



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

PDB ID : 4V7M
Title : The structures of Capreomycin bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-11-12
Resolution : 3.45 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

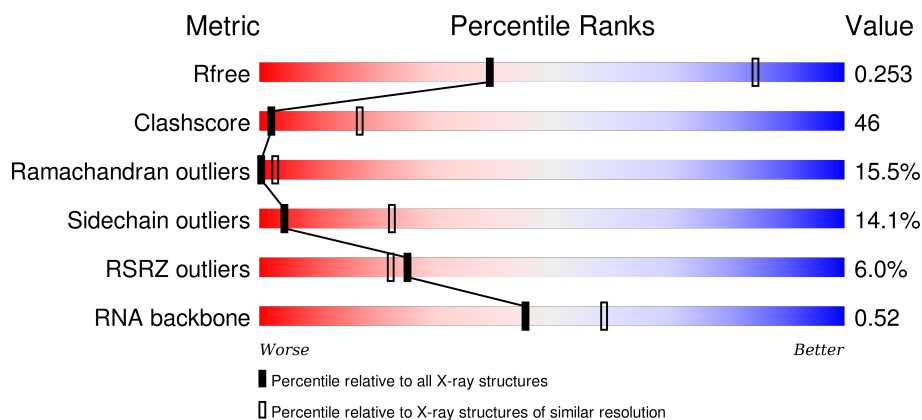
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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.





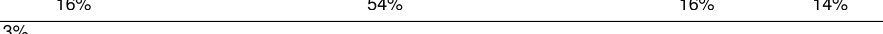
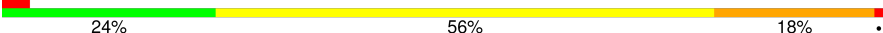
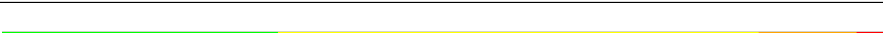
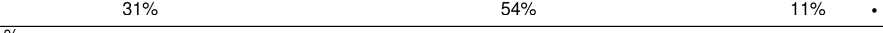
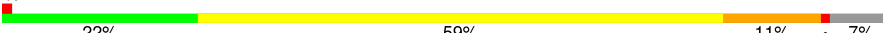
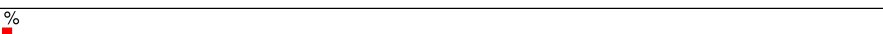
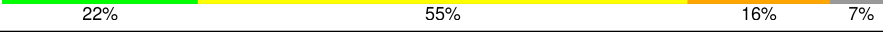
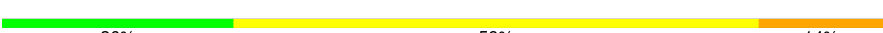
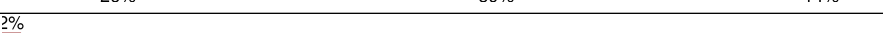
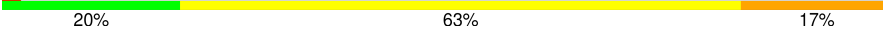

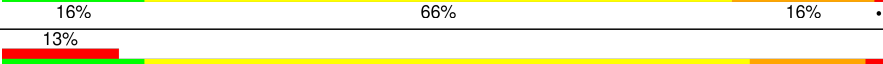
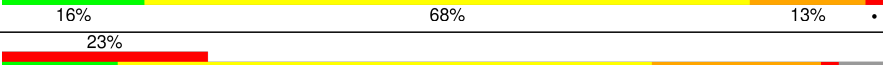

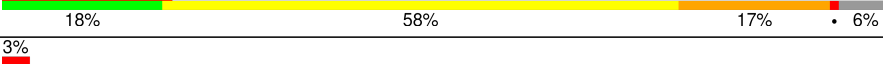
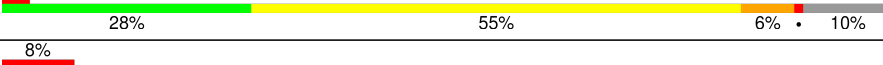

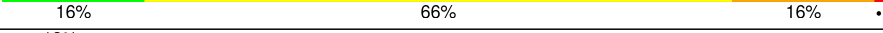
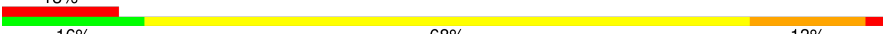



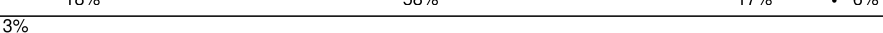
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)
RNA backbone	2183	1045 (4.10-2.80)

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	1508	<div> <div>2%</div> <div>22% 62% 13% ..</div> </div>
1	CA	1508	<div> <div>2%</div> <div>20% 63% 14% ..</div> </div>
2	AB	256	<div> <div>4%</div> <div>13% 61% 16% • 8%</div> </div>
2	CB	256	<div> <div>8%</div> <div>17% 58% 14% • 8%</div> </div>


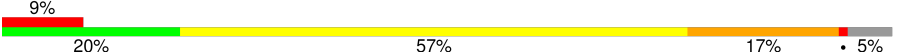

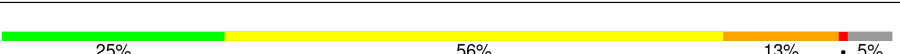
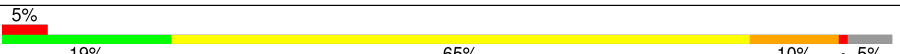
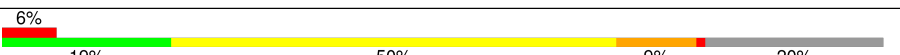
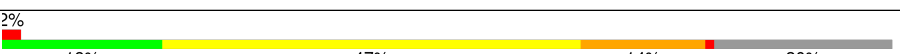
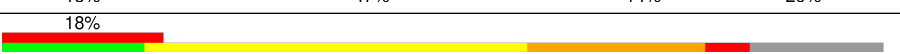
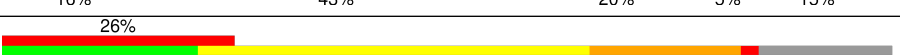
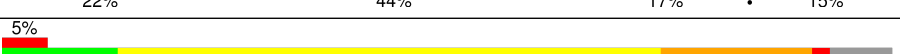
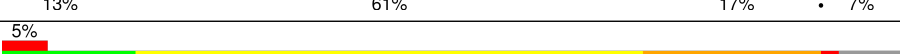
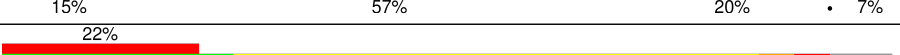

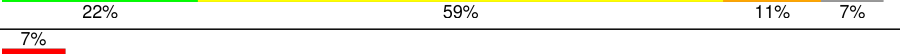


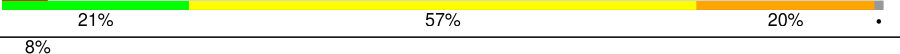
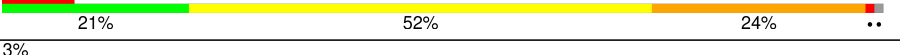
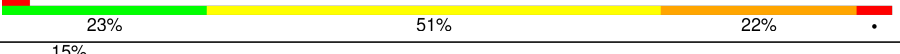
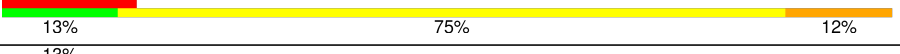
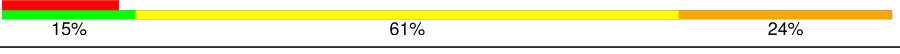
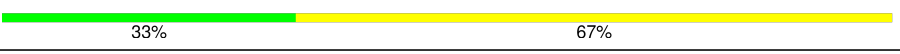

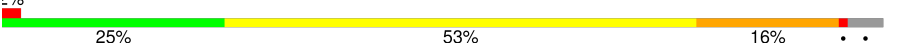
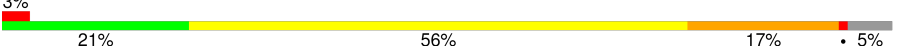
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
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	30	
22	CV	30	
23	AW	75	
23	CW	75	
24	AX	77	
25	AY	75	
25	CY	75	
26	AZ	6	
26	CZ	6	
27	BA	2915	
27	DA	2915	
28	BB	122	

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Mol	Chain	Length	Quality of chain
28	DB	122	
29	BC	229	
29	DC	229	
30	BD	276	
30	DD	276	
31	BE	206	
31	DE	206	
32	BF	210	
32	DF	210	
33	BG	182	
33	DG	182	
34	BH	180	
34	DH	180	
35	BI	148	
35	DI	148	
36	BN	140	
36	DN	140	
37	BO	122	
37	DO	122	
38	BP	150	
38	DP	150	
39	BQ	141	
39	DQ	141	
40	BR	118	
40	DR	118	


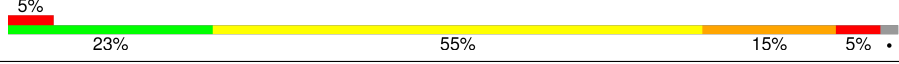
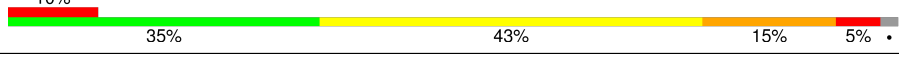

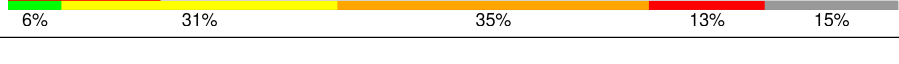
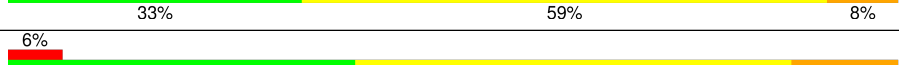
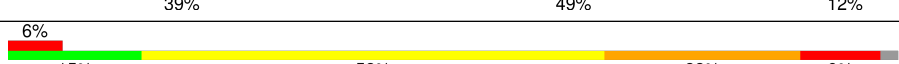
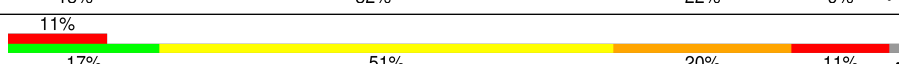
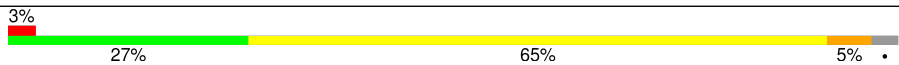

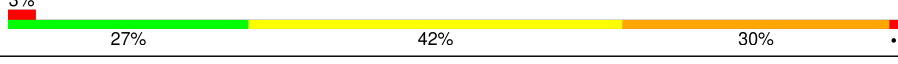

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Mol	Chain	Length	Quality of chain
41	BS	112	
41	DS	112	
42	BT	146	
42	DT	146	
43	BU	118	
43	DU	118	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	96	
46	DX	96	
47	BY	110	
47	DY	110	
48	BZ	206	
48	DZ	206	
49	B0	85	
49	D0	85	
50	B1	98	
50	D1	98	
51	B2	72	
51	D2	72	
52	B3	60	
52	D3	60	
53	B4	71	

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Mol	Chain	Length	Quality of chain
53	D4	71	
54	B5	60	
54	D5	60	
55	B6	54	
55	D6	54	
56	B7	49	
56	D7	49	
57	B8	65	
57	D8	65	
58	B9	37	
58	D9	37	
59	CX	77	

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
26	DPP	AZ	2	-	-	X	-
26	KBE	CZ	1	-	-	X	-
26	DPP	CZ	2	-	-	X	-
60	MG	AA	1615	-	-	-	X
60	MG	AA	1617	-	-	-	X
60	MG	AA	1618	-	-	-	X
60	MG	AA	1621	-	-	-	X
60	MG	AA	1633	-	-	-	X
60	MG	AA	1637	-	-	-	X
60	MG	AA	1640	-	-	-	X
60	MG	AA	1642	-	-	-	X
60	MG	AA	1643	-	-	-	X
60	MG	AA	1646	-	-	-	X
60	MG	AA	1654	-	-	-	X
60	MG	AA	1655	-	-	-	X
60	MG	AA	1675	-	-	-	X
60	MG	BA	3004	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3005	-	-	-	X
60	MG	BA	3009	-	-	-	X
60	MG	BA	3010	-	-	-	X
60	MG	BA	3013	-	-	-	X
60	MG	BA	3016	-	-	-	X
60	MG	BA	3017	-	-	-	X
60	MG	BA	3018	-	-	-	X
60	MG	BA	3020	-	-	-	X
60	MG	BA	3021	-	-	-	X
60	MG	BA	3027	-	-	-	X
60	MG	BA	3029	-	-	-	X
60	MG	BA	3030	-	-	-	X
60	MG	BA	3031	-	-	-	X
60	MG	BA	3034	-	-	-	X
60	MG	BA	3037	-	-	-	X
60	MG	BA	3042	-	-	-	X
60	MG	BA	3044	-	-	-	X
60	MG	BA	3046	-	-	-	X
60	MG	BA	3049	-	-	-	X
60	MG	BA	3055	-	-	-	X
60	MG	BA	3062	-	-	-	X
60	MG	BA	3070	-	-	-	X
60	MG	BA	3076	-	-	-	X
60	MG	BA	3077	-	-	-	X
60	MG	BA	3078	-	-	-	X
60	MG	BA	3080	-	-	-	X
60	MG	BA	3082	-	-	-	X
60	MG	BA	3083	-	-	-	X
60	MG	BA	3094	-	-	-	X
60	MG	BA	3104	-	-	-	X
60	MG	BA	3108	-	-	-	X
60	MG	BA	3117	-	-	-	X
60	MG	BA	3119	-	-	-	X
60	MG	BA	3121	-	-	-	X
60	MG	BA	3131	-	-	-	X
60	MG	BA	3133	-	-	-	X
60	MG	BA	3134	-	-	-	X
60	MG	BA	3137	-	-	-	X
60	MG	BA	3141	-	-	-	X
60	MG	BA	3142	-	-	-	X
60	MG	BA	3143	-	-	-	X
60	MG	BA	3149	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3156	-	-	-	X
60	MG	BA	3158	-	-	-	X
60	MG	BA	3162	-	-	-	X
60	MG	BA	3167	-	-	-	X
60	MG	BA	3169	-	-	-	X
60	MG	BA	3177	-	-	-	X
60	MG	BA	3178	-	-	-	X
60	MG	BA	3179	-	-	-	X
60	MG	BA	3227	-	-	-	X
60	MG	BA	3229	-	-	-	X
60	MG	BA	3232	-	-	-	X
60	MG	BA	3234	-	-	-	X
60	MG	BA	3251	-	-	-	X
60	MG	BA	3284	-	-	-	X
60	MG	BA	3293	-	-	-	X
60	MG	BA	3306	-	-	-	X
60	MG	BU	201	-	-	-	X
60	MG	CA	1610	-	-	-	X
60	MG	CA	1612	-	-	-	X
60	MG	CA	1614	-	-	-	X
60	MG	CA	1620	-	-	-	X
60	MG	CA	1622	-	-	-	X
60	MG	CA	1635	-	-	-	X
60	MG	CA	1650	-	-	-	X
60	MG	CA	1657	-	-	-	X
60	MG	CA	1673	-	-	-	X
60	MG	CA	1677	-	-	-	X
60	MG	CA	1682	-	-	-	X
60	MG	CA	1683	-	-	-	X
60	MG	CA	1686	-	-	-	X
60	MG	CA	1692	-	-	-	X
60	MG	DA	3005	-	-	-	X
60	MG	DA	3006	-	-	-	X
60	MG	DA	3008	-	-	-	X
60	MG	DA	3014	-	-	-	X
60	MG	DA	3040	-	-	-	X
60	MG	DA	3042	-	-	-	X
60	MG	DA	3061	-	-	-	X
60	MG	DA	3065	-	-	-	X
60	MG	DA	3073	-	-	-	X
60	MG	DA	3075	-	-	-	X
60	MG	DA	3078	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3084	-	-	-	X
60	MG	DA	3092	-	-	-	X
60	MG	DA	3096	-	-	-	X
60	MG	DA	3102	-	-	-	X
60	MG	DA	3111	-	-	-	X
60	MG	DA	3117	-	-	-	X
60	MG	DA	3118	-	-	-	X
60	MG	DA	3120	-	-	-	X
60	MG	DA	3128	-	-	-	X
60	MG	DA	3139	-	-	-	X
60	MG	DA	3146	-	-	-	X
60	MG	DA	3160	-	-	-	X
60	MG	DA	3167	-	-	-	X
60	MG	DA	3169	-	-	-	X
60	MG	DA	3173	-	-	-	X
60	MG	DA	3174	-	-	-	X
60	MG	DA	3180	-	-	-	X
60	MG	DA	3186	-	-	-	X
60	MG	DA	3193	-	-	-	X
60	MG	DA	3195	-	-	-	X
60	MG	DA	3205	-	-	-	X
60	MG	DA	3206	-	-	-	X
60	MG	DA	3215	-	-	-	X
60	MG	DA	3236	-	-	-	X
60	MG	DA	3237	-	-	-	X
60	MG	DF	301	-	-	-	X
60	MG	DO	201	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 293848 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1495	Total	C	N	O	P	0	0	0
			32132	14303	5953	10382	1494			
1	CA	1493	Total	C	N	O	P	0	0	0
			32098	14287	5956	10363	1492			

- 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	206	Total	C	N	O	S	0	0	1
			1604	1011	314	278	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	154	Total	C	N	O	S	0	0	0
			1249	776	251	217	5			

- 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
			1006	637	195	174			
9	CI	127	Total	C	N	O	0	0	0
			1006	637	195	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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	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	122	Total	C	N	O	S	0	0	1
			965	597	200	166	2			
13	CM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	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 RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0	0
			205	93	40	63	9			
22	CV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			

- Molecule 23 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			
23	CW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			

- Molecule 24 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 25 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			
25	CY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	33	G	C	CONFLICT	GB CP001790.1
AY	44	U	A	CONFLICT	GB CP001790.1
CY	33	G	C	CONFLICT	GB CP001790.1
CY	44	U	A	CONFLICT	GB CP001790.1

- Molecule 26 is a protein called capreomycin IA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AZ	6	Total	C	N	O	0	0	0
			47	25	14	8			
26	CZ	6	Total	C	N	O	0	0	0
			47	25	14	8			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2789	Total	C	N	O	P	0	0	0
			60072	26734	11238	19312	2788			
27	DA	2775	Total	C	N	O	P	0	0	0
			59767	26598	11176	19219	2774			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 29 is a protein called 50S ribosomal protein L1.

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

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BF	206	Total	C	N	O	S	0	0	1
			1607	1024	301	280	2			
32	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BH	161	Total	C	N	O	S	0	0	0
			1233	783	227	222	1			
34	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			
39	DQ	138	Total	C	N	O	S	0	0	0
			1094	697	205	185	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	88	Total	C	N	O	S	0	0	1
			672	432	131	105	4			
47	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

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

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			
53	D4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	48	Total	C	N	O	S	0	0	1
			402	249	83	66	4			
55	D6	46	Total	C	N	O	S	0	0	1
			390	241	80	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

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

- Molecule 57 is a protein called 50S ribosomal protein L35.

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

- Molecule 58 is a protein called 50S ribosomal protein L36.

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

- Molecule 59 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CX	46	G	A	CONFLICT	GB CP001637.1

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	334	Total	Mg	0	0
			334	334		
60	CA	102	Total	Mg	0	0
			102	102		
60	DF	1	Total	Mg	0	0
			1	1		
60	CV	1	Total	Mg	0	0
			1	1		
60	BE	3	Total	Mg	0	0
			3	3		
60	AW	4	Total	Mg	0	0
			4	4		
60	BP	2	Total	Mg	0	0
			2	2		
60	AX	9	Total	Mg	0	0
			9	9		
60	B5	1	Total	Mg	0	0
			1	1		
60	BB	5	Total	Mg	0	0
			5	5		
60	DO	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BF	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	CK	1	Total 1	Mg 1	0	0
60	D7	1	Total 1	Mg 1	0	0
60	BU	2	Total 2	Mg 2	0	0
60	AA	114	Total 114	Mg 114	0	0
60	DD	2	Total 2	Mg 2	0	0
60	D0	1	Total 1	Mg 1	0	0
60	BG	1	Total 1	Mg 1	0	0
60	BR	1	Total 1	Mg 1	0	0
60	DA	239	Total 239	Mg 239	0	0
60	AG	1	Total 1	Mg 1	0	0
60	DE	1	Total 1	Mg 1	0	0
60	CW	4	Total 4	Mg 4	0	0
60	D5	1	Total 1	Mg 1	0	0
60	BD	1	Total 1	Mg 1	0	0
60	B0	3	Total 3	Mg 3	0	0
60	CE	1	Total 1	Mg 1	0	0
60	DB	3	Total 3	Mg 3	0	0

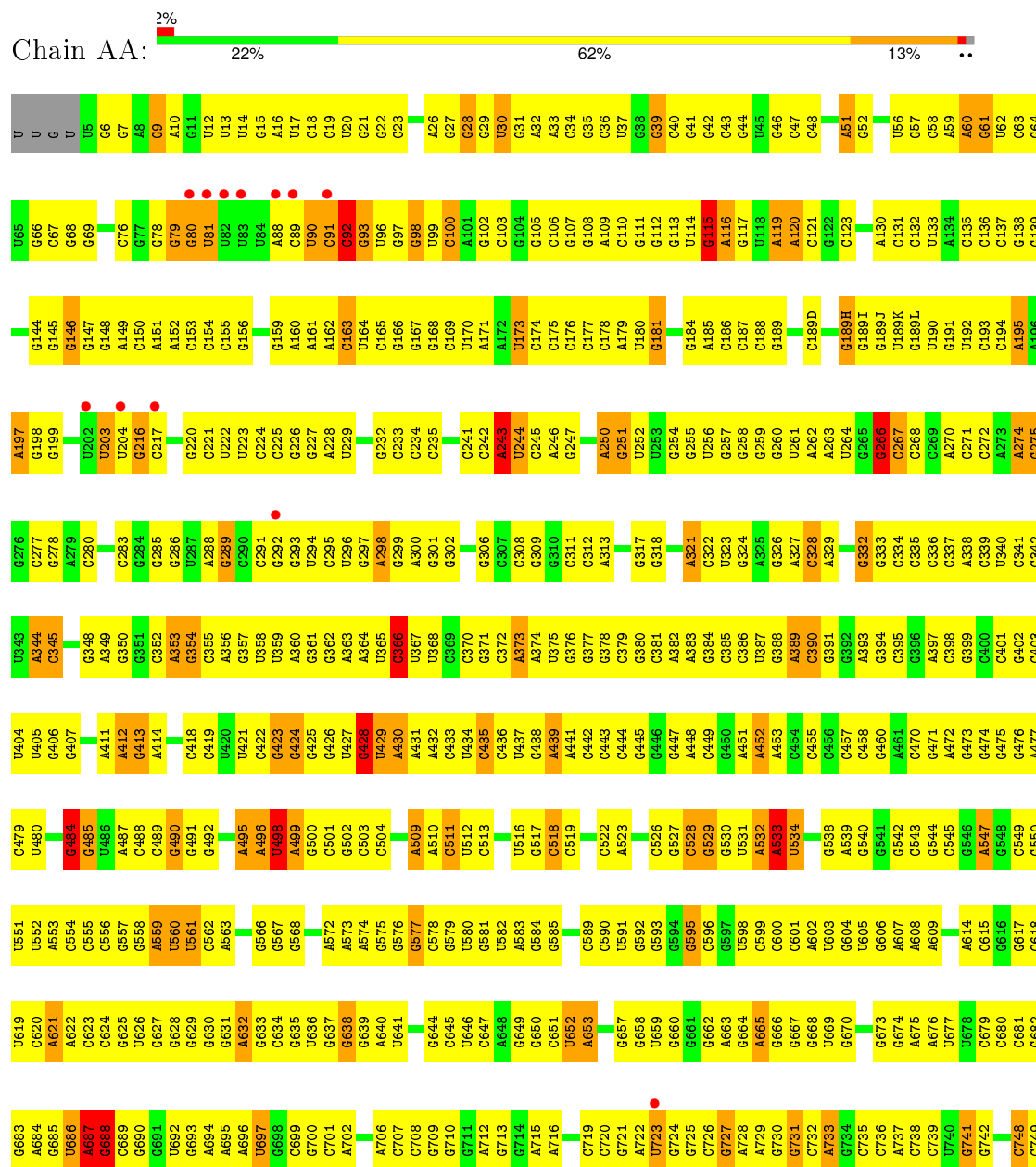
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

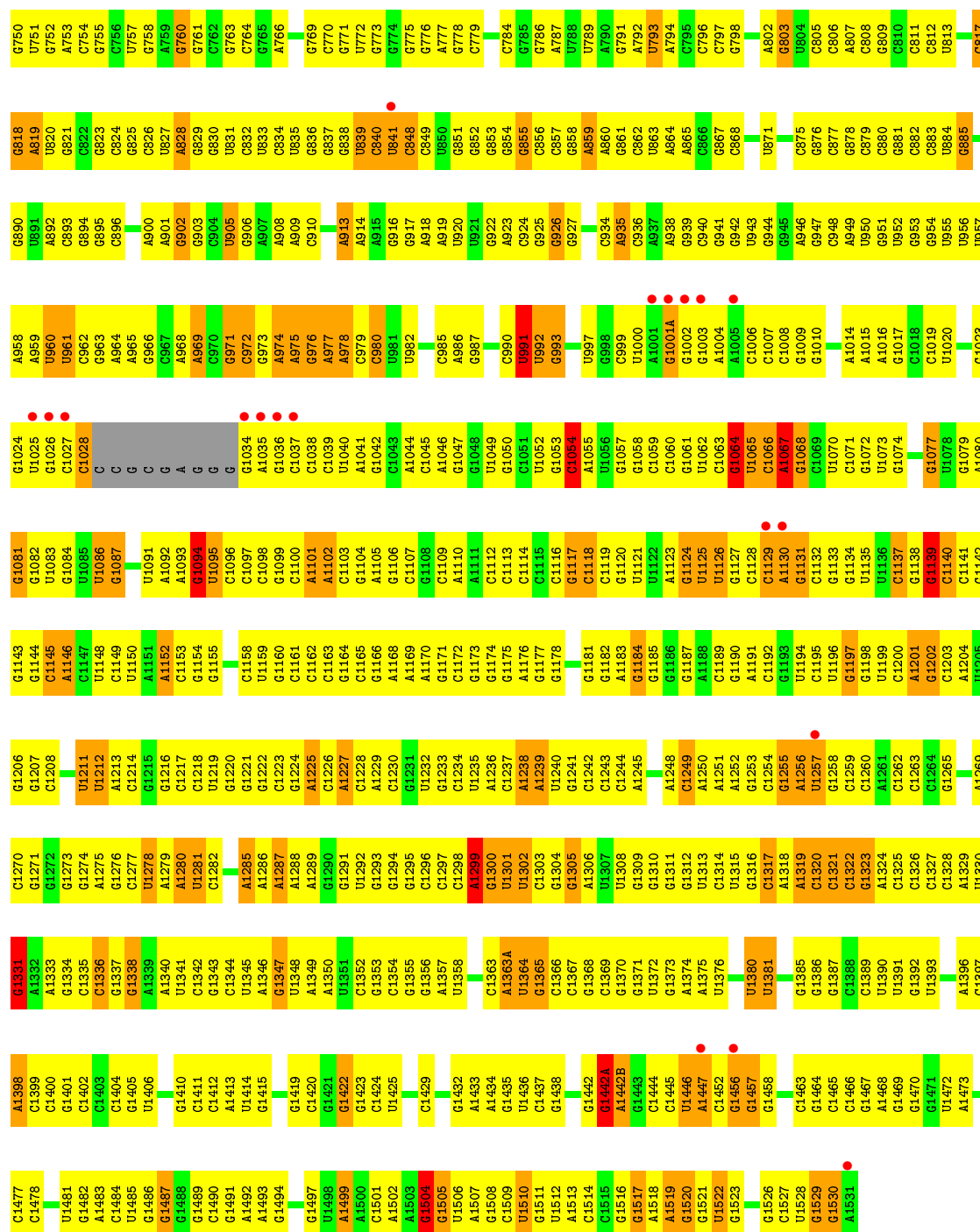
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B5	1	Total 1	Zn 1	0	0
61	B4	1	Total 1	Zn 1	0	0
61	AD	1	Total 1	Zn 1	0	0
61	B9	1	Total 1	Zn 1	0	0
61	D9	1	Total 1	Zn 1	0	0
61	D5	1	Total 1	Zn 1	0	0
61	D4	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

