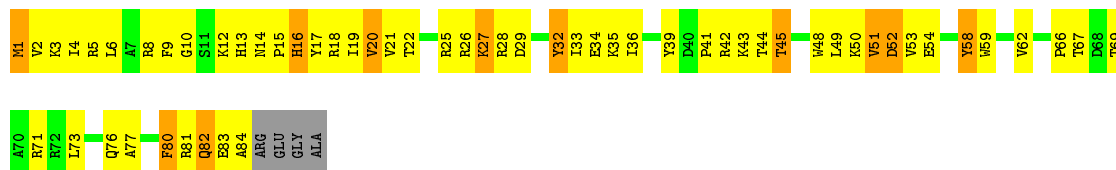
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



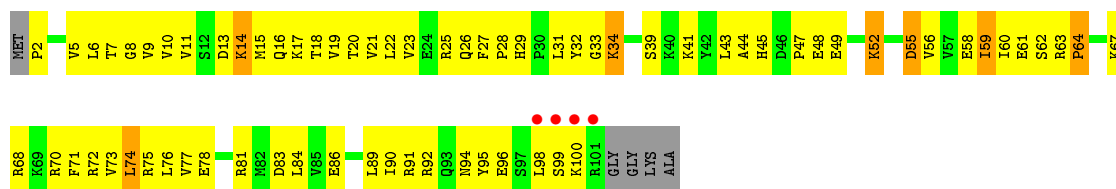
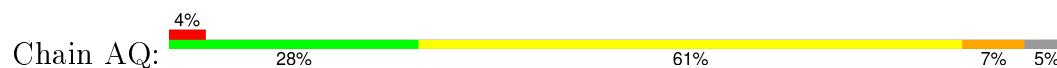
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

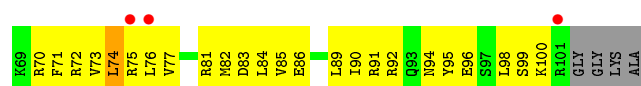


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

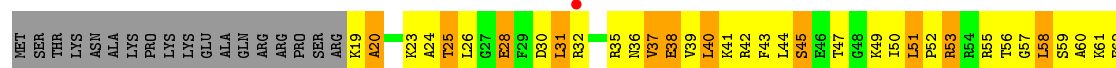
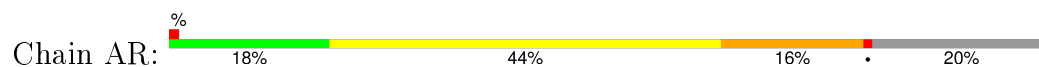


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

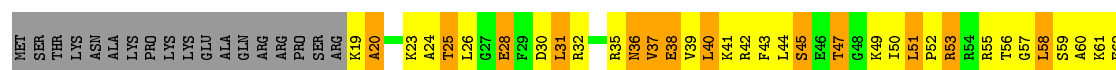
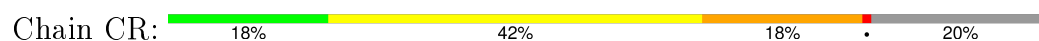




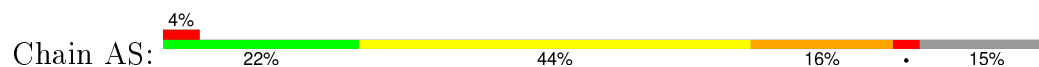
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



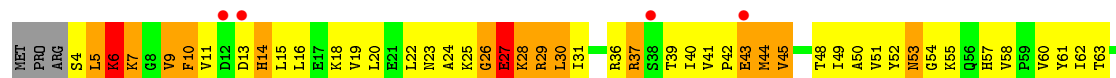
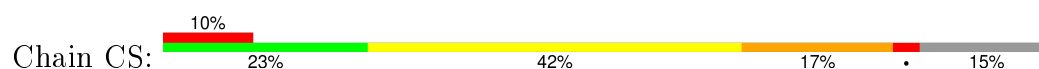
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

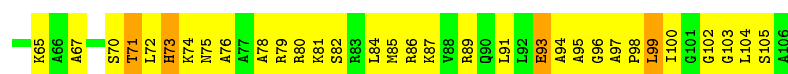


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

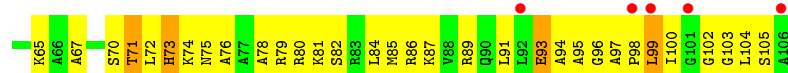


• Molecule 20: 30S RIBOSOMAL PROTEIN S20





• Molecule 20: 30S RIBOSOMAL PROTEIN S20



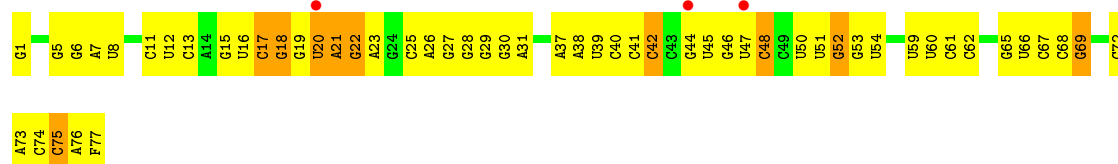
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: P AND A-SITE PHE-TRNA PHE

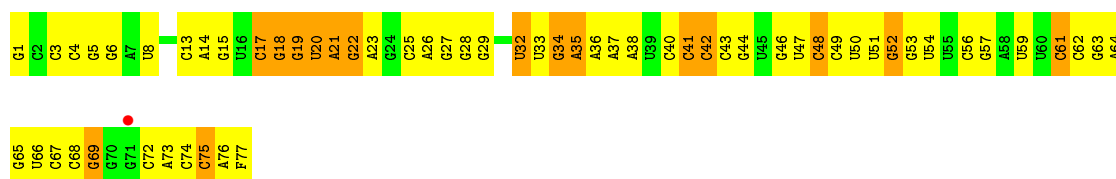


• Molecule 22: P AND A-SITE PHE-TRNA PHE

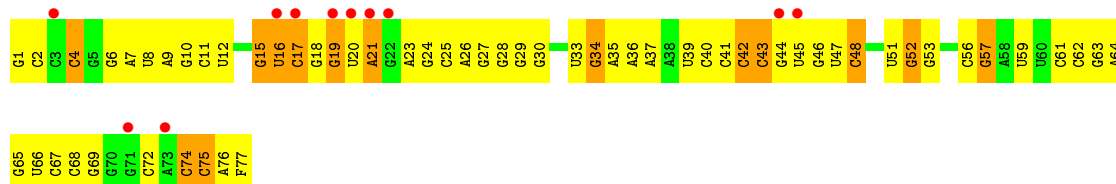


• Molecule 22: P AND A-SITE PHE-TRNA PHE

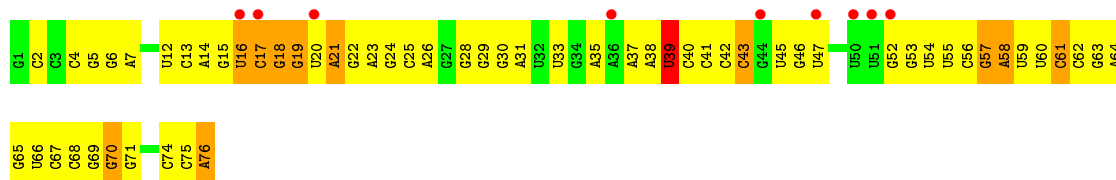




- Molecule 22: P AND A-SITE PHE-TRNA PHE



- Molecule 23: E-SITE TRNA PHE



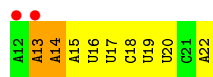
- Molecule 23: E-SITE TRNA PHE



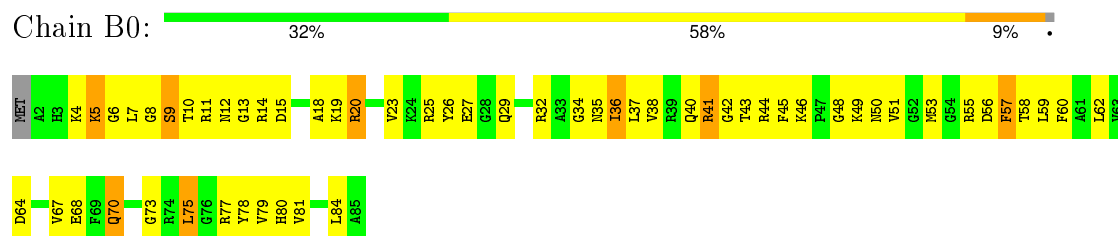
- Molecule 24: MRNA



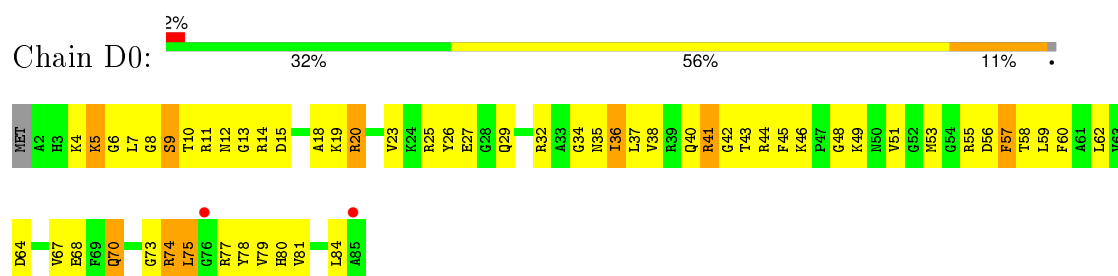
- Molecule 24: MRNA



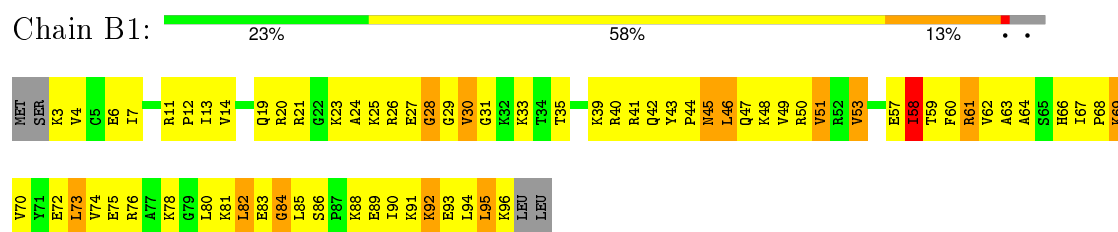
- Molecule 25: 50S RIBOSOMAL PROTEIN L27



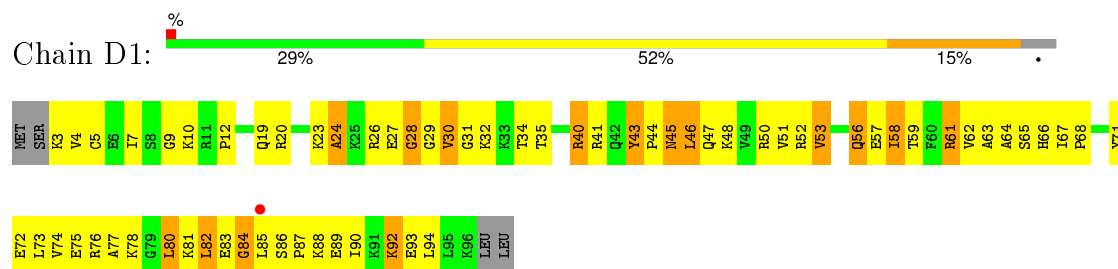
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



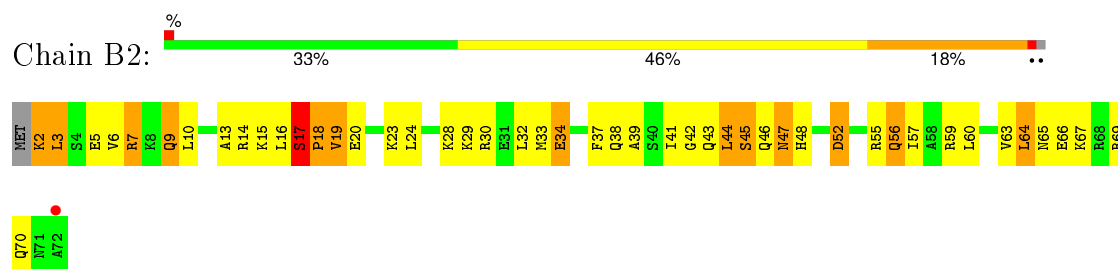
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



• Molecule 26: 50S RIBOSOMAL PROTEIN L28

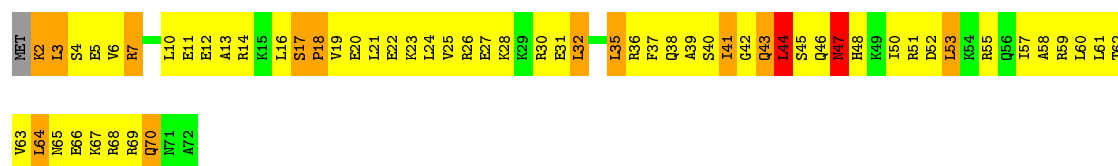


• Molecule 27: 50S RIBOSOMAL PROTEIN L29

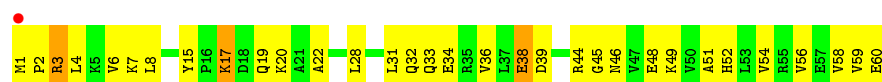


• Molecule 27: 50S RIBOSOMAL PROTEIN L29

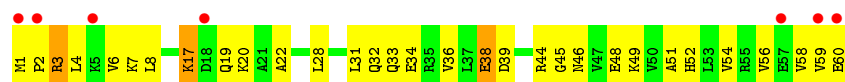




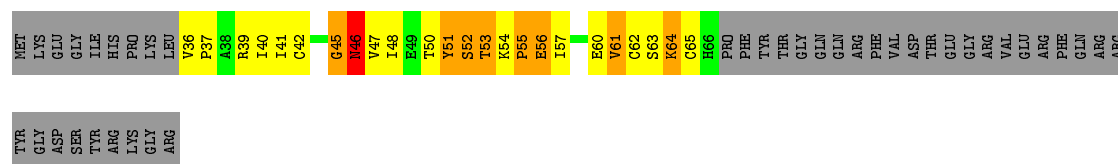
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



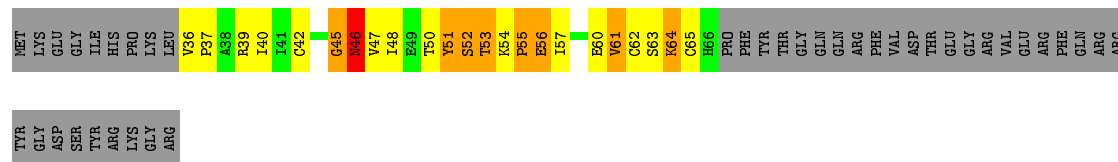
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



- Molecule 29: 50S RIBOSOMAL PROTEIN L31



- Molecule 29: 50S RIBOSOMAL PROTEIN L31

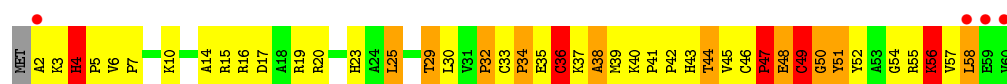


- Molecule 30: 50S RIBOSOMAL PROTEIN L32

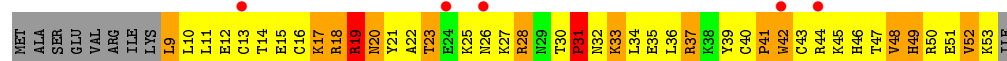


- Molecule 30: 50S RIBOSOMAL PROTEIN L32





- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 32: 50S RIBOSOMAL PROTEIN L34



- Molecule 32: 50S RIBOSOMAL PROTEIN L34



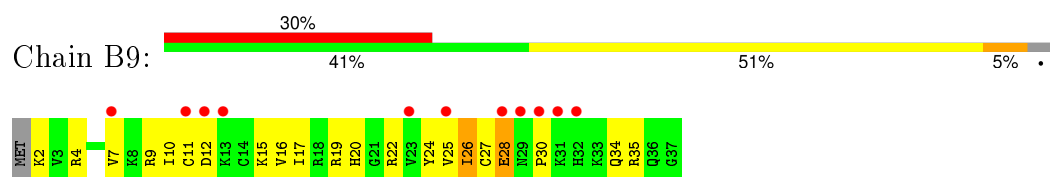
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



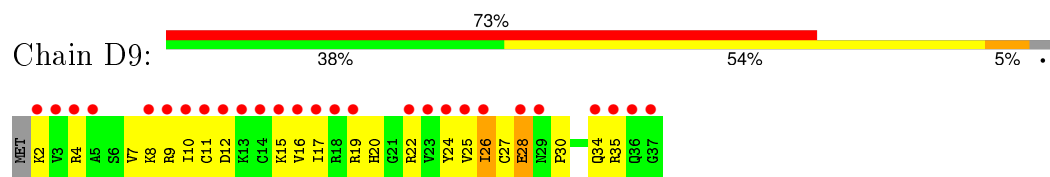
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



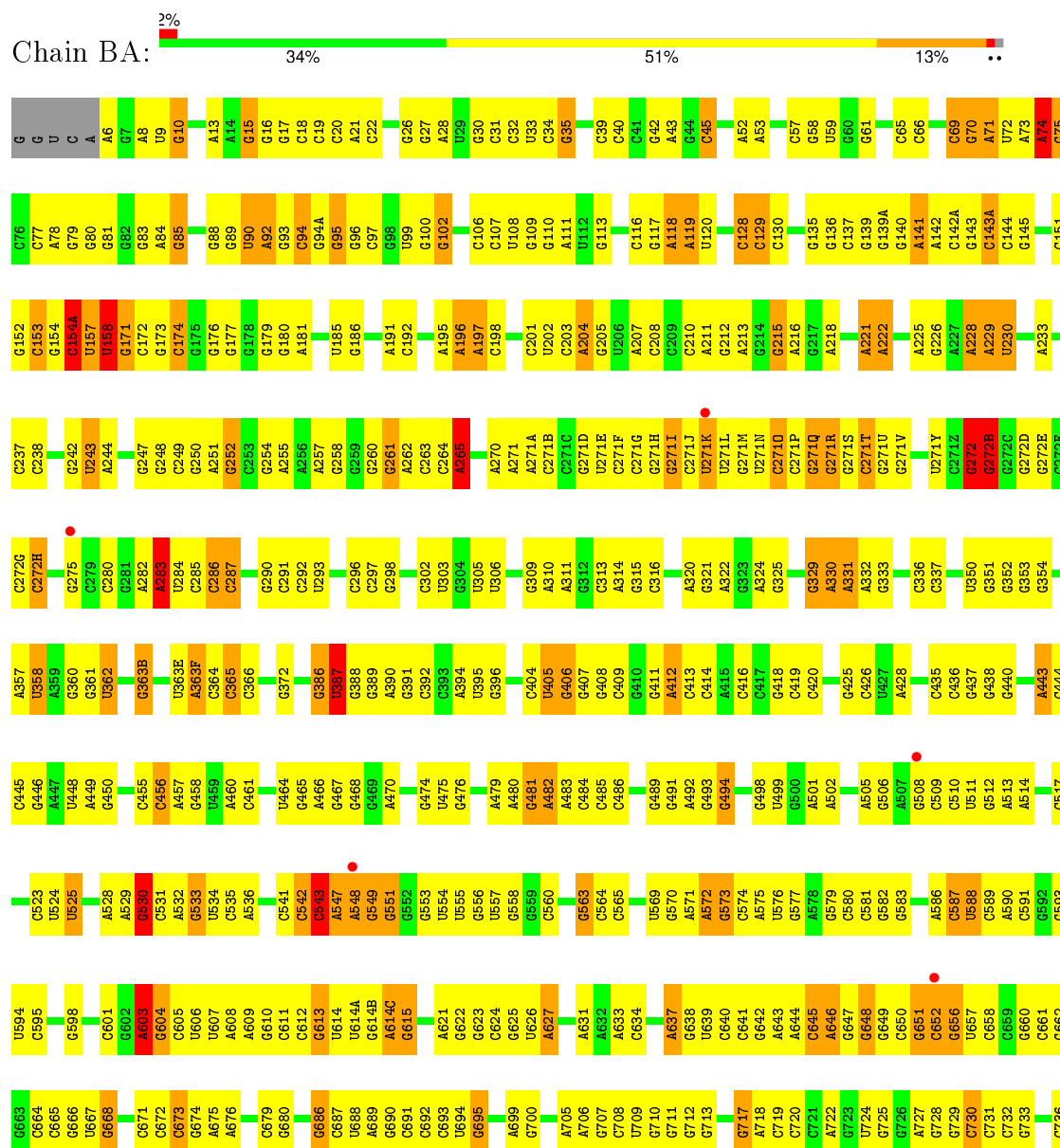
- Molecule 34: 50S RIBOSOMAL PROTEIN L36



• Molecule 34: 50S RIBOSOMAL PROTEIN L36



• Molecule 35: 23S RIBOSOMAL RNA



C1843	C1844	G1845	G1846	A1847	A1848	U1851	C1852	A1853	A1854	G1855	G1856	G1857	G1858	A1859	G1860	G1861	G1862	G1863	G1864	G1865	G1866	A1876	A1877	G1878	C1879	A1880	C1881	G1882	G1883	A1884	A1885	A1886	G1887	A1888	A1889	A1890	G1896	G1897	G1898	G1899	A1900	A1901	C1902	G1903	G1906	G1907	C1908	C1909	G1910	U1911	U1912	A1913	C1914	U1915	A1916	U1917				
C1607	G1608	A1609	A1610	A1611	A1612	G1613	G1614	A1615	A1616	A1617	A1618	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	A1641	G1642	G1647	G1648	G1651	A1652	G1653	A1654	A1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	C1663	C1664	C1665	C1666	G1667	A1668	C1669	C1670	U1671	G1674	C1675	U1676	C1677	U1678	C1679	C1681	G1682	C1683	G1684					
G1517	U1518	G1519	G1520	G1525	G1526	G1527	A1528	A1528A	G1529	G1530	C1531	C1532	G1533	C1534	A1544	G1547	A1548	G1549	U1550	C1551	A1554	G1555	A1558	G1559	G1561	G1562	A1563	A1564	A1565	G1566	G1567	G1568	A1569	A1570	A1571	A1572	G1573	C1574	U1578	A1579	A1580	G1581	C1582	A1583	A1584	A1585	A1586	A1587	C1588	G1589	U1590	G1591	C1592	A1593	U1594	G1595	C1596	G1597	G1598	A1603
C1450A	C1451	A1452	U1453	G1455	G1456	A1457	G1458	A1459	A1460	A1461	C1464	C1467	C1468	A1469	A1470	A1471	A1472	G1473	A1474	C1475	A1477	G1478	G1479	A1480	G1481	G1482	G1483	G1484	A1485	A1486	G1487	G1488	U1489	A1490	G1491	G1492	C1493	A1494	A1495	A1496	U1497	C1498	C1501	C1502	U1503	C1504	C1505	C1506	C1509	A1509A	A1509B	G1510	C1511	G1515	C1516					
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A1302	G1303	G1309	G1310	G1311	U1312	U1313	C1314	U1315	A1316	A1317	C1318	C1319	C1320	A1321	C1327	C1328	U1329	C1330	A1331	G1332	C1333	G1334	U1335	A1336	G1337	G1338	G1339	U1340	U1341	G1344	C1345	G1346	G1347	G1348	A1349	C1350	C1351	U1352	A1353	A1354	G1355	G1356	U1357	G1358	A1359	C1363	G1364	A1365	G1368	A1373	G1374	C1375	C1376							
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U807	G808	G809	U810	G811	C812	U813	G814	C815	G816	C817	G818	A819	U826	U827	U828	A829	G830	G831	G832	U833	C834	U837	G838	A839	C840	A841	G842	G843	C844	U847	G848	A849	C850	U851	G852	G853	G854	G855	C856	C857	U858	G859	U860	A861	G862	A863	G864	C865	A866	C869	A870	G874	G875	C876	U877	G8805	A878			
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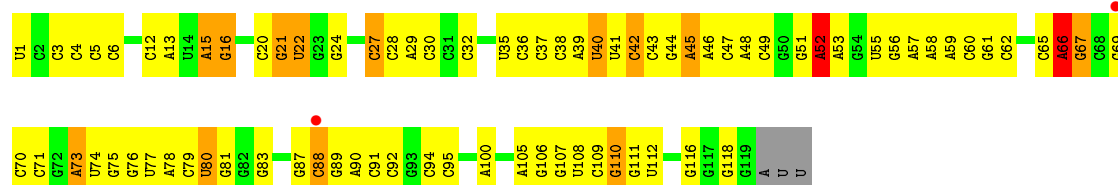
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● Molecule 35: 23S RIBOSOMAL RNA

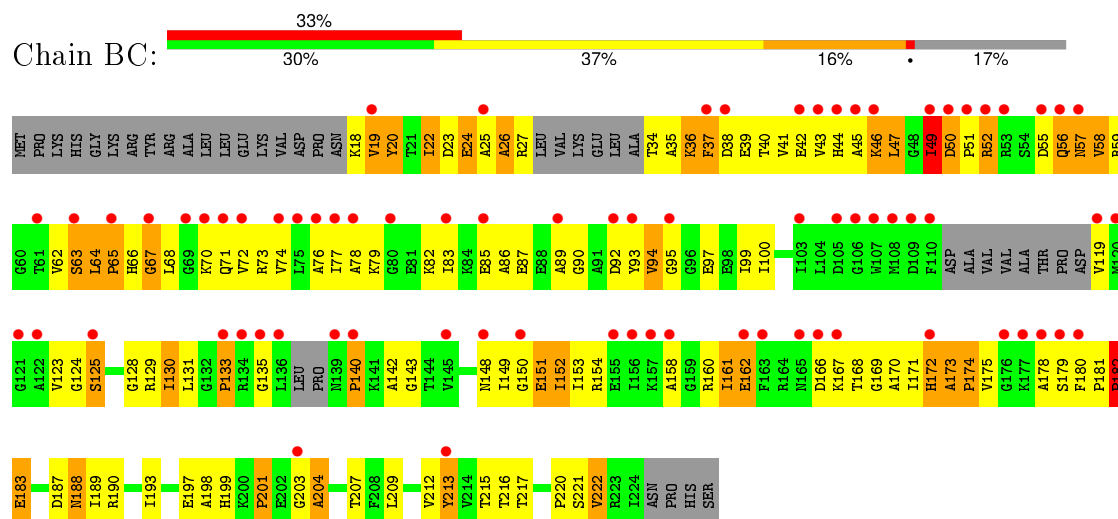


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		U1127	A1001		C856	A783	G715	A643			C417	A322	C209	A52	A52
		A1128	G1002	G932	C857	U784	A716	A644			G418	U271K	C210	A53	A53
		G1131	G1003		U858	G785	G717	C645			C419	U271L	A211	G57	C57
		A1132	U1011	A941	G859	C786	A718	A646			G425	G271M	G212	G58	G58
		C1133	G1012	G942	U860	U787	C719	G647			C271O	U271N	A213	U59	U59
		U1135	U1013	U943	A861	A788	C720	G648			G329	G271P	G214	G136	G60
		C1136	C1013	G944	G862	A789	C721	G649			A330	G271Q	G215	G137	G60
		U1019	U1019	A945	A863	C790	A722	C650			A331	G271R	G216	G139	G61
		A1020	G946	G946	G864	C791	G723	G651			A332	G271S	G217	G139A	G61
		U1021	G947	C965	G865	G792	U724	C652			A333	G271T	A218	G140	G65
		C1138	A1021	A866	A866	A793	G725	G656			A334	C271U	A219	G142	G66
		U1140	C1022	G948	G725	G794	G726	U657			C336	G271V	A221	A142	C66
		U1141	U1023	C949	C949	C795	A727	G658			C337	G271W	A222	G143	C69
		U1142	U1024	G950	G950	C796	G728	C659			U350	U271Y	A225	G144A	G70
		A1142A	G1025	G951	A870	C797	G729	G660			G351	C271Z	G226	G145	A71
		U1211	U1026	G952	G874	A802	C730	C661			G352	G272	A227	G146	U72
		G1212	A1027	G954	G875	U803	C731	G662			A443	G272B	A228	G147	A73
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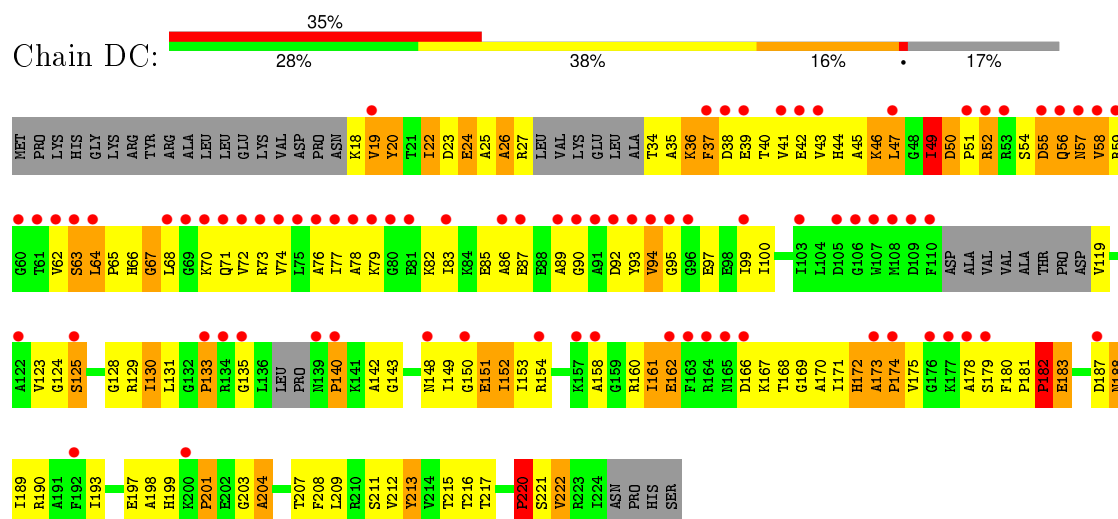




