



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:50 am GMT

PDB ID : 4V97
Title : Crystal structure of the bacterial ribosome ram mutation G299A.
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2012-04-06
Resolution : 3.52 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28683
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28972

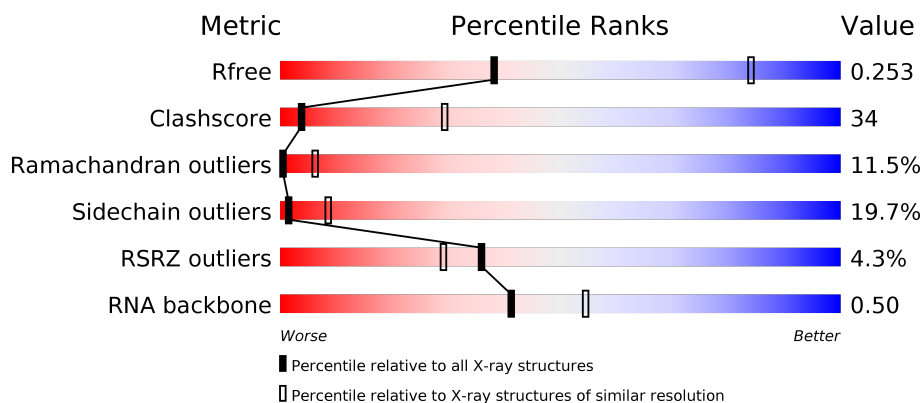
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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.




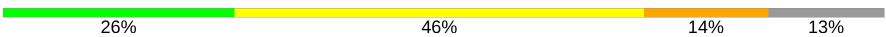
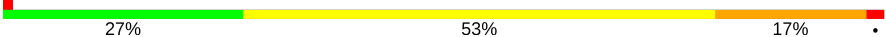


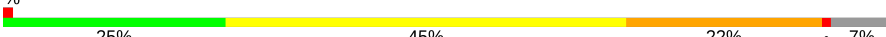
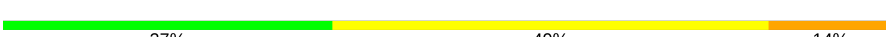
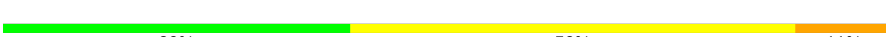
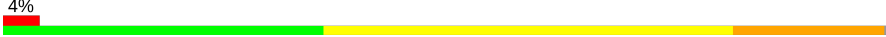

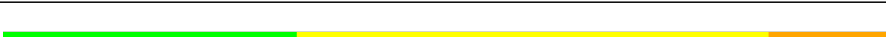


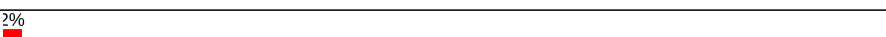





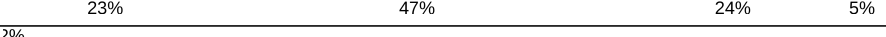
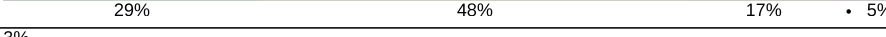
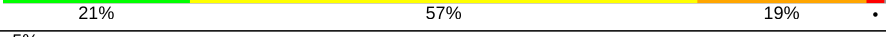
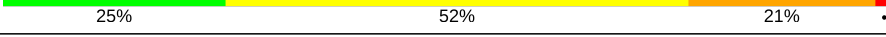

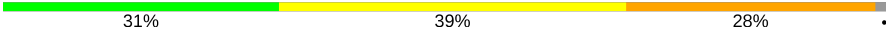
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1239 (3.64-3.40)
Clashscore	112137	1007 (3.62-3.42)
Ramachandran outliers	110173	1328 (3.64-3.40)
Sidechain outliers	110143	1329 (3.64-3.40)
RSRZ outliers	101464	1270 (3.64-3.40)
RNA backbone	2435	1027 (4.18-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>3%</div> <div>49%</div> <div>36%</div> <div>13%</div> <div>.</div> </div>
1	CA	1522	<div> <div>4%</div> <div>50%</div> <div>34%</div> <div>15%</div> <div>.</div> </div>
2	AB	256	<div> <div>2%</div> <div>21%</div> <div>50%</div> <div>19%</div> <div>8%</div> <div>.</div> </div>
2	CB	256	<div> <div>4%</div> <div>18%</div> <div>50%</div> <div>22%</div> <div>8%</div> <div>.</div> </div>


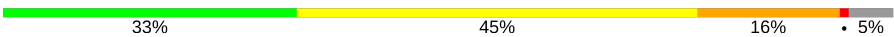
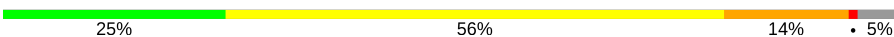


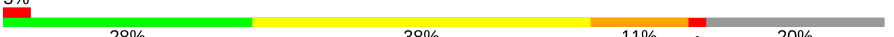
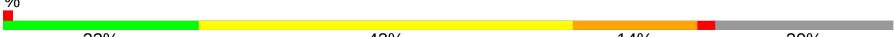
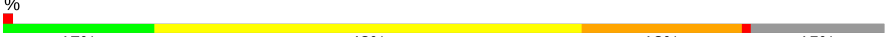
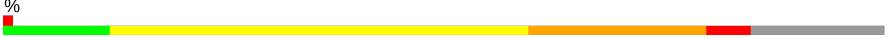