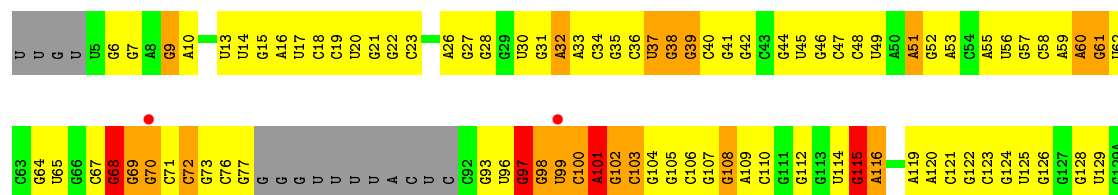
- Molecule 1: 16S ribosomal RNA



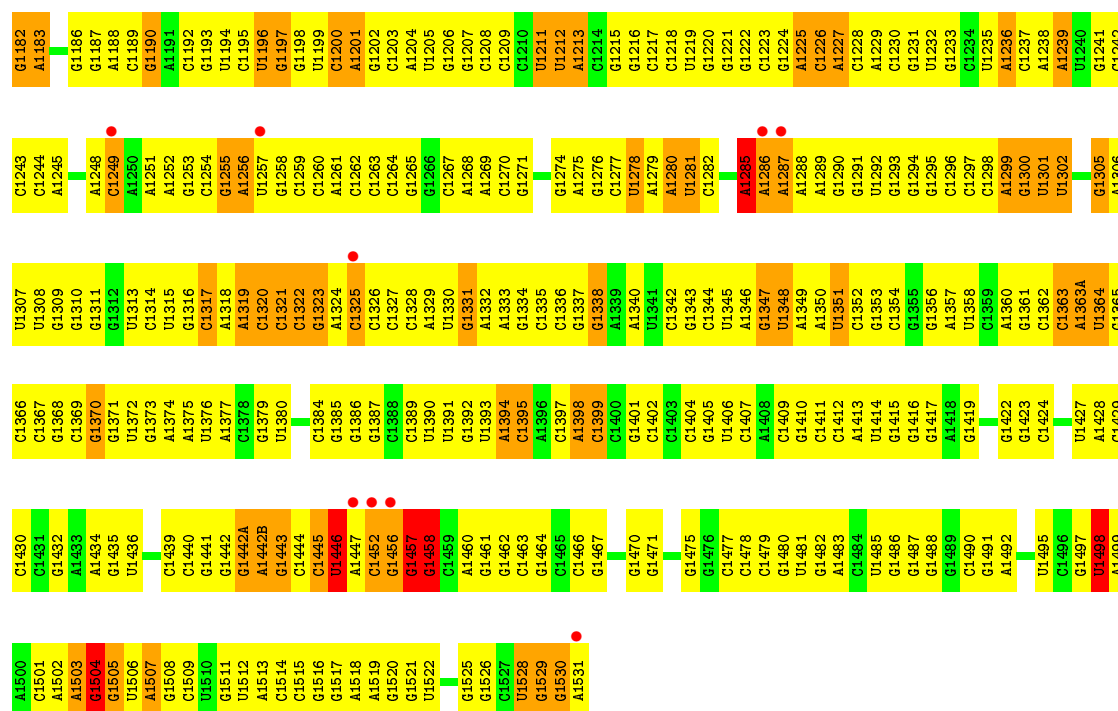


• Molecule 1: 16S ribosomal RNA

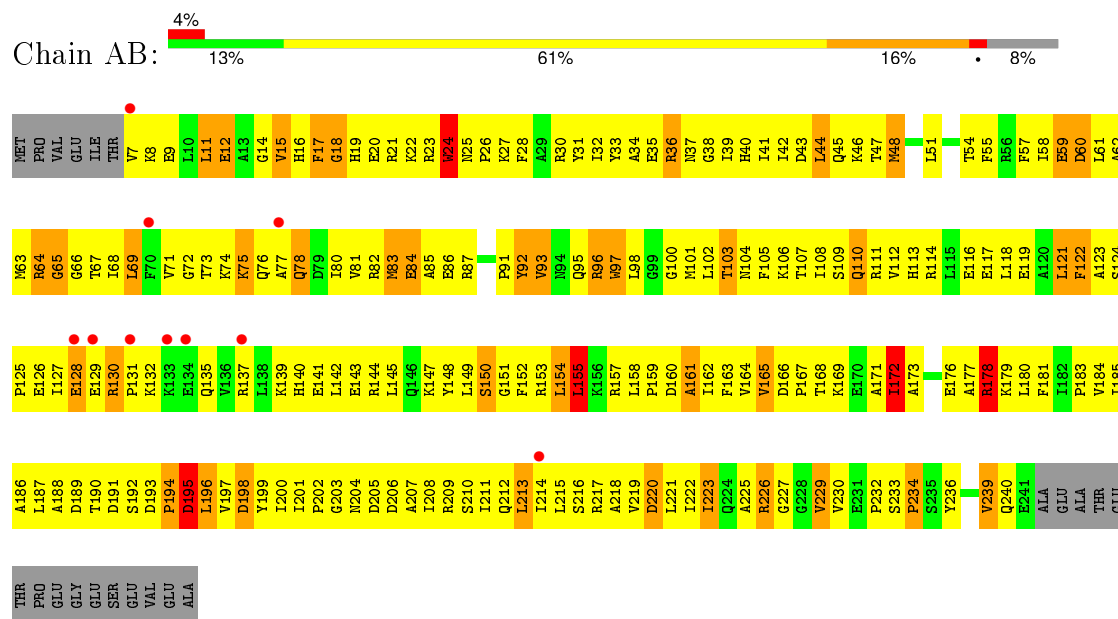
Chain CA:



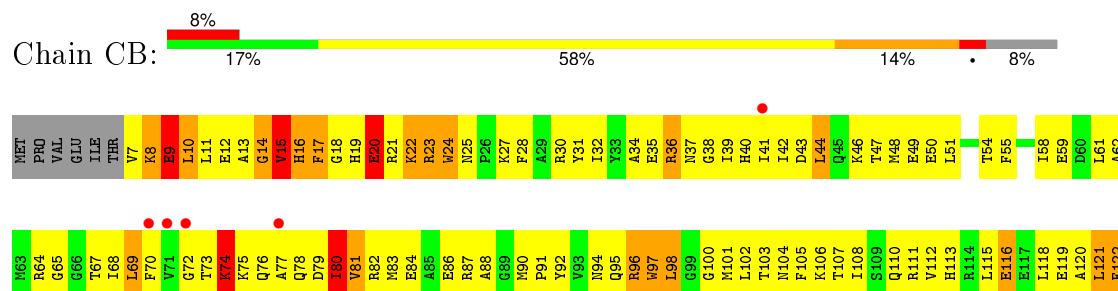


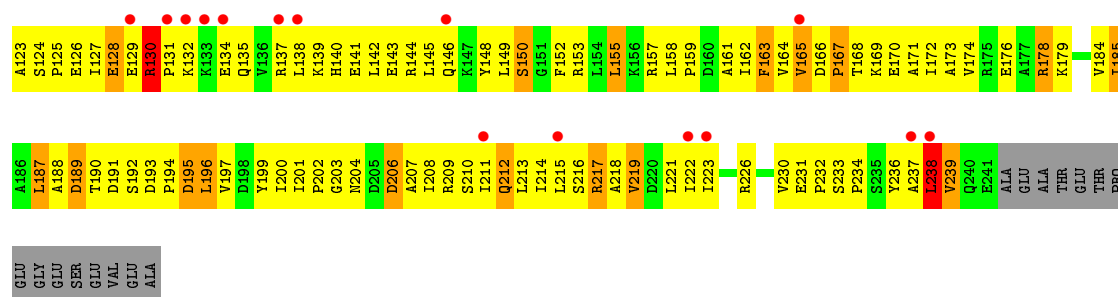


• Molecule 2: 30S ribosomal protein S2

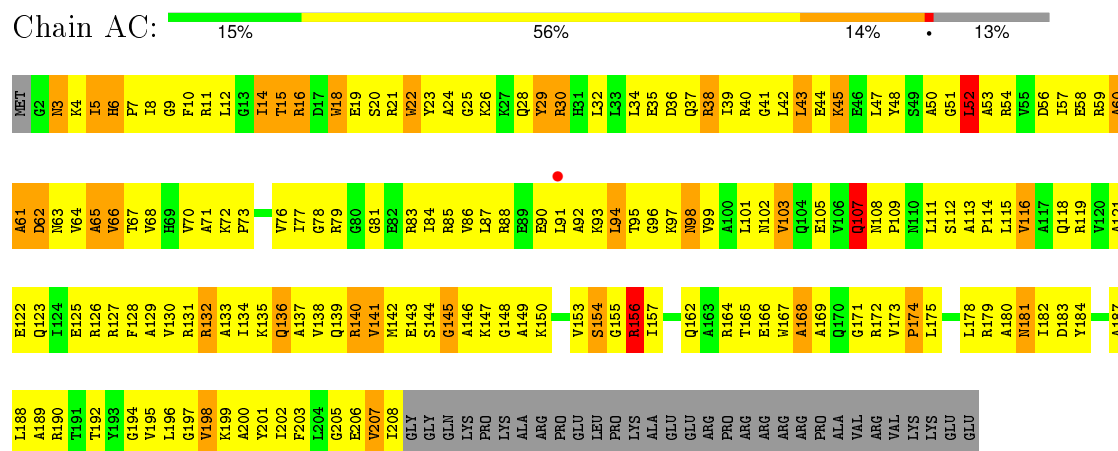


• Molecule 2: 30S ribosomal protein S2

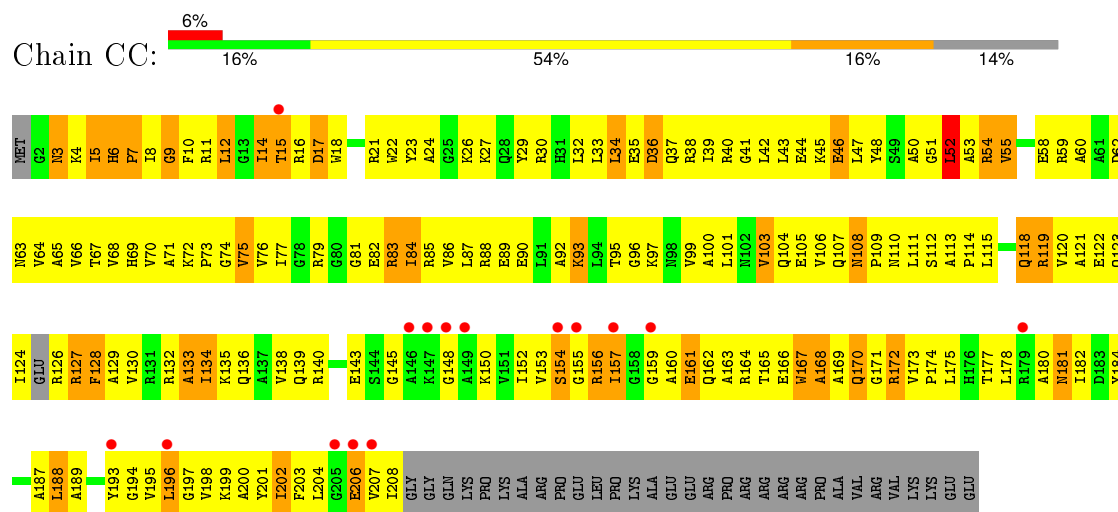




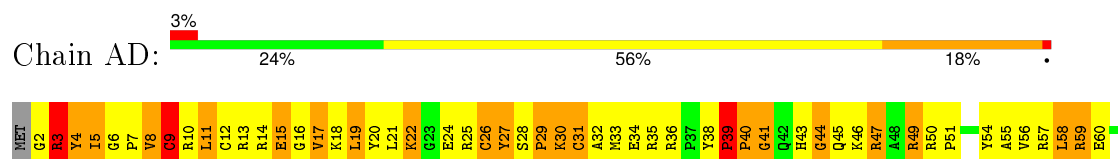
• Molecule 3: 30S ribosomal protein S3

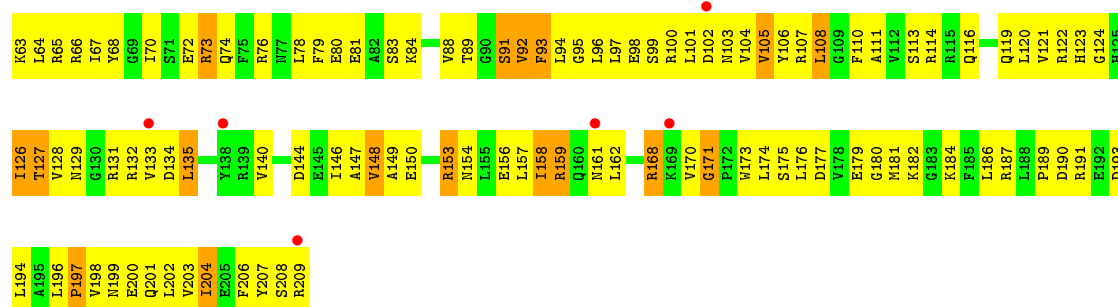


• Molecule 3: 30S ribosomal protein S3



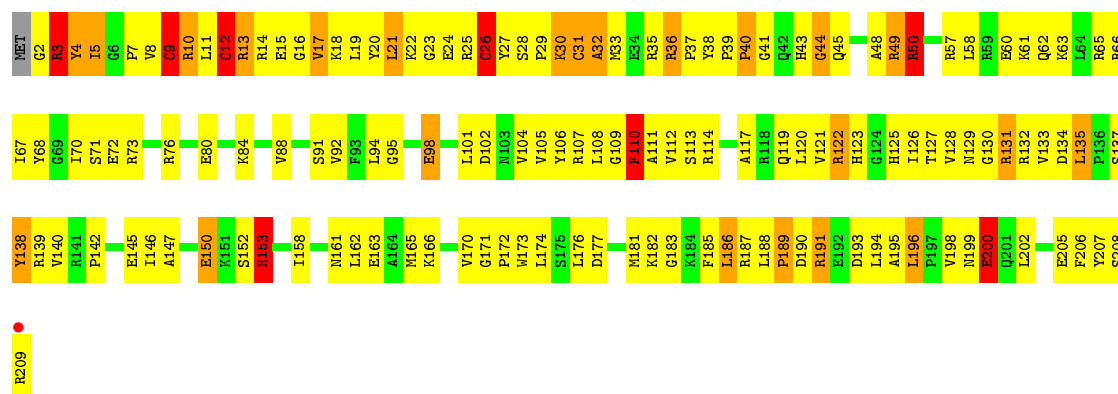
• Molecule 4: 30S ribosomal protein S4





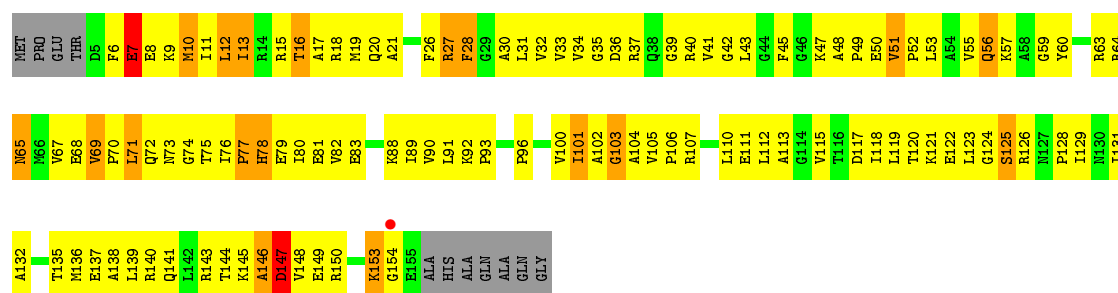
• Molecule 4: 30S ribosomal protein S4

Chain CD: 31% 54% 11% •



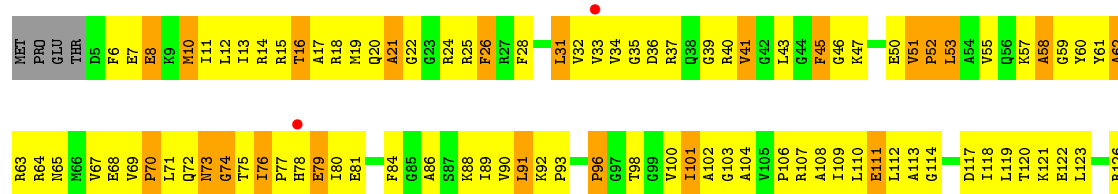
• Molecule 5: 30S ribosomal protein S5

Chain AE: 22% 59% 11% 7%



• Molecule 5: 30S ribosomal protein S5

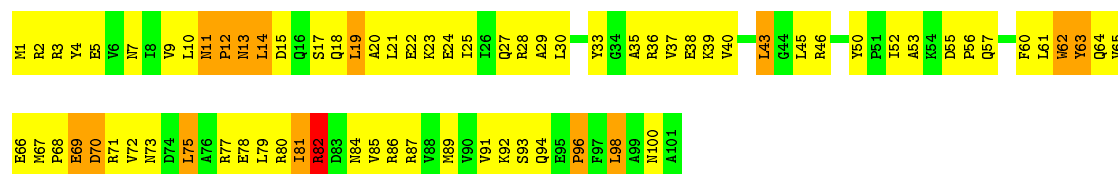
Chain CE: 22% 55% 16% 7%





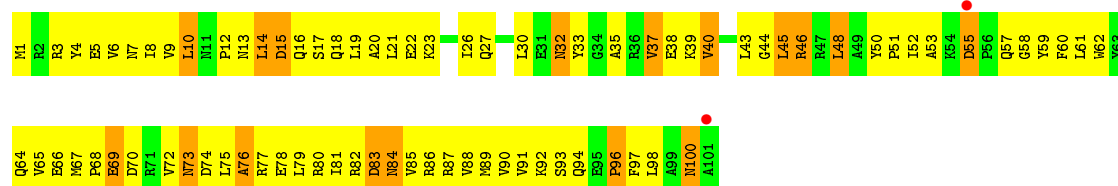
• Molecule 6: 30S ribosomal protein S6

Chain AF: 26% 59% 14%



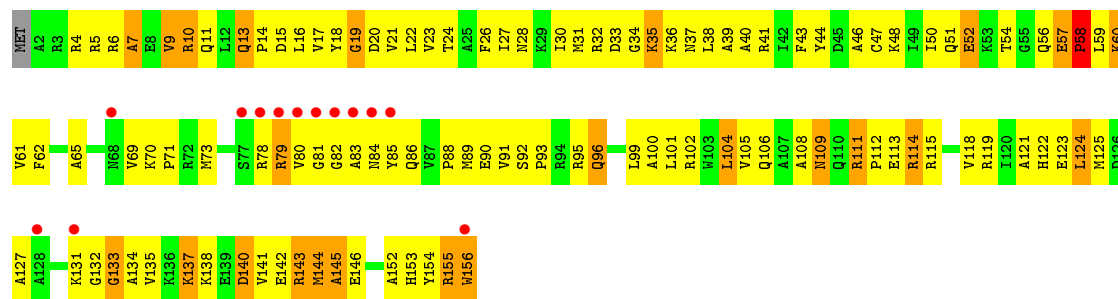
• Molecule 6: 30S ribosomal protein S6

Chain CF: 2% 20% 63% 17%



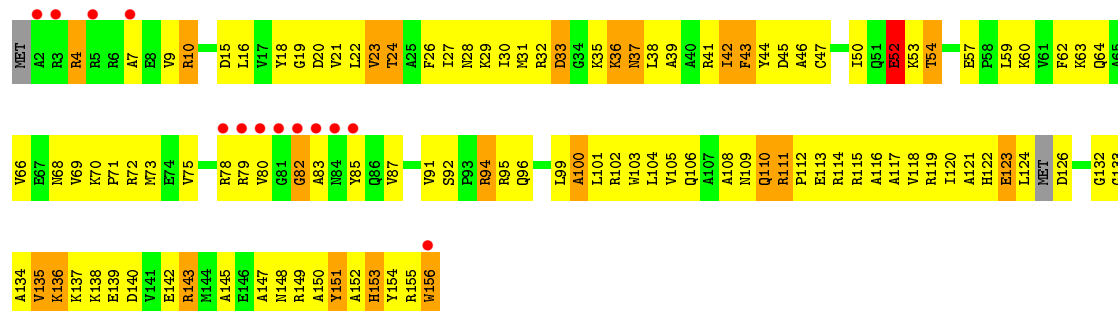
• Molecule 7: 30S ribosomal protein S7

Chain AG: 8% 27% 56% 15%

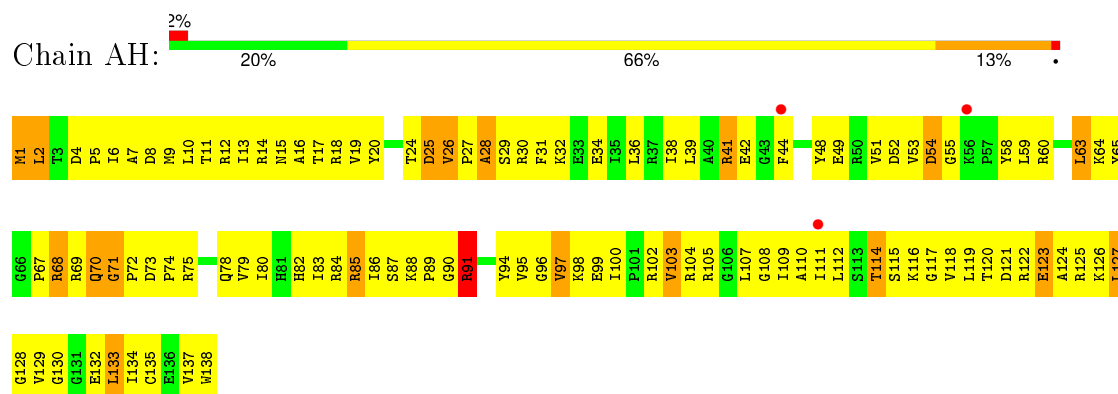


• Molecule 7: 30S ribosomal protein S7

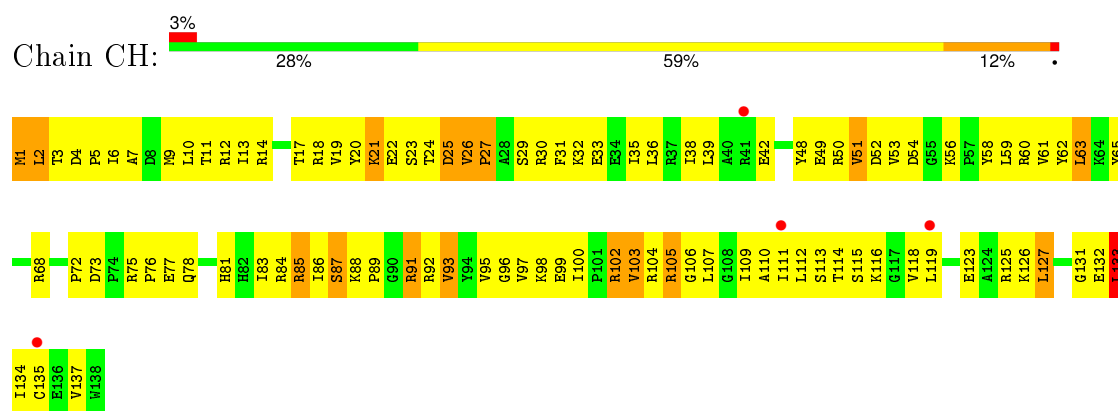
Chain CG: 8% 28% 56% 14%



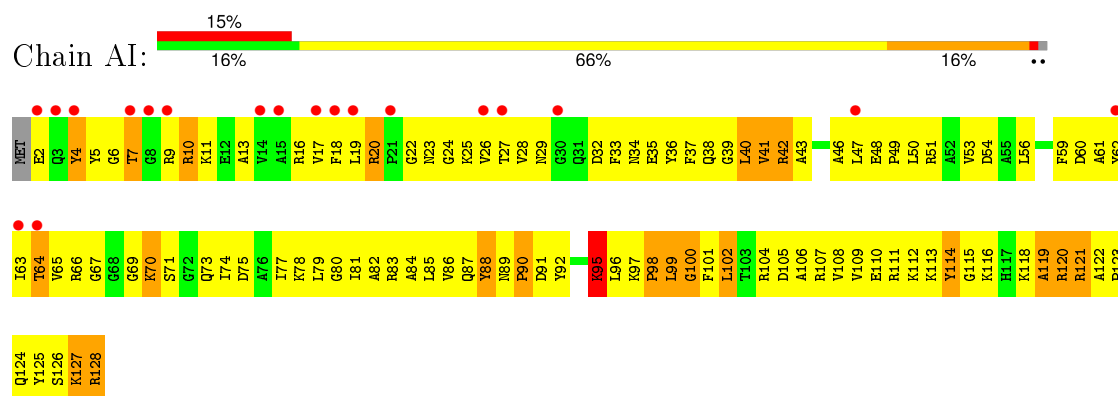
- Molecule 8: 30S ribosomal protein S8



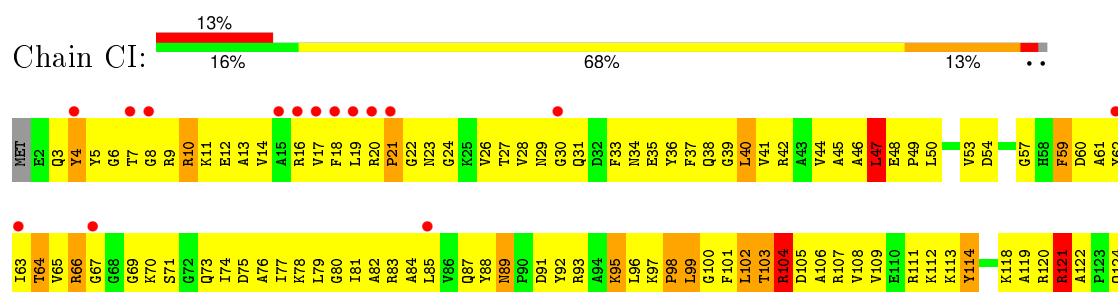
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

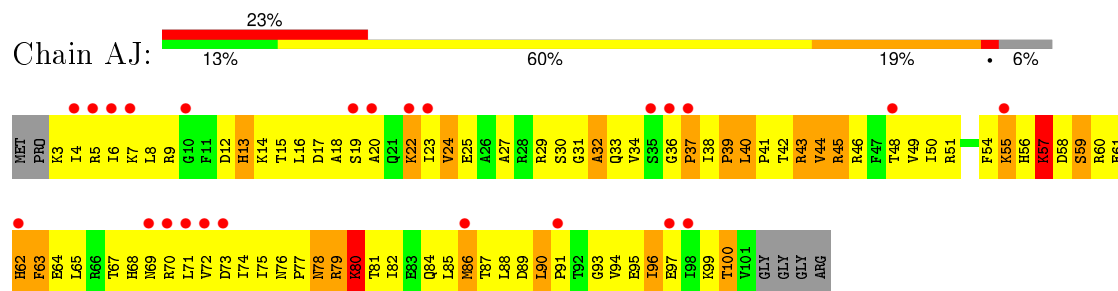


- Molecule 9: 30S ribosomal protein S9

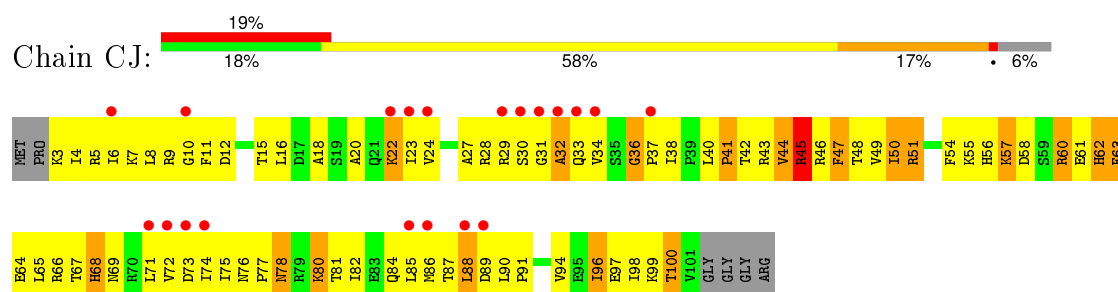




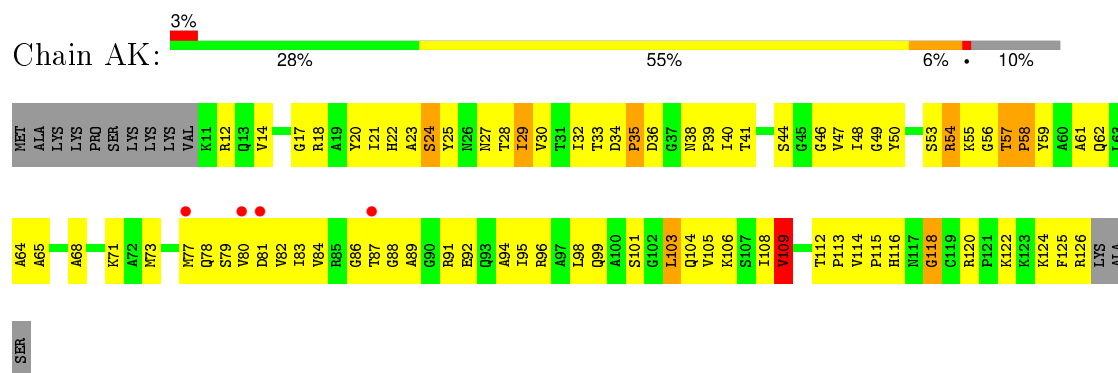
• Molecule 10: 30S ribosomal protein S10



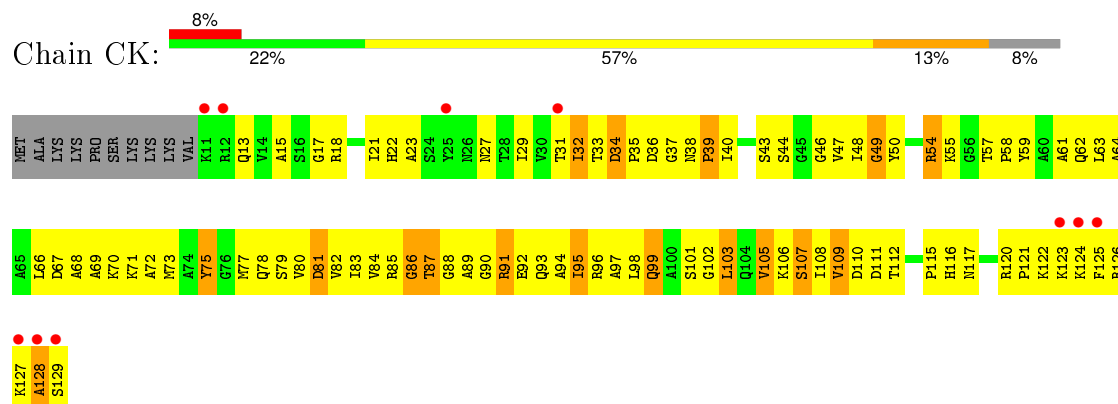
• Molecule 10: 30S ribosomal protein S10



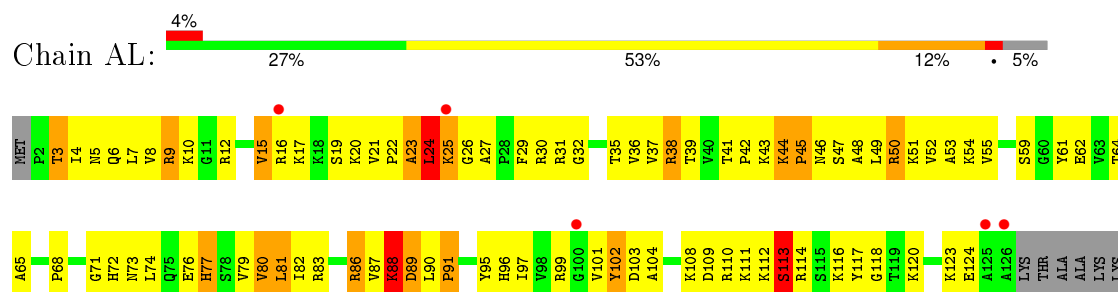
• Molecule 11: 30S ribosomal protein S11



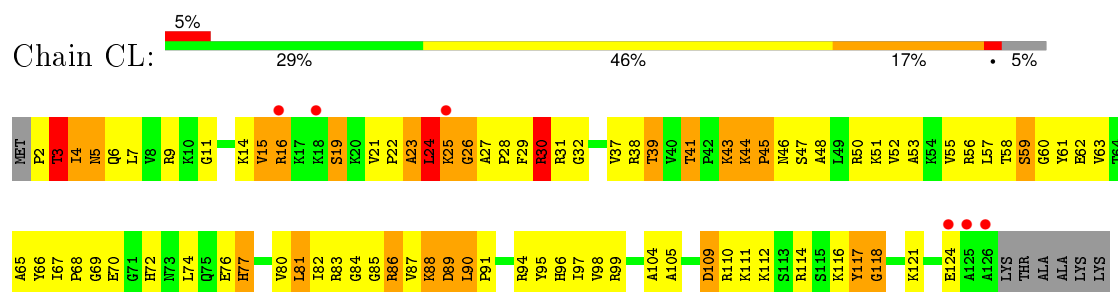
• Molecule 11: 30S ribosomal protein S11