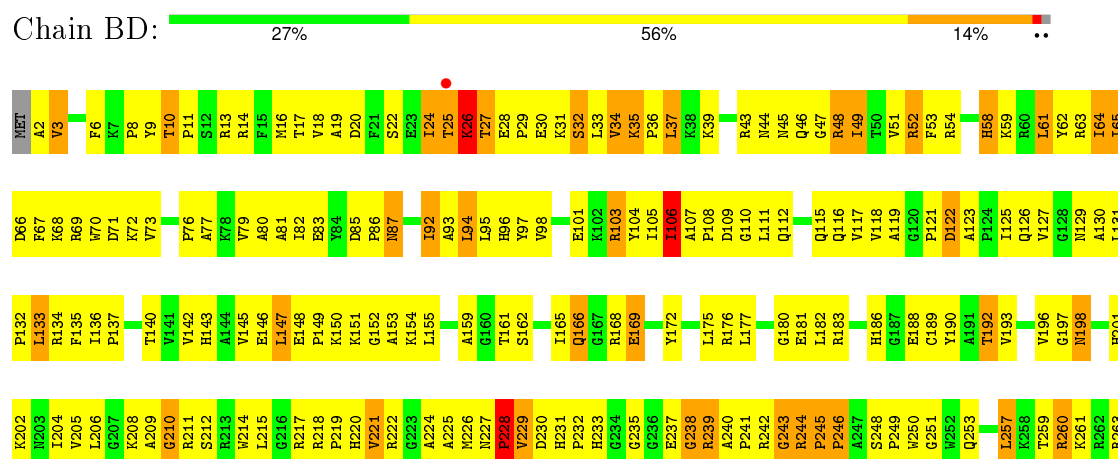
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

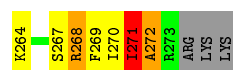


• Molecule 37: 50S RIBOSOMAL PROTEIN L1



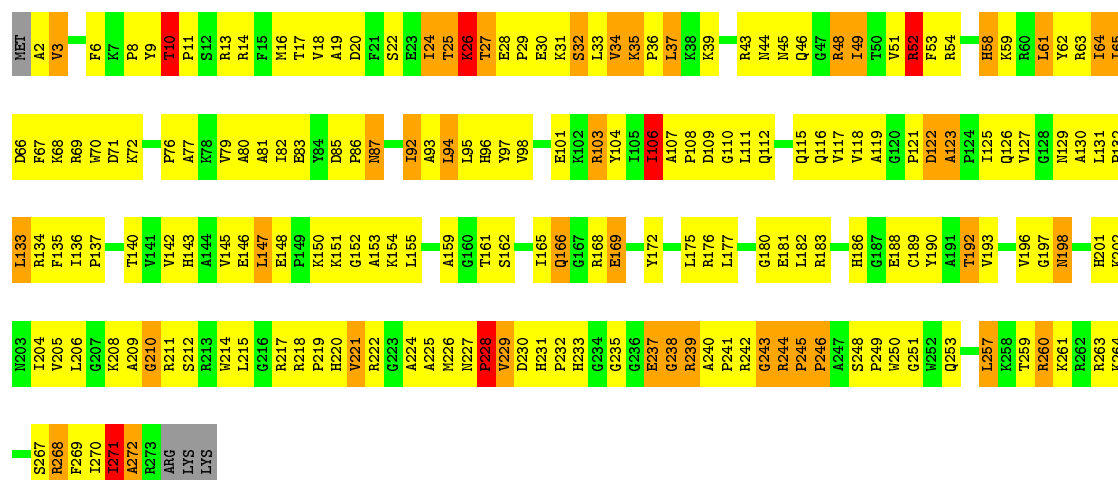
• Molecule 38: 50S RIBOSOMAL PROTEIN L2





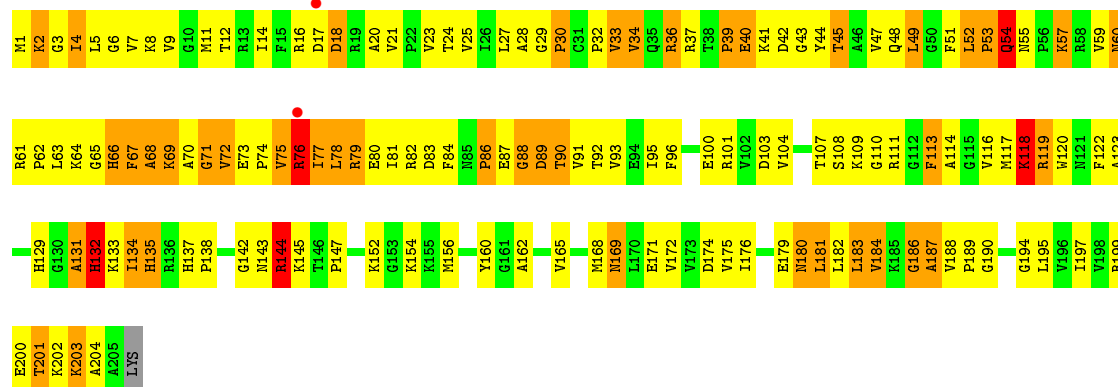
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD: 28% 54% 14%



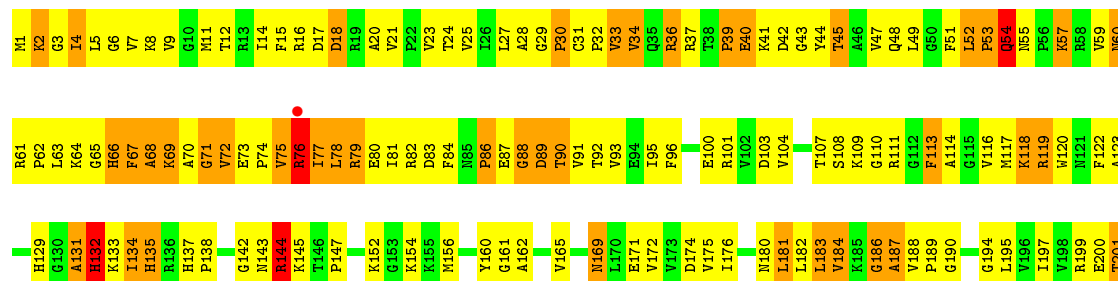
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

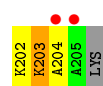
Chain BE: 29% 47% 21%



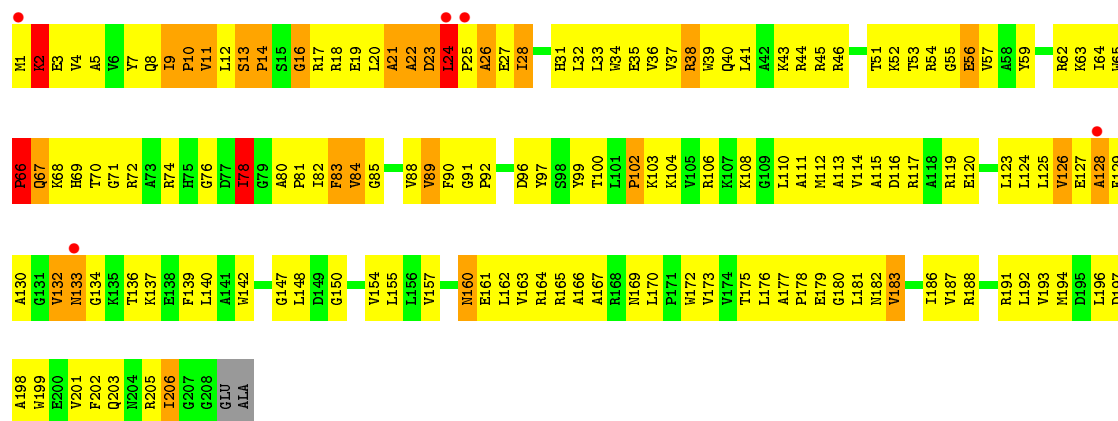
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE: 29% 49% 20%

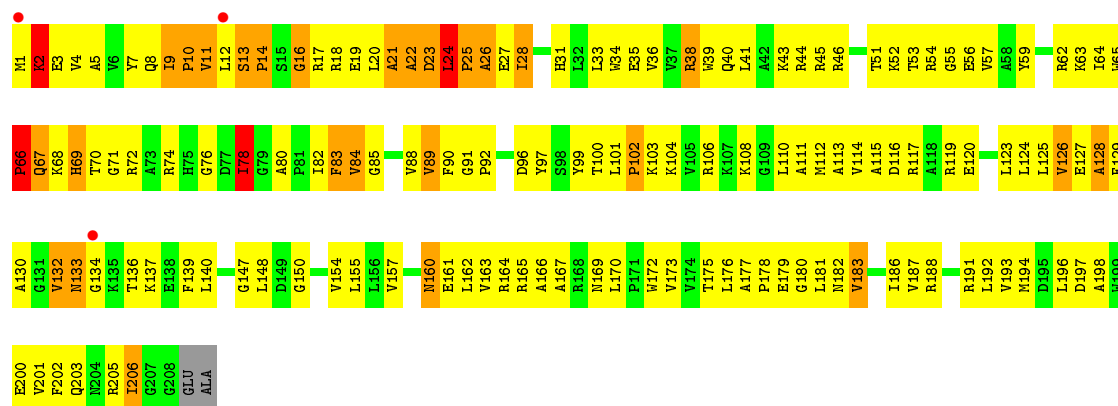




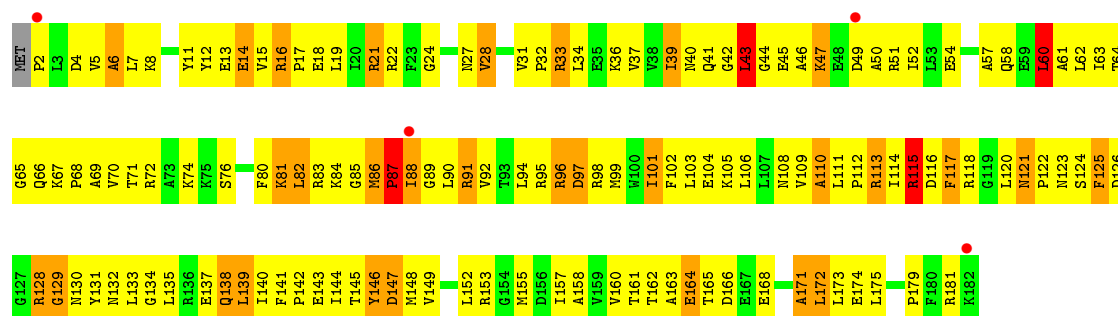
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



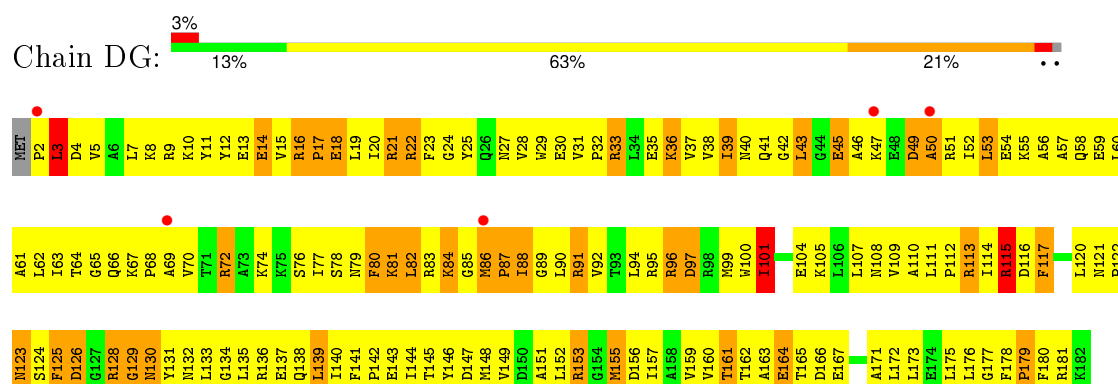
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

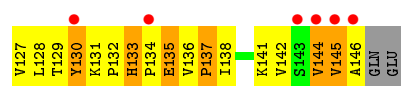


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

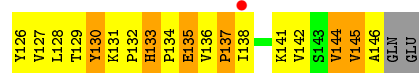
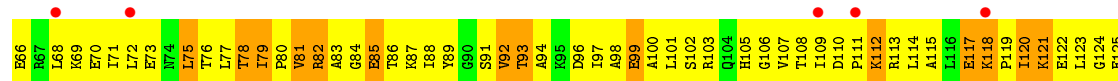
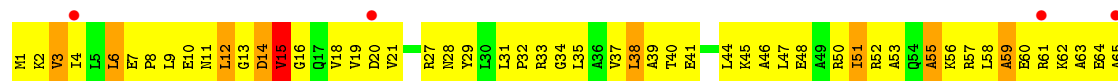


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

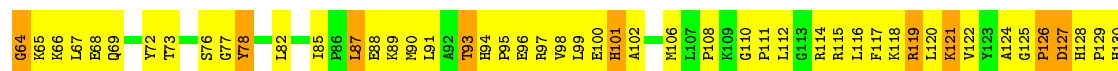
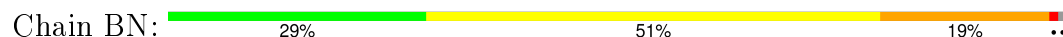




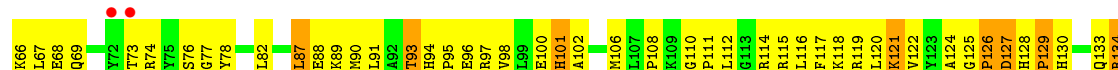
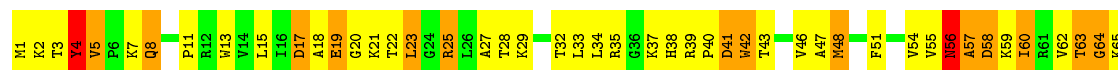
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



• Molecule 44: 50S RIBOSOMAL PROTEIN L13



• Molecule 44: 50S RIBOSOMAL PROTEIN L13



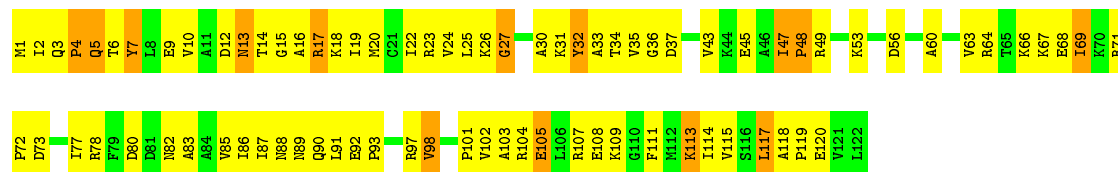
• Molecule 45: 50S RIBOSOMAL PROTEIN L14





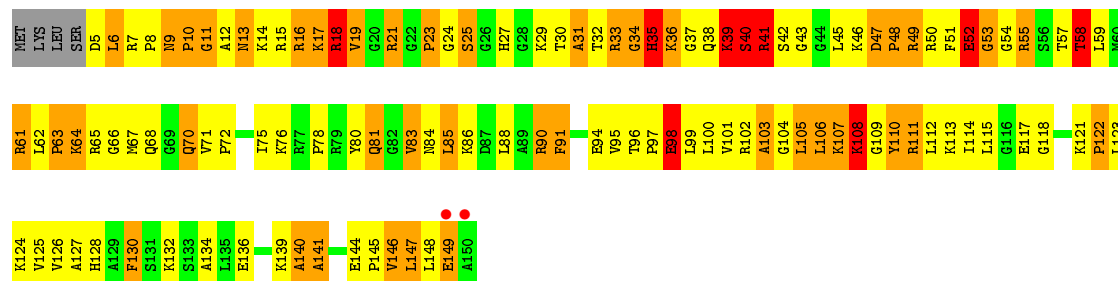
• Molecule 45: 50S RIBOSOMAL PROTEIN L14

Chain DO: 34% 55% 11%



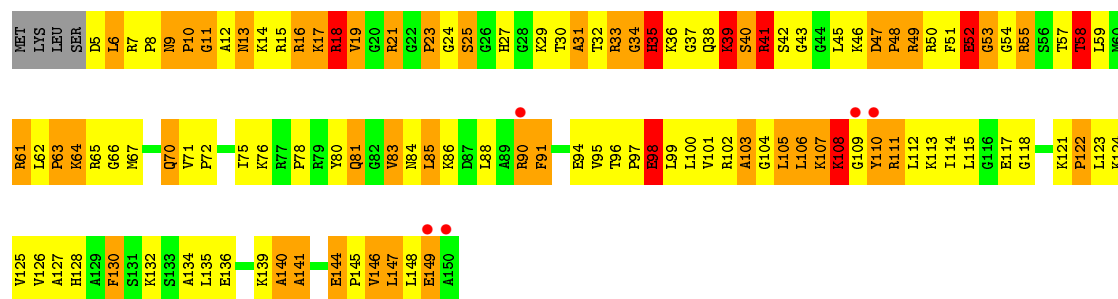
• Molecule 46: 50S RIBOSOMAL PROTEIN L15

Chain BP: 19% 44% 28% 6%



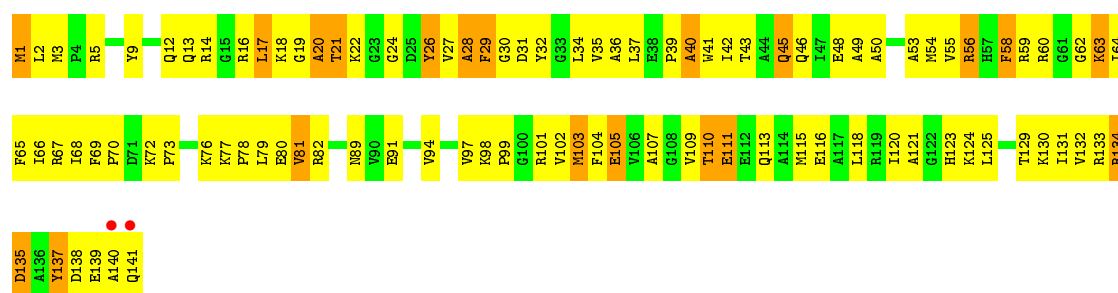
• Molecule 46: 50S RIBOSOMAL PROTEIN L15

Chain DP: 3% 19% 44% 29% 5%

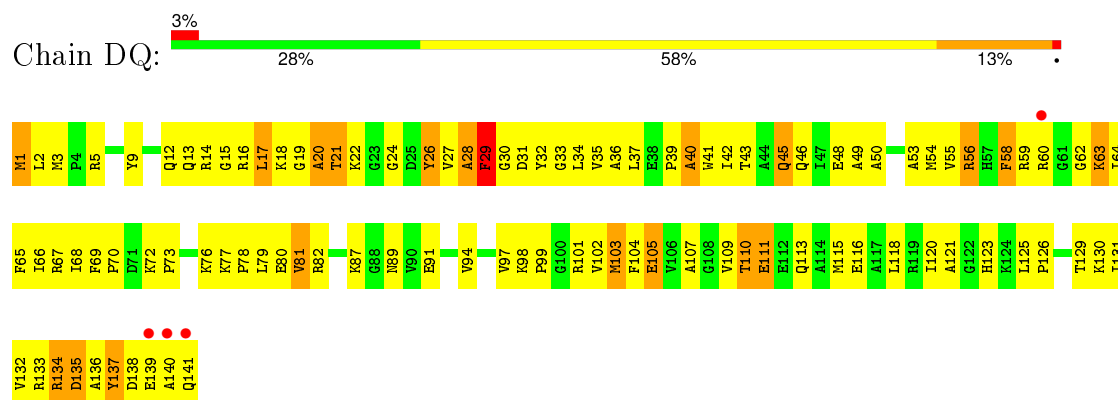


• Molecule 47: 50S RIBOSOMAL PROTEIN L16

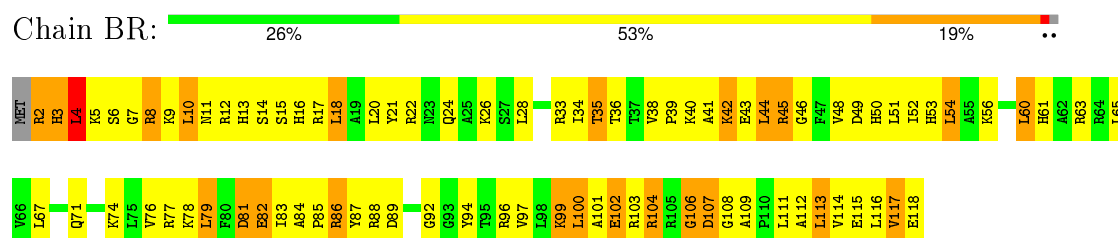
Chain BQ: 30% 55% 14%



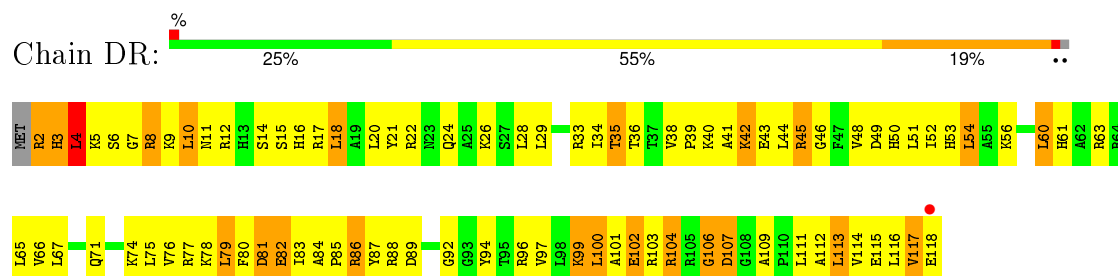
- Molecule 47: 50S RIBOSOMAL PROTEIN L16



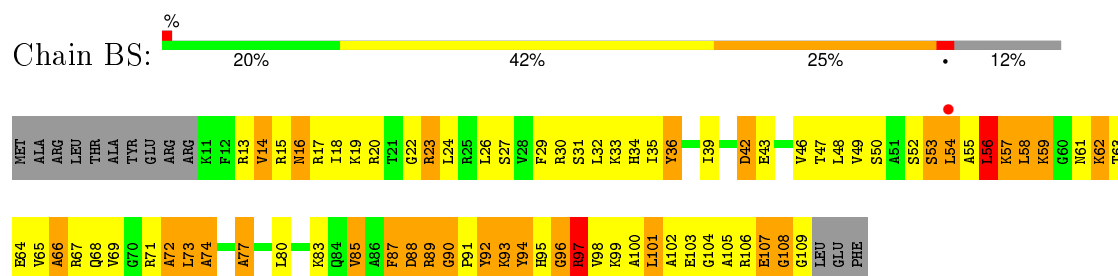
- Molecule 48: 50S RIBOSOMAL PROTEIN L17



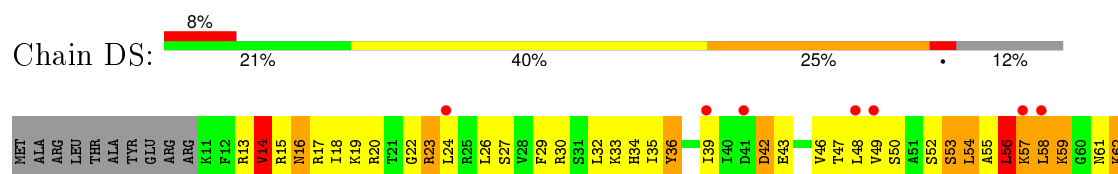
- Molecule 48: 50S RIBOSOMAL PROTEIN L17



- Molecule 49: 50S RIBOSOMAL PROTEIN L18

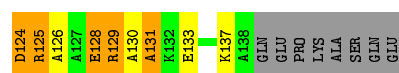
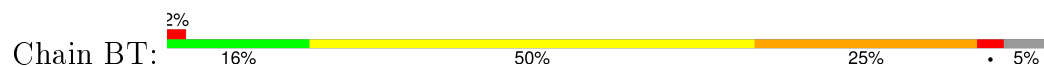


- Molecule 49: 50S RIBOSOMAL PROTEIN L18

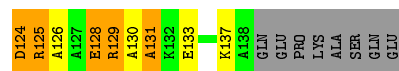
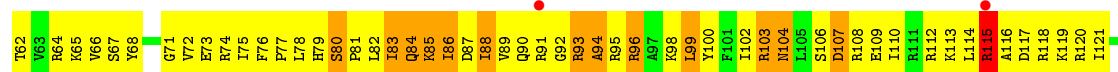
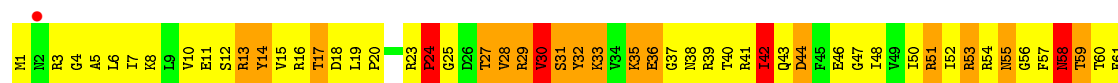
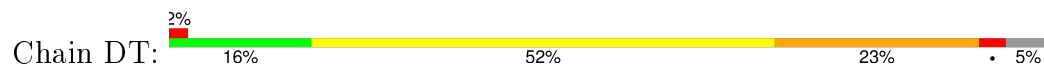




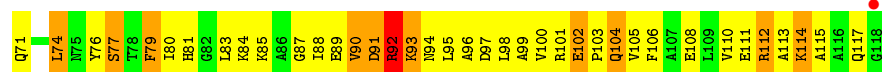
• Molecule 50: 50S RIBOSOMAL PROTEIN L19



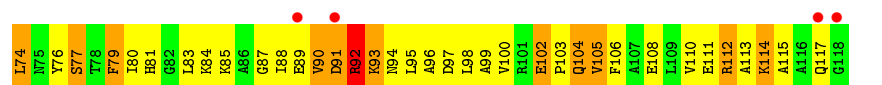
• Molecule 50: 50S RIBOSOMAL PROTEIN L19



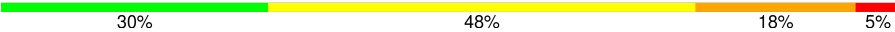
• Molecule 51: 50S RIBOSOMAL PROTEIN L20