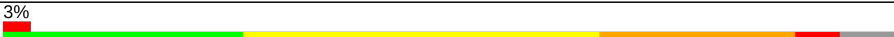


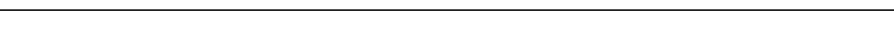




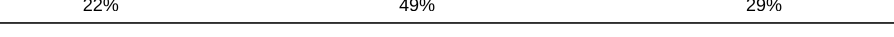

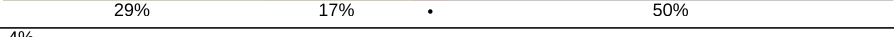

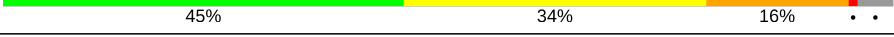


Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	CV	77	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	24	
24	CX	24	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	BC	229	
27	DC	229	
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	7006	-	-	-	X
57	MG	AA	7008	-	-	-	X
57	MG	AA	7011	-	-	-	X
57	MG	AA	7013	-	-	-	X
57	MG	AA	7016	-	-	-	X
57	MG	AA	7018	-	-	-	X
57	MG	AA	7019	-	-	-	X
57	MG	AA	7021	-	-	-	X
57	MG	AA	7026	-	-	-	X
57	MG	AA	7034	-	-	-	X
57	MG	AA	7037	-	-	-	X
57	MG	AA	7043	-	-	-	X
57	MG	AA	7044	-	-	-	X
57	MG	AA	7051	-	-	-	X
57	MG	AA	7053	-	-	-	X
57	MG	AA	7054	-	-	-	X
57	MG	AA	7056	-	-	-	X
57	MG	AA	7058	-	-	-	X
57	MG	AA	7059	-	-	-	X
57	MG	AA	7061	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	7064	-	-	-	X
57	MG	AA	7066	-	-	-	X
57	MG	AA	7067	-	-	-	X
57	MG	AA	7071	-	-	-	X
57	MG	AA	7075	-	-	-	X
57	MG	AA	7090	-	-	-	X
57	MG	AA	7091	-	-	-	X
57	MG	AA	7094	-	-	-	X
57	MG	AA	7110	-	-	-	X
57	MG	B7	101	-	-	-	X
57	MG	BA	3004	-	-	-	X
57	MG	BA	3007	-	-	-	X
57	MG	BA	3008	-	-	-	X
57	MG	BA	3020	-	-	-	X
57	MG	BA	3027	-	-	-	X
57	MG	BA	3028	-	-	-	X
57	MG	BA	3030	-	-	-	X
57	MG	BA	3041	-	-	-	X
57	MG	BA	3044	-	-	-	X
57	MG	BA	3045	-	-	-	X
57	MG	BA	3046	-	-	-	X
57	MG	BA	3047	-	-	-	X
57	MG	BA	3051	-	-	-	X
57	MG	BA	3054	-	-	-	X
57	MG	BA	3065	-	-	-	X
57	MG	BA	3066	-	-	-	X
57	MG	BA	3069	-	-	-	X
57	MG	BA	3073	-	-	-	X
57	MG	BA	3081	-	-	-	X
57	MG	BA	3084	-	-	-	X
57	MG	BA	3086	-	-	-	X
57	MG	BA	3090	-	-	-	X
57	MG	BA	3098	-	-	-	X
57	MG	BA	3099	-	-	-	X
57	MG	BA	3111	-	-	-	X
57	MG	BA	3116	-	-	-	X
57	MG	BA	3119	-	-	-	X
57	MG	BA	3120	-	-	-	X
57	MG	BA	3125	-	-	-	X
57	MG	BA	3136	-	-	-	X
57	MG	BA	3142	-	-	-	X
57	MG	BA	3144	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3145	-	-	-	X
57	MG	BA	3146	-	-	-	X
57	MG	BA	3153	-	-	-	X
57	MG	BA	3159	-	-	-	X
57	MG	BA	3160	-	-	-	X
57	MG	BA	3182	-	-	-	X
57	MG	BA	3187	-	-	-	X
57	MG	BA	3188	-	-	-	X
57	MG	BA	3191	-	-	-	X
57	MG	BA	3193	-	-	-	X
57	MG	BA	3196	-	-	-	X
57	MG	BA	3198	-	-	-	X
57	MG	BA	3201	-	-	-	X
57	MG	BA	3203	-	-	-	X
57	MG	BA	3204	-	-	-	X
57	MG	BA	3205	-	-	-	X
57	MG	BA	3210	-	-	-	X
57	MG	BA	3218	-	-	-	X
57	MG	BA	3220	-	-	-	X
57	MG	BA	3222	-	-	-	X
57	MG	BA	3225	-	-	-	X
57	MG	BA	3227	-	-	-	X
57	MG	BA	3229	-	-	-	X
57	MG	BA	3234	-	-	-	X
57	MG	BA	3235	-	-	-	X
57	MG	BA	3238	-	-	-	X
57	MG	BA	3241	-	-	-	X
57	MG	BA	3243	-	-	-	X
57	MG	BA	3248	-	-	-	X
57	MG	BA	3249	-	-	-	X
57	MG	BA	3251	-	-	-	X
57	MG	BA	3252	-	-	-	X
57	MG	BA	3255	-	-	-	X
57	MG	BA	3264	-	-	-	X
57	MG	BA	3265	-	-	-	X
57	MG	BA	3270	-	-	-	X
57	MG	BA	3272	-	-	-	X
57	MG	BA	3276	-	-	-	X
57	MG	BA	3279	-	-	-	X
57	MG	BA	3281	-	-	-	X
57	MG	BA	3297	-	-	-	X
57	MG	BA	3300	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3306	-	-	-	X
57	MG	BA	3307	-	-	-	X
57	MG	BA	3308	-	-	-	X
57	MG	BA	3309	-	-	-	X
57	MG	BA	3310	-	-	-	X
57	MG	BD	301	-	-	-	X
57	MG	BE	302	-	-	-	X
57	MG	CA	1607	-	-	-	X
57	MG	CA	1610	-	-	-	X
57	MG	CA	1617	-	-	-	X
57	MG	CA	1624	-	-	-	X
57	MG	CA	1626	-	-	-	X
57	MG	CA	1629	-	-	-	X
57	MG	CA	1630	-	-	-	X
57	MG	CA	1631	-	-	-	X
57	MG	CA	1640	-	-	-	X
57	MG	CA	1645	-	-	-	X
57	MG	CA	1651	-	-	-	X
57	MG	CA	1652	-	-	-	X
57	MG	CA	1653	-	-	-	X
57	MG	CA	1665	-	-	-	X
57	MG	CA	1667	-	-	-	X
57	MG	CA	1668	-	-	-	X
57	MG	CA	1670	-	-	-	X
57	MG	CA	1674	-	-	-	X
57	MG	CA	1683	-	-	-	X
57	MG	CA	1685	-	-	-	X
57	MG	CA	1699	-	-	-	X
57	MG	CA	1705	-	-	-	X
57	MG	CA	1709	-	-	-	X
57	MG	CA	1710	-	-	-	X
57	MG	CA	1720	-	-	-	X
57	MG	CA	1727	-	-	-	X
57	MG	CA	1737	-	-	-	X
57	MG	D0	101	-	-	-	X
57	MG	DA	9305	-	-	-	X
57	MG	DA	9308	-	-	-	X
57	MG	DA	9310	-	-	-	X
57	MG	DA	9312	-	-	-	X
57	MG	DA	9319	-	-	-	X
57	MG	DA	9324	-	-	-	X
57	MG	DA	9335	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	9340	-	-	-	X
57	MG	DA	9347	-	-	-	X
57	MG	DA	9349	-	-	-	X
57	MG	DA	9355	-	-	-	X
57	MG	DA	9356	-	-	-	X
57	MG	DA	9358	-	-	-	X
57	MG	DA	9359	-	-	-	X
57	MG	DA	9360	-	-	-	X
57	MG	DA	9363	-	-	-	X
57	MG	DA	9364	-	-	-	X
57	MG	DA	9365	-	-	-	X
57	MG	DA	9366	-	-	-	X
57	MG	DA	9369	-	-	-	X
57	MG	DA	9370	-	-	-	X
57	MG	DA	9381	-	-	-	X
57	MG	DA	9382	-	-	-	X
57	MG	DA	9383	-	-	-	X
57	MG	DA	9392	-	-	-	X
57	MG	DA	9398	-	-	-	X
57	MG	DA	9399	-	-	-	X
57	MG	DA	9402	-	-	-	X
57	MG	DA	9404	-	-	-	X
57	MG	DA	9408	-	-	-	X
57	MG	DA	9409	-	-	-	X
57	MG	DA	9417	-	-	-	X
57	MG	DA	9418	-	-	-	X
57	MG	DA	9421	-	-	-	X
57	MG	DA	9425	-	-	-	X
57	MG	DA	9428	-	-	-	X
57	MG	DA	9430	-	-	-	X
57	MG	DA	9435	-	-	-	X
57	MG	DA	9436	-	-	-	X
57	MG	DA	9437	-	-	-	X
57	MG	DA	9438	-	-	-	X
57	MG	DA	9439	-	-	-	X
57	MG	DA	9441	-	-	-	X
57	MG	DA	9443	-	-	-	X
57	MG	DA	9445	-	-	-	X
57	MG	DA	9454	-	-	-	X
57	MG	DA	9458	-	-	-	X
57	MG	DA	9459	-	-	-	X
57	MG	DA	9460	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	9461	-	-	-	X
57	MG	DA	9472	-	-	-	X
57	MG	DA	9473	-	-	-	X
57	MG	DA	9479	-	-	-	X
57	MG	DA	9483	-	-	-	X
57	MG	DA	9484	-	-	-	X
57	MG	DA	9489	-	-	-	X
57	MG	DA	9491	-	-	-	X
57	MG	DA	9493	-	-	-	X
57	MG	DA	9497	-	-	-	X
57	MG	DA	9498	-	-	-	X
57	MG	DA	9503	-	-	-	X
57	MG	DA	9508	-	-	-	X
57	MG	DA	9512	-	-	-	X
57	MG	DA	9514	-	-	-	X
57	MG	DA	9515	-	-	-	X
57	MG	DA	9516	-	-	-	X
57	MG	DA	9517	-	-	-	X
57	MG	DA	9518	-	-	-	X
57	MG	DA	9521	-	-	-	X
57	MG	DA	9523	-	-	-	X
57	MG	DA	9526	-	-	-	X
57	MG	DA	9527	-	-	-	X
57	MG	DA	9528	-	-	-	X
57	MG	DA	9529	-	-	-	X
57	MG	DA	9530	-	-	-	X
57	MG	DA	9533	-	-	-	X
57	MG	DA	9536	-	-	-	X
57	MG	DA	9537	-	-	-	X
57	MG	DA	9539	-	-	-	X
57	MG	DA	9544	-	-	-	X
57	MG	DA	9545	-	-	-	X
57	MG	DA	9546	-	-	-	X
57	MG	DA	9549	-	-	-	X
57	MG	DA	9553	-	-	-	X
57	MG	DA	9554	-	-	-	X
57	MG	DA	9557	-	-	-	X
57	MG	DA	9570	-	-	-	X
57	MG	DA	9581	-	-	-	X
57	MG	DA	9584	-	-	-	X
57	MG	DA	9587	-	-	-	X
57	MG	DA	9590	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	9597	-	-	-	X
57	MG	DA	9600	-	-	-	X
57	MG	DA	9605	-	-	-	X
57	MG	DA	9613	-	-	-	X
57	MG	DA	9614	-	-	-	X
57	MG	DA	9618	-	-	-	X
57	MG	DA	9621	-	-	-	X
57	MG	DA	9623	-	-	-	X
57	MG	DA	9647	-	-	-	X
57	MG	DA	9649	-	-	-	X
57	MG	DA	9653	-	-	-	X
57	MG	DA	9655	-	-	-	X
57	MG	DA	9672	-	-	-	X
57	MG	DA	9673	-	-	-	X
57	MG	DA	9675	-	-	-	X
57	MG	DA	9681	-	-	-	X
57	MG	DA	9696	-	-	-	X
57	MG	DD	7101	-	-	-	X
57	MG	DD	7103	-	-	-	X
57	MG	DQ	201	-	-	-	X
58	PAR	AA	7111	-	-	-	X
58	PAR	CA	1741	-	-	-	X
59	ZN	CN	101	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	299	A	G	ENGINEERED MUTATION	GB AP008226.1
CA	299	A	G	ENGINEERED MUTATION	GB AP008226.1