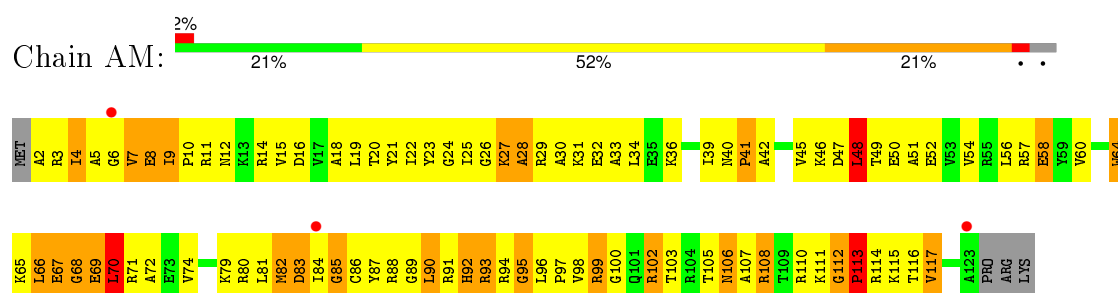
- Molecule 12: 30S ribosomal protein S12



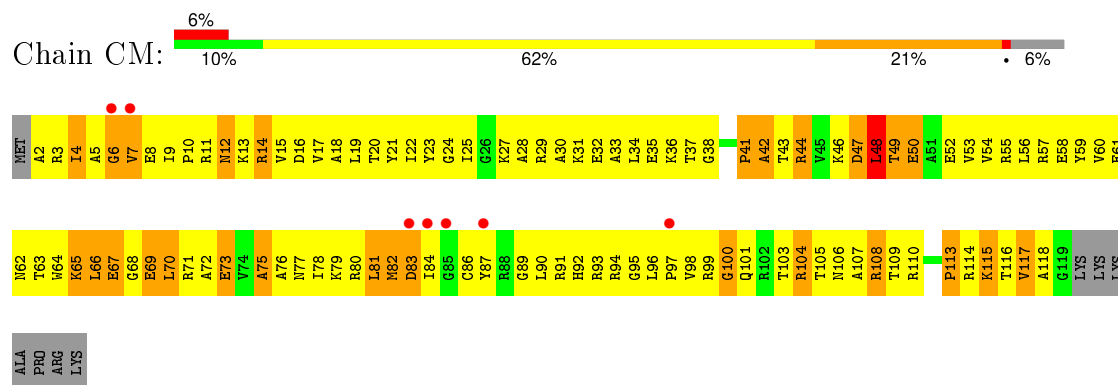
- Molecule 12: 30S ribosomal protein S12



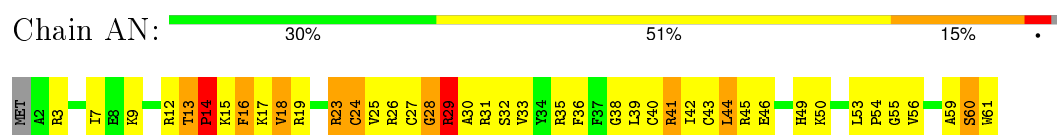
- Molecule 13: 30S ribosomal protein S13



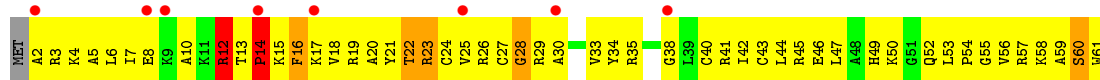
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



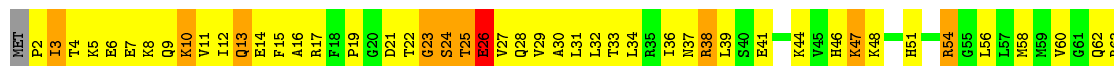
- Molecule 14: 30S ribosomal protein S14



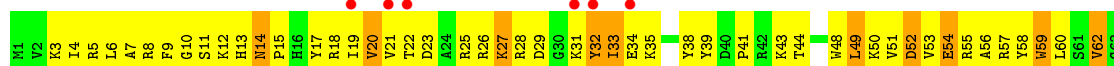
- Molecule 15: 30S ribosomal protein S15



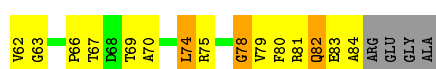
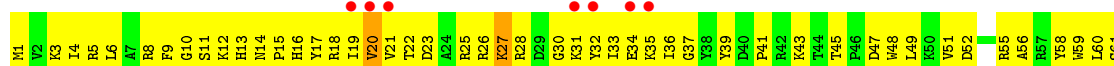
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

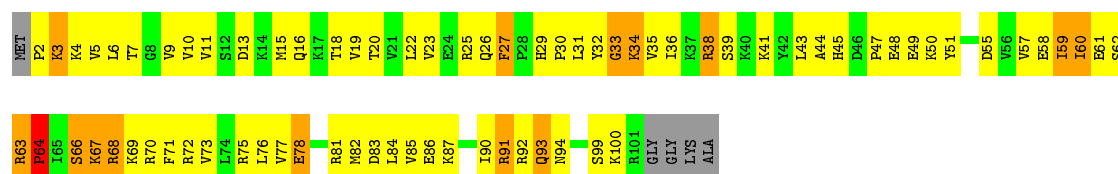


- Molecule 16: 30S ribosomal protein S16

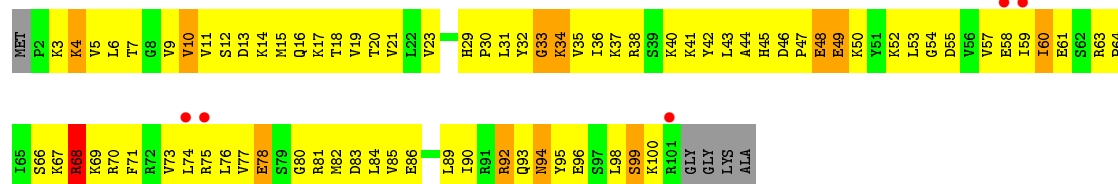


- Molecule 17: 30S ribosomal protein S17

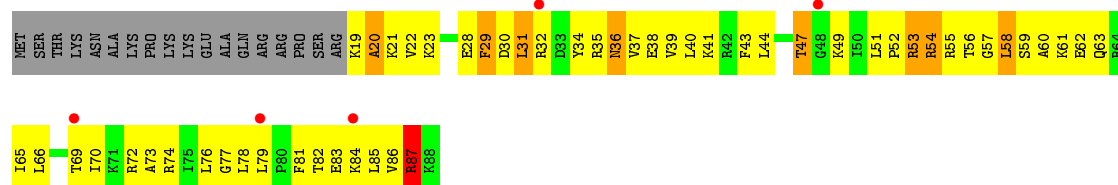
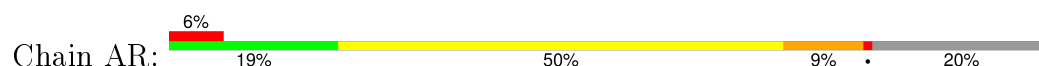




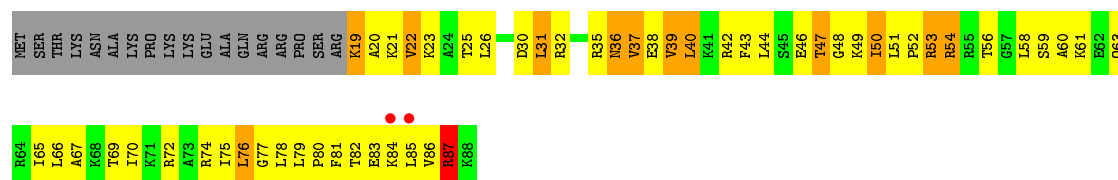
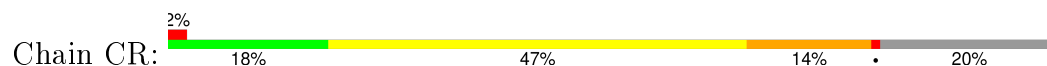
- Molecule 17: 30S ribosomal protein S17



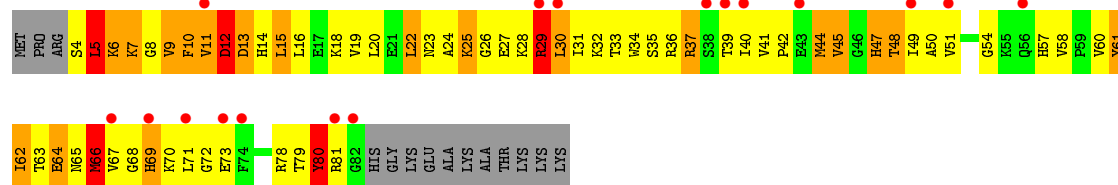
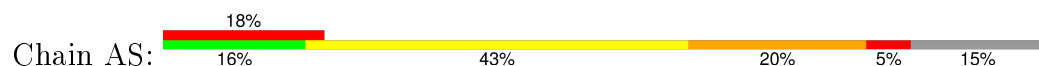
- Molecule 18: 30S ribosomal protein S18



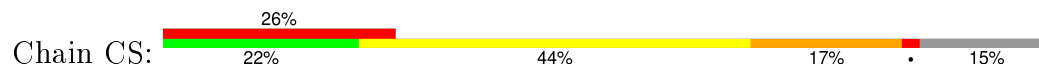
- Molecule 18: 30S ribosomal protein S18

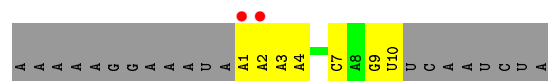


- Molecule 19: 30S ribosomal protein S19



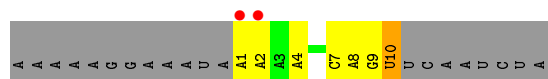
- Molecule 19: 30S ribosomal protein S19





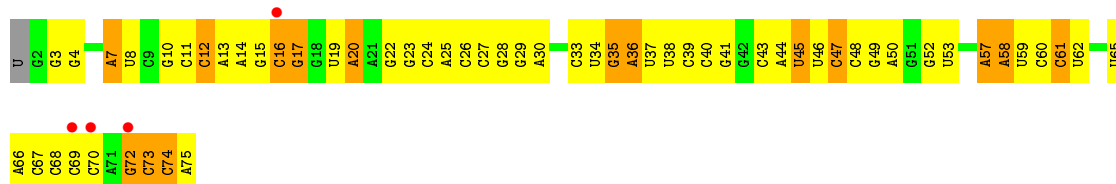
- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')

Chain CV: 



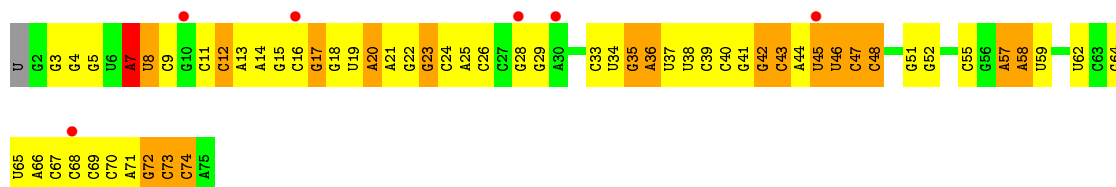
- Molecule 23: tRNA-Gln

Chain AW: 



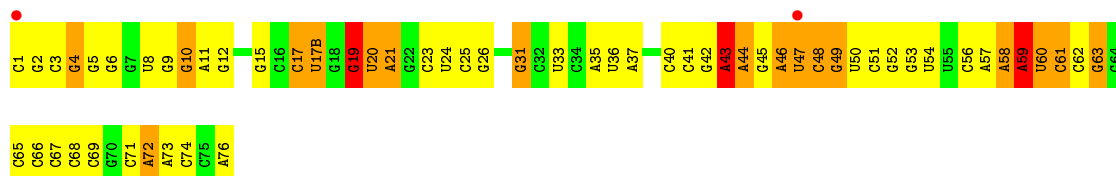
- Molecule 23: tRNA-Gln

Chain CW: 



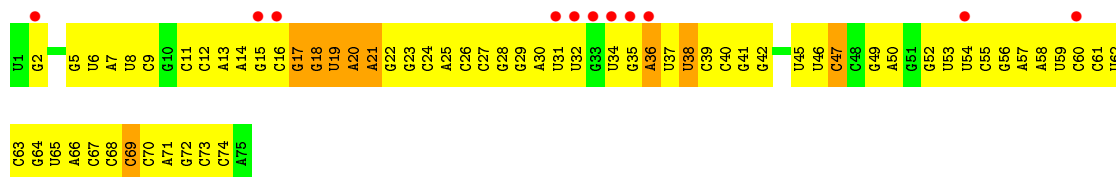
- Molecule 24: tRNA-Met

Chain AX: 

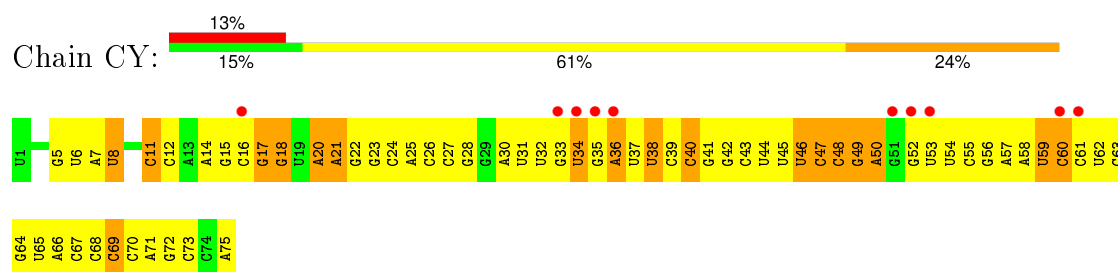


- Molecule 25: tRNA-Gln

Chain AY: 



- Molecule 25: tRNA-Gln



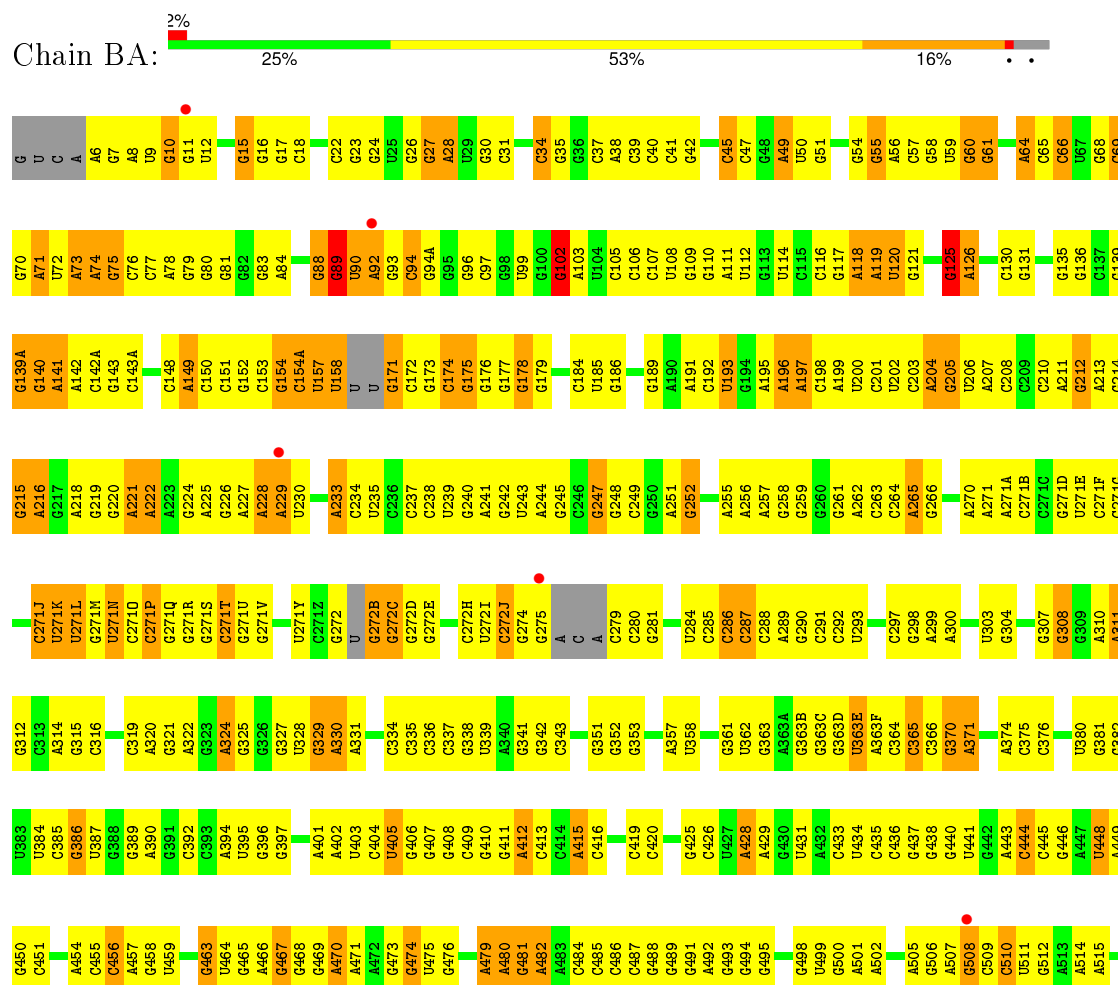
- Molecule 26: capreomycin IA



- Molecule 26: capreomycin IA

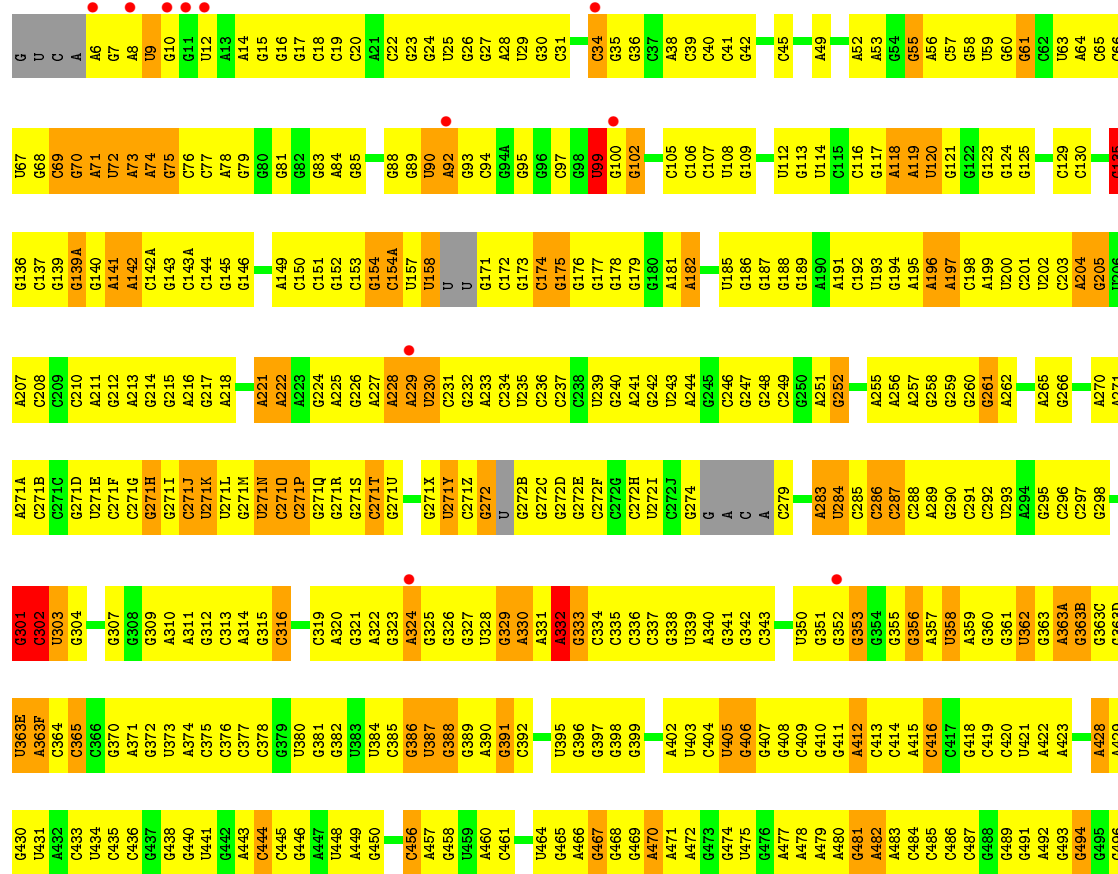


- Molecule 27: 23S ribosomal RNA



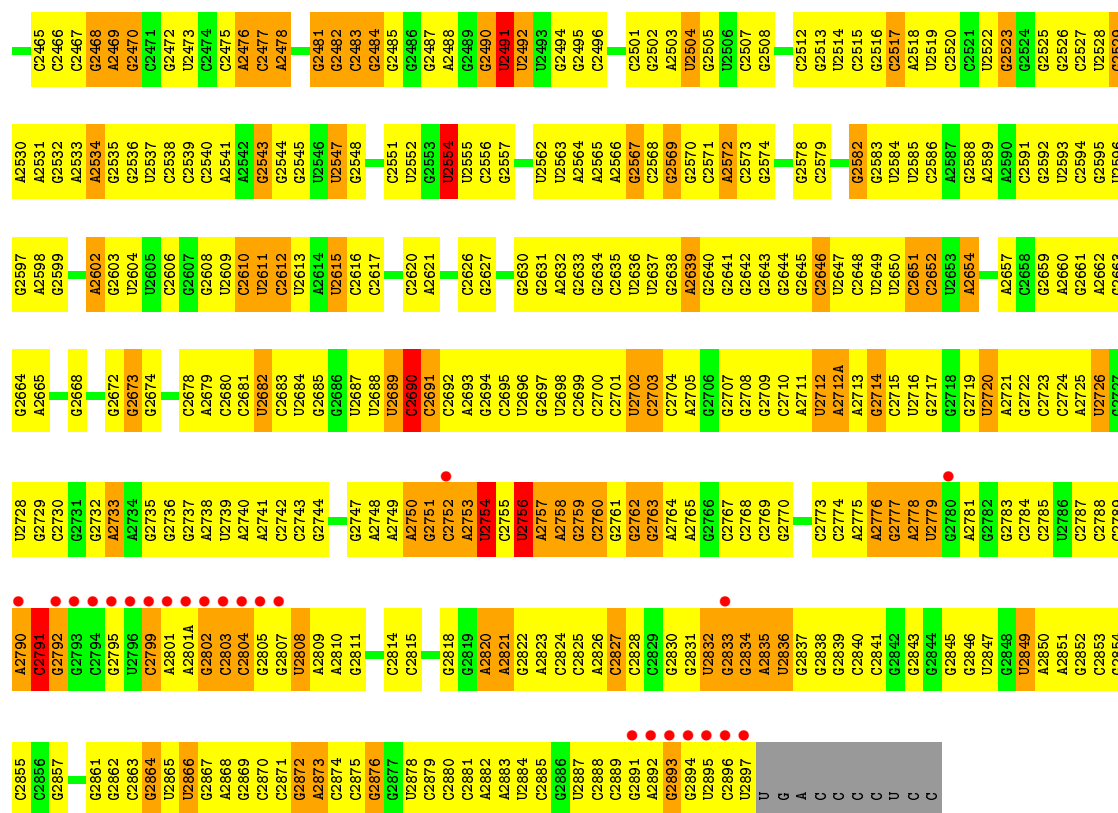


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C2394	C2395	C2396	C2397	C2398	C2399	G2400	U2401	C2402	C2403	C2404	G2405	U2406	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	A2418	U2419	G2420	G2421	A2422	U2423	G2424	A2425	A2426	G2427	G2428	A2429	A2430	A2434	A2435	U2439	C2440	G2441	C2442	G2443	G2444	U2448	U2449	A2450	A2451	C2452	A2453	U2457	G2458	A2459	U2460	C2461	U2462	C2463	U2464							
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G1559	C1560	C1561	C1562	U1563	A1568	A1569	A1570	A1571	A1572	G1573	C1574	G1575	U1576	C1577	U1578	A1579	A1580	G1581	C1582	A1583	C1584	A1586	A1587	G1588	C1589	U1590	G1592	G1593	A1594	G1595	A1596	A1597	C1598	C1599	G1600	G1601	U1602	A1603	G1607	A1608	A1609	A1610	C1611	A1544	A1545	G1546	C1547	C1548	C1549	A1618	C1550	C1551	A1554	G1555	C1556	C1557	A1558						



A1379	U1316	G1252	G1186	G1124	C	A1001	G869	G805	C737	G669	C560	A497
A1380	A1317	A1253	G1187	G1125	U	G1002	A870	C806	G738	A670		G498
A1384	G1319	G1266	U1188	A1127	U	G1003	G873	U807	U740	A632	G563	U999
G1385	G1318	G1257	A1189	A1126	U	G1004	G874	G808	G739	A633	C564	G500
G1386	C1320	G1258	G1190	U1130	G	C1005	G875	G809	G741	C634	A501	A501
G1387	A1321	G1259	G1191	G1131	A	C1006	G876		G742	C635	G570	A502
G1388	A1322	G1260	G1192	G1132	A	C1007	C976		G743	C636	A571	A503
	G1324	G1261		U1133	G	C1008		U813	G744	A637	U504	U504
	G1325	G1195	G1195	U1133	C	A1009	G880	U813	G745	A638	A505	A505
A1393	G1326	G1196	G1197	C1135	G	A1010	G881	C815	G746	C639	C574	G506
	G1327	U1263	G1198	G1136	G	G1011	G882	C816	U747	C640	A575	A507
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		G1266	G1200	G1139	A	U1014	C885	A819	A751	A643		
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C1404	U1335	A1272	G1206	G1144	U	A1020	G892	U826	U757	C649	C516	C516
A1405	A1336	U1273	C1207	C1145	A	A1021	C893	U827	C758	C650	C517	C517
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C1407	G1338	A1275	G1209	C1147	A	U1023	C895	A829	U760	C652	C589	U519
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C1409	U1340	G1277	U1211	G1149	A	G1025	C897	G831		A	C591	G521
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A1412	C1345	G1280	A1214	C1152	U	A1028	A900	C834		G	U524	U524
G1413	G1346	G1281	G1215	C1153	C		A901	G835	G766	G	U525	U525
			G1216	G1154	U	U1033	C902	G836	G767	G	G599	A526
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C1417	G1348	G1285	G1218	A1156	A	U1035	C904	G838	G771	C	C801	A528
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A1419	C1350	A1287	C1158	C1158	U	G1037	G906	C840	U773	C	A603	G530
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G1421	U1352	C1289	G1221A	G1160	C	G1039	C908	G843	G775	C	C605	A532
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G1423	C1354	C1291	G1223	G1162	U	C1041	A910	G845	A777	C	U606	G533
G1424	G1355	U1292	C1224	G1163	C	G1042	A911	C846	G778	G	A608	A536
G1425	G1356	C1293	G1225	C1164	A	C1043	C912	U847	U779	G	C537	C537
	U1357	U1294		U1165	U	G1044	U913	G848		C	G610	G538
G1426	G1358	C1295	C1230	U1167	C	A	C914	A849	A782	C	C611	G539
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G1428	A1360		G1232	G1169	G	G	G916	U851	A784	C	G613	C541
C1430	C1361		C1233	G1170	U	A	A917	G852	G785	G	U614	C542
U1431	C1362		U1234	G1171	C	C	A918	G853	C786	A	U614A	C543
C1432	C1363	U1300	G1235	G1171	G	A	G919	G854	U787	A	G	C
U1433	G1364	A1302	G1236	G	A	G	G920	G855	A722	A	G614B	A
A1434	A1365	G1303		A	C	C	G921	C856	G723	A	G615	C
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G1436	G1368		A1241	G	U	A	C923	U858	C791	C658	C618	G549
C1437	G1369	A1307	A1242	A	A	A	C924	G859	G725	G659	G619	G551
U1438	A1308	A1308	G1243	C1178	G	G	C925	U860	G726	G660	G620	G552
A1439	G1372	G1309	G1244	C1179	A	A	A926	A861	A727	C661	A821	G553
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G1441	G1374	G1311	U1246	C1181	G	G	G863	C796	C730	G663		U555
G1442	C1375	U1312	A1247	A1182	U	U	A966	G864		C664	G625	G556
G1443	G1376	U1313	A1248	A1183	U	G	G865	C965	A734	C665	U626	U557
G1444	G1377	C1314	U1249	G1184	U	G	C966	A866	A735	C666	A627	G558
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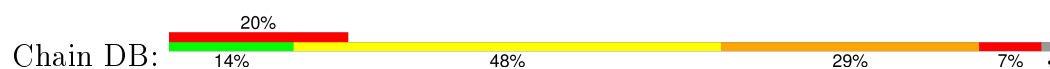




• Molecule 28: 5S ribosomal RNA

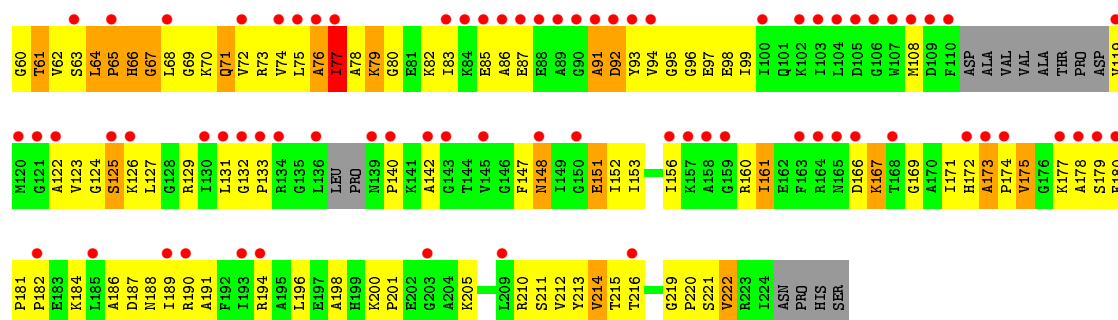


• Molecule 28: 5S ribosomal RNA

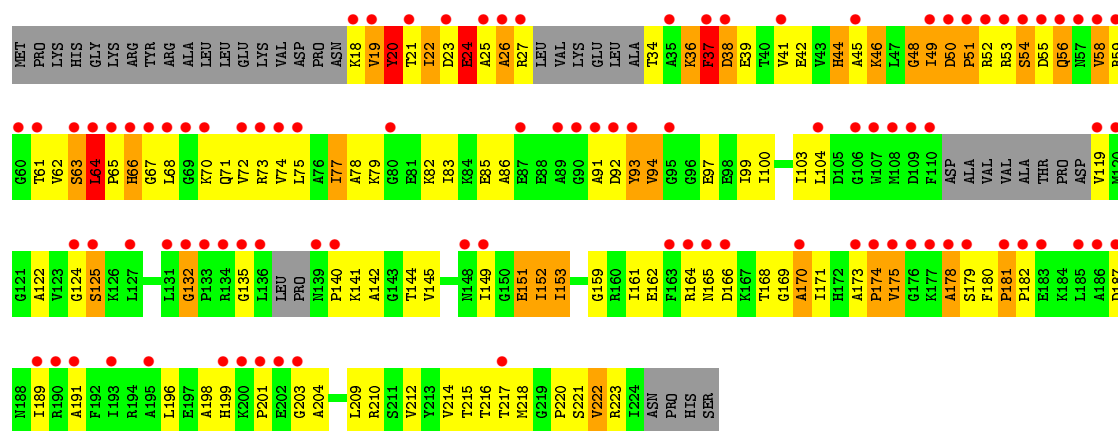
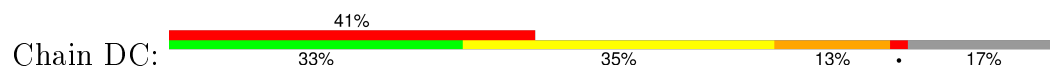