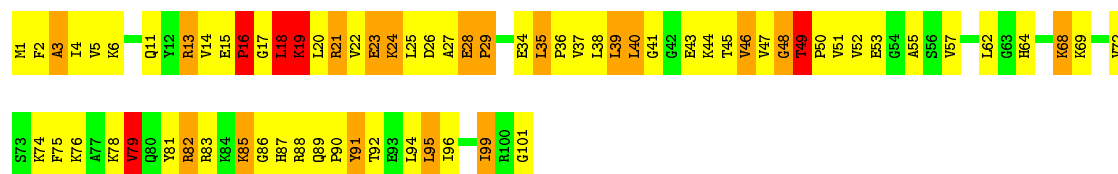


• Molecule 51: 50S RIBOSOMAL PROTEIN L20



• Molecule 52: 50S RIBOSOMAL PROTEIN L21

Chain BV: 



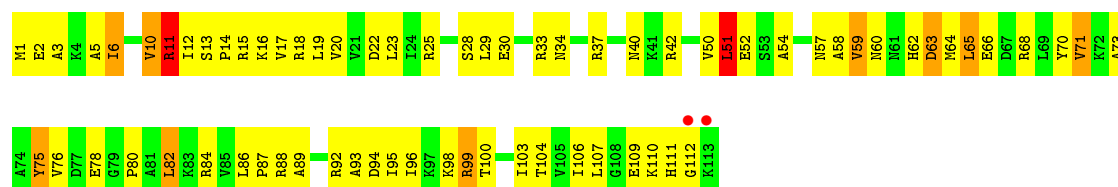
• Molecule 52: 50S RIBOSOMAL PROTEIN L21

Chain DV: 



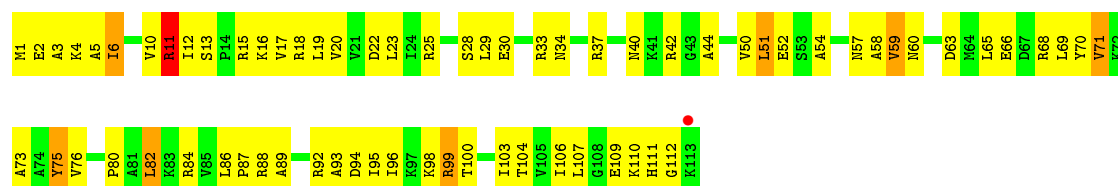
• Molecule 53: 50S RIBOSOMAL PROTEIN L22

Chain BW: 



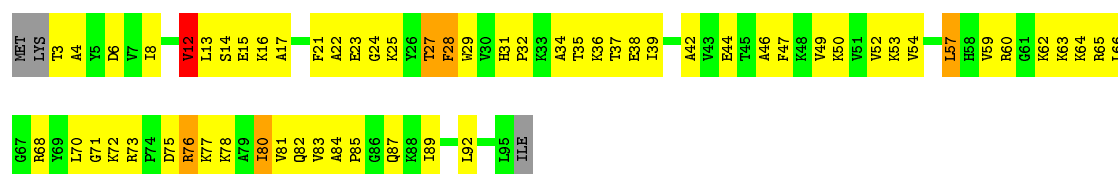
• Molecule 53: 50S RIBOSOMAL PROTEIN L22

Chain DW: 

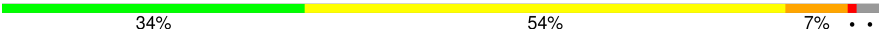


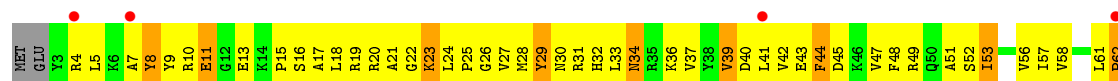
• Molecule 54: 50S RIBOSOMAL PROTEIN L23

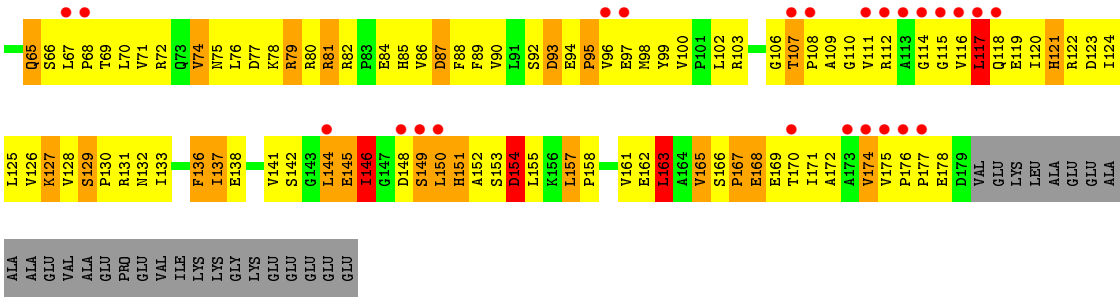
Chain BX: 



• Molecule 54: 50S RIBOSOMAL PROTEIN L23

Chain DX: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.86Å 450.46Å 628.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 49.74 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.50) 97.2 (49.74-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.256 0.210 , 0.257	Depositor DCC
R_{free} test set	33758 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 99.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 789128 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	296042	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 8AN, PHA

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	0.42	0/36190	0.70	16/56486 (0.0%)
1	CA	0.40	0/36190	0.69	14/56486 (0.0%)
2	AB	0.33	0/1936	0.60	0/2611
2	CB	0.32	0/1936	0.60	0/2611
3	AC	0.34	0/1637	0.60	0/2207
3	CC	0.33	0/1637	0.59	0/2207
4	AD	0.36	0/1733	0.64	0/2318
4	CD	0.36	0/1733	0.64	0/2318
5	AE	0.36	0/1163	0.64	0/1566
5	CE	0.35	0/1163	0.64	0/1566
6	AF	0.36	0/856	0.66	0/1154
6	CF	0.35	0/856	0.66	0/1154
7	AG	0.32	0/1276	0.57	0/1709
7	CG	0.31	0/1276	0.57	0/1709
8	AH	0.31	0/1136	0.63	0/1527
8	CH	0.30	0/1136	0.62	0/1527
9	AI	0.32	0/1027	0.59	0/1372
9	CI	0.32	0/1027	0.59	0/1372
10	AJ	0.36	0/808	0.66	0/1087
10	CJ	0.35	0/808	0.64	0/1087
11	AK	0.35	0/900	0.62	0/1213
11	CK	0.33	0/900	0.61	0/1213
12	AL	0.39	0/987	0.70	0/1322
12	CL	0.37	0/987	0.68	0/1322
13	AM	0.34	0/996	0.66	0/1329
13	CM	0.33	0/996	0.66	0/1329
14	AN	0.36	0/501	0.62	0/664
14	CN	0.33	0/501	0.61	0/664
15	AO	0.35	0/745	0.59	0/992
15	CO	0.33	0/745	0.58	0/992
16	AP	0.37	0/717	0.63	0/965
16	CP	0.37	0/717	0.63	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.36	0/837	0.61	0/1119
17	CQ	0.37	0/837	0.62	0/1119
18	AR	0.36	0/579	0.60	0/768
18	CR	0.36	0/579	0.60	0/768
19	AS	0.38	0/643	0.63	0/867
19	CS	0.36	0/643	0.62	0/867
20	AT	0.30	0/765	0.59	0/1007
20	CT	0.30	0/765	0.58	0/1007
21	AU	0.46	0/213	0.61	0/279
21	CU	0.45	0/213	0.60	0/279
22	AV	0.44	0/1784	0.75	0/2780
22	AY	0.47	0/1784	0.74	0/2780
22	CV	0.40	0/1784	0.71	0/2780
22	CY	0.41	0/1784	0.73	0/2780
23	AW	0.43	0/1809	0.71	0/2819
23	CW	0.42	0/1809	0.71	0/2819
24	AX	0.48	0/253	0.72	0/391
24	CX	0.42	0/253	0.73	1/391 (0.3%)
25	B0	0.44	0/671	0.71	0/892
25	D0	0.41	0/671	0.69	0/892
26	B1	0.48	0/739	0.85	0/983
26	D1	0.46	0/739	0.72	0/983
27	B2	0.43	0/600	0.73	0/793
27	D2	0.39	0/600	0.65	0/793
28	B3	0.43	0/473	0.68	0/636
28	D3	0.37	0/473	0.64	0/636
29	B4	0.46	0/229	0.68	0/311
29	D4	0.44	0/229	0.67	0/311
30	B5	0.62	0/473	0.96	0/639
30	D5	0.49	0/473	0.92	0/639
31	B6	0.57	0/387	0.76	0/517
31	D6	0.51	0/387	0.75	0/517
32	B7	0.52	0/427	0.67	0/563
32	D7	0.48	0/427	0.65	0/563
33	B8	0.59	0/516	0.89	2/681 (0.3%)
33	D8	0.51	0/516	0.88	2/681 (0.3%)
34	B9	0.33	0/302	0.54	0/397
34	D9	0.29	0/302	0.53	0/397
35	BA	0.59	5/67716 (0.0%)	0.76	38/105718 (0.0%)
35	DA	0.48	4/67716 (0.0%)	0.74	31/105718 (0.0%)
36	BB	0.50	0/2853	0.75	1/4451 (0.0%)
36	DB	0.42	0/2853	0.74	1/4451 (0.0%)
37	BC	0.37	0/1143	0.68	5/1552 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.37	0/1145	0.69	6/1556 (0.4%)
38	BD	0.51	0/2155	0.80	1/2907 (0.0%)
38	DD	0.47	0/2155	0.79	1/2907 (0.0%)
39	BE	0.47	0/1597	0.80	1/2155 (0.0%)
39	DE	0.41	0/1597	0.77	0/2155
40	BF	0.46	0/1659	0.71	0/2246
40	DF	0.42	0/1659	0.69	0/2246
41	BG	0.40	0/1498	0.77	2/2013 (0.1%)
41	DG	0.38	0/1498	0.71	1/2013 (0.0%)
42	BH	0.44	0/1246	0.77	0/1684
42	DH	0.37	0/1246	0.74	0/1684
43	BI	0.36	0/1147	0.65	0/1553
43	DI	0.35	0/1147	0.63	0/1553
44	BN	0.45	0/1132	0.75	0/1527
44	DN	0.38	0/1132	0.72	0/1527
45	BO	0.44	0/943	0.68	0/1269
45	DO	0.37	0/943	0.67	0/1269
46	BP	0.51	0/1131	1.01	5/1504 (0.3%)
46	DP	0.45	0/1131	0.98	5/1504 (0.3%)
47	BQ	0.45	0/1143	0.69	0/1527
47	DQ	0.40	0/1143	0.67	0/1527
48	BR	0.44	0/974	0.79	2/1302 (0.2%)
48	DR	0.39	0/974	0.76	1/1302 (0.1%)
49	BS	0.48	0/779	0.83	1/1038 (0.1%)
49	DS	0.42	0/779	0.79	2/1038 (0.2%)
50	BT	0.44	0/1156	0.79	1/1544 (0.1%)
50	DT	0.41	0/1156	0.78	1/1544 (0.1%)
51	BU	0.52	0/975	0.79	2/1297 (0.2%)
51	DU	0.42	0/975	0.74	2/1297 (0.2%)
52	BV	0.46	0/790	0.77	1/1057 (0.1%)
52	DV	0.38	0/790	0.74	1/1057 (0.1%)
53	BW	0.49	0/907	0.78	1/1216 (0.1%)
53	DW	0.42	0/907	0.75	0/1216
54	BX	0.48	0/740	0.73	1/995 (0.1%)
54	DX	0.44	0/740	0.71	1/995 (0.1%)
55	BY	0.56	0/789	0.85	0/1053
55	DY	0.49	0/789	0.83	0/1053
56	BZ	0.42	0/1436	0.72	0/1951
56	DZ	0.36	0/1436	0.65	0/1951
All	All	0.47	9/320004 (0.0%)	0.72	150/478610 (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	10
1	CA	0	8
23	AW	0	2
35	BA	4	39
35	DA	3	33
36	BB	0	3
36	DB	0	3
All	All	7	98

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	652	C	C3'-O3'	8.01	1.53	1.42
35	DA	652	C	C3'-O3'	7.44	1.52	1.42
35	BA	652	C	O3'-P	6.31	1.68	1.61
35	DA	652	C	O3'-P	5.91	1.68	1.61
35	BA	652	C	O5'-C5'	5.67	1.53	1.44

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BP	52	GLU	N-CA-C	9.63	137.00	111.00
46	DP	52	GLU	N-CA-C	9.54	136.76	111.00
35	BA	283	A	C2'-C3'-O3'	9.40	130.18	109.50
35	BA	1799	G	C2'-C3'-O3'	9.35	130.07	109.50
35	DA	1799	G	C2'-C3'-O3'	9.28	129.91	109.50

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	283	A	C3'
35	BA	1378	A	C3'
35	BA	1799	G	C3'
35	BA	1819	A	C3'
35	DA	283	A	C3'

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	21	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	484	G	Sidechain
1	AA	760	G	Sidechain
1	AA	832	C	Sidechain
1	AA	9	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	16315	1281	0
1	CA	32329	0	16312	1277	0
2	AB	1901	0	1951	273	0
2	CB	1901	0	1951	273	0
3	AC	1613	0	1677	245	0
3	CC	1613	0	1677	250	0
4	AD	1703	0	1762	166	0
4	CD	1703	0	1763	166	0
5	AE	1147	0	1207	137	0
5	CE	1147	0	1207	134	0
6	AF	843	0	857	97	0
6	CF	843	0	857	91	0
7	AG	1257	0	1296	117	0
7	CG	1257	0	1296	113	0
8	AH	1116	0	1177	127	0
8	CH	1116	0	1177	127	0
9	AI	1011	0	1041	170	0
9	CI	1011	0	1041	167	0
10	AJ	795	0	840	175	0
10	CJ	795	0	840	177	0
11	AK	885	0	904	103	0
11	CK	885	0	904	98	0
12	AL	971	0	1057	130	0
12	CL	971	0	1057	126	0
13	AM	988	0	1056	173	0
13	CM	988	0	1056	168	0
14	AN	492	0	529	74	0
14	CN	492	0	529	75	0
15	AO	734	0	771	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	77	0
16	AP	701	0	720	82	0
16	CP	701	0	720	78	0
17	AQ	824	0	891	92	0
17	CQ	824	0	891	88	0
18	AR	574	0	644	82	0
18	CR	574	0	644	86	0
19	AS	630	0	652	105	0
19	CS	630	0	652	96	0
20	AT	763	0	861	102	0
20	CT	763	0	861	102	0
21	AU	209	0	221	17	0
21	CU	209	0	221	19	0
22	AV	1630	0	831	66	0
22	AY	1630	0	831	84	0
22	CV	1630	0	831	78	0
22	CY	1630	0	831	71	0
23	AW	1619	0	822	93	0
23	CW	1619	0	821	94	0
24	AX	227	0	119	7	0
24	CX	227	0	118	10	0
25	B0	662	0	688	81	0
25	D0	662	0	688	81	0
26	B1	732	0	808	95	0
26	D1	732	0	808	88	0
27	B2	598	0	653	59	0
27	D2	598	0	653	86	0
28	B3	468	0	523	31	0
28	D3	468	0	523	30	0
29	B4	226	0	229	43	0
29	D4	226	0	229	35	0
30	B5	459	0	480	86	0
30	D5	459	0	480	86	0
31	B6	381	0	390	106	0
31	D6	381	0	390	105	0
32	B7	419	0	467	30	0
32	D7	419	0	467	30	0
33	B8	508	0	576	100	0
33	D8	508	0	576	98	0
34	B9	299	0	325	29	0
34	D9	299	0	325	31	0
35	BA	60459	0	30474	2058	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DA	60459	0	30478	2069	0
36	BB	2551	0	1294	105	0
36	DB	2551	0	1294	89	0
37	BC	1140	0	863	123	0
37	DC	1142	0	865	126	0
38	BD	2105	0	2182	327	0
38	DD	2105	0	2182	319	0
39	BE	1564	0	1629	245	0
39	DE	1564	0	1629	245	0
40	BF	1624	0	1677	211	0
40	DF	1624	0	1677	207	0
41	BG	1474	0	1534	253	0
41	DG	1474	0	1534	269	0
42	BH	1223	0	1282	173	0
42	DH	1223	0	1282	173	0
43	BI	1132	0	1218	196	0
43	DI	1132	0	1218	198	0
44	BN	1105	0	1180	138	0
44	DN	1105	0	1180	138	0
45	BO	933	0	996	121	0
45	DO	933	0	996	123	0
46	BP	1114	0	1187	280	0
46	DP	1114	0	1187	278	0
47	BQ	1122	0	1179	169	0
47	DQ	1122	0	1179	166	0
48	BR	960	0	1021	139	0
48	DR	960	0	1021	140	0
49	BS	771	0	832	152	0
49	DS	771	0	832	143	0
50	BT	1142	0	1202	241	0
50	DT	1142	0	1202	228	0
51	BU	958	0	1015	156	0
51	DU	958	0	1015	154	0
52	BV	779	0	852	159	0
52	DV	779	0	852	162	0
53	BW	896	0	953	90	0
53	DW	896	0	953	85	0
54	BX	726	0	778	87	0
54	DX	726	0	778	86	0
55	BY	776	0	870	184	0
55	DY	776	0	870	193	0
56	BZ	1404	0	1432	232	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DZ	1404	0	1432	232	0
57	AA	198	0	0	0	0
57	AD	1	0	0	0	0
57	AE	1	0	0	0	0
57	AG	1	0	0	0	0
57	AI	1	0	0	0	0
57	AL	2	0	0	0	0
57	AN	1	0	0	0	0
57	AV	5	0	0	0	0
57	AW	8	0	0	0	0
57	AX	2	0	0	0	0
57	B0	1	0	0	0	0
57	B1	1	0	0	0	0
57	B2	2	0	0	0	0
57	B5	2	0	0	0	0
57	B7	1	0	0	0	0
57	BA	422	0	0	0	0
57	BB	14	0	0	0	0
57	BD	2	0	0	0	0
57	BE	1	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BU	1	0	0	1	0
57	BV	1	0	0	0	0
57	BX	2	0	0	0	0
57	CA	199	0	0	0	0
57	CE	1	0	0	0	0
57	CI	1	0	0	0	0
57	CL	1	0	0	0	0
57	CN	1	0	0	0	0
57	CV	5	0	0	0	0
57	CW	7	0	0	0	0
57	CX	3	0	0	0	0
57	D1	1	0	0	0	0
57	D2	3	0	0	0	0
57	D5	2	0	0	0	0
57	D7	2	0	0	0	0
57	DA	421	0	0	0	0
57	DB	13	0	0	0	0
57	DC	1	0	0	0	0
57	DD	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DE	1	0	0	0	0
57	DF	2	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DS	1	0	0	0	0
57	DV	1	0	0	0	0
57	DX	3	0	0	0	0
58	AA	42	0	45	2	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D9	1	0	0	0	0
All	All	296042	0	199734	19173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

The worst 5 of 19173 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)
54:BX:63:LYS:HE3	54:BX:72:LYS:HE3	1.23	1.21
56:DZ:53:ILE:HG23	56:DZ:71:VAL:HG23	1.21	1.18
46:DP:59:LEU:HA	46:DP:61:ARG:CZ	1.73	1.18
53:BW:1:MET:HE2	53:BW:2:GLU:H	1.06	1.17
35:BA:2334:G:H21	49:BS:18:ILE:HD11	1.09	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	138 (59%)	63 (27%)	32 (14%)	0	4
2	CB	233/256 (91%)	138 (59%)	62 (27%)	33 (14%)	0	4
3	AC	205/239 (86%)	130 (63%)	55 (27%)	20 (10%)	1	10
3	CC	205/239 (86%)	128 (62%)	56 (27%)	21 (10%)	1	9
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	1	12
4	CD	206/209 (99%)	150 (73%)	38 (18%)	18 (9%)	1	12
5	AE	149/162 (92%)	115 (77%)	23 (15%)	11 (7%)	1	16
5	CE	149/162 (92%)	115 (77%)	22 (15%)	12 (8%)	1	13
6	AF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	26
6	CF	99/101 (98%)	79 (80%)	15 (15%)	5 (5%)	2	26
7	AG	153/156 (98%)	111 (72%)	36 (24%)	6 (4%)	4	34
7	CG	153/156 (98%)	111 (72%)	36 (24%)	6 (4%)	4	34
8	AH	136/138 (99%)	107 (79%)	25 (18%)	4 (3%)	6	42
8	CH	136/138 (99%)	108 (79%)	24 (18%)	4 (3%)	6	42
9	AI	121/128 (94%)	85 (70%)	23 (19%)	13 (11%)	0	8
9	CI	121/128 (94%)	83 (69%)	26 (22%)	12 (10%)	1	10
10	AJ	97/105 (92%)	62 (64%)	25 (26%)	10 (10%)	1	9
10	CJ	97/105 (92%)	63 (65%)	24 (25%)	10 (10%)	1	9
11	AK	117/129 (91%)	86 (74%)	26 (22%)	5 (4%)	3	31
11	CK	117/129 (91%)	88 (75%)	24 (20%)	5 (4%)	3	31
12	AL	123/135 (91%)	82 (67%)	27 (22%)	14 (11%)	0	7
12	CL	123/135 (91%)	83 (68%)	26 (21%)	14 (11%)	0	7
13	AM	117/126 (93%)	67 (57%)	30 (26%)	20 (17%)	0	3
13	CM	117/126 (93%)	67 (57%)	31 (26%)	19 (16%)	0	3
14	AN	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	4
14	CN	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	4
15	AO	86/89 (97%)	58 (67%)	20 (23%)	8 (9%)	1	11
15	CO	86/89 (97%)	57 (66%)	21 (24%)	8 (9%)	1	11
16	AP	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	7	47
16	CP	82/88 (93%)	59 (72%)	21 (26%)	2 (2%)	7	47
17	AQ	98/105 (93%)	74 (76%)	20 (20%)	4 (4%)	3	33
17	CQ	98/105 (93%)	76 (78%)	19 (19%)	3 (3%)	5	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	41 (60%)	14 (21%)	13 (19%)	0	2
18	CR	68/88 (77%)	41 (60%)	13 (19%)	14 (21%)	0	1
19	AS	77/93 (83%)	49 (64%)	16 (21%)	12 (16%)	0	3
19	CS	77/93 (83%)	49 (64%)	15 (20%)	13 (17%)	0	3
20	AT	97/106 (92%)	69 (71%)	18 (19%)	10 (10%)	1	9
20	CT	97/106 (92%)	71 (73%)	16 (16%)	10 (10%)	1	9
21	AU	23/27 (85%)	13 (56%)	8 (35%)	2 (9%)	1	12
21	CU	23/27 (85%)	13 (56%)	8 (35%)	2 (9%)	1	12
25	B0	82/85 (96%)	65 (79%)	14 (17%)	3 (4%)	4	36
25	D0	82/85 (96%)	61 (74%)	17 (21%)	4 (5%)	3	27
26	B1	92/98 (94%)	65 (71%)	17 (18%)	10 (11%)	0	8
26	D1	92/98 (94%)	66 (72%)	18 (20%)	8 (9%)	1	12
27	B2	69/72 (96%)	43 (62%)	19 (28%)	7 (10%)	1	9
27	D2	69/72 (96%)	37 (54%)	23 (33%)	9 (13%)	0	5
28	B3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	2	25
28	D3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	2	25
29	B4	29/71 (41%)	16 (55%)	7 (24%)	6 (21%)	0	1
29	D4	29/71 (41%)	16 (55%)	7 (24%)	6 (21%)	0	1
30	B5	57/60 (95%)	38 (67%)	8 (14%)	11 (19%)	0	2
30	D5	57/60 (95%)	39 (68%)	6 (10%)	12 (21%)	0	1
31	B6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	1
31	D6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	1
32	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
32	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	44 (71%)	9 (14%)	9 (14%)	0	4
33	D8	62/65 (95%)	43 (69%)	10 (16%)	9 (14%)	0	4
34	B9	34/37 (92%)	29 (85%)	5 (15%)	0	100	100
34	D9	34/37 (92%)	29 (85%)	5 (15%)	0	100	100
37	BC	183/229 (80%)	81 (44%)	47 (26%)	55 (30%)	0	0
37	DC	183/229 (80%)	82 (45%)	47 (26%)	54 (30%)	0	0
38	BD	270/276 (98%)	208 (77%)	38 (14%)	24 (9%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DD	270/276 (98%)	205 (76%)	38 (14%)	27 (10%)	1	9
39	BE	203/206 (98%)	130 (64%)	40 (20%)	33 (16%)	0	3
39	DE	203/206 (98%)	127 (63%)	44 (22%)	32 (16%)	0	3
40	BF	206/210 (98%)	142 (69%)	35 (17%)	29 (14%)	0	4
40	DF	206/210 (98%)	143 (69%)	35 (17%)	28 (14%)	0	4
41	BG	177/182 (97%)	107 (60%)	50 (28%)	20 (11%)	0	7
41	DG	177/182 (97%)	108 (61%)	45 (25%)	24 (14%)	0	4
42	BH	158/180 (88%)	99 (63%)	32 (20%)	27 (17%)	0	3
42	DH	158/180 (88%)	99 (63%)	32 (20%)	27 (17%)	0	3
43	BI	144/148 (97%)	87 (60%)	35 (24%)	22 (15%)	0	3
43	DI	144/148 (97%)	85 (59%)	37 (26%)	22 (15%)	0	3
44	BN	137/140 (98%)	90 (66%)	30 (22%)	17 (12%)	0	6
44	DN	137/140 (98%)	91 (66%)	29 (21%)	17 (12%)	0	6
45	BO	120/122 (98%)	91 (76%)	21 (18%)	8 (7%)	1	19
45	DO	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	1	19
46	BP	144/150 (96%)	73 (51%)	30 (21%)	41 (28%)	0	0
46	DP	144/150 (96%)	73 (51%)	30 (21%)	41 (28%)	0	0
47	BQ	139/141 (99%)	107 (77%)	24 (17%)	8 (6%)	2	23
47	DQ	139/141 (99%)	106 (76%)	23 (16%)	10 (7%)	1	17
48	BR	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	0	6
48	DR	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	0	6
49	BS	97/112 (87%)	47 (48%)	25 (26%)	25 (26%)	0	1
49	DS	97/112 (87%)	47 (48%)	25 (26%)	25 (26%)	0	1
50	BT	136/146 (93%)	82 (60%)	26 (19%)	28 (21%)	0	1
50	DT	136/146 (93%)	81 (60%)	27 (20%)	28 (21%)	0	1
51	BU	115/118 (98%)	86 (75%)	22 (19%)	7 (6%)	2	21
51	DU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	14
52	BV	99/101 (98%)	62 (63%)	22 (22%)	15 (15%)	0	3
52	DV	99/101 (98%)	63 (64%)	21 (21%)	15 (15%)	0	3
53	BW	111/113 (98%)	87 (78%)	15 (14%)	9 (8%)	1	13
53	DW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BX	91/96 (95%)	74 (81%)	14 (15%)	3 (3%)	5	39
54	DX	91/96 (95%)	74 (81%)	13 (14%)	4 (4%)	3	30
55	BY	99/110 (90%)	37 (37%)	30 (30%)	32 (32%)	0	0
55	DY	99/110 (90%)	35 (35%)	32 (32%)	32 (32%)	0	0
56	BZ	175/206 (85%)	113 (65%)	38 (22%)	24 (14%)	0	4
56	DZ	175/206 (85%)	103 (59%)	45 (26%)	27 (15%)	0	3
All	All	11670/12592 (93%)	7783 (67%)	2440 (21%)	1447 (12%)	0	6

5 of 1447 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	88	ALA
2	AB	154	LEU
2	AB	165	VAL