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

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

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

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

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

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

Continued on next page...

Continued from previous page...

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

- Molecule 22 is a RNA chain called P-SITE tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	CV	77	Total	C	N	O	P	0	0	0
			1643	732	297	537	77			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	AY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total	C	N	O	P	0	0	0
			255	115	46	82	12			
24	CX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2810	Total 60527	C 26937	N 11326	O 19455	P 2809	0	0	0
25	DA	2824	Total 60827	C 27071	N 11381	O 19552	P 2823	0	0	0

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
32	DH	168	Total	C	N	O	S	0	0	0
			1290	820	240	229	1			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
36	DP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
38	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
39	DS	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
45	DY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

Continued on next page...

Continued from previous page...

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
51	D4	40	Total	C	N	O	S	0	0	1
			298	189	50	54	5			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

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

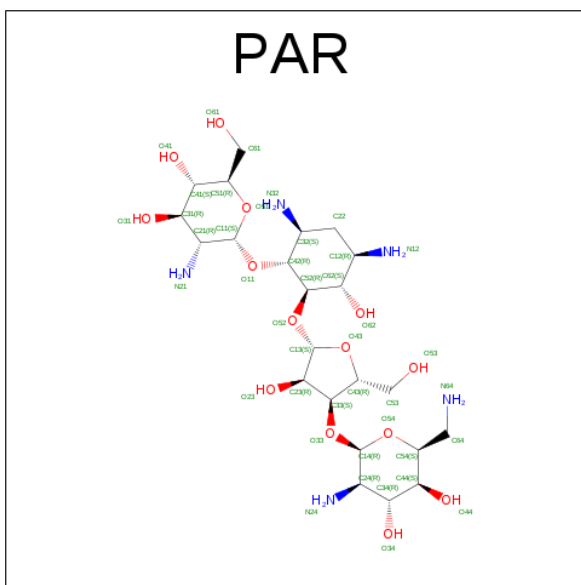
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BA	323	Total Mg 323 323	0	0
57	CA	141	Total Mg 141 141	0	0
57	DQ	1	Total Mg 1 1	0	0
57	DF	1	Total Mg 1 1	0	0
57	CV	5	Total Mg 5 5	0	0
57	D2	1	Total Mg 1 1	0	0
57	BE	3	Total Mg 3 3	0	0
57	DU	3	Total Mg 3 3	0	0
57	BP	1	Total Mg 1 1	0	0
57	AX	1	Total Mg 1 1	0	0
57	CY	1	Total Mg 1 1	0	0
57	DD	3	Total Mg 3 3	0	0
57	B5	1	Total Mg 1 1	0	0
57	BB	5	Total Mg 5 5	0	0
57	AE	1	Total Mg 1 1	0	0
57	BF	1	Total Mg 1 1	0	0
57	AV	5	Total Mg 5 5	0	0
57	D8	1	Total Mg 1 1	0	0
57	AA	110	Total Mg 110 110	0	0
57	CX	1	Total Mg 1 1	0	0
57	BU	1	Total Mg 1 1	0	0
57	BN	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D0	2	Total 2	Mg 2	0	0
57	DE	2	Total 2	Mg 2	0	0
57	DX	1	Total 1	Mg 1	0	0
57	DA	397	Total 397	Mg 397	0	0
57	DW	1	Total 1	Mg 1	0	0
57	B7	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	D1	2	Total 2	Mg 2	0	0
57	DP	3	Total 3	Mg 3	0	0
57	CW	1	Total 1	Mg 1	0	0
57	D5	2	Total 2	Mg 2	0	0
57	BD	2	Total 2	Mg 2	0	0
57	CE	2	Total 2	Mg 2	0	0
57	DB	5	Total 5	Mg 5	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