• Molecule 29: 50S ribosomal protein L1

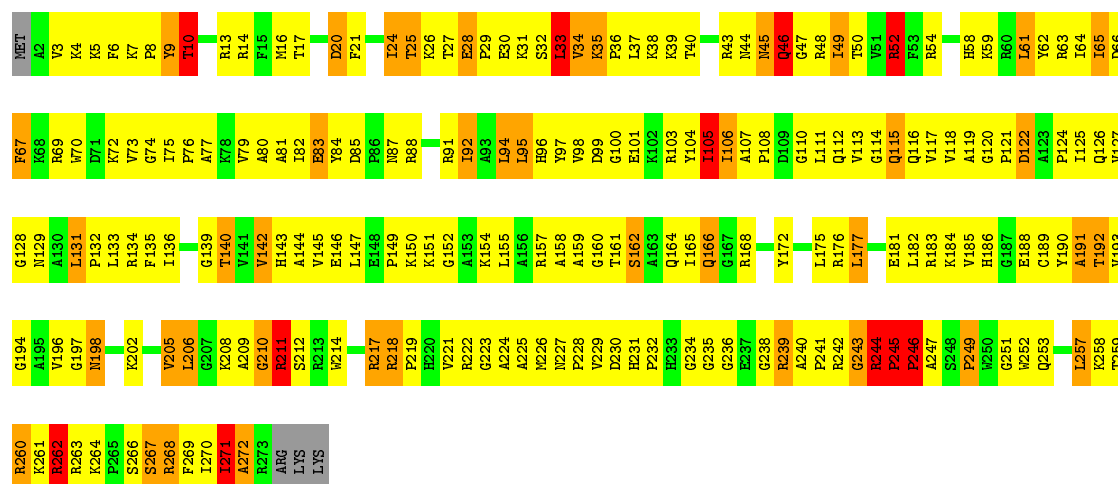




• Molecule 29: 50S ribosomal protein L1

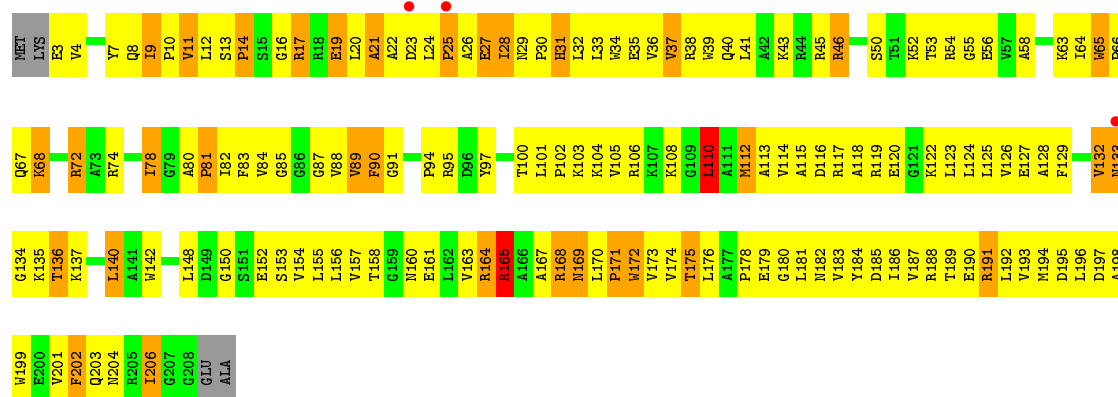


• Molecule 30: 50S ribosomal protein L2

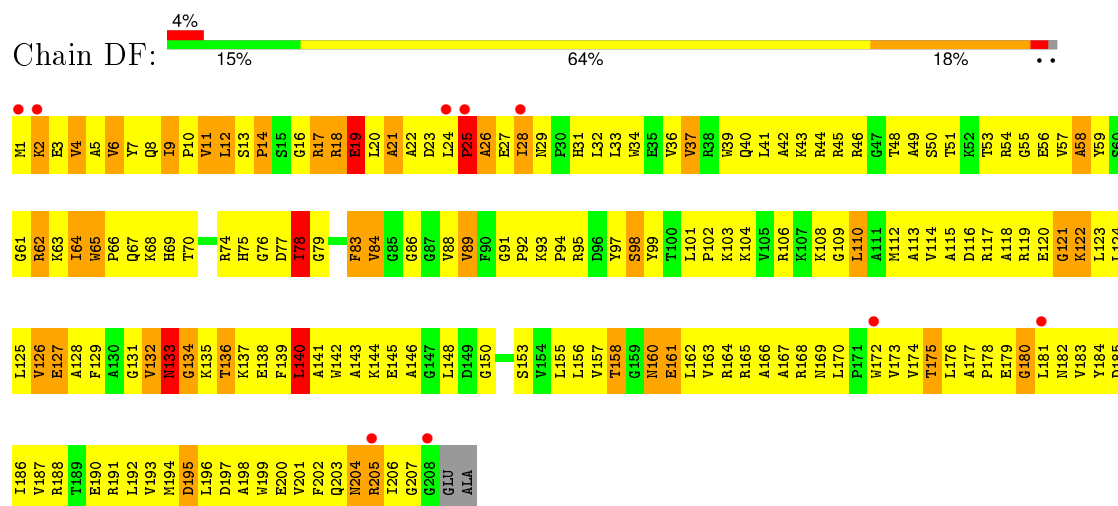


• Molecule 30: 50S ribosomal protein L2

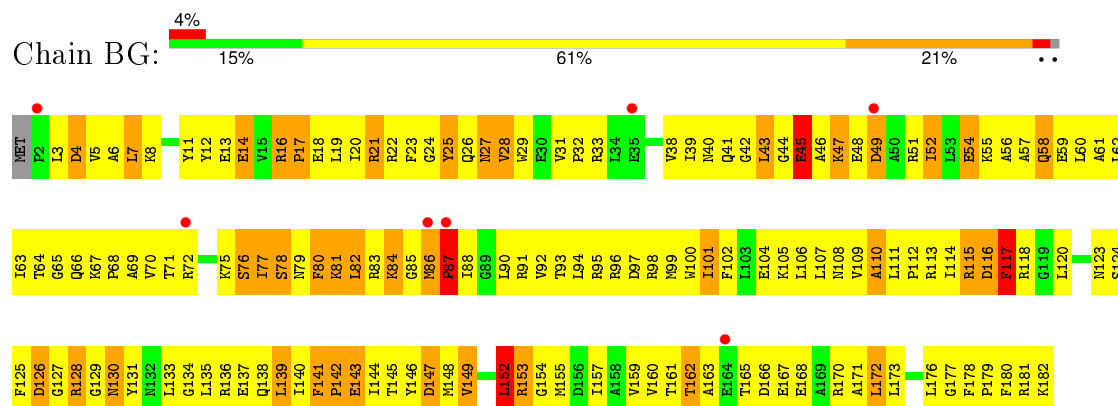




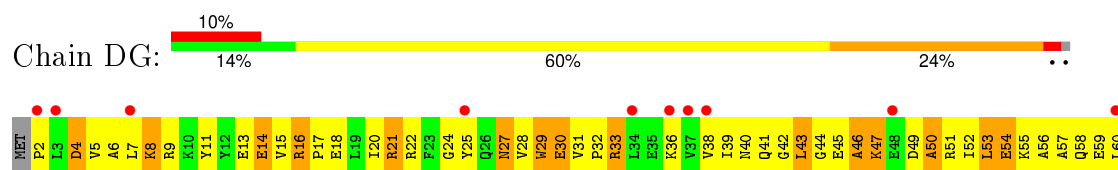
• Molecule 32: 50S ribosomal protein L4

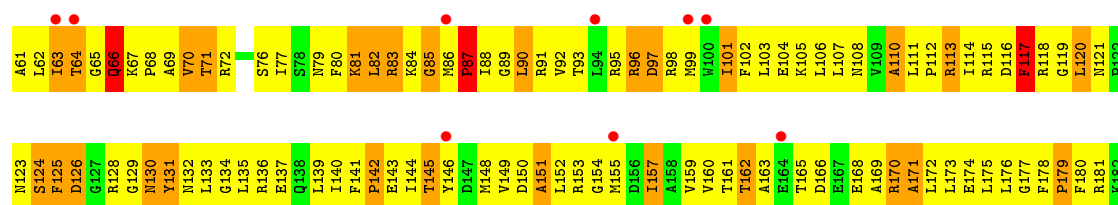


• Molecule 33: 50S ribosomal protein L5

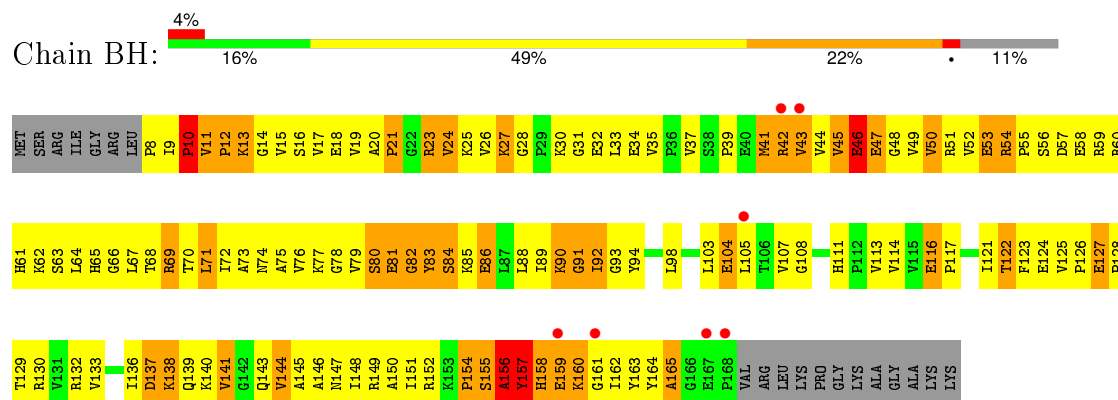


• Molecule 33: 50S ribosomal protein L5

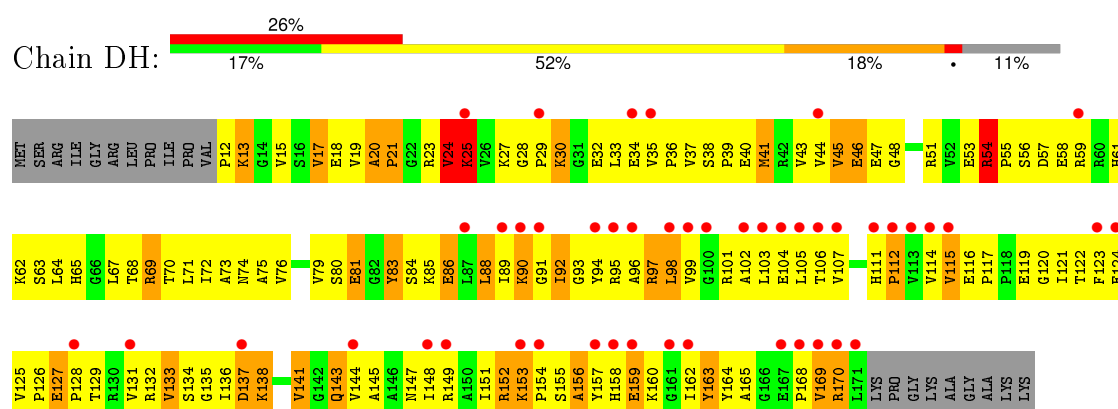




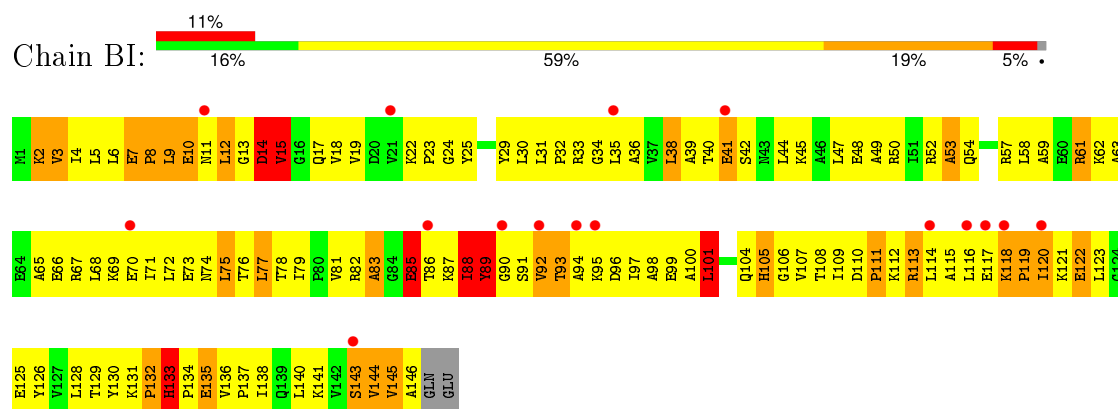
• Molecule 34: 50S ribosomal protein L6



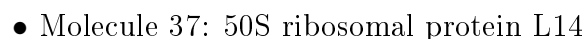
• Molecule 34: 50S ribosomal protein L6

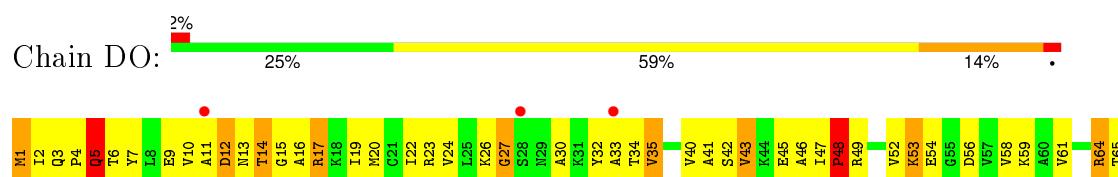


• Molecule 35: 50S ribosomal protein L9

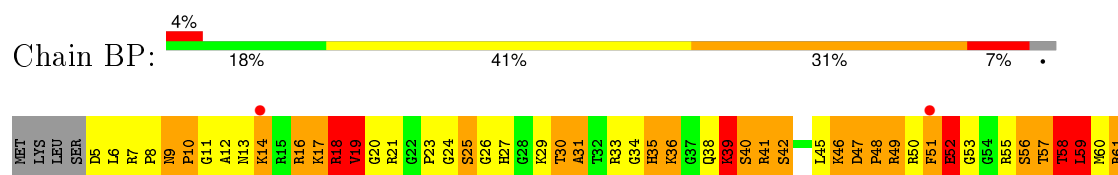


• Molecule 35: 50S ribosomal protein L9

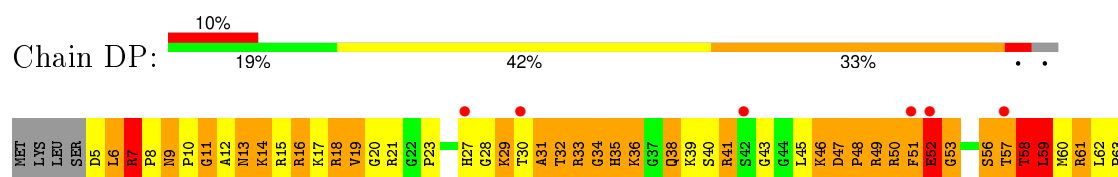




• Molecule 38: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L15



• Molecule 39: 50S ribosomal protein L16

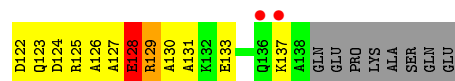
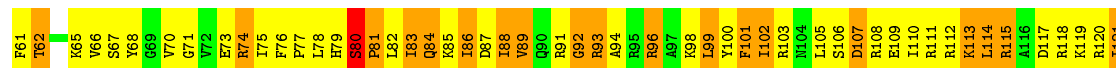
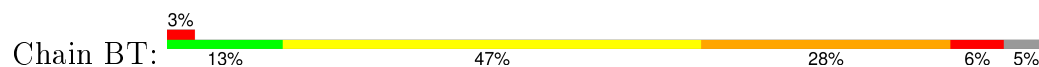


• Molecule 39: 50S ribosomal protein L16

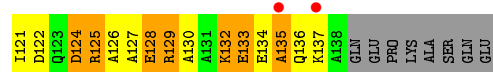
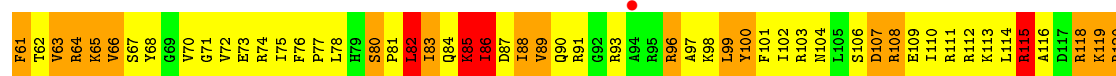
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D135
A136
Y137
D138
E139
ALA
GLN



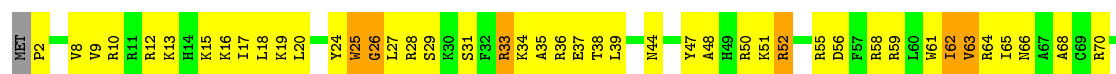
- Molecule 42: 50S ribosomal protein L19



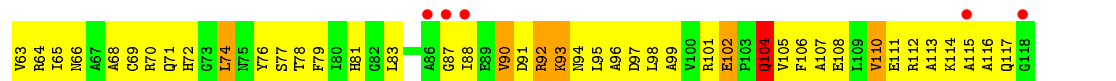
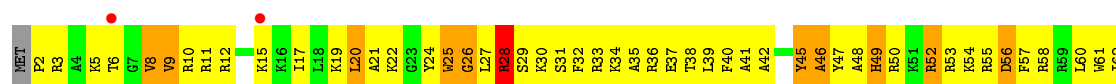
- Molecule 42: 50S ribosomal protein L19



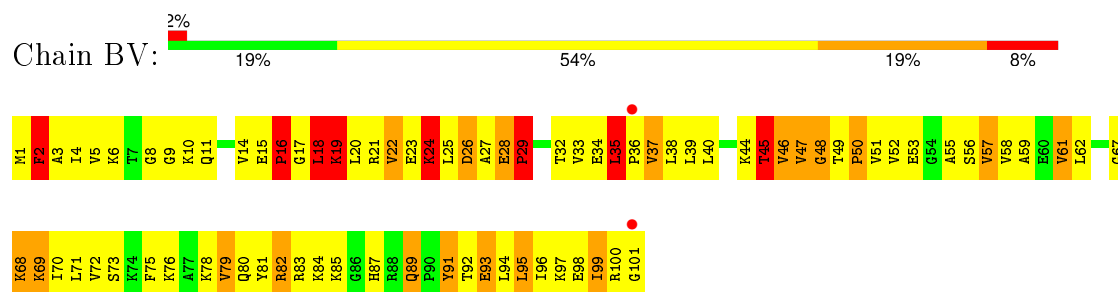
- Molecule 43: 50S ribosomal protein L20



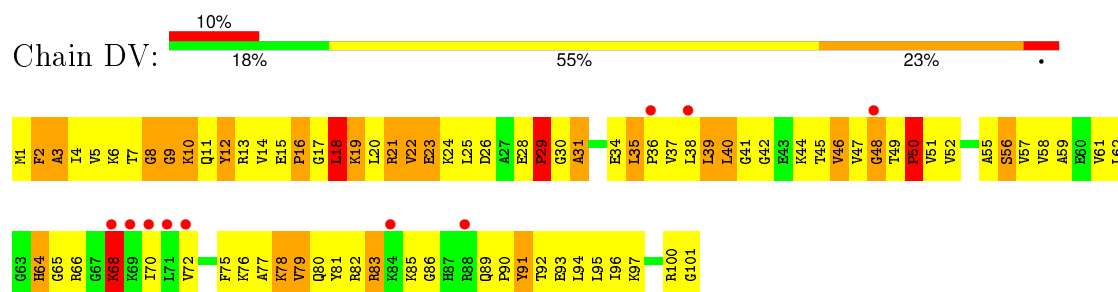
- Molecule 43: 50S ribosomal protein L20



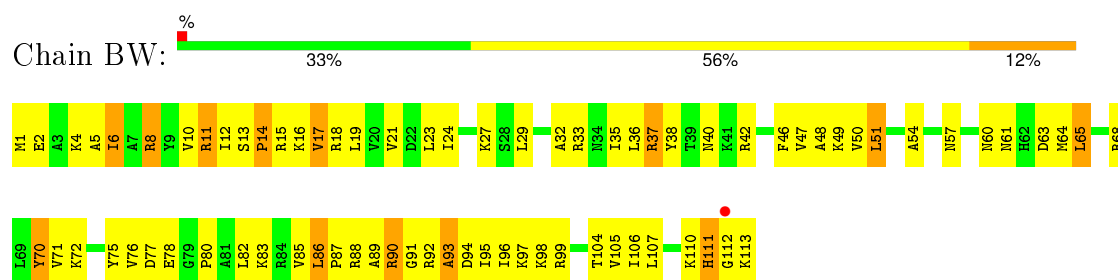
- Molecule 44: 50S ribosomal protein L21



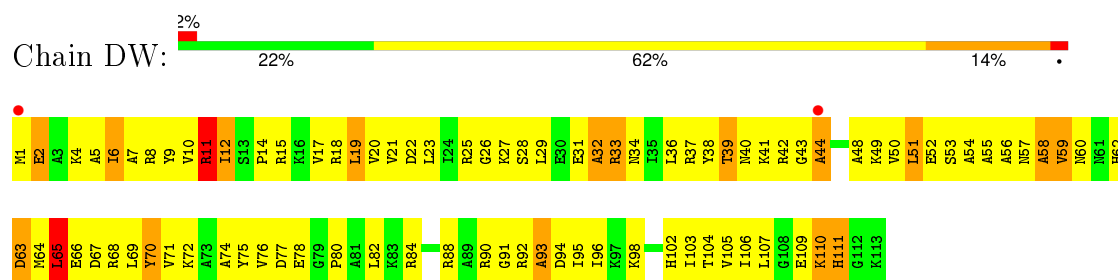
- Molecule 44: 50S ribosomal protein L21



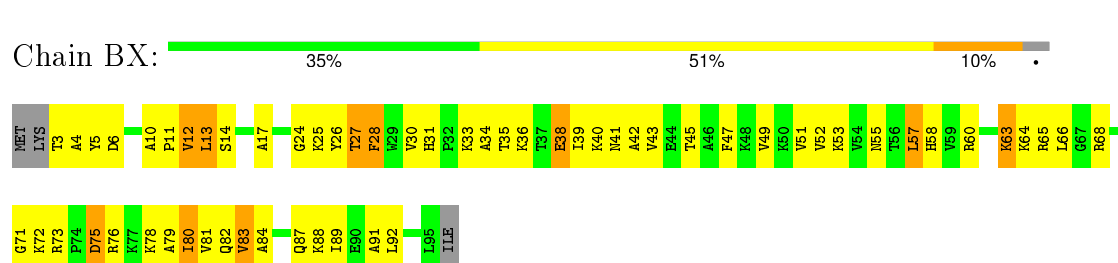
- Molecule 45: 50S ribosomal protein L22

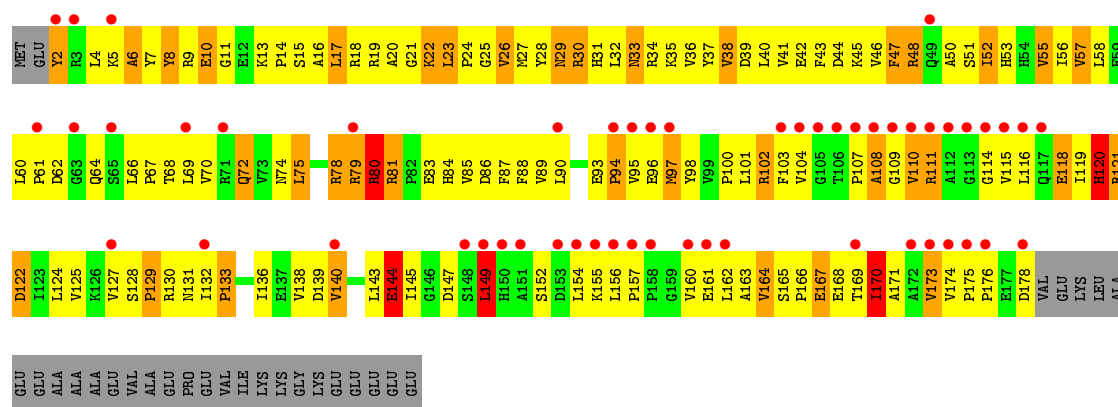


- Molecule 45: 50S ribosomal protein L22

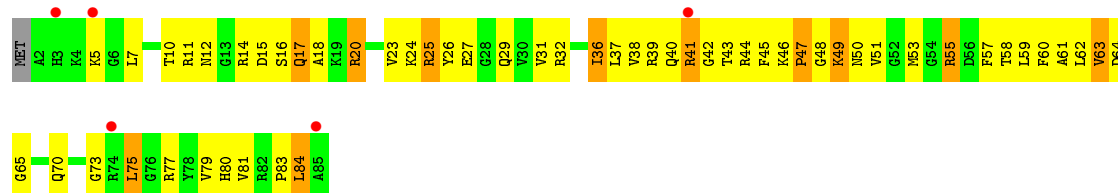


- Molecule 46: 50S ribosomal protein L23

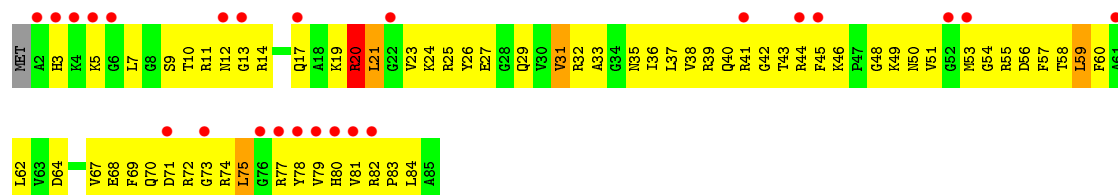




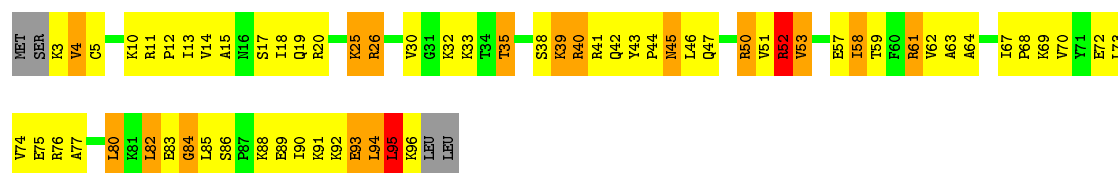
• Molecule 49: 50S ribosomal protein L27



• Molecule 49: 50S ribosomal protein L27



• Molecule 50: 50S ribosomal protein L28

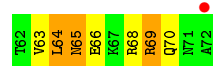
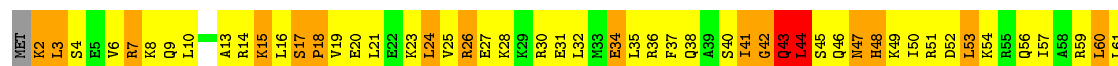
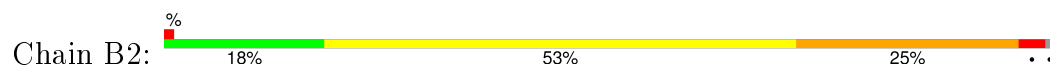


• Molecule 50: 50S ribosomal protein L28

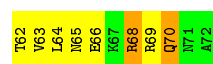
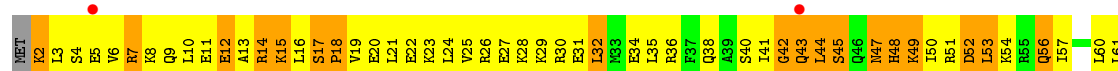
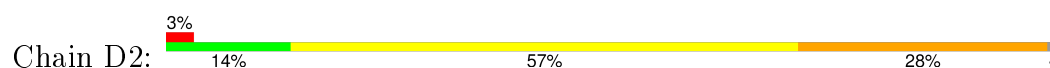




- Molecule 51: 50S ribosomal protein L29



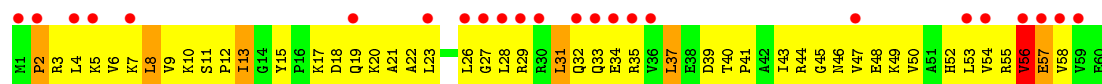
- Molecule 51: 50S ribosomal protein L29



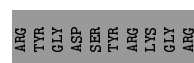
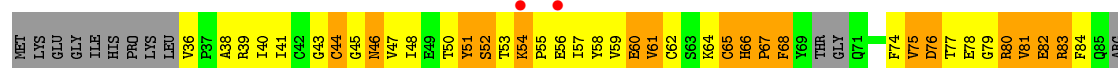
- Molecule 52: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L30

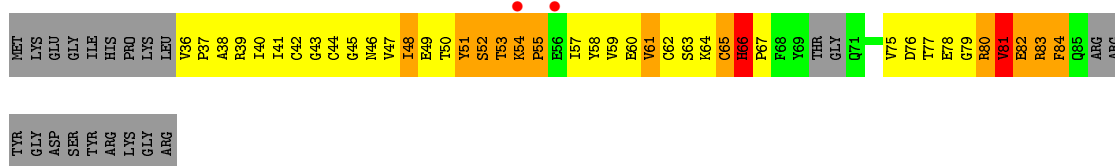


- Molecule 53: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L31





- Molecule 54: 50S ribosomal protein L32



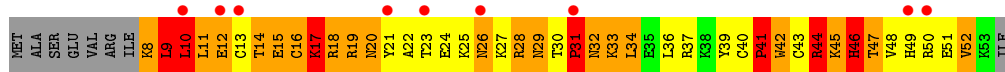
- Molecule 54: 50S ribosomal protein L32



- Molecule 55: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L33



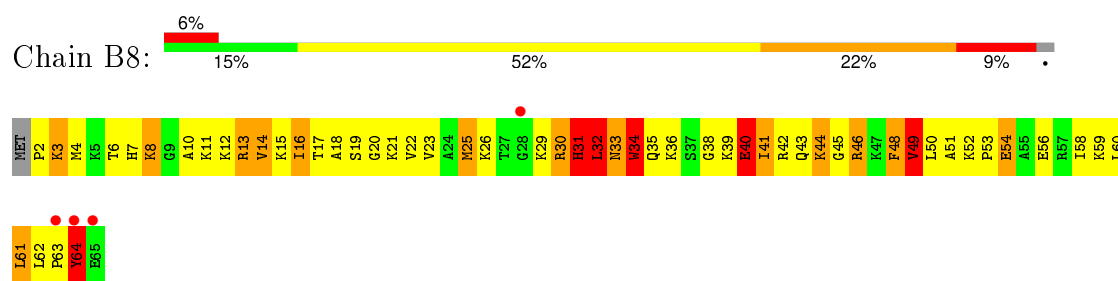
- Molecule 56: 50S ribosomal protein L34