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%)	181 (90%)	21 (10%)	9	39
2	CB	202/220 (92%)	181 (90%)	21 (10%)	9	39
3	AC	160/188 (85%)	152 (95%)	8 (5%)	30	69
3	CC	160/188 (85%)	151 (94%)	9 (6%)	26	66
4	AD	180/181 (99%)	161 (89%)	19 (11%)	8	38
4	CD	180/181 (99%)	159 (88%)	21 (12%)	7	32
5	AE	115/123 (94%)	106 (92%)	9 (8%)	16	53
5	CE	115/123 (94%)	107 (93%)	8 (7%)	19	59
6	AF	90/90 (100%)	85 (94%)	5 (6%)	26	66
6	CF	90/90 (100%)	85 (94%)	5 (6%)	26	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/127 (99%)	118 (94%)	8 (6%)	22	63
7	CG	126/127 (99%)	117 (93%)	9 (7%)	18	58
8	AH	119/119 (100%)	111 (93%)	8 (7%)	20	61
8	CH	119/119 (100%)	111 (93%)	8 (7%)	20	61
9	AI	98/99 (99%)	88 (90%)	10 (10%)	9	40
9	CI	98/99 (99%)	88 (90%)	10 (10%)	9	40
10	AJ	88/92 (96%)	76 (86%)	12 (14%)	5	26
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	6	29
11	AK	90/99 (91%)	84 (93%)	6 (7%)	20	61
11	CK	90/99 (91%)	84 (93%)	6 (7%)	20	61
12	AL	104/111 (94%)	93 (89%)	11 (11%)	8	38
12	CL	104/111 (94%)	92 (88%)	12 (12%)	7	33
13	AM	99/101 (98%)	90 (91%)	9 (9%)	12	46
13	CM	99/101 (98%)	90 (91%)	9 (9%)	12	46
14	AN	49/50 (98%)	46 (94%)	3 (6%)	23	64
14	CN	49/50 (98%)	46 (94%)	3 (6%)	23	64
15	AO	79/80 (99%)	70 (89%)	9 (11%)	7	33
15	CO	79/80 (99%)	70 (89%)	9 (11%)	7	33
16	AP	72/74 (97%)	61 (85%)	11 (15%)	3	21
16	CP	72/74 (97%)	61 (85%)	11 (15%)	3	21
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	28	67
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	28	67
18	AR	61/77 (79%)	53 (87%)	8 (13%)	5	27
18	CR	61/77 (79%)	52 (85%)	9 (15%)	4	22
19	AS	69/80 (86%)	60 (87%)	9 (13%)	5	27
19	CS	69/80 (86%)	60 (87%)	9 (13%)	5	27
20	AT	76/82 (93%)	71 (93%)	5 (7%)	21	61
20	CT	76/82 (93%)	71 (93%)	5 (7%)	21	61
21	AU	19/22 (86%)	18 (95%)	1 (5%)	28	67
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28	67
25	B0	66/67 (98%)	59 (89%)	7 (11%)	8	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	D0	66/67 (98%)	59 (89%)	7 (11%)	8	38
26	B1	78/83 (94%)	65 (83%)	13 (17%)	3	16
26	D1	78/83 (94%)	66 (85%)	12 (15%)	3	20
27	B2	66/67 (98%)	57 (86%)	9 (14%)	5	26
27	D2	66/67 (98%)	57 (86%)	9 (14%)	5	26
28	B3	51/52 (98%)	49 (96%)	2 (4%)	39	76
28	D3	51/52 (98%)	49 (96%)	2 (4%)	39	76
29	B4	27/63 (43%)	23 (85%)	4 (15%)	4	22
29	D4	27/63 (43%)	23 (85%)	4 (15%)	4	22
30	B5	51/52 (98%)	42 (82%)	9 (18%)	2	13
30	D5	51/52 (98%)	41 (80%)	10 (20%)	1	9
31	B6	43/52 (83%)	34 (79%)	9 (21%)	1	8
31	D6	43/52 (83%)	34 (79%)	9 (21%)	1	8
32	B7	41/42 (98%)	36 (88%)	5 (12%)	6	29
32	D7	41/42 (98%)	36 (88%)	5 (12%)	6	29
33	B8	53/55 (96%)	42 (79%)	11 (21%)	1	8
33	D8	53/55 (96%)	42 (79%)	11 (21%)	1	8
34	B9	33/34 (97%)	30 (91%)	3 (9%)	12	46
34	D9	33/34 (97%)	30 (91%)	3 (9%)	12	46
37	BC	61/181 (34%)	53 (87%)	8 (13%)	5	27
37	DC	61/181 (34%)	53 (87%)	8 (13%)	5	27
38	BD	213/218 (98%)	183 (86%)	30 (14%)	4	24
38	DD	213/218 (98%)	183 (86%)	30 (14%)	4	24
39	BE	165/166 (99%)	142 (86%)	23 (14%)	4	25
39	DE	165/166 (99%)	143 (87%)	22 (13%)	5	26
40	BF	165/166 (99%)	150 (91%)	15 (9%)	12	46
40	DF	165/166 (99%)	151 (92%)	14 (8%)	13	49
41	BG	155/156 (99%)	133 (86%)	22 (14%)	4	24
41	DG	155/156 (99%)	129 (83%)	26 (17%)	2	15
42	BH	132/148 (89%)	119 (90%)	13 (10%)	10	42
42	DH	132/148 (89%)	119 (90%)	13 (10%)	10	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BI	122/124 (98%)	113 (93%)	9 (7%)	17	56
43	DI	122/124 (98%)	113 (93%)	9 (7%)	17	56
44	BN	117/119 (98%)	98 (84%)	19 (16%)	3	17
44	DN	117/119 (98%)	100 (86%)	17 (14%)	4	23
45	BO	100/100 (100%)	90 (90%)	10 (10%)	9	41
45	DO	100/100 (100%)	92 (92%)	8 (8%)	15	52
46	BP	112/116 (97%)	92 (82%)	20 (18%)	2	13
46	DP	112/116 (97%)	93 (83%)	19 (17%)	2	15
47	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	21
47	DQ	111/111 (100%)	94 (85%)	17 (15%)	3	21
48	BR	100/101 (99%)	88 (88%)	12 (12%)	6	30
48	DR	100/101 (99%)	88 (88%)	12 (12%)	6	30
49	BS	77/88 (88%)	68 (88%)	9 (12%)	7	32
49	DS	77/88 (88%)	67 (87%)	10 (13%)	5	27
50	BT	120/127 (94%)	101 (84%)	19 (16%)	3	19
50	DT	120/127 (94%)	101 (84%)	19 (16%)	3	19
51	BU	92/94 (98%)	80 (87%)	12 (13%)	5	27
51	DU	92/94 (98%)	80 (87%)	12 (13%)	5	27
52	BV	82/82 (100%)	68 (83%)	14 (17%)	2	15
52	DV	82/82 (100%)	69 (84%)	13 (16%)	3	18
53	BW	91/92 (99%)	83 (91%)	8 (9%)	12	48
53	DW	91/92 (99%)	83 (91%)	8 (9%)	12	48
54	BX	74/78 (95%)	67 (90%)	7 (10%)	11	43
54	DX	74/78 (95%)	67 (90%)	7 (10%)	11	43
55	BY	84/91 (92%)	70 (83%)	14 (17%)	3	16
55	DY	84/91 (92%)	70 (83%)	14 (17%)	3	16
56	BZ	155/179 (87%)	133 (86%)	22 (14%)	4	24
56	DZ	155/179 (87%)	131 (84%)	24 (16%)	3	20
All	All	9654/10432 (92%)	8547 (88%)	1107 (12%)	7	33

5 of 1107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BV	99	ILE
7	CG	113	GLU
50	DT	99	LEU
54	BX	80	ILE
2	CB	94	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 306 such sidechains are listed below:

Mol	Chain	Res	Type
53	BW	62	HIS
6	CF	100	ASN
48	DR	53	HIS
54	BX	55	ASN
3	CC	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	215 (14%)	29 (1%)
1	CA	1503/1522 (98%)	216 (14%)	29 (1%)
22	AV	74/77 (96%)	15 (20%)	0
22	AY	74/77 (96%)	20 (27%)	1 (1%)
22	CV	74/77 (96%)	19 (25%)	1 (1%)
22	CY	74/77 (96%)	20 (27%)	1 (1%)
23	AW	75/76 (98%)	13 (17%)	0
23	CW	75/76 (98%)	15 (20%)	0
24	AX	10/11 (90%)	1 (10%)	0
24	CX	10/11 (90%)	2 (20%)	0
35	BA	2806/2822 (99%)	516 (18%)	55 (1%)
35	DA	2806/2822 (99%)	515 (18%)	53 (1%)
36	BB	118/122 (96%)	13 (11%)	1 (0%)
36	DB	118/122 (96%)	13 (11%)	1 (0%)
All	All	9320/9414 (99%)	1593 (17%)	171 (1%)

5 of 1593 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	48	C

5 of 171 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2481	G
1	CA	366	C
35	DA	2172	U
35	BA	2610	C
1	CA	30	U

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

8 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	8AN	AV	76	57,22	15,24,25	1.08	1 (6%)	11,35,38	1.18	2 (18%)
22	PHA	AV	77	22	10,11,11	0.63	0	10,13,13	0.65	0
22	8AN	AY	76	22	15,24,25	1.17	1 (6%)	11,35,38	0.59	0
22	PHA	AY	77	22	10,11,11	0.66	0	10,13,13	0.77	1 (10%)
22	8AN	CV	76	57,22	15,24,25	1.14	2 (13%)	11,35,38	0.97	1 (9%)
22	PHA	CV	77	22	10,11,11	0.64	0	10,13,13	0.58	0
22	8AN	CY	76	22	15,24,25	0.95	1 (6%)	11,35,38	0.69	0
22	PHA	CY	77	22	10,11,11	1.11	0	10,13,13	0.66	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	8AN	AV	76	57,22	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PHA	AV	77	22	-	0/4/6/6	0/1/1/1
22	8AN	AY	76	22	-	0/3/25/26	0/3/3/3
22	PHA	AY	77	22	-	0/4/6/6	0/1/1/1
22	8AN	CV	76	57,22	-	0/3/25/26	0/3/3/3
22	PHA	CV	77	22	-	0/4/6/6	0/1/1/1
22	8AN	CY	76	22	-	0/3/25/26	0/3/3/3
22	PHA	CY	77	22	-	0/4/6/6	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AY	76	8AN	C3'-N3'	-3.62	1.41	1.47
22	AV	76	8AN	C3'-N3'	-3.57	1.41	1.47
22	CV	76	8AN	C3'-N3'	-3.39	1.42	1.47
22	CY	76	8AN	C3'-N3'	-2.73	1.43	1.47
22	CV	76	8AN	C2-N3	2.07	1.35	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	76	8AN	C2'-C1'-N9	-2.47	110.51	114.29
22	AY	77	PHA	O-C-CA	-2.14	119.92	125.49
22	CV	76	8AN	O4'-C4'-C3'	2.15	107.31	104.09
22	AV	76	8AN	O4'-C4'-C3'	2.18	107.35	104.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	76	8AN	1	0
22	AV	77	PHA	1	0
22	AY	76	8AN	3	0
22	AY	77	PHA	5	0
22	CV	76	8AN	2	0
22	CV	77	PHA	2	0
22	CY	76	8AN	2	0
22	CY	77	PHA	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1354 ligands modelled in this entry, 1352 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	$\# Z > 2$
58	PAR	AA	1799	-	45,45,45	1.93	14 (31%)	59,67,67	1.36	7 (11%)
58	PAR	CA	1800	-	45,45,45	1.68	11 (24%)	59,67,67	1.29	8 (13%)

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
58	PAR	AA	1799	-	-	0/18/94/94	0/4/4/4
58	PAR	CA	1800	-	-	0/18/94/94	0/4/4/4

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CA	1800	PAR	C31-C21	2.03	1.56	1.53
58	CA	1800	PAR	C62-C52	2.09	1.58	1.52
58	AA	1799	PAR	O11-C42	2.10	1.49	1.43
58	AA	1799	PAR	O11-C11	2.10	1.47	1.41
58	AA	1799	PAR	C14-C24	2.18	1.56	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	1800	PAR	C22-C12-C62	-2.25	106.66	110.11
58	CA	1800	PAR	C11-O51-C51	2.24	118.10	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	1800	PAR	O11-C11-C21	2.28	112.19	107.96
58	AA	1799	PAR	C22-C32-C42	2.47	116.11	109.53
58	CA	1800	PAR	C22-C32-C42	2.57	116.39	109.53

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
58	AA	1799	PAR	2	0
58	CA	1800	PAR	2	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	3
13	AM	3
9	AI	2
9	CI	2
41	DG	1
41	BG	1
31	D6	1
31	B6	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D6	46:HIS	C	47:THR	N	4.60
1	B6	46:HIS	C	47:THR	N	4.59
1	BG	112:PRO	C	113:ARG	N	3.80
1	DG	112:PRO	C	113:ARG	N	3.77
1	CM	69:GLU	C	70:LEU	N	3.15

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%)	-0.01	25 (1%) 73 64	47, 104, 183, 200	0
1	CA	1504/1522 (98%)	0.11	34 (2%) 64 54	69, 117, 189, 200	0
2	AB	235/256 (91%)	0.07	7 (2%) 54 43	73, 131, 181, 200	0
2	CB	235/256 (91%)	0.20	5 (2%) 67 58	85, 154, 189, 200	0
3	AC	207/239 (86%)	-0.02	1 (0%) 91 88	71, 116, 160, 200	0
3	CC	207/239 (86%)	0.23	7 (3%) 49 40	87, 139, 180, 200	0
4	AD	208/209 (99%)	-0.23	0 100 100	60, 110, 153, 185	0
4	CD	208/209 (99%)	-0.32	0 100 100	58, 101, 142, 181	0
5	AE	151/162 (93%)	-0.16	1 (0%) 89 82	52, 101, 144, 174	0
5	CE	151/162 (93%)	0.21	5 (3%) 50 41	66, 119, 168, 200	0
6	AF	101/101 (100%)	-0.33	1 (0%) 84 76	56, 96, 142, 181	0
6	CF	101/101 (100%)	-0.23	1 (0%) 84 76	51, 107, 147, 196	0
7	AG	155/156 (99%)	0.11	9 (5%) 26 21	65, 117, 166, 200	0
7	CG	155/156 (99%)	0.20	8 (5%) 31 24	80, 129, 161, 182	0
8	AH	138/138 (100%)	-0.04	3 (2%) 65 55	62, 106, 140, 174	0
8	CH	138/138 (100%)	0.25	6 (4%) 39 30	82, 122, 160, 195	0
9	AI	127/128 (99%)	0.24	5 (3%) 43 35	79, 136, 176, 200	0
9	CI	127/128 (99%)	0.53	13 (10%) 9 8	96, 145, 188, 200	0
10	AJ	99/105 (94%)	0.65	17 (17%) 2 2	65, 140, 184, 200	0
10	CJ	99/105 (94%)	0.79	17 (17%) 2 2	70, 153, 195, 200	0
11	AK	119/129 (92%)	0.02	3 (2%) 61 50	62, 99, 159, 198	0
11	CK	119/129 (92%)	-0.13	4 (3%) 49 40	74, 111, 155, 184	0
12	AL	125/135 (92%)	-0.11	2 (1%) 74 65	51, 91, 144, 190	0
12	CL	125/135 (92%)	0.29	5 (4%) 42 33	59, 113, 161, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.17	7 (5%) 28 22	75, 120, 163, 200	0
13	CM	125/126 (99%)	0.64	15 (12%) 6 6	77, 137, 184, 200	0
14	AN	60/61 (98%)	-0.25	0 100 100	50, 109, 147, 200	0
14	CN	60/61 (98%)	0.58	4 (6%) 21 16	89, 135, 183, 200	0
15	AO	88/89 (98%)	-0.16	2 (2%) 64 54	55, 100, 144, 162	0
15	CO	88/89 (98%)	0.01	2 (2%) 64 54	69, 108, 154, 182	0
16	AP	84/88 (95%)	0.22	1 (1%) 81 72	78, 107, 147, 184	0
16	CP	84/88 (95%)	0.19	0 100 100	61, 100, 150, 179	0
17	AQ	100/105 (95%)	0.04	4 (4%) 42 33	82, 109, 150, 181	0
17	CQ	100/105 (95%)	0.12	4 (4%) 42 33	71, 115, 153, 167	0
18	AR	70/88 (79%)	-0.15	1 (1%) 78 68	59, 96, 139, 169	0
18	CR	70/88 (79%)	0.12	0 100 100	66, 111, 152, 173	0
19	AS	79/93 (84%)	0.40	4 (5%) 32 24	82, 122, 176, 200	0
19	CS	79/93 (84%)	0.81	9 (11%) 7 7	91, 145, 188, 200	0
20	AT	99/106 (93%)	0.16	1 (1%) 84 76	77, 120, 170, 195	0
20	CT	99/106 (93%)	0.21	5 (5%) 32 24	67, 116, 174, 200	0
21	AU	25/27 (92%)	1.09	5 (20%) 1 2	80, 119, 154, 178	0
21	CU	25/27 (92%)	1.71	9 (36%) 0 0	79, 141, 171, 185	0
22	AV	75/77 (97%)	0.20	3 (4%) 42 33	55, 121, 158, 197	0
22	AY	75/77 (97%)	0.78	8 (10%) 8 7	49, 162, 196, 200	0
22	CV	75/77 (97%)	0.07	1 (1%) 79 70	64, 144, 178, 192	0
22	CY	75/77 (97%)	1.17	11 (14%) 3 3	84, 181, 199, 200	0
23	AW	76/76 (100%)	0.60	9 (11%) 6 6	99, 173, 199, 200	0
23	CW	76/76 (100%)	0.60	7 (9%) 11 10	117, 178, 200, 200	0
24	AX	11/11 (100%)	0.54	1 (9%) 11 10	68, 116, 146, 168	0
24	CX	11/11 (100%)	0.79	2 (18%) 2 2	87, 126, 158, 159	0
25	B0	84/85 (98%)	-0.23	0 100 100	30, 62, 111, 143	0
25	D0	84/85 (98%)	0.27	2 (2%) 62 52	58, 106, 148, 178	0
26	B1	94/98 (95%)	-0.16	0 100 100	37, 68, 129, 162	0
26	D1	94/98 (95%)	-0.03	1 (1%) 82 73	38, 79, 131, 166	0
27	B2	71/72 (98%)	-0.24	1 (1%) 78 68	40, 80, 141, 188	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	-0.21	0 100 100	62, 97, 150, 182	0
28	B3	60/60 (100%)	-0.23	1 (1%) 73 64	31, 67, 112, 190	0
28	D3	60/60 (100%)	0.94	7 (11%) 6 6	65, 124, 163, 200	0
29	B4	31/71 (43%)	-0.26	0 100 100	67, 132, 172, 182	0
29	D4	31/71 (43%)	-0.30	0 100 100	105, 142, 184, 197	0
30	B5	59/60 (98%)	-0.27	2 (3%) 49 40	37, 60, 164, 200	0
30	D5	59/60 (98%)	-0.05	4 (6%) 20 16	52, 88, 175, 191	0
31	B6	45/54 (83%)	0.92	5 (11%) 7 7	57, 113, 166, 174	0
31	D6	45/54 (83%)	1.66	16 (35%) 0 0	92, 138, 175, 200	0
32	B7	49/49 (100%)	-0.30	0 100 100	25, 53, 112, 194	0
32	D7	49/49 (100%)	-0.05	0 100 100	41, 67, 119, 181	0
33	B8	64/65 (98%)	-0.06	1 (1%) 74 65	25, 69, 131, 198	0
33	D8	64/65 (98%)	0.10	0 100 100	45, 92, 149, 183	0
34	B9	36/37 (97%)	1.63	11 (30%) 1 1	70, 99, 142, 153	0
34	D9	36/37 (97%)	3.27	27 (75%) 0 0	120, 159, 194, 200	0
35	BA	2807/2822 (99%)	-0.02	48 (1%) 73 64	35, 64, 176, 200	0
35	DA	2807/2822 (99%)	0.06	61 (2%) 65 55	44, 93, 186, 200	0
36	BB	119/122 (97%)	-0.27	1 (0%) 87 80	57, 81, 135, 179	0
36	DB	119/122 (97%)	-0.00	2 (1%) 73 64	90, 129, 183, 197	0
37	BC	191/229 (83%)	2.01	75 (39%) 0 0	115, 175, 200, 200	0
37	DC	191/229 (83%)	1.75	80 (41%) 0 0	113, 172, 200, 200	0
38	BD	272/276 (98%)	-0.38	1 (0%) 93 90	33, 62, 106, 186	0
38	DD	272/276 (98%)	-0.26	0 100 100	40, 76, 114, 158	0
39	BE	205/206 (99%)	-0.20	2 (0%) 84 76	28, 65, 151, 200	0
39	DE	205/206 (99%)	0.16	3 (1%) 76 67	53, 105, 162, 193	0
40	BF	208/210 (99%)	-0.40	5 (2%) 62 52	26, 65, 154, 194	0
40	DF	208/210 (99%)	-0.21	3 (1%) 78 68	41, 91, 166, 200	0
41	BG	181/182 (99%)	-0.12	4 (2%) 65 55	57, 99, 158, 197	0
41	DG	181/182 (99%)	0.11	5 (2%) 56 46	78, 120, 160, 182	0
42	BH	160/180 (88%)	0.02	7 (4%) 38 29	44, 94, 160, 199	0
42	DH	160/180 (88%)	1.41	46 (28%) 1 1	107, 169, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	0.96	32 (21%) 1 1	48, 154, 200, 200	0
43	DI	146/148 (98%)	0.39	10 (6%) 20 16	74, 126, 175, 200	0
44	BN	139/140 (99%)	-0.42	0 100 100	33, 68, 138, 187	0
44	DN	139/140 (99%)	0.30	2 (1%) 78 68	75, 116, 173, 200	0
45	BO	122/122 (100%)	-0.37	0 100 100	30, 69, 107, 139	0
45	DO	122/122 (100%)	-0.17	0 100 100	59, 105, 137, 157	0
46	BP	146/150 (97%)	-0.05	2 (1%) 78 68	25, 84, 158, 188	0
46	DP	146/150 (97%)	0.18	5 (3%) 49 40	51, 108, 169, 200	0
47	BQ	141/141 (100%)	-0.30	2 (1%) 78 68	41, 69, 130, 200	0
47	DQ	141/141 (100%)	0.07	4 (2%) 56 46	66, 115, 166, 200	0
48	BR	117/118 (99%)	-0.36	0 100 100	21, 62, 114, 165	0
48	DR	117/118 (99%)	-0.13	1 (0%) 85 78	37, 89, 131, 173	0
49	BS	99/112 (88%)	0.02	1 (1%) 84 76	43, 83, 138, 181	0
49	DS	99/112 (88%)	0.56	9 (9%) 11 10	80, 128, 179, 200	0
50	BT	138/146 (94%)	-0.29	3 (2%) 65 55	40, 86, 164, 195	0
50	DT	138/146 (94%)	-0.02	3 (2%) 65 55	74, 116, 173, 200	0
51	BU	117/118 (99%)	-0.55	1 (0%) 85 78	23, 55, 106, 158	0
51	DU	117/118 (99%)	-0.12	4 (3%) 49 40	56, 101, 167, 200	0
52	BV	101/101 (100%)	-0.29	0 100 100	29, 76, 135, 200	0
52	DV	101/101 (100%)	0.48	4 (3%) 42 33	55, 135, 177, 200	0
53	BW	113/113 (100%)	-0.30	2 (1%) 71 62	26, 55, 122, 200	0
53	DW	113/113 (100%)	-0.17	1 (0%) 85 78	50, 80, 140, 194	0
54	BX	93/96 (96%)	-0.50	0 100 100	41, 66, 106, 157	0
54	DX	93/96 (96%)	-0.23	0 100 100	42, 86, 118, 150	0
55	BY	101/110 (91%)	0.31	9 (8%) 12 10	42, 88, 178, 200	0
55	DY	101/110 (91%)	0.78	17 (16%) 2 2	49, 107, 181, 200	0
56	BZ	177/206 (85%)	0.22	19 (10%) 8 7	40, 107, 185, 200	0
56	DZ	177/206 (85%)	0.90	28 (15%) 3 3	96, 152, 198, 200	0
All	All	21244/22006 (96%)	0.10	874 (4%) 41 32	21, 102, 183, 200	0

The worst 5 of 874 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BC	179	SER	14.3
1	CA	83	U	13.1
56	DZ	112	ARG	11.2
35	BA	888	C	10.4
37	BC	51	PRO	10.2