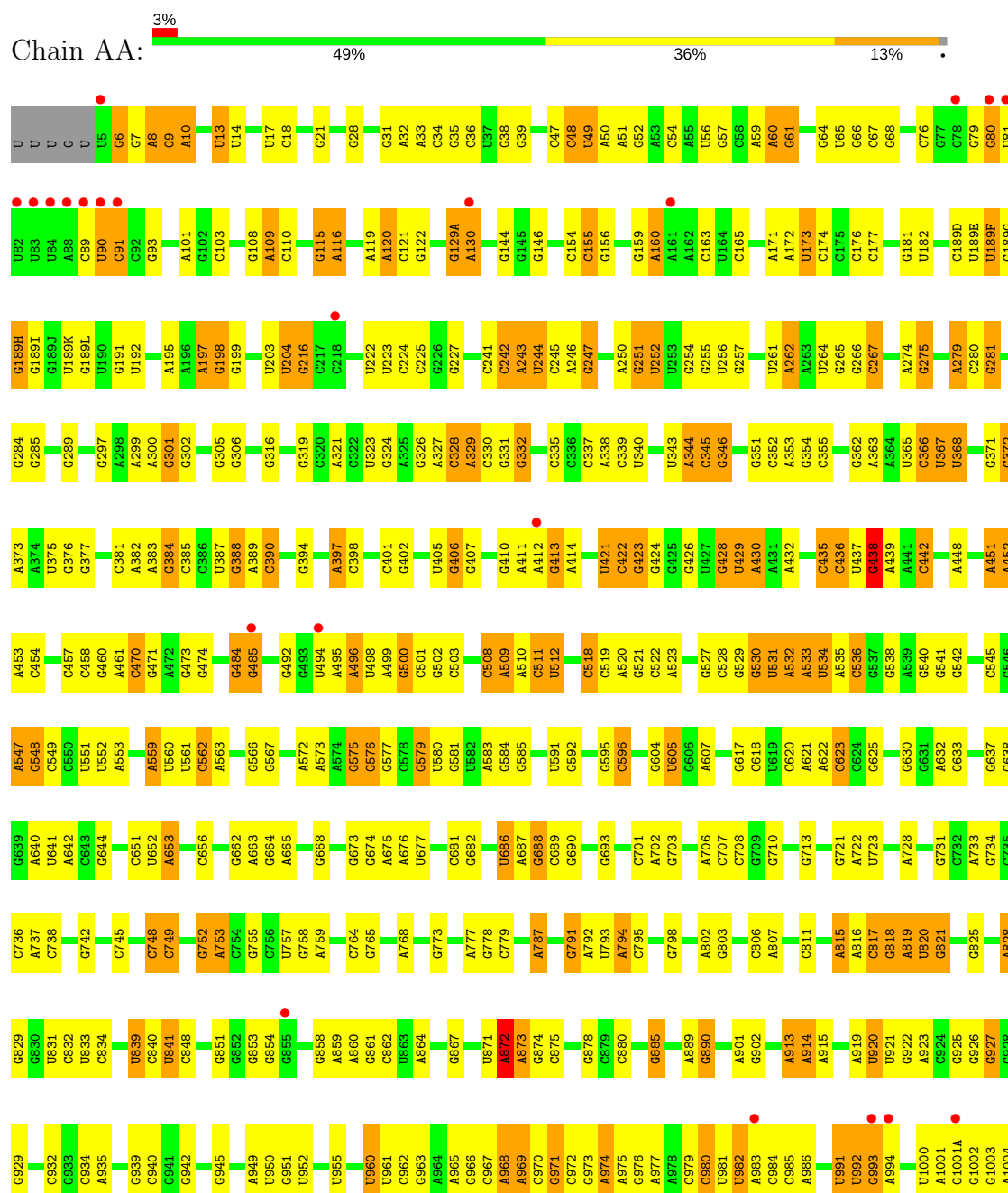
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

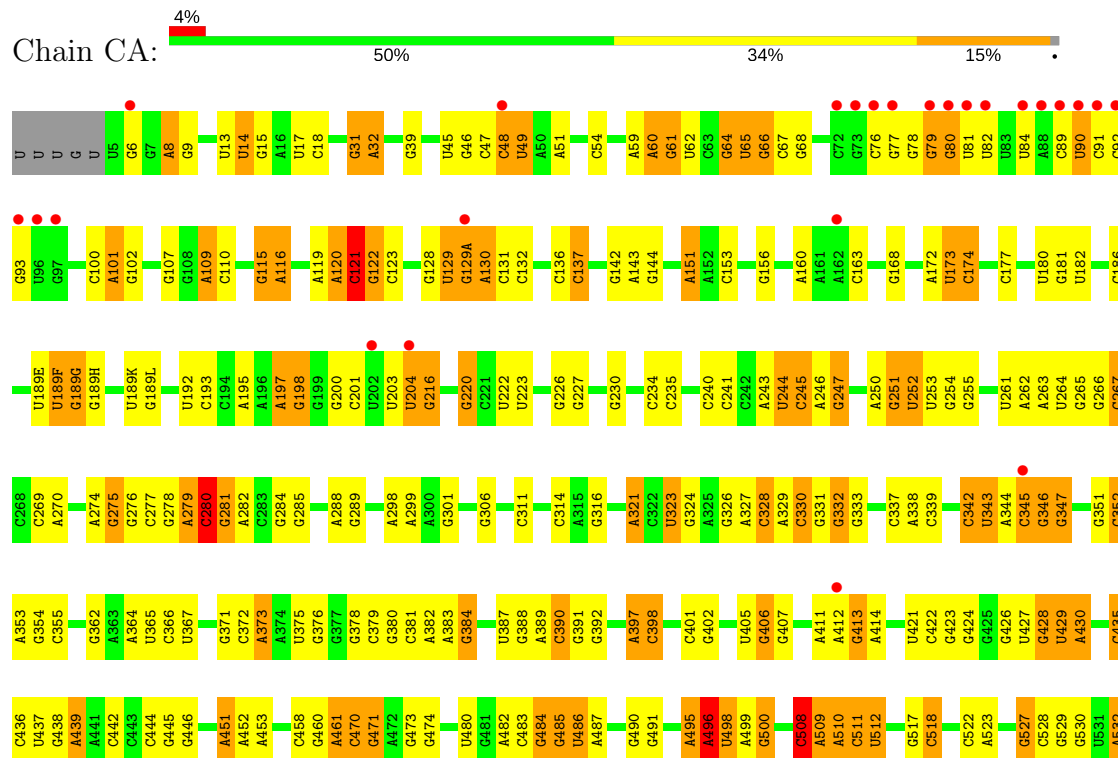
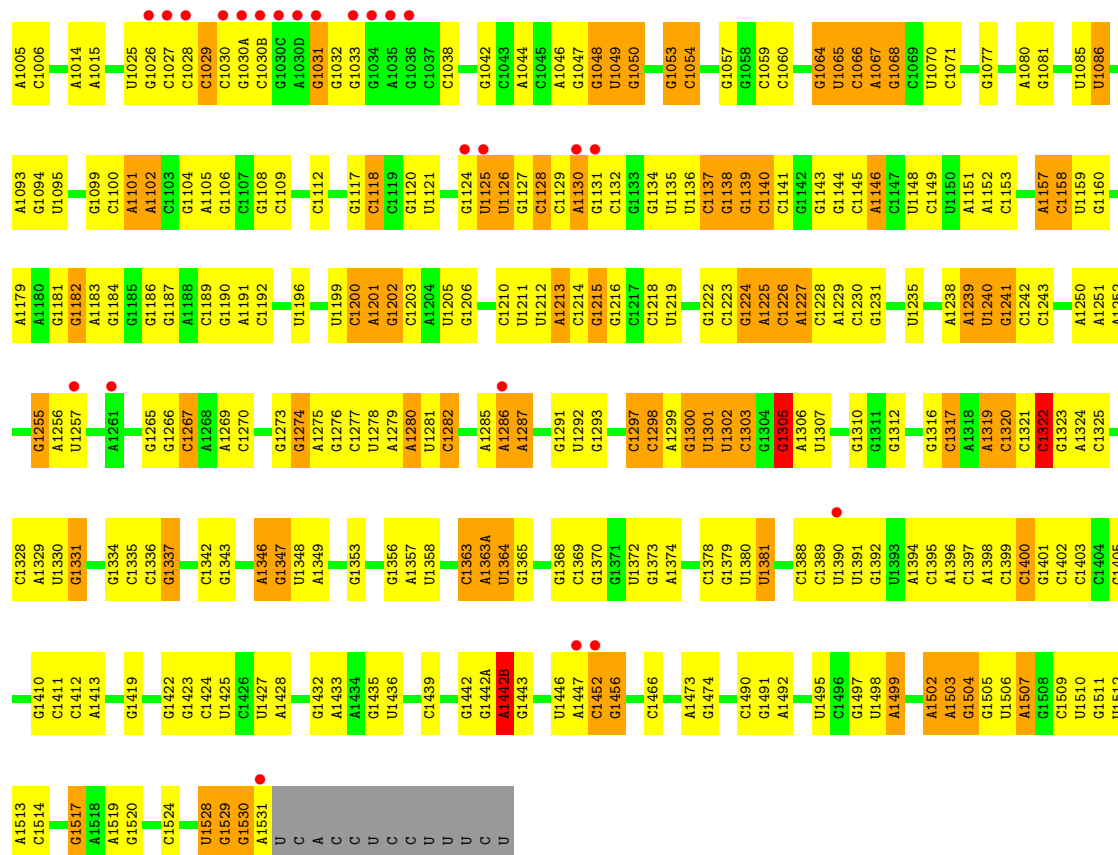
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	CN	1	Total Zn 1 1	0	0
59	AD	1	Total Zn 1 1	0	0
59	CD	1	Total Zn 1 1	0	0
59	AN	1	Total Zn 1 1	0	0