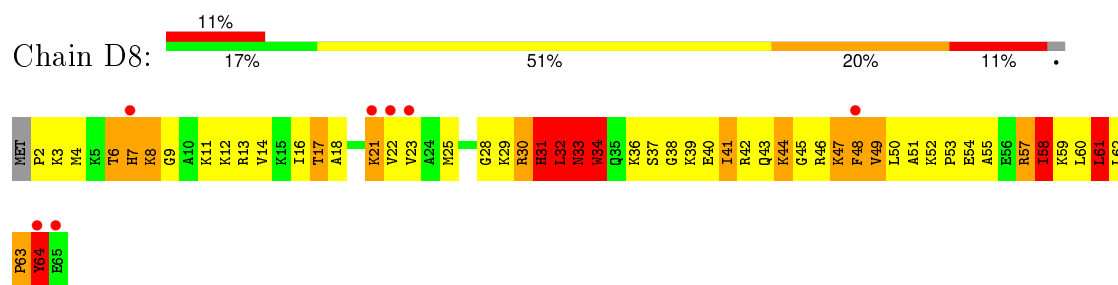
- Molecule 56: 50S ribosomal protein L34



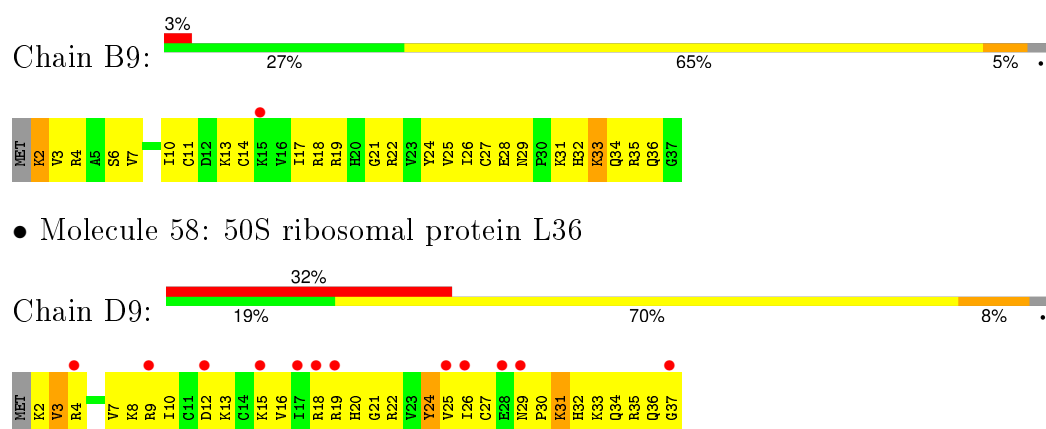
- Molecule 57: 50S ribosomal protein L35



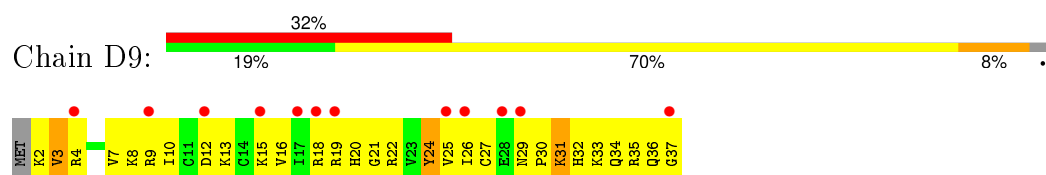
- Molecule 57: 50S ribosomal protein L35



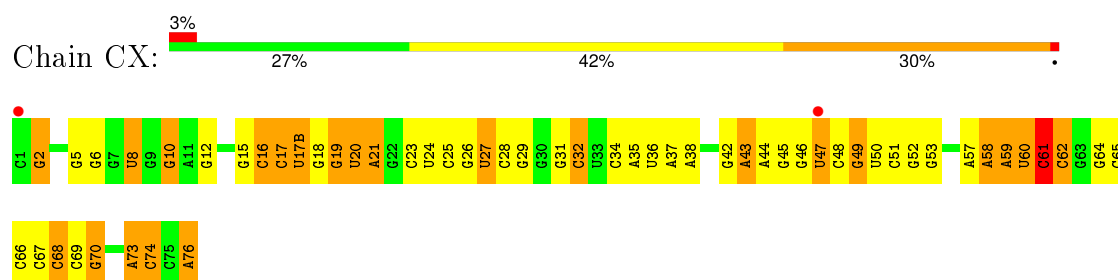
- Molecule 58: 50S ribosomal protein L36



- Molecule 58: 50S ribosomal protein L36



- Molecule 59: RNA (77-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.35Å 448.24Å 631.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.45 49.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.45) 82.3 (49.75-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.268 0.253 , 0.253	Depositor DCC
R_{free} test set	33186 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 667587 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	293848	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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, DPP, MG, KBE, UAL, MYN

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	0.48	0/35968	0.74	23/56136 (0.0%)
1	CA	0.50	9/35932 (0.0%)	0.75	27/56082 (0.0%)
2	AB	0.39	0/1936	0.68	0/2611
2	CB	0.37	0/1936	0.66	0/2611
3	AC	0.38	0/1637	0.65	0/2207
3	CC	0.37	0/1627	0.67	0/2192
4	AD	0.42	0/1733	0.71	0/2318
4	CD	0.44	0/1733	0.72	1/2318 (0.0%)
5	AE	0.41	0/1163	0.68	0/1566
5	CE	0.42	0/1163	0.68	0/1566
6	AF	0.44	0/856	0.75	1/1154 (0.1%)
6	CF	0.43	0/856	0.71	0/1154
7	AG	0.38	0/1276	0.61	0/1709
7	CG	0.39	0/1267	0.62	0/1696
8	AH	0.40	0/1136	0.72	0/1527
8	CH	0.38	0/1136	0.70	0/1527
9	AI	0.38	0/1024	0.68	0/1372
9	CI	0.36	0/1024	0.67	0/1372
10	AJ	0.36	0/808	0.66	0/1087
10	CJ	0.36	0/808	0.67	0/1087
11	AK	0.41	0/879	0.75	0/1187
11	CK	0.39	0/900	0.68	0/1213
12	AL	0.44	0/987	0.80	0/1322
12	CL	0.44	0/987	0.74	0/1322
13	AM	0.37	0/975	0.75	2/1305 (0.2%)
13	CM	0.36	0/947	0.72	0/1270
14	AN	0.41	0/501	0.69	0/664
14	CN	0.45	0/501	0.67	0/664
15	AO	0.39	0/745	0.64	0/992
15	CO	0.37	0/745	0.64	0/992
16	AP	0.40	0/717	0.70	0/965
16	CP	0.43	0/717	0.74	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	0/837	0.67	0/1119
17	CQ	0.40	0/837	0.68	0/1119
18	AR	0.48	0/579	0.75	0/768
18	CR	0.41	0/579	0.72	0/768
19	AS	0.40	0/643	0.70	1/867 (0.1%)
19	CS	0.37	0/643	0.66	0/867
20	AT	0.38	0/765	0.72	1/1007 (0.1%)
20	CT	0.37	0/765	0.70	0/1007
21	AU	0.42	0/213	0.60	0/279
21	CU	0.34	0/213	0.62	0/279
22	AV	0.48	0/230	0.65	0/357
22	CV	0.45	0/239	0.69	0/371
23	AW	0.47	0/1756	0.78	0/2734
23	CW	0.46	0/1756	0.75	2/2734 (0.1%)
24	AX	0.58	2/1831 (0.1%)	0.87	6/2853 (0.2%)
25	AY	0.37	0/1776	0.71	0/2766
25	CY	0.36	0/1776	0.71	0/2766
26	AZ	0.91	0/5	0.51	0/5
26	CZ	0.51	0/5	0.85	0/5
27	BA	0.61	3/67273 (0.0%)	0.79	62/105005 (0.1%)
27	DA	0.51	1/66930 (0.0%)	0.77	45/104469 (0.0%)
28	BB	0.57	0/2853	0.81	6/4451 (0.1%)
28	DB	0.79	6/2853 (0.2%)	0.95	13/4451 (0.3%)
29	BC	0.31	0/1145	0.60	0/1556
29	DC	0.30	0/1145	0.61	0/1556
30	BD	0.54	0/2155	0.86	3/2907 (0.1%)
30	DD	0.51	0/2155	0.82	2/2907 (0.1%)
31	BE	0.56	0/1597	0.87	2/2155 (0.1%)
31	DE	0.42	0/1597	0.75	0/2155
32	BF	0.50	0/1642	0.82	1/2225 (0.0%)
32	DF	0.42	0/1659	0.75	1/2246 (0.0%)
33	BG	0.44	0/1499	0.78	0/2016
33	DG	0.40	0/1499	0.72	0/2016
34	BH	0.59	0/1258	0.91	2/1703 (0.1%)
34	DH	0.33	0/1246	0.67	0/1684
35	BI	0.39	0/1147	0.74	0/1553
35	DI	0.37	0/1147	0.75	0/1553
36	BN	0.54	0/1132	0.91	2/1527 (0.1%)
36	DN	0.41	0/1132	0.77	1/1527 (0.1%)
37	BO	0.54	0/943	0.80	0/1269
37	DO	0.44	0/943	0.69	0/1269
38	BP	0.59	0/1131	1.16	5/1504 (0.3%)
38	DP	0.48	0/1131	1.00	5/1504 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BQ	0.53	0/1128	0.77	0/1508
39	DQ	0.42	0/1114	0.68	0/1488
40	BR	0.55	0/974	0.92	2/1302 (0.2%)
40	DR	0.43	0/974	0.81	0/1302
41	BS	0.55	0/779	0.97	2/1038 (0.2%)
41	DS	0.43	0/779	0.75	0/1038
42	BT	0.57	0/1156	0.96	5/1544 (0.3%)
42	DT	0.46	0/1156	0.83	1/1544 (0.1%)
43	BU	0.57	0/975	0.85	0/1297
43	DU	0.38	0/975	0.69	0/1297
44	BV	0.58	0/790	0.95	2/1057 (0.2%)
44	DV	0.41	0/790	0.72	0/1057
45	BW	0.53	0/907	0.77	0/1216
45	DW	0.41	0/907	0.72	0/1216
46	BX	0.51	0/740	0.78	0/995
46	DX	0.48	0/740	0.73	0/995
47	BY	0.61	0/680	0.93	1/904 (0.1%)
47	DY	0.46	0/789	0.82	1/1053 (0.1%)
48	BZ	0.41	0/1436	0.72	0/1951
48	DZ	0.36	0/1436	0.70	0/1951
49	B0	0.47	0/671	0.74	0/892
49	D0	0.41	0/671	0.67	0/892
50	B1	0.49	0/739	0.76	1/983 (0.1%)
50	D1	0.43	0/739	0.76	0/983
51	B2	0.45	0/600	0.74	0/793
51	D2	0.39	0/600	0.67	0/793
52	B3	0.48	0/473	0.76	0/636
52	D3	0.34	0/473	0.63	0/636
53	B4	0.43	0/349	0.71	0/474
53	D4	0.39	0/349	0.64	0/474
54	B5	0.62	0/473	1.04	2/639 (0.3%)
54	D5	0.50	0/473	0.82	0/639
55	B6	0.72	0/409	1.07	0/548
55	D6	0.70	0/397	1.12	4/531 (0.8%)
56	B7	0.55	0/427	0.80	0/563
56	D7	0.48	0/427	0.73	0/563
57	B8	0.63	0/516	1.02	2/681 (0.3%)
57	D8	0.51	0/516	0.87	1/681 (0.1%)
58	B9	0.53	0/302	0.80	0/397
58	D9	0.39	0/302	0.70	0/397
59	CX	0.47	0/1832	0.75	1/2855 (0.0%)
All	All	0.51	21/318243 (0.0%)	0.77	239/475835 (0.1%)

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	35
1	CA	1	31
19	AS	0	1
23	AW	0	1
23	CW	0	1
24	AX	0	1
27	BA	4	96
27	DA	0	63
28	BB	0	3
28	DB	0	6
42	BT	0	1
59	CX	0	2
All	All	5	241

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	46	A	C6-N6	-11.79	1.24	1.33
1	CA	101	A	C6-N6	-8.09	1.27	1.33
1	CA	1458	G	C5-C6	-7.73	1.34	1.42
1	CA	70	G	C5-C6	-7.36	1.34	1.42
1	CA	1446	U	N1-C2	-7.30	1.31	1.38

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	46	A	C5-C6-N1	-12.54	111.43	117.70
28	DB	53	A	O5'-P-OP2	11.96	125.06	110.70
24	AX	46	A	C6-N1-C2	10.83	125.10	118.60
24	AX	46	A	N1-C2-N3	-10.72	123.94	129.30
27	BA	1992	G	C2'-C3'-O3'	10.30	132.16	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	BA	1378	A	C3'
27	BA	1799	G	C3'
27	BA	1992	G	C3'

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Mol	Chain	Res	Type	Atom
27	BA	2497	A	C3'
1	CA	533	A	C3'

5 of 241 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	181	G	Sidechain
1	AA	298	A	Sidechain
1	AA	37	U	Sidechain
1	AA	388	G	Sidechain
1	AA	490	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32132	0	16219	1429	0
1	CA	32098	0	16199	1614	0
2	AB	1901	0	1951	312	0
2	CB	1901	0	1951	269	0
3	AC	1613	0	1677	278	0
3	CC	1604	0	1670	270	0
4	AD	1703	0	1763	264	0
4	CD	1703	0	1763	197	0
5	AE	1147	0	1207	160	0
5	CE	1147	0	1207	172	0
6	AF	843	0	857	91	0
6	CF	843	0	857	99	0
7	AG	1257	0	1296	161	0
7	CG	1249	0	1286	155	0
8	AH	1116	0	1177	165	0
8	CH	1116	0	1177	143	0
9	AI	1006	0	1034	176	0
9	CI	1006	0	1034	201	0
10	AJ	795	0	840	159	0
10	CJ	795	0	840	175	0
11	AK	864	0	881	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CK	885	0	904	117	0
12	AL	971	0	1057	122	0
12	CL	971	0	1057	128	0
13	AM	965	0	1034	166	0
13	CM	937	0	995	162	0
14	AN	492	0	533	77	0
14	CN	492	0	533	108	0
15	AO	734	0	771	94	0
15	CO	734	0	771	99	0
16	AP	701	0	720	107	0
16	CP	701	0	720	96	0
17	AQ	824	0	891	114	0
17	CQ	824	0	891	125	0
18	AR	574	0	644	87	0
18	CR	574	0	644	83	0
19	AS	630	0	652	126	0
19	CS	630	0	652	110	0
20	AT	763	0	861	134	0
20	CT	763	0	861	131	0
21	AU	209	0	221	26	0
21	CU	209	0	221	24	0
22	AV	205	0	106	7	0
22	CV	213	0	110	11	0
23	AW	1573	0	800	86	0
23	CW	1573	0	800	72	0
24	AX	1639	0	835	72	0
25	AY	1591	0	810	72	0
25	CY	1591	0	810	81	0
26	AZ	47	0	40	11	0
26	CZ	47	0	40	14	0
27	BA	60072	0	30294	2481	0
27	DA	59767	0	30140	2934	0
28	BB	2551	0	1295	107	0
28	DB	2551	0	1295	201	0
29	BC	1142	0	865	119	0
29	DC	1142	0	865	116	0
30	BD	2105	0	2182	345	0
30	DD	2105	0	2182	317	0
31	BE	1564	0	1629	250	0
31	DE	1564	0	1629	346	0
32	BF	1607	0	1652	226	0
32	DF	1624	0	1677	293	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	BG	1474	0	1535	250	0
33	DG	1474	0	1535	310	0
34	BH	1233	0	1294	217	0
34	DH	1223	0	1282	184	0
35	BI	1132	0	1218	207	0
35	DI	1132	0	1218	223	0
36	BN	1105	0	1180	153	0
36	DN	1105	0	1180	195	0
37	BO	933	0	996	114	0
37	DO	933	0	996	145	0
38	BP	1114	0	1187	303	0
38	DP	1114	0	1187	329	0
39	BQ	1107	0	1166	179	0
39	DQ	1094	0	1141	150	0
40	BR	960	0	1021	148	0
40	DR	960	0	1021	182	0
41	BS	771	0	832	185	0
41	DS	771	0	832	188	0
42	BT	1142	0	1202	236	0
42	DT	1142	0	1202	303	0
43	BU	958	0	1014	151	0
43	DU	958	0	1015	187	0
44	BV	779	0	852	162	0
44	DV	779	0	852	141	0
45	BW	896	0	953	108	0
45	DW	896	0	953	135	0
46	BX	726	0	778	75	0
46	DX	726	0	778	87	0
47	BY	672	0	766	190	0
47	DY	776	0	870	211	0
48	BZ	1404	0	1432	215	0
48	DZ	1404	0	1432	266	0
49	B0	662	0	688	83	0
49	D0	662	0	688	92	0
50	B1	732	0	808	97	0
50	D1	732	0	808	98	0
51	B2	598	0	653	75	0
51	D2	598	0	653	95	0
52	B3	468	0	523	46	0
52	D3	468	0	523	71	0
53	B4	344	0	305	69	0
53	D4	344	0	305	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	B5	459	0	476	80	0
54	D5	459	0	477	62	0
55	B6	402	0	413	109	0
55	D6	390	0	404	135	0
56	B7	419	0	467	46	0
56	D7	419	0	467	41	0
57	B8	508	0	576	130	0
57	D8	508	0	576	138	0
58	B9	299	0	323	34	0
58	D9	299	0	323	57	0
59	CX	1640	0	837	62	0
60	AA	114	0	0	0	0
60	AG	1	0	0	0	0
60	AW	4	0	0	0	0
60	AX	9	0	0	0	0
60	B0	3	0	0	0	0
60	B5	1	0	0	0	0
60	BA	334	0	0	0	0
60	BB	5	0	0	0	0
60	BD	1	0	0	0	0
60	BE	3	0	0	0	0
60	BF	1	0	0	0	0
60	BG	1	0	0	0	0
60	BP	2	0	0	0	0
60	BR	1	0	0	0	0
60	BU	2	0	0	0	0
60	BX	1	0	0	0	0
60	CA	102	0	0	0	0
60	CE	1	0	0	0	0
60	CK	1	0	0	0	0
60	CV	1	0	0	0	0
60	CW	4	0	0	0	0
60	D0	1	0	0	0	0
60	D5	1	0	0	0	0
60	D7	1	0	0	0	0
60	DA	239	0	0	0	0
60	DB	3	0	0	0	0
60	DD	2	0	0	0	0
60	DE	1	0	0	0	0
60	DF	1	0	0	0	0
60	DO	1	0	0	0	0
61	AD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B4	1	0	0	0	0
61	B5	1	0	0	0	0
61	B9	1	0	0	0	0
61	CD	1	0	0	0	0
61	D4	1	0	0	0	0
61	D5	1	0	0	0	0
61	D9	1	0	0	0	0
All	All	293848	0	198788	22560	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 46.

The worst 5 of 22560 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)
55:B6:15:GLU:CD	55:B6:18:ARG:HE	1.41	1.22
4:AD:19:LEU:HD11	4:AD:67:ILE:HG13	1.24	1.19
1:CA:1321:C:H3'	1:CA:1322:C:H5''	1.21	1.19
13:AM:90:LEU:HD23	13:AM:93:ARG:HG2	1.23	1.18
2:AB:166:ASP:HB3	2:AB:169:LYS:HB2	1.24	1.18

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%)	147 (63%)	57 (24%)	29 (12%)	0	5
2	CB	233/256 (91%)	144 (62%)	56 (24%)	33 (14%)	0	3
3	AC	205/239 (86%)	122 (60%)	53 (26%)	30 (15%)	0	3
3	CC	202/239 (84%)	116 (57%)	48 (24%)	38 (19%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	206/209 (99%)	138 (67%)	39 (19%)	29 (14%)	0	4
4	CD	206/209 (99%)	141 (68%)	39 (19%)	26 (13%)	0	5
5	AE	149/162 (92%)	98 (66%)	34 (23%)	17 (11%)	0	7
5	CE	149/162 (92%)	107 (72%)	27 (18%)	15 (10%)	1	9
6	AF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	10
6	CF	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	1	16
7	AG	153/156 (98%)	108 (71%)	28 (18%)	17 (11%)	0	7
7	CG	150/156 (96%)	93 (62%)	39 (26%)	18 (12%)	0	6
8	AH	136/138 (99%)	87 (64%)	37 (27%)	12 (9%)	1	11
8	CH	136/138 (99%)	92 (68%)	37 (27%)	7 (5%)	2	25
9	AI	125/128 (98%)	86 (69%)	26 (21%)	13 (10%)	1	8
9	CI	125/128 (98%)	72 (58%)	43 (34%)	10 (8%)	1	13
10	AJ	97/105 (92%)	59 (61%)	27 (28%)	11 (11%)	0	7
10	CJ	97/105 (92%)	52 (54%)	34 (35%)	11 (11%)	0	7
11	AK	114/129 (88%)	82 (72%)	26 (23%)	6 (5%)	2	23
11	CK	117/129 (91%)	81 (69%)	25 (21%)	11 (9%)	1	10
12	AL	123/132 (93%)	78 (63%)	29 (24%)	16 (13%)	0	4
12	CL	123/132 (93%)	82 (67%)	19 (15%)	22 (18%)	0	2
13	AM	120/126 (95%)	69 (58%)	28 (23%)	23 (19%)	0	2
13	CM	116/126 (92%)	66 (57%)	24 (21%)	26 (22%)	0	1
14	AN	58/61 (95%)	33 (57%)	17 (29%)	8 (14%)	0	4
14	CN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	6
15	AO	86/89 (97%)	61 (71%)	16 (19%)	9 (10%)	1	8
15	CO	86/89 (97%)	62 (72%)	15 (17%)	9 (10%)	1	8
16	AP	82/88 (93%)	54 (66%)	19 (23%)	9 (11%)	0	7
16	CP	82/88 (93%)	56 (68%)	24 (29%)	2 (2%)	7	45
17	AQ	98/105 (93%)	76 (78%)	13 (13%)	9 (9%)	1	10
17	CQ	98/105 (93%)	64 (65%)	23 (24%)	11 (11%)	0	7
18	AR	68/88 (77%)	48 (71%)	14 (21%)	6 (9%)	1	11
18	CR	68/88 (77%)	50 (74%)	11 (16%)	7 (10%)	1	8
19	AS	77/93 (83%)	46 (60%)	13 (17%)	18 (23%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CS	77/93 (83%)	49 (64%)	18 (23%)	10 (13%)	0	4
20	AT	97/106 (92%)	57 (59%)	25 (26%)	15 (16%)	0	3
20	CT	97/106 (92%)	64 (66%)	18 (19%)	15 (16%)	0	3
21	AU	23/27 (85%)	15 (65%)	7 (30%)	1 (4%)	3	30
21	CU	23/27 (85%)	19 (83%)	1 (4%)	3 (13%)	0	4
29	BC	183/229 (80%)	67 (37%)	66 (36%)	50 (27%)	0	0
29	DC	183/229 (80%)	62 (34%)	69 (38%)	52 (28%)	0	0
30	BD	270/276 (98%)	175 (65%)	54 (20%)	41 (15%)	0	3
30	DD	270/276 (98%)	180 (67%)	51 (19%)	39 (14%)	0	3
31	BE	203/206 (98%)	133 (66%)	38 (19%)	32 (16%)	0	2
31	DE	203/206 (98%)	115 (57%)	49 (24%)	39 (19%)	0	2
32	BF	204/210 (97%)	141 (69%)	40 (20%)	23 (11%)	0	7
32	DF	206/210 (98%)	126 (61%)	44 (21%)	36 (18%)	0	2
33	BG	179/182 (98%)	114 (64%)	31 (17%)	34 (19%)	0	2
33	DG	179/182 (98%)	98 (55%)	53 (30%)	28 (16%)	0	2
34	BH	159/180 (88%)	92 (58%)	31 (20%)	36 (23%)	0	1
34	DH	158/180 (88%)	96 (61%)	30 (19%)	32 (20%)	0	1
35	BI	144/148 (97%)	72 (50%)	37 (26%)	35 (24%)	0	1
35	DI	144/148 (97%)	73 (51%)	48 (33%)	23 (16%)	0	2
36	BN	137/140 (98%)	98 (72%)	23 (17%)	16 (12%)	0	6
36	DN	137/140 (98%)	83 (61%)	30 (22%)	24 (18%)	0	2
37	BO	120/122 (98%)	95 (79%)	19 (16%)	6 (5%)	3	25
37	DO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0	8
38	BP	144/150 (96%)	68 (47%)	33 (23%)	43 (30%)	0	0
38	DP	144/150 (96%)	69 (48%)	38 (26%)	37 (26%)	0	1
39	BQ	137/141 (97%)	99 (72%)	25 (18%)	13 (10%)	1	10
39	DQ	134/141 (95%)	86 (64%)	28 (21%)	20 (15%)	0	3
40	BR	115/118 (98%)	73 (64%)	24 (21%)	18 (16%)	0	2
40	DR	115/118 (98%)	69 (60%)	29 (25%)	17 (15%)	0	3
41	BS	97/112 (87%)	46 (47%)	25 (26%)	26 (27%)	0	0
41	DS	97/112 (87%)	44 (45%)	28 (29%)	25 (26%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BT	136/146 (93%)	81 (60%)	25 (18%)	30 (22%)	0	1
42	DT	136/146 (93%)	71 (52%)	28 (21%)	37 (27%)	0	0
43	BU	115/118 (98%)	79 (69%)	27 (24%)	9 (8%)	1	13
43	DU	115/118 (98%)	63 (55%)	36 (31%)	16 (14%)	0	4
44	BV	99/101 (98%)	59 (60%)	18 (18%)	22 (22%)	0	1
44	DV	99/101 (98%)	56 (57%)	25 (25%)	18 (18%)	0	2
45	BW	111/113 (98%)	86 (78%)	20 (18%)	5 (4%)	3	29
45	DW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	5
46	BX	91/96 (95%)	71 (78%)	19 (21%)	1 (1%)	17	62
46	DX	91/96 (95%)	63 (69%)	16 (18%)	12 (13%)	0	4
47	BY	84/110 (76%)	30 (36%)	25 (30%)	29 (34%)	0	0
47	DY	99/110 (90%)	36 (36%)	27 (27%)	36 (36%)	0	0
48	BZ	175/206 (85%)	94 (54%)	46 (26%)	35 (20%)	0	1
48	DZ	175/206 (85%)	85 (49%)	52 (30%)	38 (22%)	0	1
49	B0	82/85 (96%)	66 (80%)	11 (13%)	5 (6%)	2	19
49	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	3	26
50	B1	92/98 (94%)	72 (78%)	13 (14%)	7 (8%)	1	14
50	D1	92/98 (94%)	70 (76%)	11 (12%)	11 (12%)	0	6
51	B2	69/72 (96%)	43 (62%)	13 (19%)	13 (19%)	0	2
51	D2	69/72 (96%)	41 (59%)	16 (23%)	12 (17%)	0	2
52	B3	58/60 (97%)	49 (84%)	4 (7%)	5 (9%)	1	11
52	D3	58/60 (97%)	46 (79%)	6 (10%)	6 (10%)	1	8
53	B4	45/71 (63%)	18 (40%)	10 (22%)	17 (38%)	0	0
53	D4	45/71 (63%)	19 (42%)	11 (24%)	15 (33%)	0	0
54	B5	57/60 (95%)	41 (72%)	8 (14%)	8 (14%)	0	4
54	D5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	5
55	B6	46/54 (85%)	18 (39%)	9 (20%)	19 (41%)	0	0
55	D6	44/54 (82%)	15 (34%)	12 (27%)	17 (39%)	0	0
56	B7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	19
56	D7	47/49 (96%)	40 (85%)	5 (11%)	2 (4%)	3	30
57	B8	62/65 (95%)	30 (48%)	19 (31%)	13 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	D8	62/65 (95%)	33 (53%)	17 (27%)	12 (19%)	0	2
58	B9	34/37 (92%)	27 (79%)	5 (15%)	2 (6%)	2	21
58	D9	34/37 (92%)	24 (71%)	7 (21%)	3 (9%)	1	11
All	All	11692/12586 (93%)	7260 (62%)	2616 (22%)	1816 (16%)	0	3