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	PHA	CY	77	11/11	0.92	0.39	-	42,44,48,152	0
22	8AN	AY	76	22/23	0.97	0.24	-	29,48,67,71	0
22	8AN	CV	76	22/23	0.95	0.18	-	12,58,100,116	0
22	8AN	AV	76	22/23	0.97	0.22	-	12,58,100,116	0
22	PHA	AV	77	11/11	0.90	0.37	-	121,125,131,132	0
22	PHA	CV	77	11/11	0.87	0.28	-	121,125,131,132	0
22	8AN	CY	76	22/23	0.94	0.24	-	29,48,67,71	0
22	PHA	AY	77	11/11	0.97	0.39	-	42,44,47,48	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
57	MG	BA	3047	1/1	0.76	0.82	70.75	72,72,72,72	0
57	MG	DA	3202	1/1	0.59	1.01	42.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3090	1/1	0.76	0.87	41.62	77,77,77,77	0
57	MG	BA	3117	1/1	0.97	0.56	38.03	59,59,59,59	0
57	MG	DA	3118	1/1	0.81	0.62	36.88	62,62,62,62	0
57	MG	DA	3070	1/1	0.81	0.72	32.03	94,94,94,94	0
57	MG	DA	3124	1/1	0.96	0.62	30.41	28,28,28,28	0
57	MG	DA	3152	1/1	0.38	0.81	29.48	82,82,82,82	0
57	MG	CA	1690	1/1	0.75	0.85	28.73	110,110,110,110	0
57	MG	BA	3067	1/1	0.78	0.76	28.13	53,53,53,53	0
57	MG	AA	1715	1/1	0.76	0.67	28.01	39,39,39,39	1
57	MG	CA	1652	1/1	0.77	0.72	27.73	52,52,52,52	0
57	MG	AA	1634	1/1	0.88	0.78	27.11	73,73,73,73	0
57	MG	BA	3091	1/1	0.93	0.46	26.50	41,41,41,41	0
57	MG	BA	3340	1/1	0.76	0.61	26.46	90,90,90,90	1
57	MG	DA	3046	1/1	0.94	0.54	26.22	30,30,30,30	0
57	MG	BA	3123	1/1	0.97	0.57	25.07	29,29,29,29	0
57	MG	DA	3182	1/1	0.86	0.59	24.95	60,60,60,60	0
57	MG	BA	3062	1/1	0.91	0.56	24.64	31,31,31,31	0
57	MG	CA	1721	1/1	0.17	0.46	24.02	97,97,97,97	0
57	MG	BA	3048	1/1	0.85	0.67	23.63	33,33,33,33	0
57	MG	BA	3112	1/1	0.99	0.39	23.22	15,15,15,15	0
57	MG	DA	3048	1/1	0.94	0.67	23.07	61,61,61,61	0
57	MG	BA	3241	1/1	0.79	0.51	22.85	70,70,70,70	0
57	MG	BA	3069	1/1	0.97	0.53	22.78	63,63,63,63	0
57	MG	BA	3053	1/1	0.93	0.47	22.76	64,64,64,64	0
57	MG	BA	3410	1/1	0.98	0.45	22.62	120,120,120,120	0
57	MG	BA	3025	1/1	0.96	0.48	21.44	9,9,9,9	0
57	MG	BA	3114	1/1	0.97	0.43	21.33	3,3,3,3	0
57	MG	BA	3237	1/1	0.67	0.58	20.51	74,74,74,74	0
57	MG	DA	3409	1/1	0.98	0.55	20.37	121,121,121,121	0
57	MG	BA	3055	1/1	0.99	0.32	20.06	18,18,18,18	0
57	MG	DA	3049	1/1	0.75	0.77	19.66	71,71,71,71	0
57	MG	DA	3192	1/1	0.48	0.63	19.31	74,74,74,74	0
57	MG	DA	3066	1/1	0.96	0.42	19.23	43,43,43,43	0
57	MG	BA	3271	1/1	0.93	0.49	19.20	43,43,43,43	0
57	MG	AA	1719	1/1	0.94	0.50	18.81	52,52,52,52	0
57	MG	DA	3158	1/1	0.94	0.53	18.75	48,48,48,48	0
57	MG	CA	1634	1/1	0.89	0.59	18.50	53,53,53,53	0
57	MG	AA	1694	1/1	0.95	0.46	18.45	84,84,84,84	0
57	MG	BA	3026	1/1	0.96	0.33	17.92	8,8,8,8	0
57	MG	DA	3196	1/1	0.58	0.29	17.70	96,96,96,96	0
57	MG	BA	3023	1/1	0.95	0.34	17.54	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3150	1/1	0.81	0.42	17.07	64,64,64,64	0
57	MG	BA	3045	1/1	0.98	0.41	16.75	1,1,1,1	0
57	MG	BA	3398	1/1	0.96	0.36	16.56	84,84,84,84	0
57	MG	DA	3222	1/1	0.72	0.53	15.93	95,95,95,95	0
57	MG	DA	3054	1/1	0.90	0.46	15.76	90,90,90,90	0
57	MG	CA	1739	1/1	0.63	0.49	15.34	128,128,128,128	0
57	MG	DA	3098	1/1	0.81	0.59	15.27	38,38,38,38	0
57	MG	DN	201	1/1	0.69	2.50	14.91	129,129,129,129	0
57	MG	CA	1789	1/1	0.89	0.56	14.73	64,64,64,64	1
57	MG	DA	3006	1/1	0.78	0.42	14.48	23,23,23,23	0
57	MG	DA	3027	1/1	0.93	0.42	14.48	37,37,37,37	0
57	MG	AA	1705	1/1	0.82	0.51	14.00	63,63,63,63	0
57	MG	BA	3005	1/1	0.92	0.41	13.79	7,7,7,7	0
57	MG	BA	3064	1/1	0.98	0.34	13.74	20,20,20,20	0
57	MG	BA	3011	1/1	0.96	0.30	13.59	32,32,32,32	0
57	MG	BA	3070	1/1	0.98	0.44	13.53	2,2,2,2	0
57	MG	CA	1719	1/1	0.86	0.62	13.49	93,93,93,93	0
57	MG	BA	3233	1/1	0.99	0.40	13.47	24,24,24,24	0
57	MG	CA	1695	1/1	0.95	0.36	13.06	54,54,54,54	0
57	MG	BA	3105	1/1	0.92	0.46	12.95	50,50,50,50	0
57	MG	BA	3216	1/1	0.71	0.33	12.75	80,80,80,80	0
57	MG	AA	1623	1/1	0.84	0.54	12.72	70,70,70,70	0
57	MG	BA	3004	1/1	0.90	0.33	12.63	42,42,42,42	0
57	MG	DA	3239	1/1	0.77	0.98	12.61	79,79,79,79	0
57	MG	AA	1610	1/1	0.92	0.60	12.50	49,49,49,49	0
57	MG	DA	3071	1/1	0.93	0.55	12.26	23,23,23,23	0
57	MG	AA	1664	1/1	0.87	0.33	11.64	47,47,47,47	0
57	MG	BA	3279	1/1	0.61	0.29	11.59	53,53,53,53	0
57	MG	CA	1716	1/1	0.68	0.76	11.58	68,68,68,68	1
57	MG	DA	3029	1/1	0.93	0.41	10.90	40,40,40,40	0
57	MG	BA	3180	1/1	0.90	0.38	10.90	50,50,50,50	0
57	MG	DA	3148	1/1	0.91	0.55	10.57	46,46,46,46	0
57	MG	CA	1623	1/1	0.67	0.50	10.27	71,71,71,71	0
57	MG	BA	3065	1/1	0.98	0.24	10.21	1,1,1,1	0
57	MG	BA	3299	1/1	0.98	0.28	10.16	46,46,46,46	1
57	MG	AA	1781	1/1	0.71	0.25	10.04	63,63,63,63	0
57	MG	BA	3291	1/1	0.73	0.37	10.03	42,42,42,42	0
57	MG	BA	3301	1/1	0.90	0.37	10.02	57,57,57,57	0
57	MG	BA	3086	1/1	0.90	0.40	9.91	32,32,32,32	0
57	MG	AA	1721	1/1	0.74	0.49	9.90	90,90,90,90	0
57	MG	CA	1707	1/1	0.87	0.34	9.85	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3012	1/1	0.69	0.28	9.73	45,45,45,45	0
57	MG	D7	102	1/1	0.78	0.84	9.61	62,62,62,62	1
57	MG	DA	3106	1/1	0.64	0.45	9.59	78,78,78,78	0
57	MG	DA	3088	1/1	0.97	0.41	9.51	37,37,37,37	0
57	MG	BA	3009	1/1	0.97	0.35	9.49	17,17,17,17	0
57	MG	BA	3170	1/1	0.86	0.34	9.48	61,61,61,61	0
57	MG	DA	3380	1/1	0.92	0.41	9.44	52,52,52,52	0
57	MG	AA	1682	1/1	0.83	0.40	9.35	131,131,131,131	0
57	MG	DA	3063	1/1	0.89	0.49	9.28	32,32,32,32	0
57	MG	BA	3022	1/1	0.98	0.35	9.24	20,20,20,20	0
57	MG	BA	3295	1/1	0.76	0.44	9.02	64,64,64,64	0
57	MG	DA	3092	1/1	0.87	0.37	8.98	46,46,46,46	0
57	MG	BA	3012	1/1	0.97	0.32	8.82	16,16,16,16	0
57	MG	BA	3229	1/1	0.99	0.35	8.60	20,20,20,20	0
57	MG	BA	3376	1/1	0.71	0.45	8.59	81,81,81,81	0
57	MG	BA	3275	1/1	0.84	0.57	8.38	98,98,98,98	0
57	MG	DA	3241	1/1	0.99	0.37	8.34	32,32,32,32	0
57	MG	DA	3163	1/1	0.95	0.31	8.27	52,52,52,52	0
57	MG	CA	1783	1/1	0.87	0.37	8.26	105,105,105,105	0
57	MG	AA	1636	1/1	0.96	0.51	8.19	74,74,74,74	0
57	MG	BA	3268	1/1	0.91	0.30	8.14	34,34,34,34	0
57	MG	BA	3266	1/1	0.89	0.32	7.99	50,50,50,50	0
57	MG	DA	3297	1/1	0.82	0.45	7.95	71,71,71,71	0
57	MG	BA	3021	1/1	0.98	0.36	7.74	30,30,30,30	0
57	MG	BA	3409	1/1	0.91	0.35	7.69	20,20,20,20	0
57	MG	BA	3060	1/1	0.95	0.38	7.61	1,1,1,1	0
57	MG	DA	3056	1/1	0.98	0.34	7.58	49,49,49,49	0
57	MG	DA	3023	1/1	0.97	0.33	7.48	20,20,20,20	0
57	MG	BA	3194	1/1	0.86	0.27	7.37	42,42,42,42	0
57	MG	AA	1706	1/1	0.73	0.44	7.33	108,108,108,108	0
57	MG	CA	1709	1/1	0.73	0.35	7.31	73,73,73,73	0
57	MG	AA	1666	1/1	0.70	0.42	7.24	93,93,93,93	0
57	MG	CA	1625	1/1	0.55	0.42	7.19	96,96,96,96	0
57	MG	BA	3381	1/1	0.97	0.39	7.13	29,29,29,29	0
57	MG	DA	3101	1/1	0.82	0.35	7.06	67,67,67,67	0
57	MG	BA	3118	1/1	0.88	0.24	6.99	68,68,68,68	0
57	MG	AA	1774	1/1	0.91	0.33	6.91	88,88,88,88	0
57	MG	DA	3121	1/1	0.87	0.40	6.76	83,83,83,83	0
57	MG	CA	1678	1/1	0.71	0.41	6.64	94,94,94,94	0
57	MG	AA	1773	1/1	0.75	0.37	6.63	72,72,72,72	0
57	MG	BA	3007	1/1	0.95	0.26	6.60	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1686	1/1	0.86	0.33	6.53	43,43,43,43	0
57	MG	DA	3047	1/1	0.88	0.34	6.40	28,28,28,28	0
57	MG	DA	3024	1/1	0.96	0.21	6.30	49,49,49,49	0
57	MG	BB	203	1/1	0.95	0.48	6.26	14,14,14,14	1
57	MG	B2	602	1/1	0.94	0.51	6.16	55,55,55,55	0
57	MG	BA	3161	1/1	0.90	0.23	6.09	86,86,86,86	0
57	MG	BA	3058	1/1	0.98	0.38	6.04	19,19,19,19	0
57	MG	DA	3231	1/1	0.95	0.35	5.82	31,31,31,31	0
57	MG	BA	3082	1/1	0.95	0.30	5.79	37,37,37,37	0
57	MG	BA	3255	1/1	0.90	0.32	5.72	37,37,37,37	0
57	MG	BA	3046	1/1	0.98	0.29	5.70	4,4,4,4	0
57	MG	DA	3235	1/1	0.96	0.29	5.57	30,30,30,30	0
57	MG	DA	3005	1/1	0.94	0.27	5.50	52,52,52,52	0
57	MG	DA	3010	1/1	0.99	0.35	5.50	18,18,18,18	0
57	MG	BA	3097	1/1	0.98	0.28	5.43	7,7,7,7	0
57	MG	DF	302	1/1	0.60	0.57	5.41	91,91,91,91	0
57	MG	BN	201	1/1	0.79	0.62	5.38	64,64,64,64	0
57	MG	DA	3144	1/1	0.83	0.38	5.32	63,63,63,63	1
57	MG	DA	3341	1/1	0.83	0.27	5.27	54,54,54,54	0
57	MG	DA	3013	1/1	0.96	0.36	5.24	31,31,31,31	0
57	MG	DA	3022	1/1	0.98	0.33	5.19	34,34,34,34	0
57	MG	BA	3178	1/1	0.96	0.24	5.19	24,24,24,24	0
57	MG	DA	3074	1/1	0.95	0.28	5.16	26,26,26,26	0
57	MG	D7	101	1/1	0.65	0.40	5.05	73,73,73,73	0
57	MG	DA	3270	1/1	0.75	0.28	5.04	87,87,87,87	0
57	MG	CA	1609	1/1	0.73	0.65	5.02	61,61,61,61	0
57	MG	BA	3120	1/1	0.88	0.32	5.00	90,90,90,90	0
57	MG	DA	3061	1/1	0.95	0.28	4.99	30,30,30,30	0
57	MG	DA	3399	1/1	0.59	0.29	4.92	119,119,119,119	0
57	MG	BA	3143	1/1	0.78	0.31	4.81	49,49,49,49	1
57	MG	BA	3239	1/1	0.99	0.31	4.81	20,20,20,20	0
57	MG	DA	3146	1/1	0.86	0.31	4.72	55,55,55,55	0
57	MG	AA	1739	1/1	0.90	0.29	4.68	115,115,115,115	0
57	MG	BA	3215	1/1	0.90	0.31	4.62	33,33,33,33	0
57	MG	DA	3119	1/1	0.76	0.36	4.60	86,86,86,86	0
57	MG	DA	3378	1/1	0.96	0.31	4.54	72,72,72,72	0
57	MG	DA	3178	1/1	0.86	0.21	4.52	88,88,88,88	0
57	MG	AA	1712	1/1	0.86	0.30	4.47	61,61,61,61	0
57	MG	DB	212	1/1	0.92	0.50	4.42	99,99,99,99	1
57	MG	DA	3036	1/1	0.95	0.32	4.38	32,32,32,32	0
57	MG	BA	3200	1/1	0.78	0.25	4.34	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3113	1/1	0.91	0.24	4.28	3,3,3,3	0
57	MG	BA	3092	1/1	0.96	0.27	4.24	28,28,28,28	0
57	MG	BA	3190	1/1	0.94	0.29	4.21	51,51,51,51	0
57	MG	BA	3307	1/1	0.99	0.30	4.17	23,23,23,23	0
57	MG	BA	3366	1/1	0.82	0.45	4.16	112,112,112,112	0
57	MG	BA	3039	1/1	0.95	0.27	4.10	14,14,14,14	0
57	MG	BB	212	1/1	0.92	0.23	4.07	31,31,31,31	1
57	MG	DA	3172	1/1	0.82	0.27	4.02	58,58,58,58	0
57	MG	BA	3300	1/1	0.97	0.31	4.02	3,3,3,3	0
57	MG	BA	3272	1/1	0.96	0.27	4.00	46,46,46,46	0
57	MG	CA	1636	1/1	0.97	0.49	3.94	50,50,50,50	0
57	MG	AA	1630	1/1	0.95	0.23	3.88	55,55,55,55	0
57	MG	AA	1788	1/1	0.96	0.23	3.86	73,73,73,73	0
57	MG	BA	3382	1/1	0.89	0.23	3.86	31,31,31,31	0
57	MG	DA	3258	1/1	0.95	0.38	3.81	37,37,37,37	0
57	MG	DA	3274	1/1	0.95	0.30	3.74	60,60,60,60	0
57	MG	CA	1785	1/1	0.85	0.30	3.63	95,95,95,95	0
57	MG	BA	3035	1/1	0.99	0.26	3.63	2,2,2,2	0
58	PAR	CA	1800	42/42	0.90	0.25	3.56	86,91,109,113	0
57	MG	DA	3130	1/1	0.96	0.33	3.56	41,41,41,41	0
57	MG	BX	102	1/1	0.95	0.32	3.51	104,104,104,104	0
57	MG	BA	3256	1/1	0.98	0.34	3.50	11,11,11,11	0
57	MG	DA	3018	1/1	0.96	0.31	3.41	31,31,31,31	0
57	MG	DA	3171	1/1	0.98	0.23	3.33	43,43,43,43	0
57	MG	BA	3028	1/1	0.98	0.22	3.24	12,12,12,12	0
57	MG	AA	1786	1/1	0.91	0.27	3.20	108,108,108,108	0
57	MG	BA	3403	1/1	0.88	0.22	3.19	65,65,65,65	0
57	MG	AA	1688	1/1	0.96	0.25	3.17	35,35,35,35	0
57	MG	DA	3083	1/1	0.98	0.29	3.00	33,33,33,33	0
57	MG	D2	601	1/1	0.84	0.30	2.92	35,35,35,35	1
57	MG	DA	3283	1/1	0.89	0.26	2.90	77,77,77,77	0
57	MG	BB	205	1/1	0.98	0.20	2.88	25,25,25,25	0
57	MG	BB	204	1/1	0.92	0.25	2.88	106,106,106,106	0
57	MG	BA	3375	1/1	0.90	0.22	2.87	21,21,21,21	1
57	MG	BA	3379	1/1	0.91	0.23	2.84	36,36,36,36	0
57	MG	DA	3293	1/1	0.49	0.24	2.77	74,74,74,74	0
57	MG	CA	1638	1/1	0.90	0.27	2.77	42,42,42,42	0
57	MG	DA	3217	1/1	0.78	0.26	2.75	62,62,62,62	0
57	MG	DA	3184	1/1	0.94	0.29	2.73	36,36,36,36	0
57	MG	DA	3093	1/1	0.95	0.23	2.59	36,36,36,36	0
57	MG	DA	3165	1/1	0.89	0.20	2.58	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3001	1/1	0.86	0.22	2.52	33,33,33,33	0
57	MG	BA	3129	1/1	0.99	0.27	2.50	10,10,10,10	0
57	MG	B0	101	1/1	0.82	0.31	2.46	50,50,50,50	0
57	MG	DA	3364	1/1	1.00	0.22	2.42	52,52,52,52	0
57	MG	B7	101	1/1	0.93	0.30	2.35	45,45,45,45	1
57	MG	BA	3169	1/1	0.99	0.23	2.29	18,18,18,18	0
57	MG	BO	201	1/1	0.89	0.23	2.24	29,29,29,29	0
57	MG	DD	301	1/1	0.94	0.26	2.20	38,38,38,38	0
57	MG	DO	201	1/1	0.87	0.37	2.18	85,85,85,85	0
58	PAR	AA	1799	42/42	0.94	0.23	2.18	60,65,83,87	0
57	MG	BA	3110	1/1	0.82	0.21	2.14	44,44,44,44	0
57	MG	DA	3281	1/1	0.66	0.23	1.96	52,52,52,52	0
57	MG	DA	3395	1/1	0.93	0.41	1.96	49,49,49,49	0
57	MG	DA	3303	1/1	0.97	0.30	1.87	30,30,30,30	0
57	MG	BA	3188	1/1	0.83	0.24	1.81	64,64,64,64	0
57	MG	DA	3114	1/1	0.81	0.28	1.78	29,29,29,29	0
57	MG	BA	3185	1/1	0.98	0.22	1.77	1,1,1,1	0
57	MG	AA	1777	1/1	0.73	0.29	1.72	141,141,141,141	0
57	MG	BA	3145	1/1	0.95	0.21	1.69	27,27,27,27	0
57	MG	AA	1638	1/1	0.96	0.23	1.64	36,36,36,36	0
57	MG	DA	3294	1/1	0.82	0.26	1.58	54,54,54,54	0
57	MG	DA	3200	1/1	0.91	0.20	1.54	59,59,59,59	0
57	MG	DA	3110	1/1	0.95	0.19	1.51	41,41,41,41	0
57	MG	CW	103	1/1	0.97	0.26	1.48	87,87,87,87	0
57	MG	DA	3115	1/1	0.94	0.26	1.48	22,22,22,22	0
57	MG	AA	1608	1/1	0.98	0.20	1.45	46,46,46,46	0
57	MG	CA	1692	1/1	0.90	0.19	1.40	59,59,59,59	0
57	MG	BA	3163	1/1	0.71	0.18	1.39	42,42,42,42	0
57	MG	BA	3137	1/1	0.89	0.18	1.38	33,33,33,33	0
57	MG	DA	3026	1/1	0.95	0.24	1.32	19,19,19,19	0
57	MG	CA	1620	1/1	0.94	0.28	1.30	59,59,59,59	0
57	MG	BA	3079	1/1	0.97	0.21	1.26	31,31,31,31	0
57	MG	CA	1626	1/1	0.95	0.22	1.24	34,34,34,34	0
57	MG	DA	3273	1/1	0.73	0.19	1.24	59,59,59,59	0
57	MG	BD	301	1/1	0.99	0.21	1.19	16,16,16,16	0
57	MG	AA	1710	1/1	0.83	0.27	1.12	71,71,71,71	0
57	MG	BA	3034	1/1	0.96	0.19	1.12	40,40,40,40	0
57	MG	CA	1685	1/1	0.74	0.20	1.10	62,62,62,62	0
57	MG	CA	1704	1/1	0.91	0.34	1.07	114,114,114,114	0
57	MG	BA	3087	1/1	0.99	0.21	1.06	10,10,10,10	0
57	MG	DA	3040	1/1	0.94	0.20	1.01	25,25,25,25	0
57	MG	BA	3173	1/1	0.97	0.21	1.00	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3204	1/1	0.94	0.24	1.00	33,33,33,33	0
57	MG	DA	3175	1/1	0.87	0.20	0.93	63,63,63,63	0
57	MG	DA	3247	1/1	0.50	0.20	0.93	61,61,61,61	0
57	MG	BA	3182	1/1	0.98	0.23	0.90	62,62,62,62	0
57	MG	D2	603	1/1	0.96	0.29	0.88	95,95,95,95	0
57	MG	BA	3192	1/1	0.92	0.17	0.88	21,21,21,21	0
57	MG	BA	3076	1/1	0.96	0.20	0.82	25,25,25,25	0
57	MG	CA	1675	1/1	0.91	0.19	0.80	92,92,92,92	0
57	MG	BA	3396	1/1	0.97	0.28	0.78	11,11,11,11	0
57	MG	BA	3172	1/1	0.92	0.21	0.77	52,52,52,52	0
57	MG	DA	3073	1/1	0.88	0.19	0.75	36,36,36,36	0
57	MG	DA	3195	1/1	0.84	0.16	0.73	89,89,89,89	0
57	MG	DA	3396	1/1	0.91	0.20	0.73	145,145,145,145	0
57	MG	DA	3267	1/1	0.69	0.17	0.70	71,71,71,71	0
57	MG	DA	3322	1/1	0.97	0.22	0.66	62,62,62,62	0
57	MG	CV	101	1/1	0.99	0.21	0.63	20,20,20,20	0
57	MG	DA	3365	1/1	0.83	0.25	0.62	19,19,19,19	0
57	MG	CA	1713	1/1	0.61	0.17	0.50	73,73,73,73	0
57	MG	DA	3100	1/1	0.94	0.20	0.46	63,63,63,63	0
57	MG	BA	3193	1/1	0.92	0.18	0.44	40,40,40,40	0
57	MG	BA	3341	1/1	0.91	0.20	0.40	40,40,40,40	0
57	MG	BA	3236	1/1	0.90	0.19	0.36	44,44,44,44	0
57	MG	DA	3191	1/1	0.94	0.23	0.26	41,41,41,41	0
57	MG	DA	3075	1/1	0.97	0.21	0.24	37,37,37,37	0
57	MG	CA	1619	1/1	0.98	0.18	0.15	80,80,80,80	0
57	MG	CA	1608	1/1	0.93	0.19	0.11	39,39,39,39	0
57	MG	BA	3108	1/1	0.95	0.19	0.10	4,4,4,4	0
57	MG	DA	3078	1/1	0.97	0.21	0.09	20,20,20,20	0
57	MG	CA	1612	1/1	0.72	0.16	0.08	91,91,91,91	0
57	MG	DA	3001	1/1	0.87	0.18	0.04	42,42,42,42	0
57	MG	AN	101	1/1	0.86	0.24	-0.00	50,50,50,50	0
57	MG	BA	3367	1/1	0.81	0.37	-0.00	1,1,1,1	1
57	MG	BA	3391	1/1	0.99	0.20	-0.02	37,37,37,37	0
57	MG	AA	1674	1/1	0.97	0.16	-0.07	42,42,42,42	0
57	MG	BA	3265	1/1	0.92	0.18	-0.13	30,30,30,30	0
57	MG	BA	3400	1/1	0.93	0.15	-0.15	47,47,47,47	0
57	MG	DA	3209	1/1	0.97	0.14	-0.16	73,73,73,73	0
57	MG	BD	302	1/1	0.98	0.22	-0.16	22,22,22,22	0
57	MG	BA	3232	1/1	0.99	0.20	-0.17	27,27,27,27	0
57	MG	BA	3164	1/1	0.90	0.18	-0.19	56,56,56,56	0
57	MG	BA	3084	1/1	0.99	0.18	-0.19	12,12,12,12	0
57	MG	BA	3262	1/1	0.92	0.15	-0.23	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3365	1/1	0.91	0.19	-0.24	1,1,1,1	0
57	MG	BA	3078	1/1	0.99	0.18	-0.24	13,13,13,13	0
57	MG	CA	1603	1/1	0.89	0.20	-0.24	68,68,68,68	0
59	ZN	AD	302	1/1	0.99	0.24	-0.30	55,55,55,55	0
57	MG	DA	3333	1/1	0.97	0.16	-0.31	108,108,108,108	0
57	MG	DA	3302	1/1	0.96	0.19	-0.32	43,43,43,43	1
57	MG	DA	3309	1/1	0.98	0.21	-0.32	47,47,47,47	0
57	MG	BA	3051	1/1	0.99	0.17	-0.37	5,5,5,5	0
57	MG	DA	3180	1/1	0.94	0.17	-0.38	35,35,35,35	0
57	MG	AA	1684	1/1	0.85	0.19	-0.43	74,74,74,74	0
57	MG	DA	3308	1/1	0.93	0.17	-0.44	53,53,53,53	0
57	MG	CA	1790	1/1	0.98	0.18	-0.49	48,48,48,48	0
59	ZN	AN	102	1/1	0.99	0.18	-0.53	109,109,109,109	0
57	MG	BF	301	1/1	0.91	0.20	-0.58	41,41,41,41	0
57	MG	BA	3017	1/1	0.94	0.19	-0.58	9,9,9,9	0
57	MG	CA	1776	1/1	0.88	0.18	-0.59	46,46,46,46	0
57	MG	BA	3198	1/1	0.97	0.17	-0.60	51,51,51,51	0
57	MG	DA	3401	1/1	0.90	0.15	-0.62	57,57,57,57	0
57	MG	BA	3109	1/1	0.96	0.18	-0.65	39,39,39,39	0
57	MG	DA	3242	1/1	0.96	0.19	-0.69	18,18,18,18	0
59	ZN	CD	301	1/1	0.99	0.23	-0.74	55,55,55,55	0
57	MG	CA	1711	1/1	0.73	0.16	-0.75	74,74,74,74	0
57	MG	DA	3035	1/1	0.88	0.11	-0.76	55,55,55,55	0
57	MG	DA	3014	1/1	0.98	0.18	-0.77	31,31,31,31	0
57	MG	DA	3065	1/1	0.98	0.18	-0.78	17,17,17,17	0
57	MG	DA	3390	1/1	0.99	0.17	-0.80	48,48,48,48	0
57	MG	AA	1626	1/1	0.95	0.17	-0.83	37,37,37,37	0