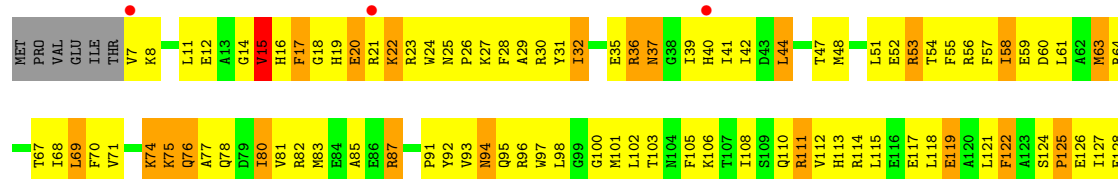
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

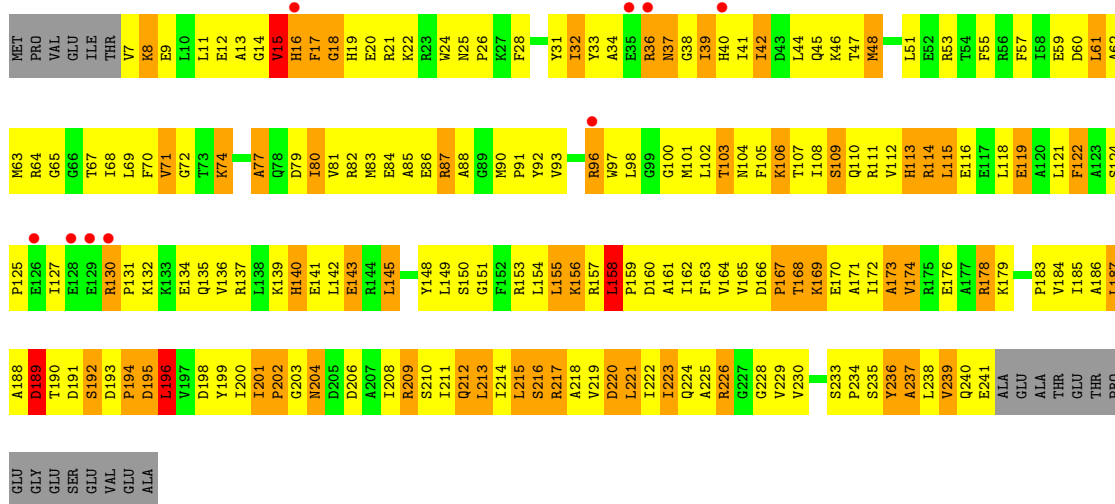
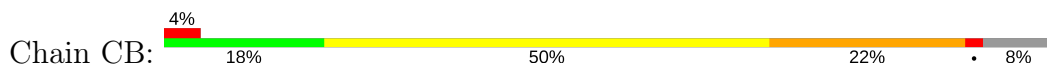
• Molecule 1: 16S rRNA