5 of 1816 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	24	TRP
2	AB	122	PHE
2	AB	128	GLU
2	AB	154	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	177 (88%)	25 (12%)	6	28
2	CB	202/220 (92%)	177 (88%)	25 (12%)	6	28
3	AC	160/188 (85%)	144 (90%)	16 (10%)	9	40
3	CC	159/188 (85%)	142 (89%)	17 (11%)	8	36
4	AD	180/181 (99%)	159 (88%)	21 (12%)	7	30
4	CD	180/181 (99%)	162 (90%)	18 (10%)	9	40
5	AE	115/123 (94%)	103 (90%)	12 (10%)	9	38
5	CE	115/123 (94%)	99 (86%)	16 (14%)	4	23
6	AF	90/90 (100%)	82 (91%)	8 (9%)	12	46
6	CF	90/90 (100%)	79 (88%)	11 (12%)	6	28
7	AG	126/127 (99%)	109 (86%)	17 (14%)	5	25
7	CG	125/127 (98%)	115 (92%)	10 (8%)	15	51
8	AH	119/119 (100%)	106 (89%)	13 (11%)	8	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	105 (88%)	14 (12%)	6	30
9	AI	97/99 (98%)	85 (88%)	12 (12%)	6	28
9	CI	97/99 (98%)	82 (84%)	15 (16%)	3	18
10	AJ	88/92 (96%)	73 (83%)	15 (17%)	2	14
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	6	28
11	AK	88/99 (89%)	82 (93%)	6 (7%)	20	59
11	CK	90/99 (91%)	83 (92%)	7 (8%)	16	52
12	AL	104/109 (95%)	92 (88%)	12 (12%)	7	31
12	CL	104/109 (95%)	92 (88%)	12 (12%)	7	31
13	AM	97/101 (96%)	84 (87%)	13 (13%)	5	25
13	CM	94/101 (93%)	82 (87%)	12 (13%)	5	27
14	AN	49/50 (98%)	43 (88%)	6 (12%)	6	28
14	CN	49/50 (98%)	47 (96%)	2 (4%)	37	74
15	AO	79/80 (99%)	71 (90%)	8 (10%)	9	39
15	CO	79/80 (99%)	69 (87%)	10 (13%)	5	27
16	AP	72/74 (97%)	62 (86%)	10 (14%)	4	23
16	CP	72/74 (97%)	65 (90%)	7 (10%)	10	41
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	13	49
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	28	67
18	AR	61/77 (79%)	57 (93%)	4 (7%)	21	61
18	CR	61/77 (79%)	53 (87%)	8 (13%)	5	26
19	AS	69/80 (86%)	55 (80%)	14 (20%)	1	7
19	CS	69/80 (86%)	55 (80%)	14 (20%)	1	7
20	AT	76/82 (93%)	63 (83%)	13 (17%)	2	14
20	CT	76/82 (93%)	66 (87%)	10 (13%)	5	26
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	37
21	CU	19/22 (86%)	17 (90%)	2 (10%)	8	37
26	AZ	1/1 (100%)	1 (100%)	0	100	100
26	CZ	1/1 (100%)	1 (100%)	0	100	100
29	BC	61/181 (34%)	55 (90%)	6 (10%)	10	41
29	DC	61/181 (34%)	52 (85%)	9 (15%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BD	213/218 (98%)	184 (86%)	29 (14%)	5	24
30	DD	213/218 (98%)	183 (86%)	30 (14%)	4	22
31	BE	165/166 (99%)	142 (86%)	23 (14%)	4	23
31	DE	165/166 (99%)	133 (81%)	32 (19%)	2	8
32	BF	163/166 (98%)	142 (87%)	21 (13%)	5	26
32	DF	165/166 (99%)	143 (87%)	22 (13%)	5	25
33	BG	155/156 (99%)	136 (88%)	19 (12%)	6	28
33	DG	155/156 (99%)	133 (86%)	22 (14%)	4	22
34	BH	134/148 (90%)	116 (87%)	18 (13%)	5	25
34	DH	132/148 (89%)	119 (90%)	13 (10%)	10	41
35	BI	122/124 (98%)	107 (88%)	15 (12%)	6	28
35	DI	122/124 (98%)	104 (85%)	18 (15%)	4	20
36	BN	117/119 (98%)	94 (80%)	23 (20%)	1	8
36	DN	117/119 (98%)	98 (84%)	19 (16%)	3	16
37	BO	100/100 (100%)	84 (84%)	16 (16%)	3	17
37	DO	100/100 (100%)	88 (88%)	12 (12%)	6	29
38	BP	112/116 (97%)	86 (77%)	26 (23%)	1	4
38	DP	112/116 (97%)	90 (80%)	22 (20%)	1	8
39	BQ	110/111 (99%)	89 (81%)	21 (19%)	2	9
39	DQ	108/111 (97%)	96 (89%)	12 (11%)	8	34
40	BR	100/101 (99%)	83 (83%)	17 (17%)	2	14
40	DR	100/101 (99%)	84 (84%)	16 (16%)	3	17
41	BS	77/88 (88%)	53 (69%)	24 (31%)	0	2
41	DS	77/88 (88%)	67 (87%)	10 (13%)	5	26
42	BT	120/127 (94%)	88 (73%)	32 (27%)	0	3
42	DT	120/127 (94%)	87 (72%)	33 (28%)	0	3
43	BU	92/94 (98%)	78 (85%)	14 (15%)	3	19
43	DU	92/94 (98%)	82 (89%)	10 (11%)	8	35
44	BV	82/82 (100%)	64 (78%)	18 (22%)	1	5
44	DV	82/82 (100%)	65 (79%)	17 (21%)	1	7
45	BW	91/92 (99%)	78 (86%)	13 (14%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DW	91/92 (99%)	84 (92%)	7 (8%)	16	53
46	BX	74/78 (95%)	63 (85%)	11 (15%)	4	20
46	DX	74/78 (95%)	58 (78%)	16 (22%)	1	6
47	BY	73/91 (80%)	59 (81%)	14 (19%)	2	8
47	DY	84/91 (92%)	69 (82%)	15 (18%)	2	11
48	BZ	155/179 (87%)	131 (84%)	24 (16%)	3	18
48	DZ	155/179 (87%)	138 (89%)	17 (11%)	8	35
49	B0	66/67 (98%)	60 (91%)	6 (9%)	12	45
49	D0	66/67 (98%)	58 (88%)	8 (12%)	6	29
50	B1	78/83 (94%)	65 (83%)	13 (17%)	3	15
50	D1	78/83 (94%)	72 (92%)	6 (8%)	16	53
51	B2	66/67 (98%)	52 (79%)	14 (21%)	1	6
51	D2	66/67 (98%)	58 (88%)	8 (12%)	6	29
52	B3	51/52 (98%)	44 (86%)	7 (14%)	4	24
52	D3	51/52 (98%)	46 (90%)	5 (10%)	10	41
53	B4	34/63 (54%)	30 (88%)	4 (12%)	6	30
53	D4	34/63 (54%)	28 (82%)	6 (18%)	2	12
54	B5	51/52 (98%)	42 (82%)	9 (18%)	2	12
54	D5	51/52 (98%)	41 (80%)	10 (20%)	1	8
55	B6	44/52 (85%)	27 (61%)	17 (39%)	0	1
55	D6	44/52 (85%)	30 (68%)	14 (32%)	0	2
56	B7	41/42 (98%)	37 (90%)	4 (10%)	10	41
56	D7	41/42 (98%)	35 (85%)	6 (15%)	4	21
57	B8	53/55 (96%)	40 (76%)	13 (24%)	1	4
57	D8	53/55 (96%)	39 (74%)	14 (26%)	0	3
58	B9	33/34 (97%)	32 (97%)	1 (3%)	48	81
58	D9	33/34 (97%)	31 (94%)	2 (6%)	23	63
All	All	9644/10430 (92%)	8280 (86%)	1364 (14%)	4	22

5 of 1364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BZ	167	GLU

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Mol	Chain	Res	Type
4	CD	138	TYR
47	DY	42	VAL
50	B1	80	LEU
56	B7	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 345 such sidechains are listed below:

Mol	Chain	Res	Type
50	B1	45	ASN
3	CC	181	ASN
46	DX	41	ASN
51	B2	43	GLN
58	B9	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1508 (99%)	234 (15%)	56 (3%)
1	CA	1491/1508 (98%)	248 (16%)	61 (4%)
22	AV	9/30 (30%)	1 (11%)	0
22	CV	9/30 (30%)	2 (22%)	0
23	AW	73/75 (97%)	15 (20%)	3 (4%)
23	CW	73/75 (97%)	20 (27%)	3 (4%)
24	AX	76/77 (98%)	24 (31%)	4 (5%)
25	AY	74/75 (98%)	19 (25%)	0
25	CY	74/75 (98%)	20 (27%)	0
27	BA	2779/2915 (95%)	539 (19%)	96 (3%)
27	DA	2765/2915 (94%)	555 (20%)	114 (4%)
28	BB	118/122 (96%)	16 (13%)	3 (2%)
28	DB	118/122 (96%)	40 (33%)	5 (4%)
59	CX	76/77 (98%)	21 (27%)	2 (2%)
All	All	9228/9604 (96%)	1754 (19%)	347 (3%)

5 of 1754 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	28	G
1	AA	31	G
1	AA	32	A

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Mol	Chain	Res	Type
1	AA	39	G

5 of 347 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	2778	A
1	CA	968	A
27	DA	2490	G
28	BB	66	A
1	CA	366	C

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

10 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$
26	KBE	AZ	1	26	8,8,9	1.38	1 (12%)	7,8,10	2.47	3 (42%)
26	DPP	AZ	2	26	3,5,6	0.56	0	1,5,7	2.67	1 (100%)
26	UAL	AZ	3	26	7,8,9	2.52	2 (28%)	4,9,11	1.73	1 (25%)
26	MYN	AZ	4	26	8,11,12	1.72	1 (12%)	8,14,16	1.68	2 (25%)
26	DPP	AZ	5	26	3,5,6	0.50	0	1,5,7	1.94	0
26	KBE	CZ	1	26	8,8,9	1.10	1 (12%)	7,8,10	2.03	1 (14%)
26	DPP	CZ	2	26	3,5,6	0.82	0	1,5,7	2.44	1 (100%)
26	UAL	CZ	3	26	7,8,9	2.53	2 (28%)	4,9,11	1.34	1 (25%)
26	MYN	CZ	4	26	8,11,12	1.39	1 (12%)	8,14,16	1.79	2 (25%)
26	DPP	CZ	5	26	3,5,6	0.75	0	1,5,7	1.58	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
26	KBE	AZ	1	26	-	0/7/7/8	0/0/0/0
26	DPP	AZ	2	26	-	0/1/4/6	0/0/0/0
26	UAL	AZ	3	26	-	0/3/7/9	0/0/0/0
26	MYN	AZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	AZ	5	26	-	0/1/4/6	0/0/0/0
26	KBE	CZ	1	26	-	0/7/7/8	0/0/0/0
26	DPP	CZ	2	26	-	0/1/4/6	0/0/0/0
26	UAL	CZ	3	26	-	0/3/7/9	0/0/0/0
26	MYN	CZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	CZ	5	26	-	0/1/4/6	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AZ	3	UAL	C1-N1	-4.01	1.33	1.40
26	CZ	3	UAL	C1-N1	-3.76	1.33	1.40
26	AZ	1	KBE	CA-C	-3.28	1.39	1.49
26	CZ	1	KBE	CA-C	-2.87	1.40	1.49
26	CZ	4	MYN	CZ-NE	3.39	1.39	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	CZ	4	MYN	CG-CB-CA	-3.44	109.33	112.70
26	AZ	3	UAL	O-C-CA	-3.18	120.72	125.40
26	AZ	2	DPP	O-C-CA	-2.67	118.53	125.49
26	AZ	4	MYN	CG-CB-CA	-2.65	110.11	112.70
26	AZ	4	MYN	CB-CA-N	-2.63	104.01	110.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	AZ	1	KBE	5	0
26	AZ	2	DPP	4	0
26	AZ	3	UAL	3	0
26	AZ	4	MYN	3	0
26	CZ	1	KBE	10	0
26	CZ	2	DPP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	CZ	3	UAL	2	0
26	CZ	4	MYN	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 850 ligands modelled in this entry, 850 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1495/1508 (99%)	-0.05	31 (2%) 67 61	32, 72, 154, 200	0
1	CA	1493/1508 (99%)	0.19	35 (2%) 64 57	38, 81, 158, 200	0
2	AB	235/256 (91%)	0.21	10 (4%) 39 33	69, 98, 133, 148	0
2	CB	235/256 (91%)	0.33	20 (8%) 13 13	74, 103, 147, 165	0
3	AC	207/239 (86%)	-0.02	1 (0%) 91 89	66, 86, 109, 114	0
3	CC	206/239 (86%)	0.29	15 (7%) 18 17	76, 98, 123, 136	0
4	AD	208/209 (99%)	0.24	6 (2%) 55 48	52, 73, 87, 92	0
4	CD	208/209 (99%)	0.13	1 (0%) 91 89	47, 68, 85, 89	0
5	AE	151/162 (93%)	-0.10	1 (0%) 89 84	49, 67, 94, 107	0
5	CE	151/162 (93%)	0.11	2 (1%) 79 72	53, 75, 94, 100	0
6	AF	101/101 (100%)	-0.35	0 100 100	54, 69, 84, 98	0
6	CF	101/101 (100%)	0.02	2 (1%) 68 62	49, 73, 83, 98	0
7	AG	155/156 (99%)	0.45	13 (8%) 14 14	62, 82, 107, 124	0
7	CG	154/156 (98%)	0.18	13 (8%) 14 14	69, 92, 116, 124	0
8	AH	138/138 (100%)	0.37	3 (2%) 65 59	54, 71, 82, 96	0
8	CH	138/138 (100%)	0.32	4 (2%) 55 48	55, 75, 87, 97	0
9	AI	127/128 (99%)	0.77	19 (14%) 3 3	57, 99, 123, 126	0
9	CI	127/128 (99%)	0.86	17 (13%) 4 5	72, 106, 123, 129	0
10	AJ	99/105 (94%)	1.13	24 (24%) 1 1	69, 108, 130, 130	0
10	CJ	99/105 (94%)	1.12	20 (20%) 1 2	79, 115, 136, 143	0
11	AK	116/129 (89%)	0.32	4 (3%) 49 42	53, 67, 89, 107	0
11	CK	119/129 (92%)	0.43	10 (8%) 14 14	56, 76, 99, 114	0
12	AL	125/132 (94%)	0.27	5 (4%) 42 36	49, 63, 80, 103	0
12	CL	125/132 (94%)	0.26	6 (4%) 34 29	51, 71, 83, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	122/126 (96%)	0.10	3 (2%) 61 54	63, 87, 97, 102	0
13	CM	118/126 (93%)	0.29	7 (5%) 26 23	77, 100, 114, 120	0
14	AN	60/61 (98%)	0.20	0 100 100	52, 77, 91, 97	0
14	CN	60/61 (98%)	1.06	8 (13%) 4 5	75, 92, 101, 105	0
15	AO	88/89 (98%)	-0.09	0 100 100	47, 65, 82, 93	0
15	CO	88/89 (98%)	-0.10	0 100 100	50, 70, 87, 92	0
16	AP	84/88 (95%)	0.69	8 (9%) 10 11	50, 68, 95, 109	0
16	CP	84/88 (95%)	0.57	7 (8%) 14 14	55, 66, 85, 109	0
17	AQ	100/105 (95%)	-0.17	0 100 100	53, 69, 84, 88	0
17	CQ	100/105 (95%)	0.27	5 (5%) 32 27	59, 73, 91, 94	0
18	AR	70/88 (79%)	0.48	5 (7%) 19 18	49, 68, 94, 100	0
18	CR	70/88 (79%)	-0.03	2 (2%) 55 48	56, 74, 99, 104	0
19	AS	79/93 (84%)	0.99	17 (21%) 1 1	63, 90, 110, 115	0
19	CS	79/93 (84%)	1.59	24 (30%) 1 1	91, 111, 132, 138	0
20	AT	99/106 (93%)	0.49	5 (5%) 32 27	54, 75, 104, 110	0
20	CT	99/106 (93%)	0.55	5 (5%) 32 27	63, 76, 111, 114	0
21	AU	25/27 (92%)	1.40	6 (24%) 1 1	74, 82, 90, 95	0
21	CU	25/27 (92%)	2.43	15 (60%) 0 0	72, 93, 105, 109	0
22	AV	10/30 (33%)	1.07	2 (20%) 1 2	51, 66, 125, 128	0
22	CV	10/30 (33%)	1.04	2 (20%) 1 2	65, 81, 134, 138	0
23	AW	74/75 (98%)	0.37	4 (5%) 29 26	49, 117, 149, 154	0
23	CW	74/75 (98%)	0.97	6 (8%) 15 14	79, 129, 148, 165	0
24	AX	77/77 (100%)	0.04	2 (2%) 59 52	35, 85, 115, 128	0
25	AY	75/75 (100%)	0.82	11 (14%) 3 4	62, 157, 189, 191	0
25	CY	75/75 (100%)	0.92	10 (13%) 4 5	76, 170, 192, 197	0
26	AZ	1/6 (16%)	-0.53	0 100 100	64, 64, 64, 64	0
26	CZ	1/6 (16%)	-0.02	0 100 100	91, 91, 91, 91	0
27	BA	2789/2915 (95%)	-0.17	57 (2%) 68 62	19, 44, 164, 200	0
27	DA	2775/2915 (95%)	0.52	82 (2%) 54 47	30, 72, 170, 200	0
28	BB	119/122 (97%)	-0.12	3 (2%) 61 54	36, 70, 127, 168	0
28	DB	119/122 (97%)	1.16	25 (21%) 1 1	109, 142, 170, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BC	191/229 (83%)	2.59	101 (52%) 0 0	103, 169, 180, 186	0
29	DC	191/229 (83%)	2.46	95 (49%) 0 0	125, 170, 183, 186	0
30	BD	272/276 (98%)	-0.26	0 100 100	18, 41, 61, 73	0
30	DD	272/276 (98%)	0.13	4 (1%) 76 70	31, 52, 69, 81	0
31	BE	205/206 (99%)	-0.22	3 (1%) 76 70	16, 42, 76, 94	0
31	DE	205/206 (99%)	0.55	9 (4%) 38 32	44, 80, 112, 119	0
32	BF	206/210 (98%)	-0.20	3 (1%) 76 70	17, 46, 110, 129	0
32	DF	208/210 (99%)	0.55	9 (4%) 39 33	40, 69, 120, 132	0
33	BG	181/182 (99%)	0.34	7 (3%) 43 37	49, 74, 102, 119	0
33	DG	181/182 (99%)	0.67	19 (10%) 8 9	75, 101, 117, 125	0
34	BH	161/180 (89%)	0.20	7 (4%) 39 33	39, 65, 81, 95	0
34	DH	160/180 (88%)	1.42	47 (29%) 1 1	106, 129, 153, 161	0
35	BI	146/148 (98%)	0.73	16 (10%) 7 8	57, 134, 150, 159	0
35	DI	146/148 (98%)	0.77	19 (13%) 5 5	62, 107, 139, 150	0
36	BN	139/140 (99%)	-0.05	1 (0%) 89 84	23, 43, 67, 73	0
36	DN	139/140 (99%)	0.94	19 (13%) 4 5	69, 86, 106, 108	0
37	BO	122/122 (100%)	-0.30	0 100 100	22, 44, 60, 67	0
37	DO	122/122 (100%)	0.35	3 (2%) 61 54	47, 72, 80, 86	0
38	BP	146/150 (97%)	0.19	6 (4%) 41 35	17, 60, 91, 121	0
38	DP	146/150 (97%)	1.02	15 (10%) 9 9	45, 82, 103, 126	0
39	BQ	139/141 (98%)	-0.09	0 100 100	29, 47, 70, 82	0
39	DQ	138/141 (97%)	0.87	15 (10%) 7 8	58, 88, 107, 136	0
40	BR	117/118 (99%)	-0.24	0 100 100	17, 37, 59, 66	0
40	DR	117/118 (99%)	0.38	1 (0%) 85 79	39, 64, 81, 88	0
41	BS	99/112 (88%)	0.32	3 (3%) 54 47	40, 65, 82, 91	0
41	DS	99/112 (88%)	1.10	17 (17%) 2 2	71, 93, 106, 109	0
42	BT	138/146 (94%)	0.08	4 (2%) 55 48	27, 53, 108, 143	0
42	DT	138/146 (94%)	0.45	10 (7%) 18 17	64, 79, 136, 142	0
43	BU	117/118 (99%)	-0.30	0 100 100	20, 37, 59, 86	0
43	DU	117/118 (99%)	0.53	7 (5%) 25 22	48, 80, 111, 120	0
44	BV	101/101 (100%)	0.11	2 (1%) 68 62	18, 49, 68, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DV	101/101 (100%)	0.57	10 (9%) 9 11	54, 100, 114, 122	0
45	BW	113/113 (100%)	-0.18	1 (0%) 85 79	21, 34, 64, 102	0
45	DW	113/113 (100%)	0.49	2 (1%) 71 64	39, 61, 93, 118	0
46	BX	93/96 (96%)	-0.13	0 100 100	31, 45, 69, 76	0
46	DX	93/96 (96%)	0.49	1 (1%) 82 76	39, 66, 79, 85	0
47	BY	88/110 (80%)	0.63	6 (6%) 20 19	41, 58, 79, 87	0
47	DY	101/110 (91%)	1.59	31 (30%) 1 1	62, 83, 144, 153	0
48	BZ	177/206 (85%)	1.08	38 (21%) 1 1	52, 85, 159, 164	0
48	DZ	177/206 (85%)	1.78	53 (29%) 1 1	93, 123, 178, 184	0
49	B0	84/85 (98%)	0.39	5 (5%) 25 22	27, 49, 71, 85	0
49	D0	84/85 (98%)	1.36	24 (28%) 1 1	66, 82, 96, 104	0
50	B1	94/98 (95%)	0.10	0 100 100	28, 49, 80, 91	0
50	D1	94/98 (95%)	0.69	6 (6%) 23 21	40, 62, 94, 101	0
51	B2	71/72 (98%)	-0.06	1 (1%) 78 71	37, 62, 93, 106	0
51	D2	71/72 (98%)	0.25	2 (2%) 56 50	59, 78, 98, 117	0
52	B3	60/60 (100%)	0.19	1 (1%) 73 66	27, 44, 69, 103	0
52	D3	60/60 (100%)	1.67	24 (40%) 0 0	70, 88, 111, 119	0
53	B4	49/71 (69%)	-0.22	2 (4%) 41 35	72, 97, 116, 119	0
53	D4	49/71 (69%)	0.14	2 (4%) 41 35	100, 115, 120, 121	0
54	B5	59/60 (98%)	-0.11	3 (5%) 32 27	21, 38, 93, 115	0
54	D5	59/60 (98%)	0.54	6 (10%) 9 9	46, 62, 116, 136	0
55	B6	48/54 (88%)	-0.04	0 100 100	29, 58, 71, 90	0
55	D6	46/54 (85%)	1.06	9 (19%) 1 2	50, 81, 91, 101	0
56	B7	49/49 (100%)	-0.13	0 100 100	20, 32, 77, 90	0
56	D7	49/49 (100%)	0.72	3 (6%) 25 22	36, 47, 84, 92	0
57	B8	64/65 (98%)	0.49	4 (6%) 23 21	26, 44, 62, 99	0
57	D8	64/65 (98%)	1.17	7 (10%) 7 8	51, 66, 85, 109	0
58	B9	36/37 (97%)	0.67	1 (2%) 56 50	15, 45, 57, 59	0
58	D9	36/37 (97%)	1.53	12 (33%) 0 0	79, 94, 99, 102	0
59	CX	77/77 (100%)	0.29	2 (2%) 59 52	63, 100, 127, 140	0
All	All	21180/22202 (95%)	0.34	1281 (6%) 25 22	15, 72, 152, 200	0