57	MG	DA	3234	1/1	0.99	0.15	-1.01	22,22,22,22	0
57	MG	DA	3264	1/1	0.60	0.13	-1.02	96,96,96,96	0
57	MG	BA	3147	1/1	0.95	0.17	-1.02	26,26,26,26	0
57	MG	AA	1703	1/1	0.89	0.14	-1.09	38,38,38,38	0
57	MG	DA	3416	1/1	0.76	0.12	-1.09	81,81,81,81	0
57	MG	CA	1714	1/1	0.85	0.12	-1.15	62,62,62,62	0
57	MG	CN	101	1/1	0.91	0.15	-1.16	57,57,57,57	0
57	MG	BA	3189	1/1	0.98	0.17	-1.19	8,8,8,8	0
59	ZN	CN	102	1/1	0.99	0.12	-1.20	120,120,120,120	0
57	MG	CE	201	1/1	0.91	0.15	-1.30	90,90,90,90	0
57	MG	AA	1699	1/1	0.91	0.15	-1.31	78,78,78,78	0
57	MG	CA	1699	1/1	0.93	0.14	-1.35	50,50,50,50	0
57	MG	CA	1697	1/1	0.92	0.16	-1.36	72,72,72,72	0
57	MG	CA	1607	1/1	0.96	0.16	-1.38	30,30,30,30	0
57	MG	CA	1792	1/1	0.92	0.12	-1.50	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1790	1/1	0.85	0.13	-1.52	63,63,63,63	0
57	MG	CA	1659	1/1	0.94	0.18	-1.55	42,42,42,42	0
57	MG	AA	1604	1/1	0.96	0.14	-1.55	55,55,55,55	0
57	MG	AA	1692	1/1	0.99	0.13	-1.80	72,72,72,72	0
57	MG	DA	3206	1/1	0.95	0.20	-1.86	33,33,33,33	0
57	MG	BA	3042	1/1	0.99	0.14	-1.87	36,36,36,36	0
57	MG	BA	3162	1/1	0.70	0.12	-1.92	79,79,79,79	0
57	MG	DA	3085	1/1	0.93	0.14	-1.94	32,32,32,32	0
57	MG	DA	3077	1/1	0.98	0.13	-1.95	29,29,29,29	0
57	MG	CI	201	1/1	0.95	0.18	-1.96	75,75,75,75	0
57	MG	CA	1779	1/1	0.82	0.26	-2.03	115,115,115,115	0
57	MG	BA	3420	1/1	0.49	0.12	-2.04	78,78,78,78	0
57	MG	AA	1620	1/1	0.90	0.15	-2.07	54,54,54,54	0
57	MG	AA	1658	1/1	0.92	0.19	-2.10	25,25,25,25	0
57	MG	DA	3080	1/1	0.93	0.14	-2.12	63,63,63,63	0
57	MG	BA	3361	1/1	0.92	0.13	-2.12	28,28,28,28	0
57	MG	DA	3381	1/1	0.90	0.14	-2.22	45,45,45,45	0
57	MG	BA	3165	1/1	0.98	0.14	-2.24	38,38,38,38	0
57	MG	DA	3257	1/1	0.92	0.14	-2.25	52,52,52,52	0
57	MG	BA	3073	1/1	0.98	0.15	-2.28	5,5,5,5	0
57	MG	BA	3156	1/1	0.91	0.12	-2.30	20,20,20,20	0
57	MG	DF	301	1/1	0.89	0.12	-2.38	56,56,56,56	0
57	MG	CA	1710	1/1	0.96	0.07	-2.43	54,54,54,54	0
57	MG	CA	1628	1/1	0.97	0.08	-2.45	81,81,81,81	0
59	ZN	D9	101	1/1	0.96	0.12	-2.45	136,136,136,136	0
57	MG	DA	3419	1/1	0.65	0.11	-2.46	115,115,115,115	0
57	MG	BA	3013	1/1	0.99	0.16	-2.47	7,7,7,7	0
57	MG	AA	1628	1/1	0.92	0.10	-2.48	37,37,37,37	0
57	MG	AA	1698	1/1	0.92	0.14	-2.61	42,42,42,42	0
57	MG	DB	205	1/1	0.88	0.12	-2.63	55,55,55,55	0
57	MG	BA	3364	1/1	1.00	0.17	-2.64	35,35,35,35	0
57	MG	CA	1670	1/1	0.98	0.11	-2.68	69,69,69,69	0
57	MG	BA	3054	1/1	0.99	0.15	-2.69	1,1,1,1	0
59	ZN	B9	101	1/1	0.99	0.04	-2.70	94,94,94,94	0
57	MG	BA	3306	1/1	0.96	0.11	-2.73	18,18,18,18	0
57	MG	BA	3201	1/1	0.90	0.11	-2.78	35,35,35,35	0
57	MG	CA	1684	1/1	0.78	0.10	-2.80	94,94,94,94	0
57	MG	AA	1691	1/1	0.98	0.11	-2.82	27,27,27,27	0
57	MG	BA	3245	1/1	0.94	0.12	-2.86	42,42,42,42	0
57	MG	AV	101	1/1	0.99	0.14	-2.86	36,36,36,36	0
57	MG	BA	3292	1/1	0.95	0.18	-2.89	23,23,23,23	0
57	MG	BA	3240	1/1	0.95	0.12	-3.02	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3194	1/1	0.90	0.12	-3.03	59,59,59,59	0
57	MG	BA	3414	1/1	0.98	0.10	-3.09	60,60,60,60	0
57	MG	BA	3402	1/1	0.91	0.11	-3.10	63,63,63,63	0
57	MG	DA	3374	1/1	0.98	0.12	-3.11	37,37,37,37	1
57	MG	DA	3079	1/1	0.98	0.14	-3.19	37,37,37,37	0
57	MG	BA	3074	1/1	0.97	0.17	-3.27	24,24,24,24	0
57	MG	AA	1662	1/1	0.91	0.08	-3.36	95,95,95,95	0
57	MG	AA	1709	1/1	0.95	0.06	-3.66	49,49,49,49	0
57	MG	AA	1637	1/1	0.98	0.11	-3.79	58,58,58,58	0
57	MG	DA	3203	1/1	0.96	0.08	-3.84	56,56,56,56	0
57	MG	CA	1689	1/1	0.98	0.16	-4.07	40,40,40,40	0
57	MG	DA	3174	1/1	0.96	0.09	-4.24	53,53,53,53	0
57	MG	CA	1637	1/1	0.94	0.12	-4.56	83,83,83,83	0
57	MG	CA	1650	1/1	0.98	0.11	-4.58	89,89,89,89	1
57	MG	DA	3117	1/1	0.98	0.09	-4.65	16,16,16,16	0
57	MG	AA	1787	1/1	0.99	0.12	-4.88	41,41,41,41	1
57	MG	DA	3268	1/1	0.99	0.08	-4.95	41,41,41,41	0
57	MG	DA	3052	1/1	0.99	0.12	-4.98	30,30,30,30	0
57	MG	CA	1693	1/1	0.93	0.12	-5.24	87,87,87,87	0
57	MG	CA	1663	1/1	0.96	0.07	-5.45	53,53,53,53	0
57	MG	BA	3072	1/1	0.97	0.10	-6.29	3,3,3,3	0
57	MG	BA	3077	1/1	0.99	0.15	-6.48	1,1,1,1	0
57	MG	BA	3397	1/1	0.99	0.10	-10.69	73,73,73,73	0
57	MG	DA	3289	1/1	0.61	1.12	-	74,74,74,74	0
57	MG	BA	3179	1/1	0.66	1.55	-	117,117,117,117	0
57	MG	CA	1775	1/1	0.81	0.22	-	79,79,79,79	0
57	MG	BA	3318	1/1	0.87	0.36	-	70,70,70,70	1
57	MG	DA	3298	1/1	0.93	0.17	-	56,56,56,56	0
57	MG	DA	3059	1/1	0.76	0.37	-	46,46,46,46	0
57	MG	BA	3102	1/1	0.95	0.38	-	13,13,13,13	0
57	MG	DA	3019	1/1	0.83	0.50	-	29,29,29,29	0
57	MG	CA	1740	1/1	0.80	0.44	-	61,61,61,61	1
57	MG	BA	3348	1/1	0.97	0.20	-	79,79,79,79	0
57	MG	CA	1761	1/1	0.54	0.61	-	74,74,74,74	0
57	MG	BA	3372	1/1	0.96	0.53	-	57,57,57,57	1
57	MG	BA	3154	1/1	0.96	0.33	-	13,13,13,13	0
57	MG	CA	1703	1/1	0.97	0.36	-	87,87,87,87	0
57	MG	BA	3224	1/1	0.76	0.34	-	91,91,91,91	0
57	MG	DA	3095	1/1	0.97	0.10	-	37,37,37,37	0
57	MG	CA	1795	1/1	0.67	0.59	-	78,78,78,78	0
57	MG	AA	1776	1/1	0.53	0.28	-	103,103,103,103	0
57	MG	AA	1642	1/1	0.98	0.19	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3358	1/1	0.98	0.24	-	24,24,24,24	0
57	MG	CA	1705	1/1	0.61	0.40	-	150,150,150,150	0
57	MG	DA	3379	1/1	0.72	0.55	-	105,105,105,105	0
57	MG	D2	602	1/1	0.75	0.32	-	99,99,99,99	0
57	MG	CA	1731	1/1	0.74	0.30	-	85,85,85,85	0
57	MG	AV	104	1/1	0.24	0.41	-	127,127,127,127	0
57	MG	BA	3334	1/1	0.89	0.35	-	79,79,79,79	0
57	MG	AA	1686	1/1	0.96	0.57	-	104,104,104,104	0
57	MG	BA	3353	1/1	0.78	0.46	-	79,79,79,79	0
57	MG	BA	3276	1/1	0.95	0.30	-	49,49,49,49	0
57	MG	CA	1610	1/1	0.91	0.10	-	88,88,88,88	0
57	MG	DA	3225	1/1	0.83	0.57	-	71,71,71,71	0
57	MG	BA	3125	1/1	0.92	0.26	-	62,62,62,62	0
57	MG	CA	1698	1/1	0.73	0.12	-	86,86,86,86	0
57	MG	DA	3249	1/1	0.86	0.37	-	60,60,60,60	0
57	MG	CA	1664	1/1	0.83	0.54	-	53,53,53,53	0
57	MG	AA	1716	1/1	0.93	0.18	-	86,86,86,86	0
57	MG	DA	3168	1/1	0.98	0.20	-	36,36,36,36	0
57	MG	BA	3100	1/1	0.82	0.47	-	49,49,49,49	0
57	MG	DA	3102	1/1	0.94	0.46	-	129,129,129,129	1
57	MG	CA	1778	1/1	0.84	0.36	-	66,66,66,66	0
57	MG	BA	3130	1/1	0.99	0.19	-	8,8,8,8	0
57	MG	DA	3043	1/1	0.97	0.19	-	51,51,51,51	0
57	MG	DA	3091	1/1	0.97	0.30	-	39,39,39,39	0
57	MG	BA	3411	1/1	0.97	0.12	-	51,51,51,51	1
57	MG	BA	3038	1/1	0.96	0.15	-	41,41,41,41	0
57	MG	AA	1758	1/1	0.82	0.30	-	97,97,97,97	0
57	MG	CA	1797	1/1	0.95	0.10	-	120,120,120,120	0
57	MG	AA	1737	1/1	0.21	1.74	-	136,136,136,136	0
57	MG	DA	3373	1/1	0.76	0.18	-	98,98,98,98	0
57	MG	CA	1666	1/1	0.73	0.67	-	87,87,87,87	0
57	MG	BA	3183	1/1	0.98	0.32	-	20,20,20,20	0
57	MG	CA	1677	1/1	0.87	0.14	-	48,48,48,48	0
57	MG	DA	3337	1/1	0.94	0.10	-	76,76,76,76	0
57	MG	BA	3324	1/1	0.71	0.44	-	39,39,39,39	1
57	MG	BA	3222	1/1	0.99	0.15	-	84,84,84,84	0
57	MG	DA	3252	1/1	0.87	0.12	-	95,95,95,95	0
57	MG	AA	1700	1/1	0.79	0.63	-	79,79,79,79	0
57	MG	DA	3243	1/1	0.79	0.73	-	76,76,76,76	0
57	MG	BA	3019	1/1	0.98	0.28	-	28,28,28,28	0
57	MG	BA	3212	1/1	0.84	0.35	-	88,88,88,88	0
57	MG	DA	3420	1/1	0.96	0.10	-	137,137,137,137	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DB	207	1/1	0.88	0.31	-	49,49,49,49	1
57	MG	BA	3030	1/1	0.99	0.23	-	18,18,18,18	0
57	MG	BA	3088	1/1	0.96	0.23	-	21,21,21,21	0
57	MG	AA	1618	1/1	0.93	0.32	-	38,38,38,38	0
57	MG	DA	3407	1/1	0.93	0.20	-	45,45,45,45	0
57	MG	AA	1685	1/1	0.91	0.23	-	42,42,42,42	0
57	MG	DA	3237	1/1	0.96	0.17	-	156,156,156,156	0
57	MG	BA	3246	1/1	0.88	0.21	-	74,74,74,74	0
57	MG	DA	3370	1/1	0.60	0.47	-	92,92,92,92	0
57	MG	BA	3006	1/1	0.80	0.91	-	66,66,66,66	0
57	MG	BA	3191	1/1	0.98	0.19	-	14,14,14,14	0
57	MG	BA	3308	1/1	0.96	0.21	-	114,114,114,114	1
57	MG	BA	3052	1/1	0.92	0.33	-	13,13,13,13	0
57	MG	CA	1767	1/1	0.84	0.23	-	97,97,97,97	0
57	MG	DA	3037	1/1	0.98	0.22	-	45,45,45,45	0
57	MG	DA	3255	1/1	0.86	0.27	-	61,61,61,61	0
57	MG	AA	1728	1/1	0.90	0.30	-	67,67,67,67	0
57	MG	CA	1672	1/1	0.93	0.23	-	59,59,59,59	0
57	MG	BA	3196	1/1	0.41	0.58	-	130,130,130,130	1
57	MG	DA	3138	1/1	0.82	0.28	-	68,68,68,68	0
57	MG	DA	3389	1/1	0.76	0.94	-	113,113,113,113	0
57	MG	DA	3307	1/1	0.78	0.44	-	51,51,51,51	0
57	MG	BA	3214	1/1	0.90	0.50	-	83,83,83,83	0
57	MG	BA	3297	1/1	0.74	0.75	-	77,77,77,77	0
57	MG	CA	1781	1/1	0.98	0.08	-	58,58,58,58	0
57	MG	CW	102	1/1	0.82	0.10	-	112,112,112,112	0
57	MG	DA	3320	1/1	0.94	0.30	-	34,34,34,34	1
57	MG	CA	1661	1/1	0.87	0.59	-	56,56,56,56	0
57	MG	DA	3363	1/1	0.99	0.14	-	68,68,68,68	0
57	MG	AA	1770	1/1	0.81	0.39	-	163,163,163,163	0
57	MG	DA	3233	1/1	0.92	0.45	-	36,36,36,36	0
57	MG	AA	1652	1/1	0.96	0.31	-	82,82,82,82	0
57	MG	DE	301	1/1	0.95	0.27	-	39,39,39,39	0
57	MG	AA	1690	1/1	0.77	0.38	-	81,81,81,81	0
57	MG	BA	3322	1/1	0.84	0.67	-	42,42,42,42	1
57	MG	DA	3062	1/1	0.98	0.32	-	33,33,33,33	0
57	MG	DA	3183	1/1	0.90	0.29	-	96,96,96,96	0
57	MG	BA	3138	1/1	0.66	1.02	-	124,124,124,124	0
57	MG	DA	3154	1/1	0.83	0.32	-	60,60,60,60	0
57	MG	AA	1747	1/1	0.97	0.13	-	135,135,135,135	0
57	MG	DA	3367	1/1	0.66	0.51	-	108,108,108,108	0
57	MG	AA	1725	1/1	0.97	0.13	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3267	1/1	0.70	0.41	-	56,56,56,56	0
57	MG	BV	201	1/1	0.96	0.26	-	64,64,64,64	0
57	MG	DA	3385	1/1	0.96	0.26	-	79,79,79,79	0
57	MG	CA	1727	1/1	0.64	0.82	-	139,139,139,139	0
57	MG	BB	214	1/1	0.51	0.58	-	75,75,75,75	1
57	MG	AA	1656	1/1	0.86	0.75	-	97,97,97,97	0
57	MG	DA	3398	1/1	0.83	0.61	-	86,86,86,86	0
57	MG	DA	3132	1/1	0.87	0.34	-	41,41,41,41	0
57	MG	CA	1736	1/1	0.83	0.53	-	73,73,73,73	0
57	MG	AA	1795	1/1	0.79	0.51	-	128,128,128,128	0
57	MG	CA	1788	1/1	0.82	0.24	-	75,75,75,75	0
57	MG	BA	3059	1/1	0.97	0.24	-	9,9,9,9	0
57	MG	AA	1668	1/1	0.84	0.29	-	51,51,51,51	0
57	MG	BA	3416	1/1	0.65	0.30	-	93,93,93,93	0
57	MG	DA	3221	1/1	0.85	0.52	-	50,50,50,50	0
57	MG	DA	3096	1/1	0.94	0.23	-	24,24,24,24	0
57	MG	DX	103	1/1	0.50	0.49	-	102,102,102,102	0
57	MG	DA	3033	1/1	0.78	0.40	-	70,70,70,70	0
57	MG	BA	3345	1/1	0.74	0.41	-	69,69,69,69	1
57	MG	CA	1762	1/1	0.91	0.41	-	84,84,84,84	0
57	MG	BB	213	1/1	0.85	0.32	-	87,87,87,87	0
57	MG	AV	105	1/1	0.82	0.77	-	89,89,89,89	0
57	MG	DA	3108	1/1	0.60	0.86	-	83,83,83,83	0
57	MG	BB	211	1/1	0.97	0.16	-	119,119,119,119	0
57	MG	BA	3040	1/1	0.98	0.33	-	20,20,20,20	0
57	MG	AA	1729	1/1	0.88	0.45	-	69,69,69,69	0
57	MG	AA	1727	1/1	0.80	0.44	-	54,54,54,54	1
57	MG	BA	3312	1/1	0.44	0.36	-	102,102,102,102	0
57	MG	CA	1752	1/1	0.71	0.19	-	112,112,112,112	1
57	MG	AA	1621	1/1	0.79	0.26	-	50,50,50,50	0
57	MG	DA	3342	1/1	0.80	0.27	-	90,90,90,90	0
57	MG	CA	1769	1/1	0.93	0.29	-	27,27,27,27	0
57	MG	DA	3141	1/1	0.88	0.43	-	67,67,67,67	0
57	MG	DA	3016	1/1	0.96	0.24	-	51,51,51,51	0
57	MG	BA	3380	1/1	0.90	0.68	-	54,54,54,54	0
57	MG	AA	1744	1/1	0.52	0.55	-	84,84,84,84	0
57	MG	CA	1772	1/1	0.94	0.24	-	77,77,77,77	0
57	MG	BA	3362	1/1	0.98	0.18	-	85,85,85,85	0
57	MG	DA	3272	1/1	0.87	0.53	-	108,108,108,108	0
57	MG	CA	1646	1/1	0.81	0.20	-	81,81,81,81	0
57	MG	AA	1743	1/1	0.51	0.61	-	86,86,86,86	0
57	MG	BA	3044	1/1	0.98	0.31	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1676	1/1	0.68	0.45	-	71,71,71,71	0
57	MG	BA	3104	1/1	0.95	0.29	-	20,20,20,20	0
57	MG	CA	1729	1/1	0.78	0.20	-	70,70,70,70	1
57	MG	DA	3123	1/1	0.85	0.40	-	89,89,89,89	0
57	MG	CA	1679	1/1	0.98	0.12	-	86,86,86,86	0
57	MG	CA	1702	1/1	0.88	0.39	-	66,66,66,66	0
57	MG	BA	3389	1/1	0.86	0.35	-	62,62,62,62	0
57	MG	DA	3008	1/1	0.93	0.26	-	36,36,36,36	0
57	MG	DA	3328	1/1	0.73	0.54	-	50,50,50,50	0
57	MG	CA	1717	1/1	0.92	0.12	-	82,82,82,82	0
57	MG	CA	1753	1/1	0.85	0.35	-	130,130,130,130	1
57	MG	BA	3220	1/1	0.85	0.49	-	95,95,95,95	0
57	MG	DA	3021	1/1	0.89	0.17	-	35,35,35,35	0
57	MG	BA	3106	1/1	0.97	0.28	-	20,20,20,20	0
57	MG	CA	1687	1/1	0.88	0.44	-	84,84,84,84	0
57	MG	DA	3404	1/1	0.98	0.07	-	97,97,97,97	1
57	MG	AA	1625	1/1	0.71	0.46	-	65,65,65,65	0
57	MG	BA	3261	1/1	0.95	0.56	-	23,23,23,23	0
57	MG	AE	201	1/1	0.93	0.10	-	101,101,101,101	0
57	MG	DA	3384	1/1	0.93	0.23	-	115,115,115,115	0
57	MG	AA	1683	1/1	0.71	0.24	-	101,101,101,101	0
57	MG	DA	3167	1/1	0.96	0.13	-	37,37,37,37	0
57	MG	CA	1618	1/1	0.94	0.28	-	53,53,53,53	0
57	MG	BA	3273	1/1	0.93	0.11	-	75,75,75,75	0
57	MG	AA	1671	1/1	0.90	0.29	-	73,73,73,73	0
57	MG	AW	108	1/1	0.23	0.23	-	82,82,82,82	1
57	MG	DA	3162	1/1	0.85	0.27	-	77,77,77,77	0
57	MG	CA	1793	1/1	0.63	0.33	-	100,100,100,100	1
57	MG	CA	1723	1/1	0.97	0.35	-	86,86,86,86	0
57	MG	BA	3061	1/1	0.98	0.31	-	10,10,10,10	0
57	MG	BA	3294	1/1	0.96	0.37	-	33,33,33,33	0
57	MG	BA	3211	1/1	0.83	0.17	-	40,40,40,40	0
57	MG	DA	3326	1/1	0.96	0.15	-	78,78,78,78	1
57	MG	DA	3411	1/1	0.92	0.08	-	46,46,46,46	0
57	MG	CA	1602	1/1	0.12	0.75	-	101,101,101,101	0
57	MG	AA	1629	1/1	0.95	0.28	-	62,62,62,62	0
57	MG	DA	3109	1/1	0.91	0.21	-	29,29,29,29	0
57	MG	DA	3111	1/1	0.79	1.59	-	111,111,111,111	0
57	MG	BA	3024	1/1	0.98	0.42	-	11,11,11,11	0
57	MG	DA	3265	1/1	0.89	0.27	-	71,71,71,71	0
57	MG	BA	3186	1/1	0.65	0.28	-	144,144,144,144	0
57	MG	BA	3399	1/1	0.79	0.58	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3384	1/1	0.86	0.35	-	53,53,53,53	0
57	MG	BA	3127	1/1	0.76	0.33	-	44,44,44,44	1
57	MG	DA	3064	1/1	0.97	0.16	-	32,32,32,32	0
57	MG	BA	3152	1/1	0.77	0.46	-	93,93,93,93	0
57	MG	DA	3250	1/1	0.98	0.40	-	63,63,63,63	1
57	MG	BA	3378	1/1	0.94	0.40	-	8,8,8,8	0
57	MG	BA	3421	1/1	0.98	0.15	-	110,110,110,110	1
57	MG	DA	3204	1/1	0.96	0.39	-	39,39,39,39	0
57	MG	DA	3245	1/1	0.96	0.20	-	69,69,69,69	0
57	MG	AA	1678	1/1	0.97	0.10	-	166,166,166,166	0
57	MG	AA	1606	1/1	0.97	0.12	-	34,34,34,34	0
57	MG	BA	3136	1/1	0.98	0.22	-	16,16,16,16	0
57	MG	CA	1701	1/1	0.50	0.99	-	93,93,93,93	0
57	MG	DA	3347	1/1	0.96	0.26	-	53,53,53,53	0
57	MG	CA	1671	1/1	0.81	0.30	-	58,58,58,58	0
57	MG	DA	3421	1/1	0.94	0.20	-	168,168,168,168	0
57	MG	DA	3084	1/1	0.96	0.42	-	44,44,44,44	0
57	MG	BA	3405	1/1	0.97	0.34	-	164,164,164,164	1
57	MG	DA	3215	1/1	0.95	0.08	-	68,68,68,68	1
57	MG	DA	3173	1/1	0.97	0.10	-	50,50,50,50	0
57	MG	CA	1724	1/1	0.96	0.20	-	80,80,80,80	0
57	MG	DA	3284	1/1	0.65	0.38	-	74,74,74,74	0
57	MG	DA	3213	1/1	0.84	0.37	-	89,89,89,89	0
57	MG	DA	3081	1/1	0.95	0.32	-	38,38,38,38	0
57	MG	DA	3038	1/1	0.99	0.21	-	49,49,49,49	0
57	MG	DA	3126	1/1	0.95	0.14	-	59,59,59,59	0
57	MG	AX	101	1/1	0.99	0.08	-	118,118,118,118	0
57	MG	DA	3263	1/1	0.89	0.85	-	69,69,69,69	0
57	MG	DA	3296	1/1	0.67	0.57	-	138,138,138,138	0
57	MG	BA	3338	1/1	0.85	0.35	-	52,52,52,52	0
57	MG	CA	1662	1/1	0.92	0.69	-	80,80,80,80	0
57	MG	BA	3203	1/1	0.96	0.13	-	30,30,30,30	0
57	MG	CA	1616	1/1	0.88	0.41	-	43,43,43,43	0
57	MG	DA	3057	1/1	0.88	0.26	-	31,31,31,31	0
57	MG	BA	3393	1/1	0.82	0.37	-	74,74,74,74	0
57	MG	BA	3157	1/1	0.94	0.38	-	74,74,74,74	0
57	MG	BA	3202	1/1	0.97	0.41	-	16,16,16,16	0
57	MG	CX	101	1/1	0.90	0.59	-	123,123,123,123	0
57	MG	DA	3400	1/1	0.70	0.34	-	77,77,77,77	0
57	MG	DA	3122	1/1	0.78	0.67	-	77,77,77,77	0
57	MG	BA	3144	1/1	0.94	0.22	-	58,58,58,58	0
57	MG	AA	1765	1/1	0.93	0.21	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3350	1/1	0.94	0.12	-	89,89,89,89	1
57	MG	BB	202	1/1	0.86	0.38	-	92,92,92,92	0
57	MG	AA	1651	1/1	0.54	0.68	-	70,70,70,70	0
57	MG	AA	1784	1/1	0.95	0.04	-	81,81,81,81	1
57	MG	BA	3244	1/1	0.86	0.36	-	88,88,88,88	0
57	MG	DA	3417	1/1	0.97	0.08	-	37,37,37,37	0
57	MG	AA	1697	1/1	0.96	0.30	-	78,78,78,78	0
57	MG	AA	1665	1/1	0.92	0.43	-	53,53,53,53	0
57	MG	CA	1780	1/1	0.74	0.55	-	32,32,32,32	1
57	MG	CA	1755	1/1	0.88	0.16	-	107,107,107,107	0
57	MG	BA	3168	1/1	0.94	0.49	-	87,87,87,87	0
57	MG	DA	3291	1/1	0.74	0.25	-	58,58,58,58	0
57	MG	AA	1768	1/1	0.94	0.43	-	71,71,71,71	0
57	MG	BA	3135	1/1	0.88	0.66	-	36,36,36,36	0
57	MG	CW	105	1/1	0.94	0.32	-	70,70,70,70	1
57	MG	BA	3350	1/1	0.98	0.18	-	81,81,81,81	1
57	MG	AA	1742	1/1	0.81	0.42	-	100,100,100,100	0
57	MG	CA	1760	1/1	0.92	0.32	-	145,145,145,145	0
57	MG	DA	3324	1/1	0.65	0.48	-	64,64,64,64	1
57	MG	AA	1741	1/1	0.46	0.73	-	124,124,124,124	0
57	MG	CA	1750	1/1	0.90	0.37	-	77,77,77,77	1
57	MG	AA	1657	1/1	0.28	0.56	-	121,121,121,121	0
57	MG	CA	1784	1/1	0.95	0.17	-	68,68,68,68	1
57	MG	BA	3377	1/1	0.99	0.14	-	126,126,126,126	0
57	MG	DA	3161	1/1	0.73	0.35	-	65,65,65,65	0
57	MG	AA	1720	1/1	0.88	0.28	-	137,137,137,137	0
57	MG	AA	1603	1/1	0.32	0.70	-	84,84,84,84	0
57	MG	AA	1757	1/1	0.31	0.85	-	87,87,87,87	1
57	MG	BA	3253	1/1	0.77	0.37	-	87,87,87,87	0
57	MG	AA	1745	1/1	0.92	0.47	-	62,62,62,62	0
57	MG	CA	1614	1/1	0.86	1.00	-	89,89,89,89	0
57	MG	DA	3271	1/1	0.95	0.34	-	47,47,47,47	0