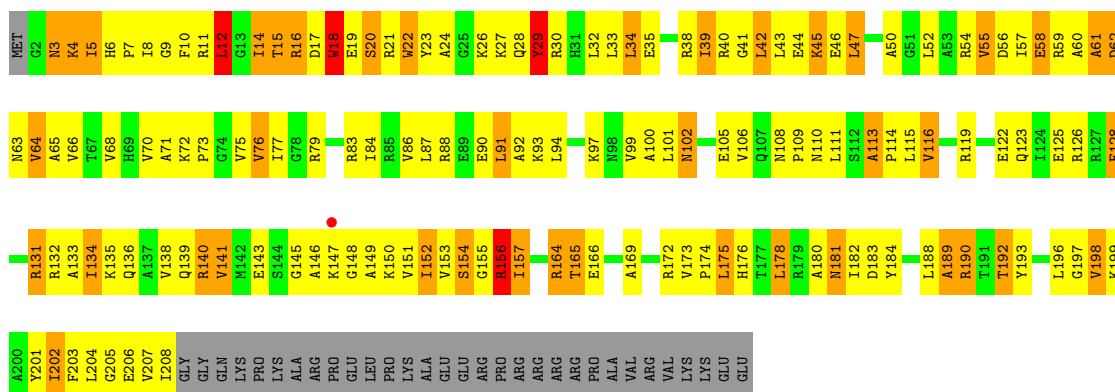




- Molecule 2: 30S ribosomal protein S2

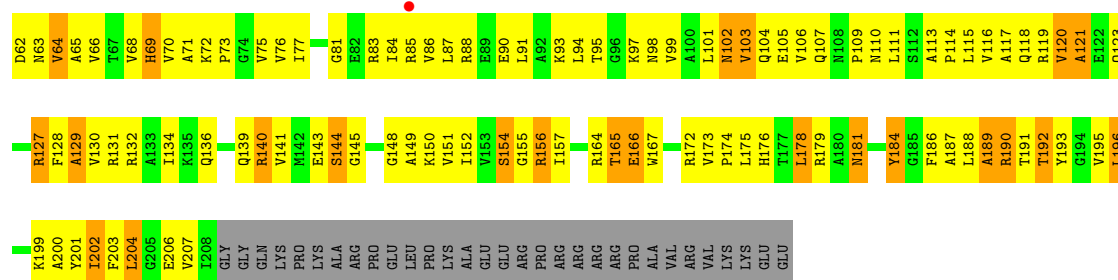


- Molecule 3: 30S ribosomal protein S3

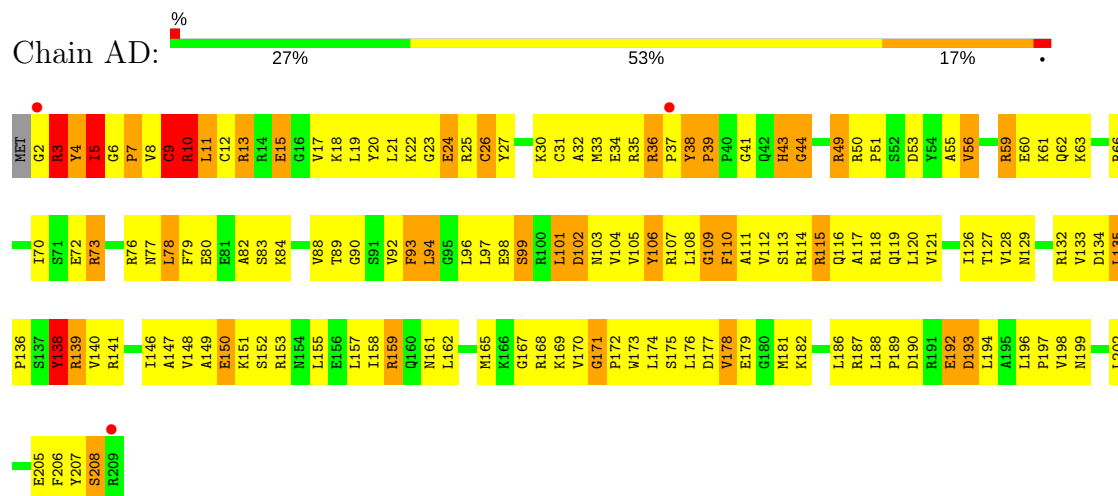


- Molecule 3: 30S ribosomal protein S3

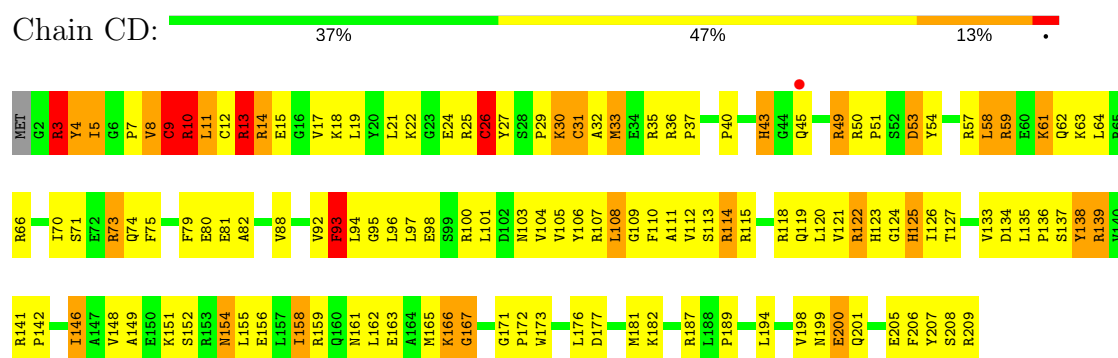




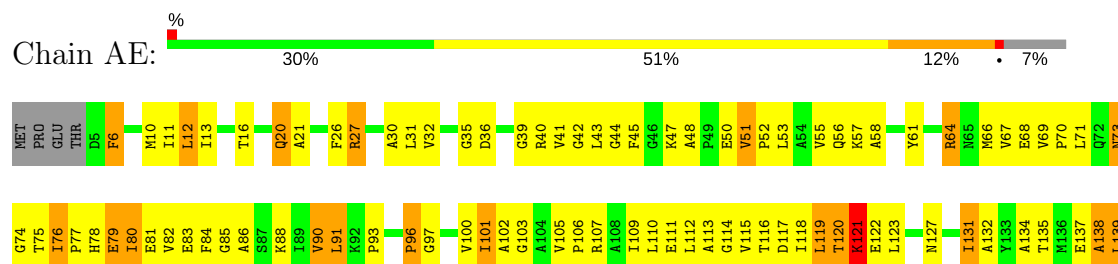
• Molecule 4: 30S ribosomal protein S4

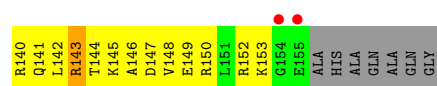


• Molecule 4: 30S ribosomal protein S4

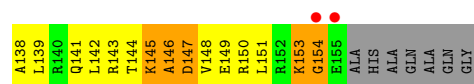


• Molecule 5: 30S ribosomal protein S5

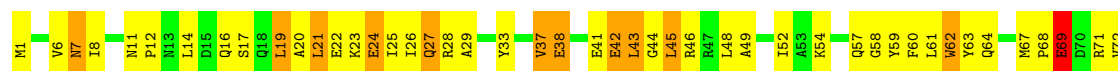




• Molecule 5: 30S ribosomal protein S5



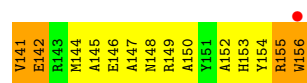
• Molecule 6: 30S ribosomal protein S6



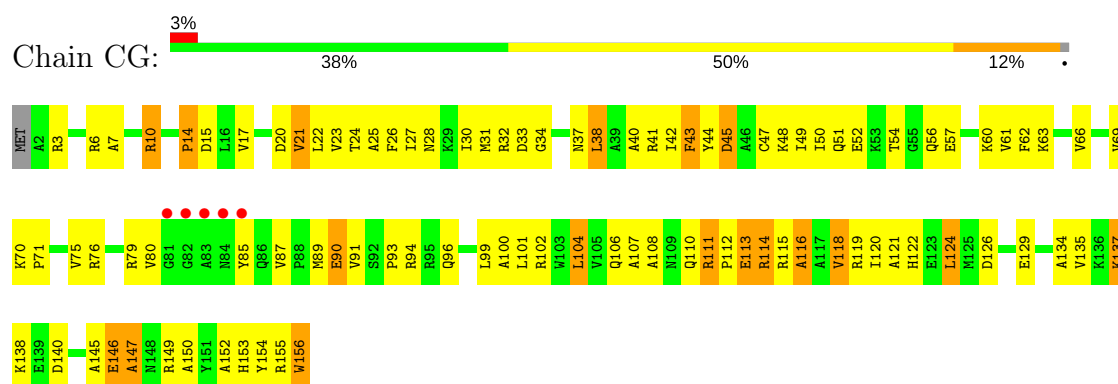
• Molecule 6: 30S ribosomal protein S6



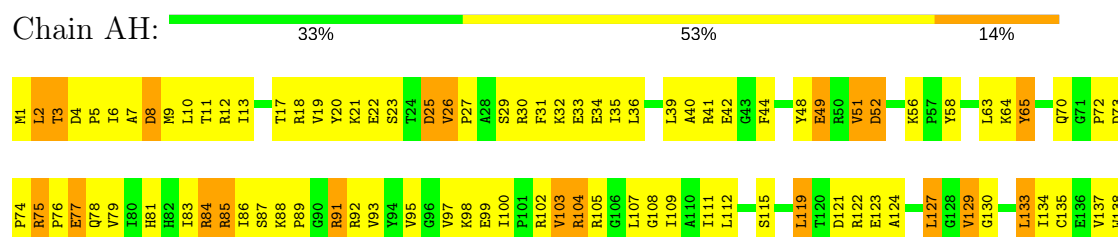