The worst 5 of 1281 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	BC	179	SER	15.4
29	DC	57	ASN	13.3
29	DC	179	SER	13.2
48	DZ	110	VAL	13.1
27	DA	2802	G	13.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
26	KBE	CZ	1	9/10	0.81	0.52	-	95,98,100,100	0
26	DPP	CZ	2	6/7	0.88	0.21	-	92,93,95,98	0
26	UAL	AZ	3	9/10	0.87	0.24	-	63,66,70,71	0
26	DPP	CZ	5	6/7	0.85	0.26	-	88,89,89,90	0
26	MYN	AZ	4	11/12	0.90	0.23	-	61,64,65,65	0
26	DPP	AZ	2	6/7	0.93	0.21	-	66,67,69,71	0
26	MYN	CZ	4	11/12	0.86	0.22	-	88,89,91,92	0
26	DPP	AZ	5	6/7	0.93	0.20	-	62,64,65,65	0
26	UAL	CZ	3	9/10	0.81	0.28	-	91,92,93,93	0
26	KBE	AZ	1	9/10	0.83	0.59	-	71,74,78,79	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
60	MG	AA	1646	1/1	0.15	1.02	56.45	71,71,71,71	0
60	MG	CA	1614	1/1	0.92	0.94	49.57	50,50,50,50	0
60	MG	AA	1621	1/1	0.90	0.66	39.83	28,28,28,28	0
60	MG	BA	3080	1/1	0.95	0.45	38.19	15,15,15,15	0
60	MG	BA	3293	1/1	0.88	0.55	28.68	45,45,45,45	0
60	MG	CA	1682	1/1	0.90	0.62	26.64	41,41,41,41	0
60	MG	BA	3021	1/1	0.94	0.39	25.54	1,1,1,1	0
60	MG	BA	3005	1/1	0.97	0.43	24.55	1,1,1,1	0
60	MG	BA	3131	1/1	0.93	0.35	24.42	1,1,1,1	0
60	MG	CA	1650	1/1	0.95	0.46	23.48	1,1,1,1	0
60	MG	AA	1642	1/1	0.91	0.41	20.64	41,41,41,41	0
60	MG	BA	3229	1/1	0.91	0.40	18.72	49,49,49,49	0
60	MG	BA	3121	1/1	0.93	0.50	18.15	23,23,23,23	0
60	MG	BA	3070	1/1	0.98	0.51	17.96	1,1,1,1	0
60	MG	BA	3177	1/1	0.78	0.43	17.68	41,41,41,41	0
60	MG	AA	1618	1/1	0.97	0.40	16.40	22,22,22,22	0
60	MG	CA	1683	1/1	0.86	0.52	16.40	53,53,53,53	0
60	MG	BA	3018	1/1	0.98	0.23	16.31	1,1,1,1	0
60	MG	BA	3142	1/1	0.83	0.36	16.23	30,30,30,30	0
60	MG	BA	3104	1/1	0.82	0.39	15.71	42,42,42,42	0
60	MG	BA	3076	1/1	0.97	0.38	15.62	1,1,1,1	0
60	MG	DA	3075	1/1	0.91	0.50	15.24	1,1,1,1	0
60	MG	BA	3227	1/1	0.91	0.37	14.50	33,33,33,33	0
60	MG	DA	3111	1/1	0.72	0.47	14.02	64,64,64,64	0
60	MG	AA	1643	1/1	0.84	0.31	13.38	29,29,29,29	0
60	MG	BA	3034	1/1	0.82	0.40	13.29	1,1,1,1	0
60	MG	BA	3020	1/1	0.97	0.40	12.97	1,1,1,1	0
60	MG	BA	3078	1/1	0.94	0.33	12.57	1,1,1,1	0
60	MG	BA	3009	1/1	0.98	0.35	12.48	1,1,1,1	0
60	MG	BA	3137	1/1	0.97	0.37	12.44	1,1,1,1	0
60	MG	DA	3120	1/1	0.85	0.38	11.95	3,3,3,3	0
60	MG	BA	3030	1/1	0.98	0.38	11.69	7,7,7,7	0
60	MG	DA	3084	1/1	0.71	0.52	11.52	71,71,71,71	0
60	MG	BA	3232	1/1	0.95	0.29	11.11	1,1,1,1	0
60	MG	DA	3180	1/1	0.96	0.57	10.83	5,5,5,5	0
60	MG	BA	3134	1/1	0.97	0.36	10.54	12,12,12,12	0
60	MG	DA	3042	1/1	0.69	0.41	9.78	46,46,46,46	0
60	MG	BA	3017	1/1	0.97	0.32	9.69	1,1,1,1	0
60	MG	BA	3306	1/1	0.95	0.29	9.55	5,5,5,5	0
60	MG	BA	3251	1/1	0.82	0.32	9.01	1,1,1,1	0
60	MG	DA	3169	1/1	0.91	0.36	8.95	16,16,16,16	0
60	MG	BA	3141	1/1	0.88	0.30	8.88	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3167	1/1	0.96	0.26	8.60	22,22,22,22	0
60	MG	DA	3206	1/1	0.92	0.33	8.57	12,12,12,12	0
60	MG	DA	3173	1/1	0.81	0.48	8.47	10,10,10,10	0
60	MG	BA	3156	1/1	0.96	0.39	8.40	7,7,7,7	0
60	MG	DA	3006	1/1	0.93	0.35	8.39	4,4,4,4	0
60	MG	BA	3108	1/1	0.99	0.41	8.34	2,2,2,2	0
60	MG	BA	3094	1/1	0.83	0.25	8.29	11,11,11,11	0
60	MG	BA	3037	1/1	0.95	0.39	8.24	33,33,33,33	0
60	MG	BA	3133	1/1	0.98	0.35	8.17	1,1,1,1	0
60	MG	DA	3160	1/1	0.91	0.36	8.13	27,27,27,27	0
60	MG	DA	3128	1/1	0.64	0.36	8.03	24,24,24,24	0
60	MG	BA	3049	1/1	0.97	0.32	7.98	1,1,1,1	0
60	MG	BA	3044	1/1	0.96	0.34	7.88	1,1,1,1	0
60	MG	BA	3169	1/1	0.96	0.30	7.74	16,16,16,16	0
60	MG	AA	1637	1/1	0.53	0.30	7.69	44,44,44,44	0
60	MG	BA	3083	1/1	0.97	0.30	7.67	1,1,1,1	0
60	MG	BA	3234	1/1	0.95	0.33	7.31	15,15,15,15	0
60	MG	DA	3096	1/1	0.81	0.40	7.26	16,16,16,16	0
60	MG	CA	1657	1/1	0.93	0.56	7.17	23,23,23,23	0
60	MG	BA	3031	1/1	0.96	0.30	7.05	1,1,1,1	0
60	MG	BA	3016	1/1	0.98	0.30	6.82	1,1,1,1	0
60	MG	DA	3195	1/1	0.89	0.38	6.45	18,18,18,18	0
60	MG	BU	201	1/1	0.97	0.43	6.44	23,23,23,23	0
60	MG	BA	3149	1/1	0.92	0.34	6.40	14,14,14,14	0
60	MG	DA	3005	1/1	0.90	0.31	6.39	28,28,28,28	0
60	MG	DA	3118	1/1	0.81	0.34	6.37	22,22,22,22	0
60	MG	BA	3013	1/1	0.96	0.32	6.19	1,1,1,1	0
60	MG	BA	3077	1/1	0.82	0.24	6.12	1,1,1,1	0
60	MG	AA	1617	1/1	0.93	0.43	6.06	13,13,13,13	0
60	MG	BA	3162	1/1	0.79	0.27	5.96	56,56,56,56	0
60	MG	BA	3027	1/1	0.97	0.28	5.86	1,1,1,1	0
60	MG	DA	3040	1/1	0.80	0.39	5.56	19,19,19,19	0
60	MG	DA	3008	1/1	0.96	0.46	5.42	13,13,13,13	0
60	MG	BA	3082	1/1	0.90	0.24	5.25	44,44,44,44	0
60	MG	BA	3143	1/1	0.97	0.22	5.11	32,32,32,32	0
60	MG	AA	1655	1/1	0.99	0.25	5.07	2,2,2,2	0
60	MG	DA	3193	1/1	0.85	0.28	4.90	29,29,29,29	0
60	MG	CA	1673	1/1	0.78	0.25	4.88	15,15,15,15	0
60	MG	BA	3117	1/1	0.96	0.28	4.79	1,1,1,1	0
60	MG	AA	1640	1/1	0.62	0.25	4.75	70,70,70,70	0
60	MG	BA	3042	1/1	0.85	0.23	4.68	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3092	1/1	0.73	0.30	4.62	17,17,17,17	0
60	MG	BA	3062	1/1	0.96	0.23	4.58	1,1,1,1	0
60	MG	DA	3237	1/1	0.85	0.36	4.55	10,10,10,10	0
60	MG	BA	3029	1/1	0.97	0.26	4.48	36,36,36,36	0
60	MG	DA	3174	1/1	0.91	0.32	4.46	6,6,6,6	0
60	MG	BA	3158	1/1	0.93	0.52	4.44	35,35,35,35	0
60	MG	DA	3014	1/1	0.80	0.36	4.40	4,4,4,4	0
60	MG	BA	3010	1/1	0.91	0.25	4.38	2,2,2,2	0
60	MG	DA	3117	1/1	0.68	0.46	4.34	49,49,49,49	0
60	MG	CA	1612	1/1	0.90	0.42	4.31	35,35,35,35	0
60	MG	AA	1633	1/1	0.87	0.24	4.23	8,8,8,8	0
60	MG	CA	1635	1/1	0.96	0.29	4.21	20,20,20,20	0
60	MG	BA	3284	1/1	0.79	0.23	4.20	21,21,21,21	0
60	MG	BA	3004	1/1	0.98	0.23	4.11	8,8,8,8	0
60	MG	BA	3119	1/1	0.95	0.23	4.08	91,91,91,91	0
60	MG	BA	3179	1/1	0.92	0.26	3.98	17,17,17,17	0
60	MG	CA	1677	1/1	0.83	0.38	3.90	51,51,51,51	0
60	MG	BA	3055	1/1	0.97	0.21	3.83	1,1,1,1	0
60	MG	DA	3205	1/1	0.86	0.36	3.82	2,2,2,2	0
60	MG	DF	301	1/1	0.56	0.56	3.77	53,53,53,53	0
60	MG	BA	3046	1/1	0.98	0.24	3.53	10,10,10,10	0
60	MG	DA	3215	1/1	0.84	0.28	3.52	23,23,23,23	0
60	MG	DO	201	1/1	0.60	0.52	3.41	65,65,65,65	0
60	MG	CA	1622	1/1	0.95	0.26	3.24	12,12,12,12	0
60	MG	CA	1610	1/1	0.93	0.26	3.15	48,48,48,48	0
60	MG	DA	3146	1/1	0.93	0.31	2.93	17,17,17,17	0
60	MG	DA	3073	1/1	0.87	0.29	2.84	58,58,58,58	0
60	MG	DA	3061	1/1	0.96	0.33	2.84	21,21,21,21	0
60	MG	DA	3167	1/1	0.88	0.26	2.77	36,36,36,36	0
60	MG	AA	1615	1/1	0.99	0.27	2.68	18,18,18,18	0
60	MG	CA	1692	1/1	0.72	0.27	2.67	32,32,32,32	0
60	MG	DA	3102	1/1	0.84	0.35	2.59	1,1,1,1	0
60	MG	AA	1675	1/1	0.98	0.25	2.48	4,4,4,4	0
60	MG	DA	3186	1/1	0.89	0.23	2.40	53,53,53,53	0
60	MG	DA	3078	1/1	0.76	0.30	2.37	26,26,26,26	0
60	MG	DA	3139	1/1	0.86	0.39	2.35	1,1,1,1	0
60	MG	BA	3178	1/1	0.97	0.22	2.27	1,1,1,1	0
60	MG	AA	1654	1/1	0.96	0.21	2.25	68,68,68,68	0
60	MG	DA	3065	1/1	0.73	0.27	2.22	28,28,28,28	0
60	MG	CA	1620	1/1	0.96	0.20	2.20	32,32,32,32	0
60	MG	CA	1686	1/1	0.49	0.28	2.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3236	1/1	0.93	0.28	2.07	39,39,39,39	0
60	MG	AA	1614	1/1	0.88	0.19	1.90	22,22,22,22	0
60	MG	DA	3041	1/1	0.77	0.31	1.90	1,1,1,1	0
60	MG	BA	3231	1/1	0.97	0.19	1.86	2,2,2,2	0
60	MG	DA	3126	1/1	0.85	0.34	1.86	7,7,7,7	0
60	MG	DA	3229	1/1	0.89	0.26	1.85	20,20,20,20	0
60	MG	AA	1604	1/1	0.88	0.27	1.82	14,14,14,14	0
60	MG	DA	3050	1/1	0.90	0.26	1.77	38,38,38,38	0
60	MG	AA	1704	1/1	0.90	0.19	1.77	13,13,13,13	0
60	MG	BD	301	1/1	0.96	0.26	1.73	12,12,12,12	0
60	MG	CA	1629	1/1	0.96	0.25	1.72	16,16,16,16	0
60	MG	BA	3114	1/1	0.82	0.21	1.71	14,14,14,14	0
60	MG	DA	3234	1/1	0.94	0.36	1.67	40,40,40,40	0
60	MG	DA	3035	1/1	0.96	0.24	1.62	1,1,1,1	0
60	MG	CA	1608	1/1	0.96	0.30	1.58	24,24,24,24	0
60	MG	BA	3040	1/1	0.98	0.20	1.47	1,1,1,1	0
60	MG	BA	3048	1/1	0.99	0.19	1.46	1,1,1,1	0
60	MG	DA	3182	1/1	0.93	0.34	1.43	23,23,23,23	0
60	MG	BA	3111	1/1	0.93	0.19	1.38	1,1,1,1	0
60	MG	DA	3016	1/1	0.72	0.28	1.30	12,12,12,12	0
60	MG	BA	3291	1/1	0.93	0.21	1.29	14,14,14,14	0
60	MG	BA	3172	1/1	0.90	0.17	1.29	18,18,18,18	0
60	MG	CA	1654	1/1	0.91	0.20	1.27	44,44,44,44	0
60	MG	DA	3091	1/1	0.84	0.29	1.22	55,55,55,55	0
60	MG	BA	3099	1/1	0.99	0.19	1.18	8,8,8,8	0
60	MG	CA	1601	1/1	0.88	0.24	1.14	1,1,1,1	0
60	MG	AA	1613	1/1	0.94	0.23	1.11	36,36,36,36	0
60	MG	DA	3052	1/1	0.82	0.22	1.02	14,14,14,14	0
60	MG	AA	1711	1/1	0.88	0.17	0.97	15,15,15,15	0
60	MG	DA	3216	1/1	0.81	0.20	0.81	24,24,24,24	0
60	MG	B0	101	1/1	0.90	0.24	0.78	4,4,4,4	0
60	MG	DA	3043	1/1	0.84	0.26	0.70	9,9,9,9	0
60	MG	DA	3210	1/1	0.86	0.28	0.70	2,2,2,2	0
60	MG	BA	3219	1/1	0.92	0.19	0.69	15,15,15,15	0
60	MG	BA	3074	1/1	0.92	0.18	0.66	4,4,4,4	0
60	MG	DA	3059	1/1	0.93	0.27	0.63	6,6,6,6	0
60	MG	DA	3099	1/1	0.98	0.24	0.62	14,14,14,14	0
60	MG	DA	3026	1/1	0.88	0.27	0.59	4,4,4,4	0
60	MG	BA	3145	1/1	0.94	0.29	0.59	31,31,31,31	0
60	MG	DA	3090	1/1	0.93	0.28	0.46	21,21,21,21	0
60	MG	DA	3055	1/1	0.98	0.23	0.45	17,17,17,17	0
60	MG	BA	3066	1/1	0.93	0.19	0.38	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3100	1/1	0.95	0.22	0.36	18,18,18,18	0
60	MG	AX	104	1/1	0.77	0.20	0.33	57,57,57,57	0
60	MG	AA	1697	1/1	0.82	0.20	0.23	27,27,27,27	0
60	MG	CA	1604	1/1	0.94	0.21	0.23	1,1,1,1	0
60	MG	AA	1635	1/1	0.93	0.20	0.20	23,23,23,23	0
60	MG	B0	103	1/1	0.92	0.23	0.17	22,22,22,22	0
60	MG	CA	1646	1/1	0.89	0.21	0.16	1,1,1,1	0
60	MG	BA	3022	1/1	0.94	0.15	0.08	19,19,19,19	0
60	MG	DA	3219	1/1	0.89	0.22	0.04	19,19,19,19	0
60	MG	AA	1665	1/1	0.92	0.15	0.02	31,31,31,31	0
60	MG	CA	1672	1/1	0.93	0.18	-0.04	21,21,21,21	0
61	ZN	AD	301	1/1	0.96	0.25	-0.05	46,46,46,46	0
60	MG	CA	1627	1/1	0.88	0.23	-0.10	9,9,9,9	0
60	MG	DA	3089	1/1	0.88	0.21	-0.16	27,27,27,27	0
60	MG	DA	3142	1/1	0.72	0.25	-0.16	37,37,37,37	0
61	ZN	CD	301	1/1	0.95	0.26	-0.27	49,49,49,49	0
60	MG	DA	3033	1/1	0.94	0.20	-0.30	4,4,4,4	0
60	MG	DD	302	1/1	0.90	0.23	-0.36	6,6,6,6	0
60	MG	BA	3267	1/1	0.96	0.15	-0.36	6,6,6,6	0
60	MG	CA	1701	1/1	0.93	0.18	-0.39	53,53,53,53	0
60	MG	BU	202	1/1	0.94	0.20	-0.43	1,1,1,1	0
60	MG	AA	1641	1/1	0.97	0.17	-0.50	13,13,13,13	0
60	MG	CA	1689	1/1	0.93	0.15	-0.54	7,7,7,7	0
60	MG	CA	1631	1/1	0.67	0.18	-0.54	19,19,19,19	0
60	MG	DA	3196	1/1	0.92	0.20	-0.59	1,1,1,1	0
60	MG	DA	3122	1/1	0.73	0.20	-0.65	40,40,40,40	0
60	MG	BE	302	1/1	0.97	0.15	-0.69	1,1,1,1	0
60	MG	AA	1674	1/1	0.99	0.14	-0.74	32,32,32,32	0
60	MG	BA	3324	1/1	0.96	0.15	-0.75	1,1,1,1	0
60	MG	DA	3070	1/1	0.94	0.21	-0.76	14,14,14,14	0
60	MG	BA	3224	1/1	0.90	0.12	-0.82	20,20,20,20	0
60	MG	DA	3037	1/1	0.94	0.20	-0.84	24,24,24,24	0
60	MG	AA	1603	1/1	0.96	0.17	-0.85	32,32,32,32	0
60	MG	BA	3323	1/1	0.97	0.14	-0.88	2,2,2,2	0
60	MG	AA	1689	1/1	0.94	0.16	-0.93	2,2,2,2	0
60	MG	AA	1658	1/1	0.96	0.15	-0.97	1,1,1,1	0
60	MG	DA	3067	1/1	0.95	0.18	-0.99	23,23,23,23	0
60	MG	DA	3153	1/1	0.78	0.18	-1.00	13,13,13,13	0
60	MG	BA	3058	1/1	0.96	0.13	-1.12	1,1,1,1	0
60	MG	BA	3325	1/1	0.90	0.13	-1.17	19,19,19,19	0
60	MG	AA	1713	1/1	0.74	0.13	-1.19	43,43,43,43	0
60	MG	DA	3077	1/1	0.82	0.18	-1.21	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3002	1/1	0.92	0.15	-1.23	9,9,9,9	0
60	MG	AA	1693	1/1	0.98	0.14	-1.24	31,31,31,31	0
60	MG	DA	3101	1/1	0.95	0.17	-1.29	20,20,20,20	0
60	MG	DA	3015	1/1	0.90	0.16	-1.34	1,1,1,1	0
60	MG	BF	301	1/1	0.94	0.13	-1.37	14,14,14,14	0
60	MG	B5	101	1/1	0.95	0.11	-1.39	16,16,16,16	0
60	MG	DA	3105	1/1	0.94	0.19	-1.44	59,59,59,59	0
60	MG	DA	3045	1/1	0.97	0.16	-1.44	11,11,11,11	0
60	MG	AA	1659	1/1	0.96	0.15	-1.48	23,23,23,23	0
60	MG	BB	204	1/1	0.96	0.14	-1.50	21,21,21,21	0
61	ZN	B4	101	1/1	0.91	0.05	-1.55	89,89,89,89	0
60	MG	AA	1639	1/1	0.96	0.11	-1.56	29,29,29,29	0
60	MG	AA	1634	1/1	0.97	0.13	-1.57	1,1,1,1	0
60	MG	AA	1668	1/1	0.98	0.13	-1.58	24,24,24,24	0
61	ZN	B5	102	1/1	0.89	0.09	-1.60	51,51,51,51	0
60	MG	BA	3011	1/1	0.98	0.16	-1.63	1,1,1,1	0
60	MG	BA	3332	1/1	0.96	0.13	-1.67	1,1,1,1	0
61	ZN	D9	101	1/1	0.91	0.07	-1.69	93,93,93,93	0
60	MG	BA	3309	1/1	0.80	0.13	-1.71	1,1,1,1	0
60	MG	DA	3076	1/1	0.94	0.12	-1.74	25,25,25,25	0
60	MG	DA	3179	1/1	0.84	0.15	-1.84	19,19,19,19	0
60	MG	BA	3115	1/1	0.95	0.14	-1.95	1,1,1,1	0
60	MG	DA	3133	1/1	0.86	0.18	-2.00	16,16,16,16	0
61	ZN	B9	101	1/1	0.97	0.07	-2.01	44,44,44,44	0
60	MG	BA	3218	1/1	0.94	0.12	-2.06	9,9,9,9	0
60	MG	CA	1663	1/1	0.98	0.12	-2.07	31,31,31,31	0
61	ZN	D5	102	1/1	0.90	0.09	-2.09	75,75,75,75	0
60	MG	BR	201	1/1	0.99	0.06	-2.12	1,1,1,1	0
60	MG	AA	1688	1/1	0.89	0.12	-2.15	49,49,49,49	0
60	MG	AA	1611	1/1	0.97	0.13	-2.25	33,33,33,33	0
60	MG	BA	3147	1/1	0.99	0.12	-2.28	8,8,8,8	0
60	MG	DA	3011	1/1	0.88	0.18	-2.35	4,4,4,4	0
60	MG	BA	3245	1/1	0.94	0.11	-2.37	25,25,25,25	0
60	MG	BA	3233	1/1	0.96	0.12	-2.47	1,1,1,1	0
61	ZN	D4	101	1/1	0.90	0.05	-2.52	113,113,113,113	0
60	MG	DA	3009	1/1	0.93	0.18	-2.55	12,12,12,12	0
60	MG	CA	1630	1/1	0.96	0.14	-2.57	57,57,57,57	0
60	MG	DA	3030	1/1	0.93	0.14	-2.76	8,8,8,8	0
60	MG	BA	3163	1/1	0.91	0.09	-2.79	12,12,12,12	0
60	MG	DB	203	1/1	0.82	0.11	-2.97	54,54,54,54	0
60	MG	CK	201	1/1	0.91	0.09	-3.04	19,19,19,19	0
60	MG	BA	3154	1/1	0.93	0.11	-3.05	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3054	1/1	0.94	0.12	-3.26	6,6,6,6	0
60	MG	CA	1617	1/1	0.96	0.16	-3.32	1,1,1,1	0
60	MG	CA	1699	1/1	0.96	0.08	-3.54	30,30,30,30	0
60	MG	AA	1667	1/1	0.96	0.17	-3.59	15,15,15,15	0
60	MG	DA	3232	1/1	0.84	0.14	-3.60	3,3,3,3	0
60	MG	AA	1678	1/1	0.94	0.13	-3.74	29,29,29,29	0
60	MG	DA	3156	1/1	0.70	0.11	-3.77	47,47,47,47	0
60	MG	BA	3087	1/1	0.97	0.09	-3.78	6,6,6,6	0
60	MG	BA	3112	1/1	0.97	0.13	-3.87	11,11,11,11	0
60	MG	DA	3187	1/1	0.97	0.09	-3.96	27,27,27,27	0
60	MG	AX	107	1/1	0.97	0.11	-4.05	8,8,8,8	0
60	MG	DA	3046	1/1	0.97	0.08	-4.10	28,28,28,28	0
60	MG	DA	3023	1/1	0.90	0.10	-4.12	14,14,14,14	0
60	MG	CA	1628	1/1	0.98	0.10	-4.36	12,12,12,12	0
60	MG	DA	3114	1/1	0.92	0.12	-5.20	34,34,34,34	0
60	MG	BA	3273	1/1	0.94	0.09	-5.51	1,1,1,1	0
60	MG	DA	3208	1/1	0.85	0.15	-6.01	12,12,12,12	0
60	MG	BA	3257	1/1	0.99	0.06	-7.11	22,22,22,22	0
60	MG	AA	1609	1/1	0.98	0.22	-	1,1,1,1	0
60	MG	DA	3027	1/1	0.88	0.92	-	38,38,38,38	0
60	MG	BA	3095	1/1	0.89	0.72	-	47,47,47,47	0
60	MG	BA	3221	1/1	0.96	0.48	-	35,35,35,35	0
60	MG	DA	3131	1/1	0.81	0.86	-	63,63,63,63	0
60	MG	DA	3140	1/1	0.80	0.34	-	24,24,24,24	0
60	MG	BA	3303	1/1	0.75	0.56	-	32,32,32,32	0
60	MG	BA	3209	1/1	0.94	0.37	-	24,24,24,24	0
60	MG	DA	3034	1/1	0.80	0.19	-	1,1,1,1	0
60	MG	BA	3305	1/1	0.94	0.25	-	32,32,32,32	0
60	MG	DA	3138	1/1	0.75	0.17	-	63,63,63,63	0
60	MG	BA	3150	1/1	0.96	0.42	-	9,9,9,9	0
60	MG	DA	3082	1/1	0.92	0.24	-	15,15,15,15	0
60	MG	BA	3191	1/1	0.84	0.33	-	6,6,6,6	0
60	MG	BA	3226	1/1	0.91	0.24	-	39,39,39,39	0
60	MG	BA	3072	1/1	0.96	0.12	-	6,6,6,6	0
60	MG	BA	3283	1/1	0.91	0.60	-	38,38,38,38	0
60	MG	DA	3224	1/1	0.93	0.11	-	18,18,18,18	0
60	MG	BA	3097	1/1	0.91	0.32	-	44,44,44,44	0
60	MG	AA	1652	1/1	0.93	0.38	-	28,28,28,28	0
60	MG	BA	3198	1/1	0.90	0.19	-	5,5,5,5	0
60	MG	DA	3158	1/1	0.91	0.55	-	49,49,49,49	0
60	MG	CA	1680	1/1	0.96	0.07	-	44,44,44,44	0
60	MG	BA	3281	1/1	0.94	0.26	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1626	1/1	0.75	0.24	-	51,51,51,51	0
60	MG	DA	3207	1/1	0.93	0.16	-	1,1,1,1	0
60	MG	CA	1659	1/1	0.96	0.62	-	46,46,46,46	0
60	MG	BA	3206	1/1	0.97	0.33	-	6,6,6,6	0
60	MG	BB	203	1/1	0.94	0.25	-	35,35,35,35	0
60	MG	CA	1670	1/1	0.90	0.26	-	26,26,26,26	0
60	MG	CA	1668	1/1	0.88	0.32	-	30,30,30,30	0
60	MG	DA	3147	1/1	0.94	0.20	-	26,26,26,26	0
60	MG	DA	3202	1/1	0.75	0.22	-	18,18,18,18	0
60	MG	CA	1688	1/1	0.97	0.09	-	37,37,37,37	0
60	MG	DA	3060	1/1	0.71	0.35	-	23,23,23,23	0
60	MG	BA	3238	1/1	0.80	0.41	-	29,29,29,29	0
60	MG	BA	3298	1/1	0.89	0.32	-	13,13,13,13	0
60	MG	BA	3067	1/1	0.96	0.10	-	1,1,1,1	0
60	MG	DA	3141	1/1	0.78	0.62	-	36,36,36,36	0
60	MG	DA	3031	1/1	0.85	0.14	-	9,9,9,9	0
60	MG	BA	3246	1/1	0.92	0.26	-	1,1,1,1	0
60	MG	DA	3053	1/1	0.81	0.55	-	32,32,32,32	0
60	MG	AA	1650	1/1	0.98	0.14	-	15,15,15,15	0
60	MG	AA	1632	1/1	0.93	0.42	-	48,48,48,48	0
60	MG	CA	1690	1/1	0.96	0.28	-	31,31,31,31	0
60	MG	DD	301	1/1	0.96	0.08	-	21,21,21,21	0
60	MG	BA	3132	1/1	0.98	0.31	-	1,1,1,1	0
60	MG	CA	1662	1/1	0.95	0.13	-	38,38,38,38	0
60	MG	DA	3004	1/1	0.96	0.29	-	7,7,7,7	0
60	MG	BA	3152	1/1	0.97	0.41	-	6,6,6,6	0
60	MG	BA	3278	1/1	0.98	0.10	-	15,15,15,15	0
60	MG	BA	3159	1/1	0.92	0.21	-	20,20,20,20	0
60	MG	DA	3171	1/1	0.73	0.44	-	52,52,52,52	0
60	MG	AA	1677	1/1	0.90	0.24	-	30,30,30,30	0
60	MG	BA	3122	1/1	0.88	0.33	-	12,12,12,12	0
60	MG	BA	3186	1/1	0.72	0.30	-	60,60,60,60	0
60	MG	DA	3058	1/1	0.89	0.22	-	1,1,1,1	0
60	MG	CA	1700	1/1	0.60	0.40	-	36,36,36,36	0
60	MG	AA	1616	1/1	0.90	0.25	-	32,32,32,32	0
60	MG	CA	1698	1/1	0.81	0.51	-	29,29,29,29	0
60	MG	AW	101	1/1	0.86	0.30	-	48,48,48,48	0
60	MG	DA	3235	1/1	0.84	0.44	-	61,61,61,61	0
60	MG	CA	1693	1/1	0.93	0.23	-	20,20,20,20	0
60	MG	BA	3073	1/1	0.98	0.30	-	1,1,1,1	0
60	MG	CA	1616	1/1	0.76	0.48	-	52,52,52,52	0
60	MG	BA	3318	1/1	0.84	0.24	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3330	1/1	0.95	0.20	-	12,12,12,12	0
60	MG	CV	601	1/1	0.73	0.47	-	16,16,16,16	0
60	MG	CA	1694	1/1	0.85	0.71	-	51,51,51,51	0
60	MG	DA	3165	1/1	0.79	0.27	-	14,14,14,14	0
60	MG	BA	3160	1/1	0.88	0.43	-	29,29,29,29	0
60	MG	DA	3098	1/1	0.81	0.35	-	27,27,27,27	0
60	MG	DA	3211	1/1	0.87	0.24	-	23,23,23,23	0
60	MG	DA	3177	1/1	0.89	0.30	-	13,13,13,13	0
60	MG	AX	103	1/1	0.71	0.20	-	51,51,51,51	0
60	MG	BA	3051	1/1	0.82	0.38	-	14,14,14,14	0
60	MG	CA	1636	1/1	0.87	0.24	-	26,26,26,26	0
60	MG	DA	3001	1/1	0.78	0.40	-	51,51,51,51	0
60	MG	BA	3197	1/1	0.90	0.21	-	24,24,24,24	0
60	MG	BA	3205	1/1	0.88	0.36	-	30,30,30,30	0
60	MG	CA	1697	1/1	0.94	0.27	-	27,27,27,27	0
60	MG	CA	1649	1/1	0.69	0.31	-	54,54,54,54	0
60	MG	BA	3173	1/1	0.89	0.19	-	50,50,50,50	0
60	MG	CA	1625	1/1	0.95	0.25	-	3,3,3,3	0
60	MG	BA	3228	1/1	0.93	0.64	-	52,52,52,52	0
60	MG	BA	3090	1/1	0.97	0.05	-	13,13,13,13	0
60	MG	BA	3313	1/1	0.89	0.45	-	45,45,45,45	0
60	MG	DA	3072	1/1	0.93	0.32	-	8,8,8,8	0
60	MG	AA	1666	1/1	0.97	0.09	-	9,9,9,9	0
60	MG	BA	3063	1/1	0.96	0.20	-	1,1,1,1	0
60	MG	BA	3220	1/1	0.98	0.17	-	1,1,1,1	0
60	MG	CA	1684	1/1	0.83	0.18	-	33,33,33,33	0
60	MG	BA	3059	1/1	0.84	0.50	-	25,25,25,25	0
60	MG	DA	3161	1/1	0.65	0.18	-	33,33,33,33	0
60	MG	BA	3155	1/1	0.94	0.35	-	14,14,14,14	0
60	MG	BA	3148	1/1	0.89	0.15	-	1,1,1,1	0
60	MG	AA	1629	1/1	0.82	0.22	-	51,51,51,51	0
60	MG	DA	3143	1/1	0.90	0.62	-	54,54,54,54	0
60	MG	DA	3108	1/1	0.94	0.26	-	18,18,18,18	0
60	MG	BA	3161	1/1	0.93	0.50	-	24,24,24,24	0
60	MG	BA	3001	1/1	0.87	0.26	-	43,43,43,43	0
60	MG	DA	3151	1/1	0.95	0.34	-	26,26,26,26	0
60	MG	BA	3190	1/1	0.86	0.12	-	39,39,39,39	0
60	MG	BA	3035	1/1	0.94	0.19	-	1,1,1,1	0
60	MG	BA	3047	1/1	0.93	0.14	-	1,1,1,1	0
60	MG	DA	3109	1/1	0.69	0.20	-	50,50,50,50	0
60	MG	DA	3223	1/1	0.84	0.33	-	13,13,13,13	0
60	MG	DA	3137	1/1	0.84	0.72	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3271	1/1	0.85	0.14	-	28,28,28,28	0
60	MG	BA	3157	1/1	0.96	0.25	-	10,10,10,10	0
60	MG	BA	3212	1/1	0.97	0.28	-	11,11,11,11	0
60	MG	AA	1622	1/1	0.88	0.32	-	12,12,12,12	0
60	MG	AA	1671	1/1	0.59	0.42	-	49,49,49,49	0
60	MG	BA	3255	1/1	0.78	0.33	-	19,19,19,19	0
60	MG	BA	3327	1/1	0.98	0.32	-	17,17,17,17	0
60	MG	AX	105	1/1	0.94	0.08	-	12,12,12,12	0
60	MG	BA	3012	1/1	0.97	0.27	-	1,1,1,1	0
60	MG	AA	1601	1/1	0.85	0.29	-	47,47,47,47	0
60	MG	DA	3021	1/1	0.67	0.28	-	27,27,27,27	0
60	MG	DA	3095	1/1	0.70	0.15	-	61,61,61,61	0
60	MG	BA	3182	1/1	0.95	0.24	-	1,1,1,1	0
60	MG	BA	3107	1/1	0.94	0.46	-	65,65,65,65	0
60	MG	DA	3106	1/1	0.95	0.12	-	23,23,23,23	0
60	MG	BA	3075	1/1	0.95	0.32	-	2,2,2,2	0
60	MG	BA	3280	1/1	0.84	0.18	-	7,7,7,7	0
60	MG	AA	1663	1/1	0.96	0.28	-	14,14,14,14	0
60	MG	DA	3022	1/1	0.94	0.28	-	11,11,11,11	0
60	MG	CW	102	1/1	0.90	0.15	-	40,40,40,40	0
60	MG	DA	3222	1/1	0.89	0.29	-	24,24,24,24	0
60	MG	CA	1613	1/1	0.88	0.47	-	36,36,36,36	0
60	MG	CA	1695	1/1	0.93	0.14	-	40,40,40,40	0
60	MG	AA	1664	1/1	0.88	0.29	-	46,46,46,46	0
60	MG	BA	3038	1/1	0.98	0.25	-	1,1,1,1	0
60	MG	DA	3064	1/1	0.90	0.48	-	12,12,12,12	0
60	MG	BA	3263	1/1	0.93	0.19	-	47,47,47,47	0
60	MG	AA	1610	1/1	0.91	0.16	-	36,36,36,36	0
60	MG	DA	3007	1/1	0.88	0.31	-	1,1,1,1	0
60	MG	BA	3312	1/1	0.85	0.25	-	22,22,22,22	0
60	MG	BA	3213	1/1	0.92	0.48	-	49,49,49,49	0
60	MG	BA	3002	1/1	0.94	0.31	-	17,17,17,17	0