57	MG	BA	3219	1/1	0.92	0.58	-	30,30,30,30	0
57	MG	DA	3190	1/1	0.81	0.26	-	67,67,67,67	0
57	MG	BA	3332	1/1	0.93	0.49	-	29,29,29,29	0
57	MG	DA	3186	1/1	0.99	0.21	-	48,48,48,48	0
57	MG	BA	3146	1/1	0.93	0.21	-	57,57,57,57	0
57	MG	DA	3359	1/1	0.99	0.07	-	62,62,62,62	1
57	MG	BA	3083	1/1	0.94	0.38	-	30,30,30,30	0
57	MG	DA	3413	1/1	0.86	0.21	-	84,84,84,84	0
57	MG	DA	3343	1/1	0.97	0.19	-	71,71,71,71	0
57	MG	CA	1770	1/1	0.91	0.41	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1696	1/1	0.94	0.09	-	47,47,47,47	0
57	MG	AA	1644	1/1	0.88	0.32	-	110,110,110,110	0
57	MG	CA	1799	1/1	0.86	0.33	-	75,75,75,75	0
57	MG	CA	1622	1/1	0.76	0.46	-	117,117,117,117	0
57	MG	CA	1629	1/1	0.59	0.22	-	59,59,59,59	0
57	MG	BA	3228	1/1	0.84	0.41	-	51,51,51,51	0
57	MG	DA	3351	1/1	0.88	0.49	-	94,94,94,94	0
57	MG	DA	3278	1/1	0.91	0.29	-	54,54,54,54	0
57	MG	BA	3321	1/1	0.98	0.14	-	80,80,80,80	0
57	MG	DA	3193	1/1	0.99	0.33	-	48,48,48,48	0
57	MG	CA	1737	1/1	0.86	0.26	-	87,87,87,87	0
57	MG	BA	3020	1/1	0.97	0.25	-	28,28,28,28	0
57	MG	DB	202	1/1	0.69	0.29	-	113,113,113,113	0
57	MG	BA	3302	1/1	0.93	0.24	-	26,26,26,26	0
57	MG	BA	3014	1/1	0.83	0.23	-	61,61,61,61	0
57	MG	BA	3231	1/1	0.92	0.67	-	38,38,38,38	0
57	MG	DA	3112	1/1	0.91	0.36	-	39,39,39,39	0
57	MG	AA	1735	1/1	0.85	0.29	-	108,108,108,108	0
57	MG	DA	3133	1/1	0.99	0.22	-	35,35,35,35	0
57	MG	DA	3262	1/1	0.80	0.55	-	73,73,73,73	0
57	MG	CA	1613	1/1	0.79	0.54	-	51,51,51,51	0
57	MG	AA	1793	1/1	0.76	0.34	-	91,91,91,91	0
57	MG	CA	1715	1/1	0.98	0.12	-	66,66,66,66	0
57	MG	BB	206	1/1	0.94	0.15	-	105,105,105,105	0
57	MG	DA	3189	1/1	0.93	0.31	-	69,69,69,69	0
57	MG	AA	1702	1/1	0.77	1.05	-	126,126,126,126	0
57	MG	DA	3406	1/1	0.83	0.18	-	51,51,51,51	0
57	MG	AA	1641	1/1	0.58	0.69	-	83,83,83,83	0
57	MG	DA	3050	1/1	0.91	0.17	-	69,69,69,69	1
57	MG	DA	3275	1/1	0.93	0.10	-	98,98,98,98	0
57	MG	BA	3404	1/1	0.92	0.19	-	56,56,56,56	0
57	MG	AA	1754	1/1	0.75	0.33	-	64,64,64,64	0
57	MG	CA	1645	1/1	0.75	0.72	-	66,66,66,66	0
57	MG	BA	3394	1/1	0.85	0.41	-	81,81,81,81	1
57	MG	DA	3226	1/1	0.82	0.32	-	88,88,88,88	0
57	MG	DA	3403	1/1	0.96	0.17	-	55,55,55,55	0
57	MG	BA	3089	1/1	0.96	0.63	-	43,43,43,43	0
57	MG	BA	3176	1/1	0.78	0.39	-	97,97,97,97	0
57	MG	BA	3018	1/1	0.96	0.48	-	9,9,9,9	0
57	MG	AA	1736	1/1	0.94	0.24	-	87,87,87,87	0
57	MG	BA	3234	1/1	0.97	0.54	-	56,56,56,56	0
57	MG	AA	1731	1/1	0.82	0.54	-	73,73,73,73	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3208	1/1	0.97	0.18	-	32,32,32,32	0
57	MG	DA	3060	1/1	0.96	0.30	-	30,30,30,30	0
57	MG	AA	1753	1/1	0.78	0.16	-	103,103,103,103	0
57	MG	BA	3283	1/1	0.73	0.24	-	33,33,33,33	0
57	MG	BA	3116	1/1	0.98	0.12	-	4,4,4,4	0
57	MG	CA	1771	1/1	0.56	0.75	-	98,98,98,98	0
57	MG	DA	3147	1/1	0.82	0.31	-	59,59,59,59	0
57	MG	BA	3363	1/1	0.99	0.15	-	73,73,73,73	0
57	MG	AA	1782	1/1	0.97	0.17	-	96,96,96,96	1
57	MG	BA	3238	1/1	0.97	0.30	-	51,51,51,51	0
57	MG	DA	3340	1/1	0.65	0.59	-	98,98,98,98	1
57	MG	DB	201	1/1	0.97	0.24	-	74,74,74,74	0
57	MG	DA	3261	1/1	0.97	0.27	-	95,95,95,95	0
57	MG	BA	3033	1/1	0.92	0.37	-	33,33,33,33	0
57	MG	DA	3287	1/1	0.91	0.28	-	148,148,148,148	0
57	MG	DA	3331	1/1	0.66	0.32	-	155,155,155,155	1
57	MG	DA	3185	1/1	0.96	0.30	-	33,33,33,33	0
57	MG	BA	3208	1/1	0.94	0.43	-	61,61,61,61	0
57	MG	BA	3016	1/1	0.94	0.46	-	28,28,28,28	0
57	MG	DA	3251	1/1	0.94	0.17	-	96,96,96,96	0
57	MG	CA	1751	1/1	0.97	0.16	-	66,66,66,66	1
57	MG	DA	3368	1/1	0.91	0.39	-	45,45,45,45	1
57	MG	AA	1675	1/1	0.96	0.59	-	63,63,63,63	0
57	MG	BA	3142	1/1	0.96	0.48	-	20,20,20,20	0
57	MG	DA	3352	1/1	0.88	0.49	-	20,20,20,20	1
57	MG	CA	1725	1/1	0.78	0.35	-	116,116,116,116	1
57	MG	DA	3025	1/1	0.92	0.48	-	13,13,13,13	0
57	MG	BA	3383	1/1	0.66	1.01	-	101,101,101,101	0
57	MG	AA	1778	1/1	0.96	0.57	-	65,65,65,65	1
57	MG	CA	1648	1/1	0.81	0.55	-	83,83,83,83	0
57	MG	DA	3415	1/1	0.65	0.31	-	96,96,96,96	0
57	MG	BA	3096	1/1	0.98	0.15	-	1,1,1,1	0
57	MG	DA	3004	1/1	0.71	0.69	-	86,86,86,86	0
57	MG	CA	1749	1/1	0.91	0.16	-	98,98,98,98	0
57	MG	BA	3314	1/1	0.89	0.43	-	92,92,92,92	1
57	MG	BA	3122	1/1	0.93	0.51	-	94,94,94,94	0
57	MG	DA	3285	1/1	0.81	0.21	-	71,71,71,71	0
57	MG	DA	3067	1/1	0.97	0.56	-	46,46,46,46	0
57	MG	AA	1726	1/1	0.77	0.26	-	71,71,71,71	0
57	MG	AA	1794	1/1	0.94	0.16	-	126,126,126,126	0
57	MG	BA	3343	1/1	0.97	0.13	-	37,37,37,37	0
57	MG	B2	601	1/1	0.92	0.22	-	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3235	1/1	0.14	0.61	-	156,156,156,156	0
57	MG	DA	3266	1/1	0.87	0.24	-	84,84,84,84	0
57	MG	DA	3149	1/1	0.93	0.29	-	57,57,57,57	0
57	MG	AA	1663	1/1	0.94	0.57	-	47,47,47,47	0
57	MG	BA	3132	1/1	0.98	0.21	-	14,14,14,14	0
57	MG	DA	3198	1/1	0.78	0.38	-	58,58,58,58	1
57	MG	AA	1785	1/1	0.98	0.18	-	105,105,105,105	0
57	MG	DA	3311	1/1	0.67	0.15	-	65,65,65,65	1
57	MG	DA	3246	1/1	0.60	0.48	-	97,97,97,97	0
57	MG	BA	3080	1/1	0.84	0.29	-	26,26,26,26	0
57	MG	DA	3015	1/1	0.84	0.45	-	79,79,79,79	0
57	MG	DA	3031	1/1	0.91	0.34	-	41,41,41,41	0
57	MG	AA	1707	1/1	0.75	0.31	-	116,116,116,116	0
57	MG	DA	3248	1/1	0.71	0.24	-	90,90,90,90	0
57	MG	DA	3288	1/1	0.92	0.66	-	37,37,37,37	0
57	MG	BA	3305	1/1	0.83	1.33	-	101,101,101,101	0
57	MG	BA	3418	1/1	0.78	0.08	-	59,59,59,59	0
57	MG	DA	3176	1/1	0.94	0.35	-	69,69,69,69	0
57	MG	AX	102	1/1	0.71	0.35	-	83,83,83,83	0
57	MG	CA	1708	1/1	0.87	0.11	-	89,89,89,89	0
57	MG	DA	3301	1/1	0.86	0.78	-	84,84,84,84	0
57	MG	DA	3230	1/1	0.90	0.68	-	71,71,71,71	0
57	MG	CA	1627	1/1	0.92	0.34	-	78,78,78,78	0
57	MG	CA	1748	1/1	0.99	0.24	-	63,63,63,63	0
57	MG	AA	1701	1/1	0.40	0.76	-	92,92,92,92	0
57	MG	AA	1733	1/1	0.23	0.87	-	141,141,141,141	0
57	MG	DB	209	1/1	0.80	0.56	-	7,7,7,7	1
57	MG	BA	3209	1/1	0.97	0.39	-	14,14,14,14	0
57	MG	BA	3151	1/1	0.76	0.44	-	45,45,45,45	1
57	MG	DA	3357	1/1	0.99	0.16	-	111,111,111,111	0
57	MG	CA	1630	1/1	0.84	0.29	-	84,84,84,84	0
57	MG	BA	3249	1/1	0.91	0.41	-	114,114,114,114	0
57	MG	CA	1791	1/1	0.95	0.11	-	85,85,85,85	1
57	MG	BA	3225	1/1	0.78	0.67	-	128,128,128,128	0
57	MG	DA	3306	1/1	0.90	0.17	-	51,51,51,51	0
57	MG	AW	107	1/1	0.61	0.40	-	101,101,101,101	0
57	MG	BA	3407	1/1	0.94	0.20	-	52,52,52,52	0
57	MG	BA	3320	1/1	0.89	0.25	-	141,141,141,141	0
57	MG	BA	3313	1/1	0.85	0.31	-	162,162,162,162	0
57	MG	CA	1605	1/1	0.95	0.14	-	47,47,47,47	0
57	MG	DA	3207	1/1	0.94	0.26	-	67,67,67,67	0
57	MG	DA	3386	1/1	0.93	0.76	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3181	1/1	0.97	0.20	-	100,100,100,100	0
57	MG	CL	201	1/1	0.68	0.74	-	91,91,91,91	0
57	MG	DA	3032	1/1	0.61	0.52	-	66,66,66,66	0
57	MG	DA	3376	1/1	0.81	0.46	-	110,110,110,110	0
57	MG	DC	301	1/1	0.72	0.23	-	91,91,91,91	1
57	MG	DA	3055	1/1	0.98	0.15	-	31,31,31,31	0
57	MG	BA	3327	1/1	0.56	0.85	-	67,67,67,67	0
57	MG	DS	201	1/1	0.67	0.26	-	74,74,74,74	1
57	MG	DA	3366	1/1	0.98	0.08	-	29,29,29,29	1
57	MG	BA	3274	1/1	0.93	0.71	-	85,85,85,85	0
57	MG	BA	3412	1/1	0.98	0.10	-	30,30,30,30	0
57	MG	DA	3197	1/1	0.59	0.59	-	106,106,106,106	0
57	MG	DA	3051	1/1	0.82	0.26	-	75,75,75,75	0
57	MG	BB	209	1/1	0.95	0.51	-	1,1,1,1	1
57	MG	DA	3387	1/1	0.89	0.52	-	66,66,66,66	0
57	MG	CA	1763	1/1	0.70	0.24	-	98,98,98,98	0
57	MG	BA	3247	1/1	0.69	0.34	-	49,49,49,49	0
57	MG	CA	1624	1/1	0.96	0.25	-	55,55,55,55	0
57	MG	D5	101	1/1	0.87	0.24	-	51,51,51,51	0
57	MG	AW	101	1/1	0.87	0.26	-	157,157,157,157	0
57	MG	CA	1728	1/1	0.41	0.64	-	101,101,101,101	0
57	MG	AA	1798	1/1	0.49	0.55	-	90,90,90,90	0
57	MG	AA	1759	1/1	0.82	0.36	-	96,96,96,96	0
57	MG	BA	3392	1/1	0.97	0.14	-	139,139,139,139	0
57	MG	AA	1673	1/1	0.79	1.32	-	76,76,76,76	1
57	MG	CW	106	1/1	0.81	0.17	-	86,86,86,86	1
57	MG	DA	3279	1/1	0.43	0.92	-	49,49,49,49	1
57	MG	BA	3155	1/1	0.69	0.85	-	116,116,116,116	0
57	MG	AA	1631	1/1	0.72	0.38	-	54,54,54,54	0
57	MG	AA	1724	1/1	0.81	0.29	-	68,68,68,68	1
57	MG	DA	3360	1/1	0.99	0.10	-	83,83,83,83	0
57	MG	CA	1766	1/1	0.88	0.15	-	96,96,96,96	0
57	MG	CA	1765	1/1	0.78	0.26	-	60,60,60,60	0
57	MG	AA	1750	1/1	0.87	0.30	-	62,62,62,62	1
57	MG	CA	1651	1/1	0.96	0.17	-	85,85,85,85	0
57	MG	CA	1746	1/1	0.50	0.46	-	91,91,91,91	0
57	MG	BA	3119	1/1	0.97	0.24	-	35,35,35,35	0
57	MG	BA	3071	1/1	0.89	0.30	-	52,52,52,52	0
57	MG	B5	102	1/1	0.84	0.49	-	58,58,58,58	1
57	MG	CA	1745	1/1	0.41	0.87	-	115,115,115,115	0
57	MG	DA	3199	1/1	0.91	0.99	-	101,101,101,101	0
57	MG	DA	3290	1/1	0.71	1.14	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3317	1/1	0.84	0.16	-	167,167,167,167	0
57	MG	AA	1797	1/1	0.88	0.53	-	53,53,53,53	0
57	MG	DA	3315	1/1	0.80	0.32	-	85,85,85,85	1
57	MG	BA	3095	1/1	0.96	0.34	-	27,27,27,27	0
57	MG	DA	3134	1/1	0.94	0.20	-	57,57,57,57	0
57	MG	DA	3042	1/1	0.65	0.30	-	89,89,89,89	0
57	MG	BA	3010	1/1	0.85	0.40	-	41,41,41,41	0
57	MG	AA	1752	1/1	0.89	0.32	-	120,120,120,120	1
57	MG	DA	3372	1/1	0.65	0.44	-	120,120,120,120	1
57	MG	DA	3394	1/1	0.96	0.13	-	103,103,103,103	0
57	MG	BA	3419	1/1	0.68	1.19	-	90,90,90,90	1
57	MG	BA	3103	1/1	0.95	0.21	-	31,31,31,31	0
57	MG	DA	3345	1/1	0.92	0.43	-	43,43,43,43	1
57	MG	DA	3327	1/1	0.82	0.98	-	64,64,64,64	1
57	MG	AA	1672	1/1	-0.07	0.98	-	125,125,125,125	1
57	MG	DA	3003	1/1	0.94	0.22	-	91,91,91,91	0
57	MG	AA	1779	1/1	0.99	0.13	-	90,90,90,90	0
57	MG	DA	3325	1/1	0.86	0.30	-	83,83,83,83	1
57	MG	DA	3219	1/1	0.93	0.35	-	99,99,99,99	0
57	MG	DA	3229	1/1	0.74	0.62	-	92,92,92,92	0
57	MG	CA	1655	1/1	0.61	0.56	-	94,94,94,94	1
57	MG	BA	3158	1/1	0.57	0.71	-	55,55,55,55	0
57	MG	AD	301	1/1	0.54	0.45	-	155,155,155,155	0
57	MG	DA	3371	1/1	0.98	0.12	-	61,61,61,61	1
57	MG	BA	3329	1/1	0.97	0.15	-	126,126,126,126	0
57	MG	BA	3357	1/1	1.00	0.17	-	84,84,84,84	0
57	MG	BA	3270	1/1	0.50	0.46	-	76,76,76,76	0
57	MG	AA	1614	1/1	0.95	0.40	-	14,14,14,14	0
57	MG	CA	1611	1/1	0.89	0.35	-	110,110,110,110	0
57	MG	BA	3330	1/1	0.92	0.24	-	85,85,85,85	1
57	MG	CA	1644	1/1	0.40	0.45	-	102,102,102,102	0
57	MG	DA	3388	1/1	0.85	0.25	-	68,68,68,68	0
57	MG	AA	1740	1/1	0.70	0.30	-	87,87,87,87	0
57	MG	DA	3361	1/1	0.94	0.15	-	64,64,64,64	0
57	MG	AA	1677	1/1	0.65	0.29	-	89,89,89,89	0
57	MG	DA	3007	1/1	0.87	0.71	-	59,59,59,59	0
57	MG	DA	3205	1/1	0.81	0.25	-	37,37,37,37	0
57	MG	BA	3339	1/1	0.36	0.60	-	125,125,125,125	1
57	MG	DA	3072	1/1	0.58	0.47	-	94,94,94,94	0
57	MG	DA	3087	1/1	0.75	0.40	-	84,84,84,84	0
57	MG	BA	3107	1/1	0.81	0.45	-	44,44,44,44	0
57	MG	BA	3199	1/1	0.95	0.68	-	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3143	1/1	0.94	0.41	-	18,18,18,18	0
57	MG	BA	3280	1/1	0.94	0.11	-	28,28,28,28	0
57	MG	BA	3344	1/1	0.96	0.14	-	57,57,57,57	0
57	MG	BA	3131	1/1	0.88	0.26	-	31,31,31,31	0
57	MG	DA	3286	1/1	0.95	0.82	-	75,75,75,75	0
57	MG	BA	3175	1/1	0.90	0.34	-	46,46,46,46	0
57	MG	AA	1713	1/1	0.87	0.15	-	53,53,53,53	0
57	MG	DA	3153	1/1	0.67	0.43	-	60,60,60,60	1
57	MG	AA	1796	1/1	0.62	0.56	-	121,121,121,121	0
57	MG	AA	1771	1/1	0.86	0.53	-	40,40,40,40	0
57	MG	DA	3299	1/1	0.78	0.52	-	93,93,93,93	0
57	MG	AA	1738	1/1	0.61	0.36	-	55,55,55,55	1
57	MG	BA	3149	1/1	0.96	0.25	-	13,13,13,13	1
57	MG	BA	3248	1/1	0.81	0.28	-	50,50,50,50	1
57	MG	DB	206	1/1	0.91	0.11	-	75,75,75,75	0
57	MG	AA	1605	1/1	0.96	0.12	-	120,120,120,120	0
57	MG	BA	3221	1/1	0.94	0.59	-	80,80,80,80	1
57	MG	DA	3053	1/1	0.93	0.17	-	26,26,26,26	0
57	MG	AA	1619	1/1	0.95	0.50	-	65,65,65,65	0
57	MG	AA	1780	1/1	0.99	0.35	-	115,115,115,115	0
57	MG	BA	3386	1/1	0.96	0.09	-	76,76,76,76	0
57	MG	DD	302	1/1	0.94	0.32	-	46,46,46,46	0
57	MG	DA	3408	1/1	0.85	0.38	-	44,44,44,44	0
57	MG	DA	3017	1/1	0.96	0.44	-	31,31,31,31	0
57	MG	BA	3335	1/1	0.98	0.10	-	62,62,62,62	0
57	MG	DA	3099	1/1	0.94	0.29	-	40,40,40,40	0
57	MG	BA	3081	1/1	0.99	0.20	-	7,7,7,7	0
57	MG	BA	3309	1/1	0.93	0.12	-	112,112,112,112	1
57	MG	AA	1767	1/1	0.99	0.29	-	44,44,44,44	0
57	MG	BA	3184	1/1	0.97	0.34	-	38,38,38,38	0
57	MG	B1	101	1/1	0.94	0.11	-	41,41,41,41	1
57	MG	BA	3160	1/1	0.65	0.46	-	74,74,74,74	0
57	MG	CA	1741	1/1	0.94	0.20	-	53,53,53,53	0
57	MG	CA	1758	1/1	0.97	0.27	-	64,64,64,64	1
57	MG	DA	3170	1/1	0.68	0.62	-	60,60,60,60	0
57	MG	DA	3120	1/1	0.97	0.19	-	39,39,39,39	0
57	MG	DA	3160	1/1	0.72	0.44	-	67,67,67,67	0
57	MG	BE	301	1/1	0.91	0.21	-	30,30,30,30	0
57	MG	AA	1763	1/1	0.68	0.17	-	62,62,62,62	0
57	MG	CA	1688	1/1	0.41	0.67	-	15,15,15,15	1
57	MG	DA	3418	1/1	0.95	0.40	-	47,47,47,47	1
57	MG	AG	201	1/1	0.57	0.44	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3177	1/1	0.84	0.48	-	77,77,77,77	0
57	MG	AA	1633	1/1	0.98	0.14	-	40,40,40,40	0
57	MG	BA	3230	1/1	0.67	0.48	-	97,97,97,97	0
57	MG	BA	3351	1/1	0.85	0.26	-	135,135,135,135	0
57	MG	BA	3347	1/1	0.98	0.29	-	42,42,42,42	0
57	MG	AA	1687	1/1	0.98	0.13	-	9,9,9,9	1
57	MG	DA	3355	1/1	0.95	0.17	-	95,95,95,95	0
57	MG	AA	1730	1/1	0.91	0.27	-	107,107,107,107	0
57	MG	CA	1668	1/1	0.61	0.98	-	99,99,99,99	0
57	MG	BA	3207	1/1	0.93	0.17	-	45,45,45,45	0
57	MG	BA	3063	1/1	0.96	0.15	-	1,1,1,1	0
57	MG	AW	103	1/1	0.94	0.10	-	106,106,106,106	0
57	MG	BA	3205	1/1	0.96	0.30	-	17,17,17,17	0
57	MG	DA	3319	1/1	0.76	0.54	-	102,102,102,102	1
57	MG	AA	1654	1/1	0.85	0.29	-	52,52,52,52	1
57	MG	CA	1643	1/1	0.73	0.19	-	157,157,157,157	0
57	MG	BA	3250	1/1	0.83	0.23	-	76,76,76,76	0
57	MG	DA	3044	1/1	0.95	0.20	-	40,40,40,40	0
57	MG	CA	1734	1/1	0.91	0.69	-	67,67,67,67	0
57	MG	BA	3075	1/1	0.98	0.36	-	31,31,31,31	0
57	MG	CA	1691	1/1	0.67	0.24	-	110,110,110,110	0
57	MG	CA	1667	1/1	0.88	0.48	-	55,55,55,55	0
57	MG	BA	3277	1/1	0.87	0.78	-	35,35,35,35	1
57	MG	CX	103	1/1	0.91	0.23	-	108,108,108,108	0
57	MG	DA	3232	1/1	0.93	0.27	-	93,93,93,93	0
57	MG	CA	1647	1/1	0.79	0.52	-	68,68,68,68	0
57	MG	BA	3269	1/1	0.92	0.27	-	38,38,38,38	0
57	MG	DA	3045	1/1	0.96	0.30	-	35,35,35,35	0
57	MG	CA	1732	1/1	0.96	0.09	-	82,82,82,82	0
57	MG	AA	1762	1/1	0.82	0.40	-	80,80,80,80	1
57	MG	AA	1648	1/1	0.80	0.32	-	87,87,87,87	0
57	MG	BA	3328	1/1	0.98	0.18	-	168,168,168,168	0
57	MG	CA	1798	1/1	0.73	0.23	-	55,55,55,55	0
57	MG	DA	3097	1/1	0.97	0.08	-	25,25,25,25	0
57	MG	BA	3388	1/1	0.97	0.36	-	12,12,12,12	0
57	MG	BA	3323	1/1	0.89	0.35	-	86,86,86,86	1
57	MG	DA	3142	1/1	0.91	0.46	-	65,65,65,65	0
57	MG	BA	3141	1/1	0.90	0.27	-	56,56,56,56	0
57	MG	DA	3356	1/1	0.95	0.15	-	57,57,57,57	0
57	MG	CA	1756	1/1	0.72	0.36	-	53,53,53,53	0
57	MG	DA	3335	1/1	0.90	0.26	-	80,80,80,80	0
57	MG	CA	1653	1/1	0.96	0.13	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3104	1/1	0.96	0.47	-	37,37,37,37	0
57	MG	CA	1649	1/1	0.31	0.41	-	95,95,95,95	0
57	MG	DA	3317	1/1	0.80	0.33	-	55,55,55,55	1
57	MG	BA	3316	1/1	0.97	0.22	-	55,55,55,55	1
57	MG	DA	3254	1/1	0.95	0.13	-	99,99,99,99	0
57	MG	AA	1681	1/1	0.79	1.02	-	86,86,86,86	0
57	MG	CA	1606	1/1	0.77	0.32	-	78,78,78,78	0
57	MG	BA	3415	1/1	0.81	0.37	-	77,77,77,77	0
57	MG	BA	3094	1/1	0.98	0.18	-	24,24,24,24	0
57	MG	AA	1670	1/1	0.85	0.38	-	49,49,49,49	0
57	MG	BA	3315	1/1	0.98	0.06	-	83,83,83,83	0
57	MG	BA	3002	1/1	1.00	0.16	-	139,139,139,139	0
57	MG	BA	3252	1/1	0.86	0.27	-	79,79,79,79	0
57	MG	BA	3401	1/1	0.93	0.29	-	81,81,81,81	0
57	MG	CA	1673	1/1	-0.08	0.63	-	128,128,128,128	1
57	MG	DA	3312	1/1	0.84	0.20	-	56,56,56,56	1
57	MG	DA	3082	1/1	0.97	0.28	-	59,59,59,59	0
57	MG	DA	3145	1/1	0.95	0.44	-	90,90,90,90	0
57	MG	CA	1733	1/1	0.81	0.52	-	81,81,81,81	1
57	MG	BA	3093	1/1	0.99	0.07	-	7,7,7,7	0
57	MG	CA	1754	1/1	0.63	0.52	-	105,105,105,105	1
57	MG	BA	3213	1/1	0.98	0.09	-	93,93,93,93	1
57	MG	AA	1772	1/1	0.77	0.33	-	85,85,85,85	0
57	MG	BA	3325	1/1	0.98	0.13	-	88,88,88,88	1
57	MG	DA	3339	1/1	0.86	0.28	-	57,57,57,57	1
57	MG	BA	3333	1/1	0.96	0.21	-	40,40,40,40	0
57	MG	DA	3236	1/1	0.98	0.33	-	47,47,47,47	0
57	MG	CA	1720	1/1	0.80	0.23	-	89,89,89,89	0
57	MG	BA	3210	1/1	0.92	1.03	-	84,84,84,84	0
57	MG	AA	1711	1/1	0.96	0.13	-	73,73,73,73	0
57	MG	BA	3298	1/1	0.91	0.47	-	69,69,69,69	0
57	MG	DA	3318	1/1	0.91	0.19	-	138,138,138,138	0
57	MG	CA	1694	1/1	0.82	0.38	-	116,116,116,116	0
57	MG	DA	3346	1/1	0.88	0.22	-	54,54,54,54	0
57	MG	DA	3353	1/1	0.58	0.59	-	107,107,107,107	0
57	MG	CA	1683	1/1	0.47	0.47	-	110,110,110,110	0
57	MG	AA	1722	1/1	0.87	0.15	-	75,75,75,75	0
57	MG	AA	1659	1/1	0.88	0.36	-	42,42,42,42	0
57	MG	BA	3167	1/1	0.86	0.37	-	32,32,32,32	1
57	MG	B5	101	1/1	0.97	0.17	-	42,42,42,42	0
57	MG	AA	1643	1/1	0.79	0.30	-	84,84,84,84	0
57	MG	BA	3282	1/1	0.84	0.51	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1679	1/1	0.77	0.48	-	56,56,56,56	0
57	MG	DA	3334	1/1	0.93	0.24	-	72,72,72,72	0