• Molecule 7: 30S ribosomal protein S7



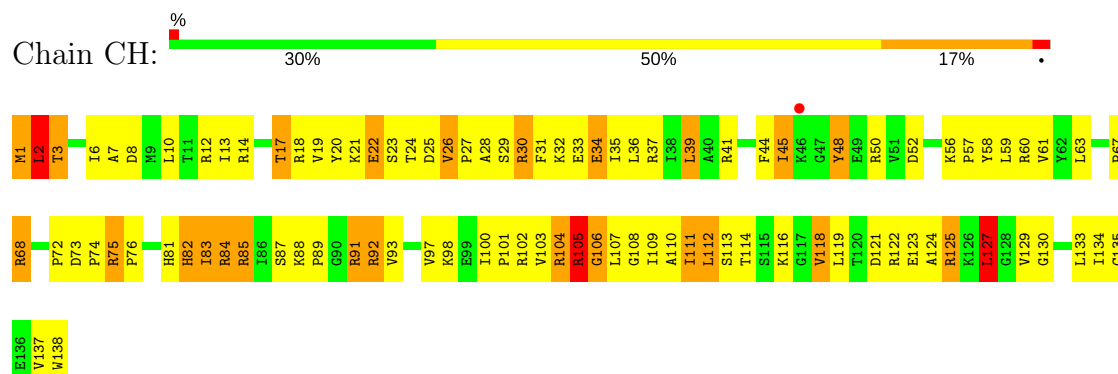
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

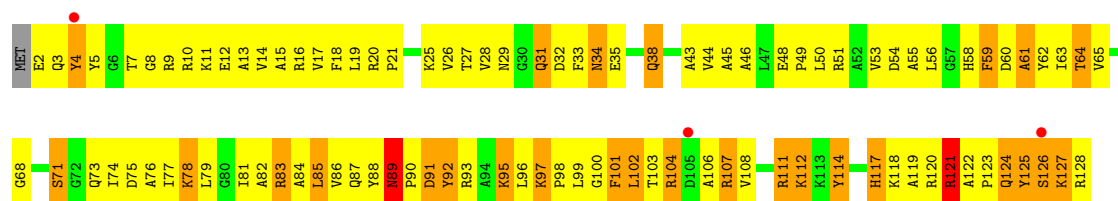


• Molecule 9: 30S ribosomal protein S9

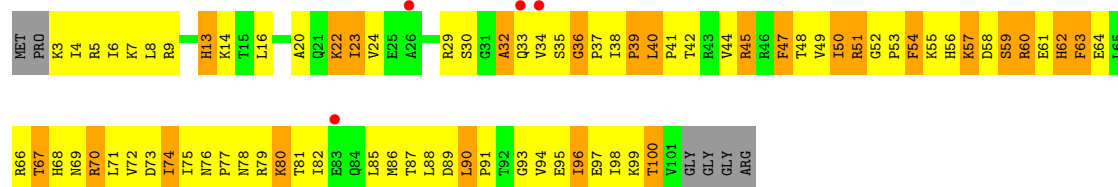
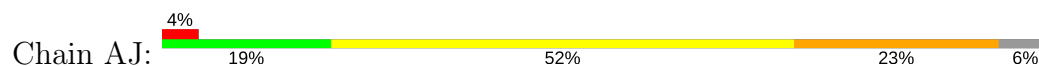


• Molecule 9: 30S ribosomal protein S9

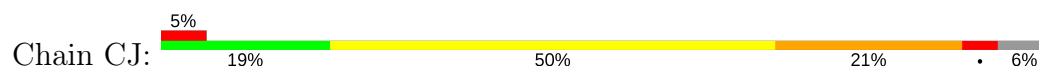




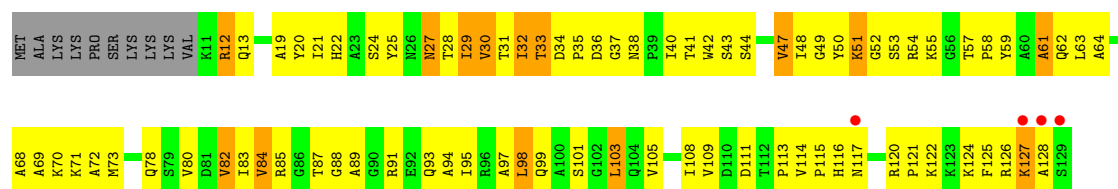
• Molecule 10: 30S ribosomal protein S10



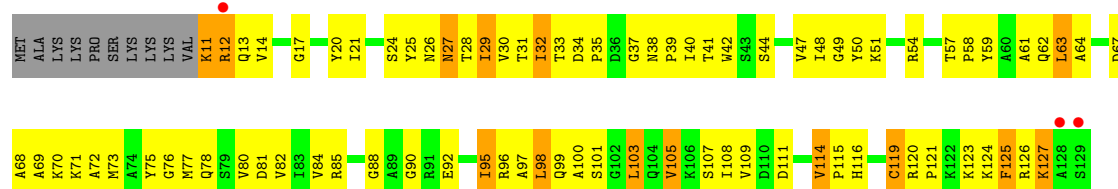
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

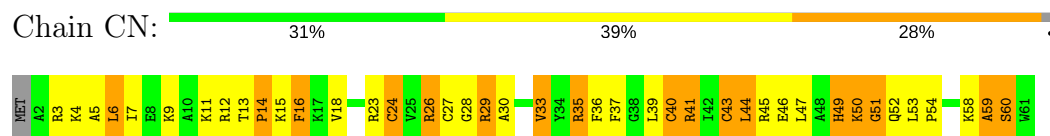


• Molecule 11: 30S ribosomal protein S11

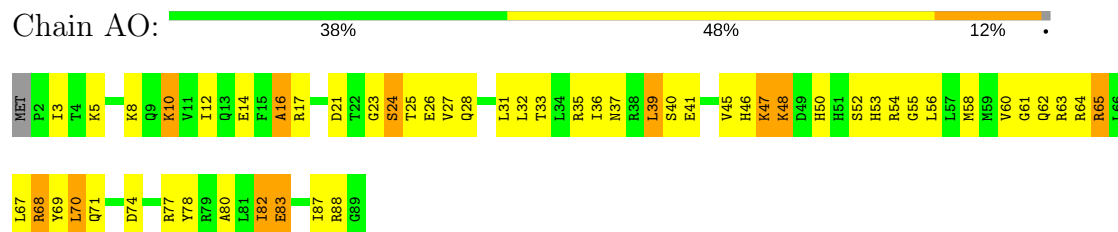


• Molecule 12: 30S ribosomal protein S12

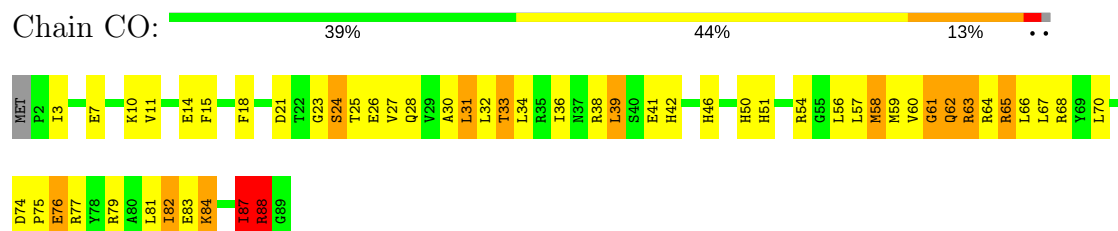
- Molecule 14: 30S ribosomal protein S14 type Z