60	MG	CA	1653	1/1	0.86	0.23	-	36,36,36,36	0
60	MG	AA	1712	1/1	0.96	0.48	-	36,36,36,36	0
60	MG	BA	3129	1/1	0.96	0.21	-	1,1,1,1	0
60	MG	CA	1634	1/1	0.90	0.19	-	16,16,16,16	0
60	MG	BA	3210	1/1	0.76	0.29	-	33,33,33,33	0
60	MG	BA	3253	1/1	0.95	0.30	-	39,39,39,39	0
60	MG	BA	3085	1/1	0.64	0.39	-	70,70,70,70	0
60	MG	AW	103	1/1	0.19	0.63	-	72,72,72,72	0
60	MG	BA	3302	1/1	0.86	0.17	-	11,11,11,11	0
60	MG	BA	3170	1/1	0.83	0.38	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3051	1/1	0.94	0.51	-	18,18,18,18	0
60	MG	AX	109	1/1	0.96	0.12	-	16,16,16,16	0
60	MG	DA	3010	1/1	0.95	0.46	-	1,1,1,1	0
60	MG	AA	1623	1/1	0.96	0.33	-	10,10,10,10	0
60	MG	BA	3249	1/1	0.94	0.54	-	13,13,13,13	0
60	MG	DA	3157	1/1	0.73	0.24	-	58,58,58,58	0
60	MG	BA	3244	1/1	0.96	0.21	-	34,34,34,34	0
60	MG	DA	3226	1/1	0.86	0.10	-	30,30,30,30	0
60	MG	AA	1692	1/1	0.97	0.29	-	19,19,19,19	0
60	MG	DA	3132	1/1	0.97	0.26	-	6,6,6,6	0
60	MG	BA	3194	1/1	0.90	0.57	-	54,54,54,54	0
60	MG	CA	1602	1/1	0.93	0.31	-	26,26,26,26	0
60	MG	DA	3221	1/1	0.91	0.50	-	52,52,52,52	0
60	MG	BA	3297	1/1	0.95	0.16	-	42,42,42,42	0
60	MG	BA	3333	1/1	0.88	0.35	-	1,1,1,1	0
60	MG	BA	3101	1/1	0.91	0.41	-	31,31,31,31	0
60	MG	BA	3064	1/1	0.87	0.70	-	45,45,45,45	0
60	MG	CA	1651	1/1	0.95	0.15	-	35,35,35,35	0
60	MG	AA	1698	1/1	0.95	0.29	-	23,23,23,23	0
60	MG	DA	3228	1/1	0.68	0.69	-	34,34,34,34	0
60	MG	AA	1708	1/1	0.76	0.26	-	41,41,41,41	0
60	MG	DA	3081	1/1	0.94	0.34	-	3,3,3,3	0
60	MG	BA	3052	1/1	0.97	0.33	-	1,1,1,1	0
60	MG	DA	3107	1/1	0.89	0.41	-	37,37,37,37	0
60	MG	DA	3028	1/1	0.93	0.20	-	1,1,1,1	0
60	MG	CA	1640	1/1	0.74	0.27	-	41,41,41,41	0
60	MG	BA	3320	1/1	0.96	0.10	-	23,23,23,23	0
60	MG	DA	3047	1/1	0.89	0.45	-	29,29,29,29	0
60	MG	CA	1638	1/1	0.68	0.38	-	31,31,31,31	0
60	MG	BA	3174	1/1	0.89	0.09	-	7,7,7,7	0
60	MG	BA	3050	1/1	0.93	0.30	-	1,1,1,1	0
60	MG	BA	3091	1/1	0.98	0.31	-	1,1,1,1	0
60	MG	DA	3213	1/1	0.86	0.21	-	31,31,31,31	0
60	MG	CA	1685	1/1	0.71	0.48	-	59,59,59,59	0
60	MG	CW	104	1/1	0.69	0.17	-	57,57,57,57	0
60	MG	BA	3311	1/1	0.91	0.42	-	40,40,40,40	0
60	MG	BA	3329	1/1	0.68	0.16	-	45,45,45,45	0
60	MG	AA	1706	1/1	0.98	0.14	-	28,28,28,28	0
60	MG	BA	3192	1/1	0.88	0.44	-	31,31,31,31	0
60	MG	CA	1681	1/1	0.96	0.47	-	44,44,44,44	0
60	MG	BA	3256	1/1	0.97	0.15	-	23,23,23,23	0
60	MG	BB	202	1/1	0.94	0.12	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3144	1/1	0.80	0.30	-	59,59,59,59	0
60	MG	DA	3013	1/1	0.85	0.38	-	30,30,30,30	0
60	MG	BA	3140	1/1	0.80	0.52	-	26,26,26,26	0
60	MG	CA	1609	1/1	0.75	0.51	-	50,50,50,50	0
60	MG	BA	3266	1/1	0.92	0.30	-	12,12,12,12	0
60	MG	DA	3159	1/1	0.69	0.39	-	32,32,32,32	0
60	MG	CA	1702	1/1	0.80	0.43	-	27,27,27,27	0
60	MG	AW	102	1/1	0.91	0.13	-	36,36,36,36	0
60	MG	BA	3033	1/1	0.96	0.42	-	1,1,1,1	0
60	MG	AA	1649	1/1	0.97	0.25	-	25,25,25,25	0
60	MG	BA	3239	1/1	0.98	0.23	-	2,2,2,2	0
60	MG	DA	3238	1/1	0.94	0.69	-	42,42,42,42	0
60	MG	DA	3113	1/1	0.94	0.47	-	2,2,2,2	0
60	MG	BA	3310	1/1	0.85	0.28	-	38,38,38,38	0
60	MG	AX	101	1/1	0.88	0.15	-	41,41,41,41	0
60	MG	BA	3248	1/1	0.96	0.21	-	34,34,34,34	0
60	MG	AA	1682	1/1	0.72	0.13	-	48,48,48,48	0
60	MG	CA	1660	1/1	0.91	0.16	-	21,21,21,21	0
60	MG	BA	3039	1/1	0.98	0.22	-	1,1,1,1	0
60	MG	AA	1691	1/1	0.94	0.39	-	23,23,23,23	0
60	MG	BA	3110	1/1	0.96	0.33	-	6,6,6,6	0
60	MG	DA	3071	1/1	0.94	0.27	-	19,19,19,19	0
60	MG	AA	1636	1/1	0.96	0.41	-	28,28,28,28	0
60	MG	BA	3081	1/1	0.95	0.13	-	19,19,19,19	0
60	MG	CA	1678	1/1	0.90	0.53	-	25,25,25,25	0
60	MG	BA	3041	1/1	0.96	0.29	-	1,1,1,1	0
60	MG	BA	3241	1/1	0.80	1.36	-	80,80,80,80	0
60	MG	AX	102	1/1	0.91	0.16	-	57,57,57,57	0
60	MG	CA	1679	1/1	0.93	0.16	-	43,43,43,43	0
60	MG	CW	103	1/1	0.30	0.34	-	73,73,73,73	0
60	MG	AA	1672	1/1	0.80	0.24	-	53,53,53,53	0
60	MG	BA	3225	1/1	0.94	0.27	-	9,9,9,9	0
60	MG	DA	3184	1/1	0.67	0.86	-	35,35,35,35	0
60	MG	BX	101	1/1	0.83	0.23	-	31,31,31,31	0
60	MG	B0	102	1/1	0.80	0.40	-	40,40,40,40	0
60	MG	BG	201	1/1	0.95	0.20	-	30,30,30,30	0
60	MG	BA	3236	1/1	0.94	0.36	-	11,11,11,11	0
60	MG	CA	1641	1/1	0.46	0.29	-	66,66,66,66	0
60	MG	BA	3057	1/1	0.96	0.11	-	3,3,3,3	0
60	MG	DA	3123	1/1	0.85	0.42	-	40,40,40,40	0
60	MG	BA	3193	1/1	0.96	0.26	-	22,22,22,22	0
60	MG	DA	3087	1/1	0.96	0.47	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3128	1/1	0.94	0.19	-	16,16,16,16	0
60	MG	BA	3126	1/1	0.96	0.11	-	5,5,5,5	0
60	MG	DA	3129	1/1	0.82	0.23	-	20,20,20,20	0
60	MG	DA	3130	1/1	0.81	0.43	-	27,27,27,27	0
60	MG	AA	1680	1/1	0.80	0.62	-	70,70,70,70	0
60	MG	BA	3237	1/1	0.97	0.19	-	1,1,1,1	0
60	MG	DA	3134	1/1	0.89	0.25	-	59,59,59,59	0
60	MG	BA	3065	1/1	0.99	0.16	-	2,2,2,2	0
60	MG	DA	3170	1/1	0.78	0.51	-	33,33,33,33	0
60	MG	BA	3102	1/1	0.95	0.17	-	1,1,1,1	0
60	MG	BA	3287	1/1	0.93	0.11	-	7,7,7,7	0
60	MG	CW	101	1/1	0.85	0.12	-	55,55,55,55	0
60	MG	BA	3292	1/1	0.94	0.31	-	27,27,27,27	0
60	MG	CA	1632	1/1	0.89	0.35	-	6,6,6,6	0
60	MG	BA	3250	1/1	0.93	0.32	-	12,12,12,12	0
60	MG	AA	1683	1/1	0.87	0.14	-	16,16,16,16	0
60	MG	AA	1628	1/1	0.98	0.17	-	10,10,10,10	0
60	MG	CA	1615	1/1	0.95	0.46	-	28,28,28,28	0
60	MG	CA	1603	1/1	0.86	0.23	-	38,38,38,38	0
60	MG	AA	1714	1/1	0.98	0.18	-	6,6,6,6	0
60	MG	DA	3199	1/1	0.56	0.44	-	35,35,35,35	0
60	MG	AA	1670	1/1	0.84	0.30	-	54,54,54,54	0
60	MG	DA	3214	1/1	0.87	0.37	-	21,21,21,21	0
60	MG	BA	3184	1/1	0.84	0.62	-	40,40,40,40	0
60	MG	AA	1700	1/1	0.92	0.30	-	74,74,74,74	0
60	MG	CA	1676	1/1	0.78	0.20	-	25,25,25,25	0
60	MG	BA	3300	1/1	0.92	0.18	-	22,22,22,22	0
60	MG	DA	3020	1/1	0.88	0.46	-	40,40,40,40	0
60	MG	DA	3063	1/1	0.92	0.21	-	24,24,24,24	0
60	MG	BA	3208	1/1	0.96	0.27	-	1,1,1,1	0
60	MG	DA	3163	1/1	0.95	0.49	-	32,32,32,32	0
60	MG	DA	3104	1/1	0.77	0.44	-	42,42,42,42	0
60	MG	BA	3285	1/1	0.95	0.12	-	1,1,1,1	0
60	MG	BA	3328	1/1	0.93	0.27	-	34,34,34,34	0
60	MG	DA	3191	1/1	0.94	0.41	-	31,31,31,31	0
60	MG	BA	3014	1/1	0.98	0.49	-	1,1,1,1	0
60	MG	DA	3125	1/1	0.74	0.19	-	49,49,49,49	0
60	MG	BA	3093	1/1	0.96	0.30	-	1,1,1,1	0
60	MG	AA	1651	1/1	0.88	0.51	-	53,53,53,53	0
60	MG	DA	3185	1/1	0.85	0.62	-	10,10,10,10	0
60	MG	BA	3222	1/1	0.86	0.29	-	26,26,26,26	0
60	MG	AA	1648	1/1	0.83	0.45	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3136	1/1	0.94	0.27	-	42,42,42,42	0
60	MG	BA	3165	1/1	0.85	0.15	-	48,48,48,48	0
60	MG	DA	3217	1/1	0.70	0.56	-	27,27,27,27	0
60	MG	DA	3115	1/1	0.83	0.29	-	36,36,36,36	0
60	MG	BA	3151	1/1	0.98	0.17	-	22,22,22,22	0
60	MG	DA	3074	1/1	0.81	0.62	-	48,48,48,48	0
60	MG	DA	3150	1/1	0.93	0.23	-	28,28,28,28	0
60	MG	AA	1624	1/1	0.99	0.35	-	1,1,1,1	0
60	MG	DA	3145	1/1	0.81	0.49	-	35,35,35,35	0
60	MG	AA	1657	1/1	0.87	0.45	-	37,37,37,37	0
60	MG	BA	3086	1/1	0.98	0.14	-	4,4,4,4	0
60	MG	BA	3123	1/1	0.97	0.14	-	6,6,6,6	0
60	MG	BA	3211	1/1	0.93	0.33	-	36,36,36,36	0
60	MG	BA	3043	1/1	0.97	0.40	-	1,1,1,1	0
60	MG	BA	3036	1/1	0.93	0.56	-	8,8,8,8	0
60	MG	DA	3239	1/1	0.59	0.34	-	34,34,34,34	0
60	MG	BA	3168	1/1	0.93	0.34	-	60,60,60,60	0
60	MG	BA	3282	1/1	0.90	0.32	-	20,20,20,20	0
60	MG	BE	303	1/1	0.96	0.32	-	58,58,58,58	0
60	MG	BA	3294	1/1	0.76	0.71	-	90,90,90,90	0
60	MG	DA	3038	1/1	0.94	0.57	-	8,8,8,8	0
60	MG	AA	1679	1/1	0.90	0.15	-	36,36,36,36	0
60	MG	DA	3192	1/1	0.85	0.18	-	10,10,10,10	0
60	MG	BA	3272	1/1	0.89	0.23	-	15,15,15,15	0
60	MG	AA	1684	1/1	0.95	0.36	-	69,69,69,69	0
60	MG	AA	1608	1/1	0.88	0.46	-	22,22,22,22	0
60	MG	CA	1626	1/1	0.94	0.42	-	31,31,31,31	0
60	MG	AA	1627	1/1	0.92	0.24	-	22,22,22,22	0
60	MG	BA	3199	1/1	0.99	0.19	-	1,1,1,1	0
60	MG	CA	1652	1/1	0.58	0.28	-	61,61,61,61	0
60	MG	DA	3025	1/1	0.77	0.39	-	1,1,1,1	0
60	MG	DA	3066	1/1	0.78	0.56	-	40,40,40,40	0
60	MG	D7	101	1/1	0.66	0.30	-	36,36,36,36	0
60	MG	BA	3204	1/1	0.83	0.33	-	25,25,25,25	0
60	MG	AA	1656	1/1	0.97	0.25	-	10,10,10,10	0
60	MG	BA	3321	1/1	0.96	0.42	-	1,1,1,1	0
60	MG	BA	3243	1/1	0.86	0.51	-	45,45,45,45	0
60	MG	CA	1674	1/1	0.77	0.45	-	55,55,55,55	0
60	MG	BA	3202	1/1	0.97	0.22	-	1,1,1,1	0
60	MG	BA	3008	1/1	0.95	0.20	-	4,4,4,4	0
60	MG	BA	3331	1/1	0.85	0.69	-	35,35,35,35	0
60	MG	DA	3154	1/1	0.56	0.81	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1639	1/1	0.94	0.31	-	16,16,16,16	0
60	MG	BA	3032	1/1	0.95	0.23	-	1,1,1,1	0
60	MG	AA	1607	1/1	0.90	0.72	-	51,51,51,51	0
60	MG	BA	3166	1/1	0.96	0.28	-	8,8,8,8	0
60	MG	BA	3088	1/1	0.96	0.13	-	1,1,1,1	0
60	MG	BA	3028	1/1	0.98	0.13	-	1,1,1,1	0
60	MG	DA	3152	1/1	0.94	0.32	-	8,8,8,8	0
60	MG	BA	3261	1/1	0.92	0.31	-	16,16,16,16	0
60	MG	AA	1606	1/1	0.99	0.29	-	1,1,1,1	0
60	MG	DA	3119	1/1	0.91	0.34	-	5,5,5,5	0
60	MG	DA	3188	1/1	0.15	0.27	-	72,72,72,72	0
60	MG	BA	3214	1/1	0.92	0.17	-	54,54,54,54	0
60	MG	DA	3003	1/1	0.88	0.27	-	17,17,17,17	0
60	MG	DA	3220	1/1	0.85	0.45	-	30,30,30,30	0
60	MG	BA	3295	1/1	0.87	0.29	-	41,41,41,41	0
60	MG	CA	1675	1/1	0.92	0.34	-	31,31,31,31	0
60	MG	AA	1602	1/1	0.98	0.05	-	1,1,1,1	0
60	MG	DA	3083	1/1	0.84	0.57	-	35,35,35,35	0
60	MG	BA	3277	1/1	0.92	0.39	-	1,1,1,1	0
60	MG	BA	3216	1/1	0.95	0.17	-	25,25,25,25	0
60	MG	AA	1699	1/1	0.91	0.19	-	21,21,21,21	0
60	MG	BA	3105	1/1	0.94	0.17	-	8,8,8,8	0
60	MG	BA	3098	1/1	0.94	0.44	-	1,1,1,1	0
60	MG	AA	1612	1/1	0.94	0.25	-	15,15,15,15	0
60	MG	BA	3125	1/1	0.95	0.21	-	1,1,1,1	0
60	MG	BA	3164	1/1	0.96	0.35	-	33,33,33,33	0
60	MG	BA	3270	1/1	0.89	0.24	-	32,32,32,32	0
60	MG	DA	3069	1/1	0.94	0.66	-	6,6,6,6	0
60	MG	DA	3085	1/1	0.84	0.51	-	1,1,1,1	0
60	MG	DA	3200	1/1	0.86	0.51	-	42,42,42,42	0
60	MG	BA	3025	1/1	0.94	0.33	-	31,31,31,31	0
60	MG	CA	1647	1/1	0.89	0.31	-	44,44,44,44	0
60	MG	DA	3019	1/1	0.79	0.29	-	6,6,6,6	0
60	MG	DA	3218	1/1	0.83	0.56	-	50,50,50,50	0
60	MG	CA	1655	1/1	0.94	0.31	-	29,29,29,29	0
60	MG	DA	3017	1/1	0.96	0.26	-	1,1,1,1	0
60	MG	DA	3135	1/1	0.91	0.45	-	11,11,11,11	0
60	MG	DA	3056	1/1	0.92	0.16	-	2,2,2,2	0
60	MG	BA	3118	1/1	0.93	0.83	-	46,46,46,46	0
60	MG	BA	3146	1/1	0.96	0.19	-	13,13,13,13	0
60	MG	DA	3178	1/1	0.84	0.22	-	22,22,22,22	0
60	MG	BA	3153	1/1	0.95	0.51	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3149	1/1	0.55	0.37	-	39,39,39,39	0
60	MG	BA	3279	1/1	0.90	0.23	-	29,29,29,29	0
60	MG	DA	3068	1/1	0.79	0.22	-	9,9,9,9	0
60	MG	DA	3230	1/1	0.97	0.05	-	17,17,17,17	0
60	MG	BA	3247	1/1	0.98	0.17	-	35,35,35,35	0
60	MG	DA	3201	1/1	0.67	0.33	-	36,36,36,36	0
60	MG	BA	3258	1/1	0.91	0.23	-	32,32,32,32	0
60	MG	BA	3185	1/1	0.83	0.10	-	3,3,3,3	0
60	MG	CA	1691	1/1	0.91	0.27	-	21,21,21,21	0
60	MG	AA	1681	1/1	0.92	0.24	-	58,58,58,58	0
60	MG	BA	3188	1/1	0.94	0.10	-	30,30,30,30	0
60	MG	CA	1664	1/1	0.96	0.10	-	83,83,83,83	0
60	MG	CA	1661	1/1	0.97	0.21	-	9,9,9,9	0
60	MG	AA	1695	1/1	0.79	0.18	-	30,30,30,30	0
60	MG	BA	3183	1/1	0.95	0.20	-	1,1,1,1	0
60	MG	AA	1653	1/1	0.92	0.21	-	38,38,38,38	0
60	MG	BA	3196	1/1	0.91	0.31	-	21,21,21,21	0
60	MG	AG	201	1/1	0.85	0.21	-	42,42,42,42	0
60	MG	BA	3135	1/1	0.98	0.13	-	20,20,20,20	0
60	MG	AA	1660	1/1	0.89	0.42	-	49,49,49,49	0
60	MG	CA	1658	1/1	0.82	0.27	-	30,30,30,30	0
60	MG	AA	1647	1/1	0.95	0.29	-	39,39,39,39	0
60	MG	BA	3203	1/1	0.86	0.20	-	17,17,17,17	0
60	MG	CA	1687	1/1	0.95	0.25	-	17,17,17,17	0
60	MG	DA	3231	1/1	0.82	0.69	-	49,49,49,49	0
60	MG	BA	3240	1/1	0.89	0.39	-	75,75,75,75	0
60	MG	DA	3227	1/1	0.82	0.26	-	36,36,36,36	0
60	MG	DA	3148	1/1	0.76	0.58	-	42,42,42,42	0
60	MG	AA	1710	1/1	0.96	0.60	-	29,29,29,29	0
60	MG	D0	101	1/1	0.87	0.29	-	12,12,12,12	0
60	MG	BA	3264	1/1	0.92	0.28	-	32,32,32,32	0
60	MG	AA	1707	1/1	0.62	0.39	-	52,52,52,52	0
60	MG	BB	205	1/1	0.97	0.24	-	1,1,1,1	0
60	MG	BA	3019	1/1	0.96	0.34	-	1,1,1,1	0
60	MG	DA	3225	1/1	0.68	0.41	-	39,39,39,39	0
60	MG	BA	3023	1/1	0.98	0.08	-	1,1,1,1	0
60	MG	DA	3144	1/1	0.90	0.29	-	53,53,53,53	0
60	MG	AW	104	1/1	0.92	0.25	-	31,31,31,31	0
60	MG	BA	3296	1/1	0.95	0.28	-	26,26,26,26	0
60	MG	BA	3103	1/1	0.86	0.26	-	1,1,1,1	0
60	MG	CA	1656	1/1	0.73	0.29	-	39,39,39,39	0
60	MG	BA	3084	1/1	0.87	0.22	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BE	301	1/1	0.97	0.14	-	1,1,1,1	0
60	MG	DE	301	1/1	0.87	0.23	-	1,1,1,1	0
60	MG	BA	3252	1/1	0.99	0.06	-	4,4,4,4	0
60	MG	DA	3088	1/1	0.91	0.29	-	22,22,22,22	0
60	MG	CA	1633	1/1	0.63	0.46	-	62,62,62,62	0
60	MG	AA	1662	1/1	0.96	0.14	-	21,21,21,21	0
60	MG	BA	3180	1/1	0.94	0.42	-	40,40,40,40	0
60	MG	CA	1644	1/1	0.58	0.64	-	67,67,67,67	0
60	MG	CA	1621	1/1	0.89	0.44	-	30,30,30,30	0
60	MG	DA	3057	1/1	0.87	0.13	-	32,32,32,32	0
60	MG	CA	1643	1/1	0.94	0.28	-	7,7,7,7	0
60	MG	AA	1638	1/1	0.51	0.74	-	76,76,76,76	0
60	MG	DA	3197	1/1	0.92	0.46	-	21,21,21,21	0
60	MG	CA	1667	1/1	0.91	0.25	-	5,5,5,5	0
60	MG	AA	1694	1/1	0.94	0.28	-	5,5,5,5	0
60	MG	BA	3200	1/1	0.96	0.20	-	14,14,14,14	0
60	MG	BA	3045	1/1	0.99	0.24	-	2,2,2,2	0
60	MG	BA	3130	1/1	0.94	0.41	-	1,1,1,1	0
60	MG	BA	3116	1/1	0.98	0.11	-	26,26,26,26	0
60	MG	CA	1606	1/1	0.90	0.64	-	45,45,45,45	0
60	MG	CA	1696	1/1	0.87	0.18	-	91,91,91,91	0
60	MG	DA	3189	1/1	0.66	0.17	-	57,57,57,57	0
60	MG	BA	3113	1/1	0.90	0.22	-	1,1,1,1	0
60	MG	CA	1671	1/1	0.94	0.14	-	24,24,24,24	0
60	MG	BA	3259	1/1	0.97	0.20	-	16,16,16,16	0
60	MG	BA	3289	1/1	0.61	0.37	-	42,42,42,42	0
60	MG	BA	3187	1/1	0.82	0.46	-	17,17,17,17	0
60	MG	DA	3172	1/1	0.86	0.33	-	6,6,6,6	0
60	MG	CA	1618	1/1	0.94	0.16	-	14,14,14,14	0
60	MG	DA	3097	1/1	0.78	0.24	-	51,51,51,51	0
60	MG	AA	1669	1/1	0.97	0.18	-	35,35,35,35	0
60	MG	AX	106	1/1	0.93	0.28	-	25,25,25,25	0
60	MG	AA	1644	1/1	0.85	0.40	-	39,39,39,39	0
60	MG	BA	3262	1/1	0.97	0.17	-	3,3,3,3	0
60	MG	DA	3093	1/1	0.79	0.47	-	31,31,31,31	0
60	MG	DA	3103	1/1	0.91	0.62	-	26,26,26,26	0
60	MG	DA	3190	1/1	0.69	0.25	-	43,43,43,43	0
60	MG	BA	3235	1/1	0.94	0.18	-	1,1,1,1	0
60	MG	DA	3094	1/1	0.84	0.47	-	16,16,16,16	0
60	MG	DA	3116	1/1	0.67	0.39	-	47,47,47,47	0
60	MG	BA	3254	1/1	0.99	0.06	-	72,72,72,72	0
60	MG	BA	3223	1/1	0.92	0.35	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3198	1/1	0.57	0.20	-	32,32,32,32	0
60	MG	DA	3049	1/1	0.90	0.26	-	36,36,36,36	0
60	MG	DA	3175	1/1	0.53	0.26	-	72,72,72,72	0
60	MG	BA	3026	1/1	0.91	0.31	-	7,7,7,7	0
60	MG	DA	3162	1/1	0.83	0.43	-	44,44,44,44	0
60	MG	AA	1701	1/1	0.86	0.31	-	11,11,11,11	0
60	MG	BA	3304	1/1	0.93	0.21	-	36,36,36,36	0
60	MG	DA	3039	1/1	0.84	0.18	-	53,53,53,53	0
60	MG	DA	3121	1/1	0.97	0.59	-	34,34,34,34	0
60	MG	DA	3212	1/1	0.83	0.19	-	4,4,4,4	0
60	MG	BA	3175	1/1	0.91	0.20	-	26,26,26,26	0
60	MG	DA	3124	1/1	0.73	0.39	-	36,36,36,36	0
60	MG	DA	3194	1/1	0.83	0.43	-	44,44,44,44	0
60	MG	BA	3106	1/1	0.91	0.30	-	3,3,3,3	0
60	MG	BA	3109	1/1	0.68	0.24	-	58,58,58,58	0
60	MG	BA	3201	1/1	0.89	0.69	-	53,53,53,53	0
60	MG	DA	3036	1/1	0.94	0.27	-	5,5,5,5	0
60	MG	BA	3334	1/1	0.93	0.20	-	1,1,1,1	0
60	MG	BA	3308	1/1	0.96	0.33	-	30,30,30,30	0
60	MG	DA	3176	1/1	0.55	0.45	-	54,54,54,54	0
60	MG	AA	1687	1/1	0.94	0.18	-	20,20,20,20	0
60	MG	AA	1709	1/1	0.86	0.35	-	36,36,36,36	0
60	MG	DA	3209	1/1	0.51	0.36	-	5,5,5,5	0
60	MG	DB	201	1/1	0.88	0.68	-	51,51,51,51	0
60	MG	BA	3061	1/1	0.93	0.20	-	17,17,17,17	0
60	MG	BA	3171	1/1	0.59	0.20	-	36,36,36,36	0
60	MG	DA	3155	1/1	0.76	0.56	-	31,31,31,31	0
60	MG	CA	1607	1/1	0.68	0.51	-	29,29,29,29	0
60	MG	BA	3260	1/1	0.88	0.96	-	65,65,65,65	0
60	MG	BA	3307	1/1	0.92	0.24	-	19,19,19,19	0
60	MG	AA	1620	1/1	0.82	0.42	-	31,31,31,31	0
60	MG	BA	3217	1/1	0.95	0.14	-	1,1,1,1	0
60	MG	DA	3080	1/1	0.84	0.49	-	36,36,36,36	0
60	MG	AA	1690	1/1	0.95	0.43	-	23,23,23,23	0
60	MG	BA	3316	1/1	0.76	0.44	-	35,35,35,35	0
60	MG	CA	1611	1/1	0.90	0.37	-	66,66,66,66	0
60	MG	BA	3181	1/1	0.93	0.36	-	16,16,16,16	0
60	MG	DA	3166	1/1	0.75	0.39	-	36,36,36,36	0
60	MG	CA	1642	1/1	0.88	0.10	-	28,28,28,28	0
60	MG	BA	3092	1/1	0.93	0.41	-	3,3,3,3	0
60	MG	DB	202	1/1	0.56	0.77	-	80,80,80,80	0
60	MG	AA	1630	1/1	0.66	0.68	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1624	1/1	0.86	0.58	-	40,40,40,40	0
60	MG	DA	3112	1/1	0.96	0.45	-	7,7,7,7	0
60	MG	DA	3029	1/1	0.94	0.43	-	1,1,1,1	0
60	MG	DA	3164	1/1	0.64	0.21	-	64,64,64,64	0
60	MG	AA	1673	1/1	0.89	0.18	-	39,39,39,39	0
60	MG	BA	3315	1/1	0.95	0.35	-	29,29,29,29	0
60	MG	AA	1703	1/1	0.98	0.24	-	35,35,35,35	0
60	MG	AX	108	1/1	0.87	0.38	-	34,34,34,34	0
60	MG	BA	3096	1/1	0.93	0.39	-	34,34,34,34	0
60	MG	DA	3168	1/1	0.89	0.65	-	55,55,55,55	0
60	MG	BA	3230	1/1	0.90	0.26	-	19,19,19,19	0
60	MG	BA	3100	1/1	0.97	0.11	-	10,10,10,10	0
60	MG	BA	3317	1/1	0.97	0.15	-	22,22,22,22	0
60	MG	DA	3079	1/1	0.91	0.34	-	19,19,19,19	0
60	MG	D5	101	1/1	0.87	0.19	-	10,10,10,10	0
60	MG	DA	3062	1/1	0.78	0.42	-	8,8,8,8	0
60	MG	AA	1625	1/1	0.88	0.25	-	21,21,21,21	0
60	MG	DA	3203	1/1	0.78	0.44	-	38,38,38,38	0
60	MG	BA	3269	1/1	0.93	0.40	-	12,12,12,12	0
60	MG	AA	1686	1/1	0.87	0.29	-	34,34,34,34	0
60	MG	CA	1648	1/1	0.95	0.35	-	24,24,24,24	0
60	MG	CA	1619	1/1	0.95	0.43	-	20,20,20,20	0
60	MG	DA	3024	1/1	0.93	0.35	-	5,5,5,5	0
60	MG	CA	1623	1/1	0.88	0.52	-	33,33,33,33	0
60	MG	AA	1685	1/1	0.89	0.27	-	69,69,69,69	0
60	MG	BA	3060	1/1	0.94	0.27	-	4,4,4,4	0
60	MG	DA	3018	1/1	0.96	0.18	-	15,15,15,15	0
60	MG	BP	202	1/1	0.96	0.28	-	1,1,1,1	0
60	MG	AA	1605	1/1	0.89	0.20	-	35,35,35,35	0
60	MG	BA	3024	1/1	0.96	0.13	-	11,11,11,11	0
60	MG	BA	3007	1/1	0.94	0.28	-	1,1,1,1	0
60	MG	BA	3290	1/1	0.86	0.44	-	24,24,24,24	0
60	MG	BA	3276	1/1	0.92	0.37	-	16,16,16,16	0
60	MG	BA	3299	1/1	0.94	0.18	-	13,13,13,13	0
60	MG	BA	3138	1/1	0.89	0.20	-	1,1,1,1	0
60	MG	DA	3044	1/1	0.96	0.19	-	1,1,1,1	0
60	MG	AA	1645	1/1	0.82	0.41	-	22,22,22,22	0
60	MG	BA	3242	1/1	0.96	0.48	-	49,49,49,49	0
60	MG	BA	3056	1/1	0.89	0.19	-	1,1,1,1	0
60	MG	BA	3015	1/1	0.83	0.14	-	5,5,5,5	0
60	MG	BA	3215	1/1	0.68	0.71	-	60,60,60,60	0
60	MG	BA	3120	1/1	0.90	0.53	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3012	1/1	0.91	0.33	-	1,1,1,1	0
60	MG	DA	3032	1/1	0.93	0.14	-	1,1,1,1	0
60	MG	BA	3265	1/1	0.86	0.38	-	13,13,13,13	0
60	MG	DA	3086	1/1	0.58	0.83	-	58,58,58,58	0
60	MG	BA	3068	1/1	0.96	0.07	-	11,11,11,11	0
60	MG	BA	3319	1/1	0.87	0.32	-	31,31,31,31	0
60	MG	BA	3127	1/1	0.95	0.27	-	1,1,1,1	0
60	MG	DA	3054	1/1	0.87	0.33	-	21,21,21,21	0
60	MG	CE	201	1/1	0.95	0.13	-	56,56,56,56	0
60	MG	DA	3048	1/1	0.84	0.31	-	23,23,23,23	0
60	MG	AA	1702	1/1	0.79	0.34	-	41,41,41,41	0
60	MG	CA	1645	1/1	0.94	0.78	-	56,56,56,56	0
60	MG	CA	1669	1/1	0.91	0.12	-	16,16,16,16	0
60	MG	DA	3204	1/1	0.76	0.48	-	67,67,67,67	0
60	MG	BA	3189	1/1	0.74	0.21	-	40,40,40,40	0
60	MG	BA	3139	1/1	0.94	0.25	-	1,1,1,1	0
60	MG	DA	3136	1/1	0.53	0.44	-	31,31,31,31	0
60	MG	AA	1676	1/1	0.96	0.31	-	11,11,11,11	0
60	MG	AA	1631	1/1	0.93	0.39	-	12,12,12,12	0
60	MG	BA	3176	1/1	0.97	0.37	-	1,1,1,1	0
60	MG	BA	3274	1/1	0.87	0.19	-	21,21,21,21	0
60	MG	AA	1661	1/1	0.95	0.25	-	21,21,21,21	0
60	MG	BA	3053	1/1	0.97	0.18	-	1,1,1,1	0
60	MG	BA	3326	1/1	0.98	0.13	-	21,21,21,21	0
60	MG	CA	1665	1/1	0.87	0.30	-	33,33,33,33	0
60	MG	CA	1605	1/1	0.95	0.41	-	6,6,6,6	0
60	MG	AA	1705	1/1	0.95	0.15	-	4,4,4,4	0
60	MG	DA	3110	1/1	0.39	0.52	-	48,48,48,48	0
60	MG	BA	3069	1/1	0.97	0.18	-	1,1,1,1	0
60	MG	BA	3322	1/1	0.98	0.30	-	10,10,10,10	0
60	MG	BA	3079	1/1	0.74	0.31	-	7,7,7,7	0
60	MG	DA	3127	1/1	0.66	0.32	-	20,20,20,20	0
60	MG	BA	3314	1/1	0.91	0.17	-	35,35,35,35	0
60	MG	CA	1666	1/1	0.96	0.20	-	9,9,9,9	0
60	MG	BP	201	1/1	0.96	0.18	-	11,11,11,11	0
60	MG	BA	3195	1/1	0.82	0.61	-	49,49,49,49	0
60	MG	DA	3181	1/1	0.88	0.51	-	50,50,50,50	0
60	MG	BB	201	1/1	0.92	0.24	-	46,46,46,46	0
60	MG	CA	1637	1/1	0.82	0.73	-	57,57,57,57	0
60	MG	BA	3268	1/1	0.98	0.20	-	1,1,1,1	0
60	MG	BA	3288	1/1	0.97	0.24	-	29,29,29,29	0
60	MG	BA	3003	1/1	0.91	0.25	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3006	1/1	0.93	0.38	-	37,37,37,37	0
60	MG	BA	3124	1/1	0.96	0.41	-	13,13,13,13	0
60	MG	DA	3233	1/1	0.90	0.21	-	1,1,1,1	0
60	MG	BA	3275	1/1	0.90	0.19	-	7,7,7,7	0
60	MG	BA	3207	1/1	0.90	0.22	-	21,21,21,21	0
60	MG	DA	3183	1/1	0.90	0.30	-	9,9,9,9	0
60	MG	BA	3089	1/1	0.95	0.20	-	12,12,12,12	0
60	MG	BA	3286	1/1	0.93	0.49	-	18,18,18,18	0
60	MG	AA	1696	1/1	0.98	0.46	-	20,20,20,20	0
60	MG	BA	3071	1/1	0.97	0.34	-	1,1,1,1	0
60	MG	AA	1619	1/1	0.94	0.20	-	10,10,10,10	0
60	MG	BA	3301	1/1	0.90	0.31	-	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.