57	MG	CA	1681	1/1	0.81	0.53	-	49,49,49,49	0
57	MG	BA	3134	1/1	0.91	0.19	-	10,10,10,10	0
57	MG	BA	3304	1/1	0.96	0.16	-	81,81,81,81	0
57	MG	CA	1777	1/1	0.86	1.29	-	135,135,135,135	0
57	MG	DA	3169	1/1	0.88	0.52	-	43,43,43,43	1
57	MG	CA	1744	1/1	0.93	0.66	-	63,63,63,63	0
57	MG	BA	3413	1/1	0.94	0.55	-	33,33,33,33	0
57	MG	DB	203	1/1	0.44	0.96	-	33,33,33,33	1
57	MG	BA	3258	1/1	0.95	0.35	-	32,32,32,32	0
57	MG	BA	3286	1/1	0.98	0.67	-	16,16,16,16	0
57	MG	BB	210	1/1	0.97	0.32	-	27,27,27,27	0
57	MG	CA	1764	1/1	0.71	0.23	-	68,68,68,68	1
57	MG	CA	1730	1/1	0.95	0.26	-	43,43,43,43	0
57	MG	BA	3206	1/1	0.97	0.25	-	22,22,22,22	0
57	MG	DA	3397	1/1	0.94	0.74	-	101,101,101,101	0
57	MG	AA	1791	1/1	0.95	0.23	-	26,26,26,26	1
57	MG	BA	3115	1/1	0.98	0.32	-	27,27,27,27	0
57	MG	DA	3375	1/1	0.89	0.16	-	83,83,83,83	0
57	MG	DA	3240	1/1	0.82	0.46	-	56,56,56,56	0
57	MG	AA	1627	1/1	0.92	0.26	-	54,54,54,54	0
57	MG	DA	3344	1/1	0.97	0.46	-	64,64,64,64	0
57	MG	DA	3041	1/1	0.91	0.21	-	46,46,46,46	0
57	MG	DA	3223	1/1	0.84	0.64	-	46,46,46,46	1
57	MG	DA	3076	1/1	0.98	0.33	-	45,45,45,45	0
57	MG	BA	3349	1/1	0.61	0.70	-	94,94,94,94	1
57	MG	CV	104	1/1	0.10	0.41	-	163,163,163,163	0
57	MG	BA	3050	1/1	0.95	0.27	-	30,30,30,30	0
57	MG	BA	3254	1/1	0.66	0.19	-	44,44,44,44	0
57	MG	AA	1746	1/1	0.96	0.36	-	95,95,95,95	0
57	MG	CA	1682	1/1	0.73	0.73	-	90,90,90,90	0
57	MG	AA	1764	1/1	0.67	0.34	-	64,64,64,64	0
57	MG	BA	3278	1/1	0.98	0.09	-	127,127,127,127	0
57	MG	BA	3395	1/1	0.96	0.21	-	113,113,113,113	0
57	MG	DA	3414	1/1	0.64	0.39	-	84,84,84,84	0
57	MG	AW	102	1/1	0.33	0.21	-	135,135,135,135	0
57	MG	CA	1768	1/1	0.88	0.35	-	72,72,72,72	0
57	MG	DA	3128	1/1	0.21	1.30	-	73,73,73,73	1
57	MG	DA	3218	1/1	0.88	0.39	-	94,94,94,94	0
57	MG	CV	103	1/1	0.85	0.59	-	74,74,74,74	0
57	MG	CA	1615	1/1	0.82	1.51	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3125	1/1	0.92	0.18	-	53,53,53,53	0
57	MG	D1	101	1/1	0.90	0.21	-	29,29,29,29	1
57	MG	AI	201	1/1	0.93	0.24	-	109,109,109,109	0
57	MG	BB	201	1/1	0.73	0.38	-	87,87,87,87	0
57	MG	BA	3223	1/1	0.72	0.50	-	64,64,64,64	0
57	MG	DA	3349	1/1	0.82	0.32	-	41,41,41,41	1
57	MG	DA	3244	1/1	0.92	0.35	-	62,62,62,62	0
57	MG	DA	3220	1/1	0.98	0.38	-	26,26,26,26	0
57	MG	DA	3129	1/1	0.94	0.13	-	22,22,22,22	0
57	MG	DA	3094	1/1	0.94	0.14	-	22,22,22,22	0
57	MG	AA	1689	1/1	0.71	0.48	-	118,118,118,118	0
57	MG	BA	3285	1/1	0.82	0.54	-	89,89,89,89	0
57	MG	BA	3181	1/1	0.95	0.32	-	49,49,49,49	0
57	MG	DA	3210	1/1	0.70	0.54	-	96,96,96,96	0
57	MG	DA	3277	1/1	0.88	0.67	-	63,63,63,63	0
57	MG	BA	3422	1/1	0.92	0.30	-	120,120,120,120	0
57	MG	DA	3260	1/1	0.78	0.98	-	81,81,81,81	0
57	MG	AA	1723	1/1	0.91	0.73	-	79,79,79,79	1
57	MG	DA	3227	1/1	0.77	1.36	-	136,136,136,136	0
57	MG	DA	3116	1/1	0.88	0.75	-	50,50,50,50	0
57	MG	CA	1712	1/1	0.98	0.12	-	81,81,81,81	0
57	MG	BA	3259	1/1	0.98	0.18	-	24,24,24,24	0
57	MG	DA	3113	1/1	0.93	0.40	-	27,27,27,27	0
57	MG	DA	3131	1/1	0.98	0.21	-	23,23,23,23	0
57	MG	CV	102	1/1	0.97	0.20	-	46,46,46,46	1
57	MG	BA	3355	1/1	0.97	0.16	-	92,92,92,92	0
57	MG	DA	3089	1/1	0.97	0.29	-	26,26,26,26	0
57	MG	CA	1633	1/1	0.98	0.14	-	42,42,42,42	0
57	MG	AL	201	1/1	0.91	0.38	-	81,81,81,81	0
57	MG	DA	3295	1/1	0.97	0.09	-	78,78,78,78	0
57	MG	BU	201	1/1	0.74	0.40	-	166,166,166,166	1
57	MG	AA	1676	1/1	0.97	0.13	-	48,48,48,48	0
57	MG	AA	1714	1/1	0.97	0.10	-	29,29,29,29	0
57	MG	BA	3374	1/1	0.93	0.07	-	92,92,92,92	0
57	MG	BA	3128	1/1	0.93	0.16	-	27,27,27,27	0
57	MG	BA	3068	1/1	0.96	0.15	-	38,38,38,38	0
57	MG	BA	3177	1/1	0.27	0.40	-	112,112,112,112	0
57	MG	BA	3174	1/1	0.92	0.25	-	55,55,55,55	0
57	MG	AA	1632	1/1	0.94	0.42	-	34,34,34,34	1
57	MG	DA	3151	1/1	0.96	0.33	-	57,57,57,57	1
57	MG	BA	3041	1/1	0.82	0.29	-	96,96,96,96	0
57	MG	AA	1640	1/1	0.71	0.34	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3289	1/1	0.76	0.23	-	79,79,79,79	0
57	MG	DA	3214	1/1	0.84	0.26	-	129,129,129,129	0
57	MG	BX	101	1/1	0.97	0.39	-	58,58,58,58	0
57	MG	DA	3020	1/1	0.86	0.33	-	59,59,59,59	0
57	MG	AA	1669	1/1	0.93	0.28	-	57,57,57,57	0
57	MG	DA	3391	1/1	0.98	0.10	-	120,120,120,120	0
57	MG	CA	1631	1/1	0.97	0.30	-	65,65,65,65	0
57	MG	DA	3280	1/1	0.96	0.35	-	109,109,109,109	0
57	MG	BA	3360	1/1	0.77	0.39	-	140,140,140,140	0
57	MG	DA	3137	1/1	0.96	0.18	-	21,21,21,21	0
57	MG	DA	3002	1/1	0.84	0.23	-	69,69,69,69	0
57	MG	BA	3354	1/1	0.97	0.14	-	129,129,129,129	0
57	MG	CW	107	1/1	0.45	0.21	-	113,113,113,113	1
57	MG	AV	102	1/1	0.96	0.15	-	93,93,93,93	1
57	MG	BA	3099	1/1	0.98	0.20	-	37,37,37,37	0
57	MG	DA	3392	1/1	0.48	0.62	-	107,107,107,107	0
57	MG	BA	3251	1/1	0.46	0.37	-	136,136,136,136	1
57	MG	BA	3293	1/1	0.99	0.10	-	87,87,87,87	0
57	MG	DB	204	1/1	0.96	0.21	-	90,90,90,90	0
57	MG	DA	3329	1/1	0.85	0.42	-	140,140,140,140	0
57	MG	DA	3103	1/1	0.92	0.43	-	34,34,34,34	0
57	MG	AA	1615	1/1	0.96	0.57	-	65,65,65,65	0
57	MG	BA	3390	1/1	0.91	0.27	-	37,37,37,37	0
57	MG	BA	3406	1/1	0.82	0.27	-	38,38,38,38	1
57	MG	DV	201	1/1	0.87	0.28	-	70,70,70,70	0
57	MG	DX	101	1/1	0.90	0.34	-	45,45,45,45	0
57	MG	BA	3140	1/1	0.96	0.36	-	66,66,66,66	0
57	MG	CA	1669	1/1	0.83	0.33	-	81,81,81,81	0
57	MG	DA	3362	1/1	0.94	0.35	-	112,112,112,112	0
57	MG	BA	3257	1/1	0.87	0.58	-	61,61,61,61	0
57	MG	DA	3369	1/1	0.32	0.40	-	112,112,112,112	0
57	MG	CW	104	1/1	0.95	0.11	-	130,130,130,130	1
57	MG	CA	1782	1/1	0.84	0.33	-	77,77,77,77	0
57	MG	AA	1612	1/1	0.92	0.31	-	67,67,67,67	0
57	MG	BA	3090	1/1	0.99	0.36	-	29,29,29,29	0
57	MG	DA	3405	1/1	0.56	0.65	-	53,53,53,53	1
57	MG	AA	1639	1/1	0.95	0.29	-	99,99,99,99	0
57	MG	DA	3393	1/1	0.75	0.52	-	109,109,109,109	1
57	MG	CA	1657	1/1	0.74	0.35	-	86,86,86,86	0
57	MG	AA	1647	1/1	0.91	0.21	-	74,74,74,74	0
57	MG	DA	3348	1/1	0.96	0.10	-	64,64,64,64	0
57	MG	D5	102	1/1	0.91	0.31	-	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3410	1/1	0.98	0.31	-	87,87,87,87	1
57	MG	AA	1732	1/1	0.77	0.52	-	61,61,61,61	0
57	MG	BA	3371	1/1	0.60	0.70	-	101,101,101,101	0
57	MG	BA	3037	1/1	0.95	0.25	-	23,23,23,23	0
57	MG	BA	3057	1/1	0.91	0.47	-	85,85,85,85	0
57	MG	BA	3171	1/1	0.91	0.11	-	31,31,31,31	0
57	MG	AA	1789	1/1	0.98	0.32	-	81,81,81,81	1
57	MG	AA	1749	1/1	0.62	0.38	-	100,100,100,100	1
57	MG	CA	1786	1/1	0.71	0.12	-	71,71,71,71	1
57	MG	CA	1680	1/1	0.46	1.13	-	94,94,94,94	0
57	MG	CA	1654	1/1	0.79	0.58	-	69,69,69,69	0
57	MG	DA	3354	1/1	0.77	0.13	-	84,84,84,84	0
57	MG	BA	3159	1/1	0.80	0.32	-	37,37,37,37	0
57	MG	AA	1616	1/1	0.80	0.84	-	70,70,70,70	0
57	MG	DA	3058	1/1	0.97	0.37	-	88,88,88,88	0
57	MG	BA	3227	1/1	0.95	0.28	-	74,74,74,74	0
57	MG	AA	1646	1/1	0.76	0.64	-	82,82,82,82	0
57	MG	BA	3043	1/1	0.97	0.20	-	20,20,20,20	0
57	MG	AA	1617	1/1	0.82	0.71	-	51,51,51,51	0
57	MG	CA	1640	1/1	0.22	0.92	-	121,121,121,121	0
57	MG	BA	3031	1/1	0.95	0.45	-	44,44,44,44	0
57	MG	DA	3269	1/1	0.87	0.36	-	47,47,47,47	0
57	MG	CA	1674	1/1	0.65	0.47	-	63,63,63,63	1
57	MG	CA	1635	1/1	0.91	0.19	-	74,74,74,74	0
57	MG	BB	208	1/1	0.92	1.03	-	61,61,61,61	1
57	MG	BA	3008	1/1	0.98	0.26	-	3,3,3,3	0
57	MG	DA	3323	1/1	0.96	0.64	-	53,53,53,53	1
57	MG	DA	3256	1/1	0.84	0.26	-	79,79,79,79	0
57	MG	AA	1661	1/1	0.38	0.57	-	84,84,84,84	0
57	MG	AA	1650	1/1	0.94	0.22	-	99,99,99,99	0
57	MG	BA	3359	1/1	0.99	0.16	-	86,86,86,86	1
57	MG	BA	3126	1/1	0.93	0.27	-	39,39,39,39	0
57	MG	CA	1742	1/1	0.82	0.21	-	70,70,70,70	0
57	MG	DA	3187	1/1	0.91	0.17	-	55,55,55,55	0
57	MG	AA	1653	1/1	0.67	0.90	-	82,82,82,82	0
57	MG	CA	1601	1/1	0.92	0.29	-	140,140,140,140	0
57	MG	AA	1607	1/1	0.71	0.31	-	64,64,64,64	0
57	MG	BA	3352	1/1	0.93	0.73	-	23,23,23,23	1
57	MG	DA	3030	1/1	0.96	0.23	-	47,47,47,47	0
57	MG	CA	1642	1/1	0.97	0.26	-	74,74,74,74	0
57	MG	AA	1695	1/1	0.88	0.16	-	52,52,52,52	0
57	MG	BA	3264	1/1	0.75	0.27	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3304	1/1	0.74	0.42	-	49,49,49,49	0
57	MG	BA	3373	1/1	0.57	0.61	-	83,83,83,83	1
57	MG	BA	3342	1/1	0.65	0.29	-	84,84,84,84	0
57	MG	CA	1665	1/1	0.76	0.35	-	68,68,68,68	0
57	MG	BA	3217	1/1	0.91	0.25	-	78,78,78,78	0
57	MG	DA	3140	1/1	0.92	0.26	-	90,90,90,90	0
57	MG	AA	1755	1/1	0.88	0.35	-	84,84,84,84	0
57	MG	DA	3300	1/1	0.58	0.29	-	95,95,95,95	0
57	MG	CA	1735	1/1	0.77	0.49	-	90,90,90,90	0
57	MG	DA	3321	1/1	0.64	0.62	-	126,126,126,126	0
57	MG	DA	3224	1/1	0.90	0.17	-	85,85,85,85	0
57	MG	AA	1751	1/1	0.78	0.42	-	72,72,72,72	1
57	MG	BA	3195	1/1	0.75	1.13	-	79,79,79,79	0
57	MG	BA	3263	1/1	0.93	0.63	-	77,77,77,77	0
57	MG	DA	3282	1/1	0.76	0.21	-	50,50,50,50	0
57	MG	DA	3009	1/1	0.96	0.15	-	45,45,45,45	0
57	MG	DA	3253	1/1	0.81	0.53	-	86,86,86,86	1
57	MG	DA	3276	1/1	0.61	0.76	-	115,115,115,115	0
57	MG	BA	3049	1/1	0.98	0.28	-	84,84,84,84	1
57	MG	DA	3305	1/1	0.97	0.56	-	100,100,100,100	1
57	MG	AA	1704	1/1	0.57	0.29	-	103,103,103,103	0
57	MG	AA	1792	1/1	0.90	0.51	-	58,58,58,58	0
57	MG	AV	103	1/1	0.73	0.44	-	81,81,81,81	0
57	MG	AA	1775	1/1	0.80	0.57	-	92,92,92,92	0
57	MG	DX	102	1/1	0.30	1.07	-	126,126,126,126	0
57	MG	BA	3385	1/1	0.96	0.12	-	87,87,87,87	0
57	MG	DA	3188	1/1	0.74	1.99	-	111,111,111,111	0
57	MG	CA	1706	1/1	0.66	0.70	-	80,80,80,80	0
57	MG	BA	3218	1/1	0.97	0.35	-	6,6,6,6	0
57	MG	DA	3127	1/1	0.84	0.46	-	67,67,67,67	0
57	MG	CA	1641	1/1	0.95	0.42	-	64,64,64,64	0
57	MG	DA	3069	1/1	0.92	0.27	-	75,75,75,75	0
57	MG	DA	3179	1/1	0.87	0.18	-	80,80,80,80	0
57	MG	BA	3346	1/1	0.94	0.38	-	67,67,67,67	0
57	MG	CW	101	1/1	0.89	0.41	-	144,144,144,144	0
57	MG	AA	1756	1/1	0.93	0.27	-	47,47,47,47	1
57	MG	BA	3287	1/1	0.99	0.51	-	31,31,31,31	0
57	MG	AA	1667	1/1	0.44	0.49	-	72,72,72,72	0
57	MG	AA	1783	1/1	0.29	0.34	-	105,105,105,105	0
57	MG	CA	1718	1/1	0.93	0.15	-	67,67,67,67	0
57	MG	BA	3197	1/1	0.95	0.32	-	46,46,46,46	0
57	MG	BA	3226	1/1	0.80	0.17	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1760	1/1	0.93	0.43	-	90,90,90,90	0
57	MG	BA	3310	1/1	0.67	0.19	-	102,102,102,102	1
57	MG	BA	3370	1/1	0.95	0.40	-	113,113,113,113	0
57	MG	DA	3402	1/1	0.91	0.41	-	125,125,125,125	0
57	MG	BA	3029	1/1	0.98	0.12	-	40,40,40,40	0
57	MG	CA	1794	1/1	0.92	0.60	-	81,81,81,81	0
57	MG	BA	3111	1/1	0.97	0.41	-	23,23,23,23	0
57	MG	DA	3314	1/1	0.92	0.20	-	141,141,141,141	0
57	MG	AA	1660	1/1	0.92	0.38	-	43,43,43,43	0
57	MG	DA	3039	1/1	0.98	0.05	-	70,70,70,70	0
57	MG	BA	3098	1/1	0.95	0.20	-	6,6,6,6	0
57	MG	BA	3243	1/1	0.90	0.16	-	65,65,65,65	0
57	MG	AA	1635	1/1	0.68	0.26	-	92,92,92,92	0
57	MG	DA	3028	1/1	0.92	0.44	-	47,47,47,47	0
57	MG	AA	1602	1/1	0.76	0.28	-	97,97,97,97	0
57	MG	DA	3164	1/1	0.85	0.21	-	84,84,84,84	0
57	MG	DA	3216	1/1	0.87	0.50	-	74,74,74,74	0
57	MG	DA	3336	1/1	0.93	0.17	-	77,77,77,77	1
57	MG	CA	1743	1/1	0.98	0.50	-	65,65,65,65	0
57	MG	BA	3153	1/1	0.89	0.40	-	20,20,20,20	1
57	MG	AL	202	1/1	-0.37	0.33	-	165,165,165,165	0
57	MG	DB	210	1/1	0.93	0.27	-	74,74,74,74	0
57	MG	AA	1645	1/1	0.89	0.53	-	41,41,41,41	0
57	MG	CA	1639	1/1	0.97	0.16	-	62,62,62,62	0
57	MG	DA	3383	1/1	0.86	0.39	-	67,67,67,67	0
57	MG	CA	1604	1/1	0.90	0.18	-	63,63,63,63	0
57	MG	BA	3336	1/1	0.99	0.09	-	105,105,105,105	1
57	MG	DA	3159	1/1	0.95	0.58	-	70,70,70,70	0
57	MG	CA	1738	1/1	0.88	0.24	-	62,62,62,62	0
57	MG	CA	1621	1/1	0.97	0.08	-	58,58,58,58	0
57	MG	DA	3330	1/1	0.97	0.13	-	51,51,51,51	1
57	MG	AA	1748	1/1	0.80	0.35	-	144,144,144,144	1
57	MG	BA	3166	1/1	0.92	0.07	-	31,31,31,31	0
57	MG	AW	104	1/1	0.76	0.11	-	60,60,60,60	1
57	MG	BA	3133	1/1	0.93	0.22	-	19,19,19,19	0
57	MG	DA	3201	1/1	0.87	1.31	-	88,88,88,88	0
57	MG	DA	3211	1/1	0.90	0.30	-	45,45,45,45	0
57	MG	DB	213	1/1	0.78	0.51	-	93,93,93,93	0
57	MG	AA	1734	1/1	0.72	0.80	-	102,102,102,102	0
57	MG	BB	207	1/1	0.84	0.42	-	29,29,29,29	1
57	MG	DA	3157	1/1	0.51	0.61	-	79,79,79,79	0
57	MG	DA	3332	1/1	0.94	0.43	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1747	1/1	0.92	0.49	-	62,62,62,62	0
57	MG	AA	1693	1/1	0.89	0.15	-	54,54,54,54	0
57	MG	DA	3150	1/1	0.89	0.31	-	65,65,65,65	1
57	MG	AA	1761	1/1	0.23	0.92	-	122,122,122,122	0
57	MG	BA	3260	1/1	0.97	0.50	-	30,30,30,30	0
57	MG	CA	1696	1/1	0.93	0.55	-	108,108,108,108	0
57	MG	BA	3296	1/1	0.89	0.21	-	66,66,66,66	0
57	MG	AA	1601	1/1	0.72	0.26	-	90,90,90,90	0
57	MG	CX	102	1/1	0.99	0.09	-	110,110,110,110	0
57	MG	BA	3284	1/1	0.94	0.65	-	53,53,53,53	0
57	MG	BA	3101	1/1	0.07	0.77	-	72,72,72,72	1
57	MG	DA	3156	1/1	0.95	0.49	-	38,38,38,38	0
57	MG	AA	1718	1/1	0.93	0.18	-	72,72,72,72	0
57	MG	DA	3068	1/1	0.90	0.35	-	98,98,98,98	0
57	MG	BA	3290	1/1	0.84	0.62	-	78,78,78,78	1
57	MG	BA	3288	1/1	0.90	0.74	-	59,59,59,59	0
57	MG	BA	3036	1/1	0.98	0.22	-	29,29,29,29	0
57	MG	DA	3338	1/1	0.77	0.30	-	74,74,74,74	0
57	MG	BA	3337	1/1	0.96	0.14	-	162,162,162,162	0
57	MG	BA	3139	1/1	0.99	0.16	-	85,85,85,85	0
57	MG	DA	3212	1/1	0.84	0.94	-	91,91,91,91	0
57	MG	DB	208	1/1	0.80	1.58	-	76,76,76,76	1
57	MG	AA	1766	1/1	0.91	0.27	-	67,67,67,67	0
57	MG	DB	211	1/1	0.87	0.25	-	119,119,119,119	0
57	MG	DA	3155	1/1	0.92	0.40	-	21,21,21,21	1
57	MG	DA	3238	1/1	0.83	0.33	-	56,56,56,56	0
57	MG	AA	1624	1/1	0.95	0.39	-	52,52,52,52	0
57	MG	CA	1660	1/1	0.75	0.35	-	59,59,59,59	0
57	MG	BA	3417	1/1	0.59	0.11	-	72,72,72,72	0
57	MG	DA	3259	1/1	0.78	0.34	-	56,56,56,56	0
57	MG	CA	1722	1/1	0.93	0.47	-	121,121,121,121	0
57	MG	DA	3292	1/1	0.90	0.89	-	51,51,51,51	1
57	MG	CA	1632	1/1	0.79	0.34	-	54,54,54,54	1
57	MG	AA	1609	1/1	0.96	0.20	-	36,36,36,36	0
57	MG	BA	3311	1/1	0.69	0.24	-	74,74,74,74	1
57	MG	BA	3326	1/1	0.85	0.28	-	46,46,46,46	1
57	MG	DA	3086	1/1	0.87	0.29	-	56,56,56,56	0
57	MG	AA	1622	1/1	0.36	0.55	-	135,135,135,135	0
57	MG	CA	1700	1/1	0.85	0.09	-	101,101,101,101	0
57	MG	CV	105	1/1	0.84	0.14	-	65,65,65,65	0
57	MG	BA	3319	1/1	0.91	0.24	-	3,3,3,3	1
57	MG	BA	3368	1/1	0.82	0.22	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3032	1/1	0.93	0.23	-	45,45,45,45	0
57	MG	BA	3408	1/1	0.92	0.19	-	43,43,43,43	0
57	MG	AA	1649	1/1	0.98	0.13	-	56,56,56,56	1
57	MG	DA	3382	1/1	0.98	0.13	-	74,74,74,74	0
57	MG	BA	3303	1/1	0.98	0.18	-	49,49,49,49	1
57	MG	DA	3139	1/1	0.71	1.40	-	112,112,112,112	0
57	MG	DA	3011	1/1	0.97	0.48	-	52,52,52,52	0
57	MG	CA	1759	1/1	0.77	0.67	-	67,67,67,67	1
57	MG	DA	3412	1/1	0.81	0.36	-	74,74,74,74	0
57	MG	CA	1787	1/1	0.92	0.13	-	66,66,66,66	0
57	MG	CA	1617	1/1	0.72	0.55	-	81,81,81,81	0
57	MG	BA	3242	1/1	0.88	0.49	-	60,60,60,60	0
57	MG	BA	3369	1/1	0.95	0.33	-	53,53,53,53	1
57	MG	AA	1611	1/1	0.88	0.20	-	63,63,63,63	0
57	MG	BA	3085	1/1	0.94	0.24	-	21,21,21,21	0
57	MG	CA	1774	1/1	0.95	0.19	-	121,121,121,121	0
57	MG	BA	3387	1/1	0.90	0.66	-	119,119,119,119	0
57	MG	CA	1757	1/1	0.84	0.49	-	128,128,128,128	0
57	MG	DA	3135	1/1	0.78	0.28	-	39,39,39,39	0
57	MG	BA	3066	1/1	0.95	0.33	-	26,26,26,26	0
57	MG	BA	3331	1/1	0.64	0.43	-	65,65,65,65	1
57	MG	AA	1717	1/1	0.95	0.32	-	61,61,61,61	0
57	MG	DA	3107	1/1	0.96	0.09	-	32,32,32,32	0
57	MG	BA	3015	1/1	0.95	0.35	-	33,33,33,33	0
57	MG	BA	3281	1/1	0.81	0.38	-	53,53,53,53	0
57	MG	DA	3310	1/1	0.92	0.41	-	54,54,54,54	1
57	MG	CA	1773	1/1	0.86	0.76	-	55,55,55,55	0
57	MG	AA	1680	1/1	0.92	0.58	-	53,53,53,53	0
57	MG	AW	106	1/1	0.72	0.27	-	102,102,102,102	1
57	MG	AW	105	1/1	0.72	0.41	-	154,154,154,154	1
57	MG	CA	1726	1/1	0.39	0.58	-	104,104,104,104	1
57	MG	DA	3377	1/1	0.96	0.33	-	24,24,24,24	0
57	MG	BA	3148	1/1	0.95	0.22	-	57,57,57,57	0
57	MG	CA	1658	1/1	0.92	0.23	-	78,78,78,78	0
57	MG	BA	3056	1/1	0.92	0.34	-	17,17,17,17	0
57	MG	DA	3228	1/1	0.53	0.28	-	83,83,83,83	0
57	MG	AA	1613	1/1	0.97	0.19	-	81,81,81,81	0
57	MG	BA	3121	1/1	0.87	0.34	-	40,40,40,40	0
57	MG	BA	3124	1/1	0.93	0.25	-	46,46,46,46	0
57	MG	CA	1656	1/1	0.65	0.54	-	120,120,120,120	0
57	MG	AA	1655	1/1	0.83	0.36	-	74,74,74,74	0
57	MG	BA	3187	1/1	0.85	0.41	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3027	1/1	0.94	0.19	-	30,30,30,30	0
57	MG	BA	3003	1/1	0.88	0.88	-	85,85,85,85	0
57	MG	DA	3316	1/1	0.99	0.09	-	88,88,88,88	0
57	MG	AA	1769	1/1	0.65	0.52	-	80,80,80,80	0
57	MG	DA	3358	1/1	0.71	0.77	-	94,94,94,94	0
57	MG	CA	1796	1/1	0.95	0.25	-	119,119,119,119	0
57	MG	AA	1708	1/1	0.81	0.41	-	72,72,72,72	0
57	MG	DA	3034	1/1	0.90	0.51	-	52,52,52,52	0
57	MG	DA	3313	1/1	0.98	0.32	-	80,80,80,80	0
57	MG	DA	3136	1/1	0.61	0.88	-	63,63,63,63	0
57	MG	DA	3105	1/1	0.93	0.28	-	54,54,54,54	0
57	MG	DA	3166	1/1	0.69	0.41	-	75,75,75,75	0
57	MG	BA	3356	1/1	0.85	0.19	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.