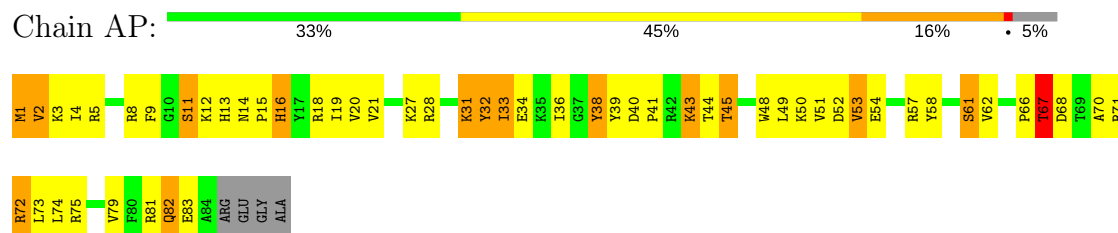
- Molecule 15: 30S ribosomal protein S15



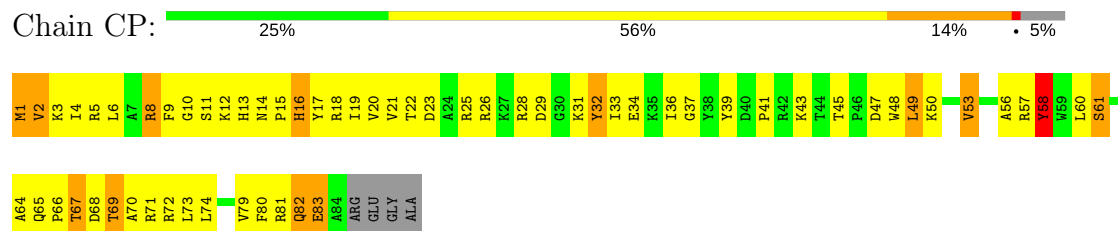
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

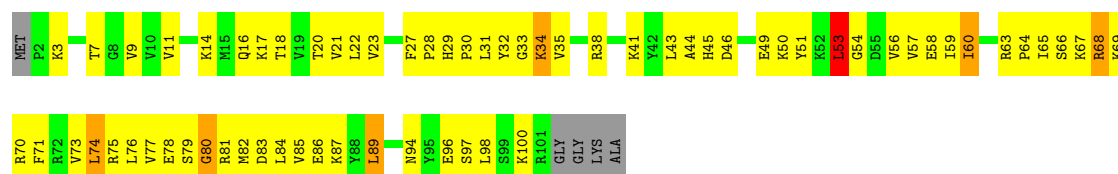


- Molecule 16: 30S ribosomal protein S16

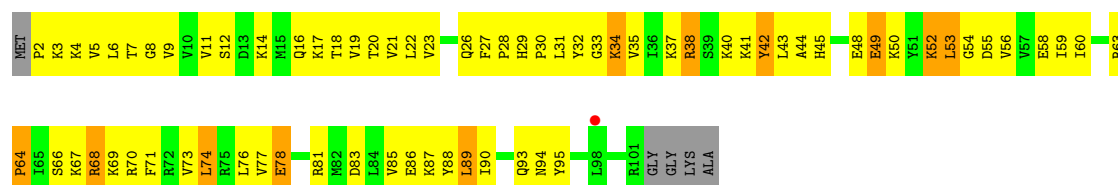


- Molecule 17: 30S ribosomal protein S17

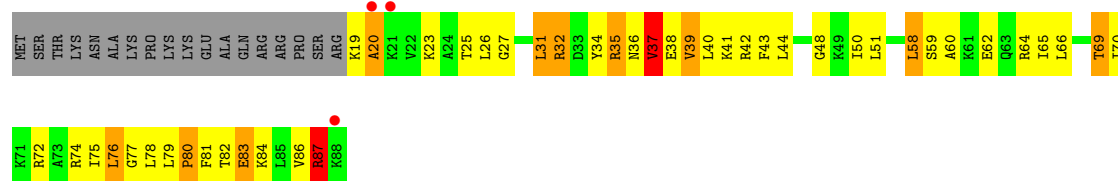




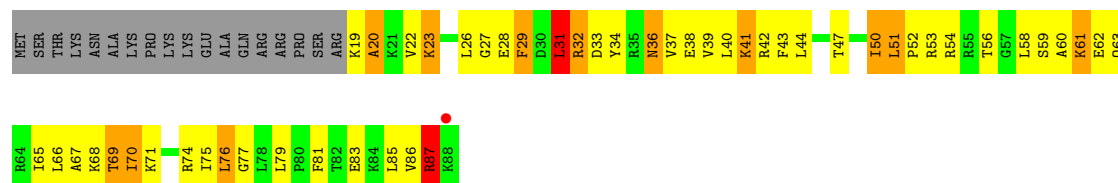
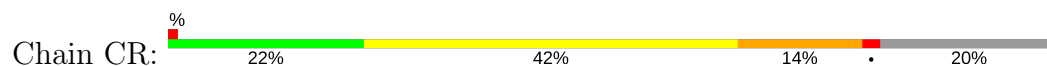
• Molecule 17: 30S ribosomal protein S17



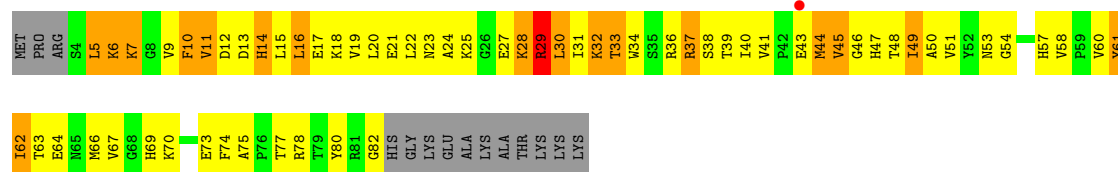
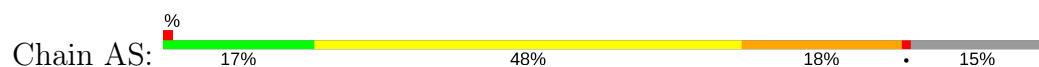
• Molecule 18: 30S ribosomal protein S18



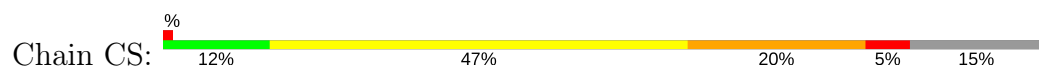
• Molecule 18: 30S ribosomal protein S18



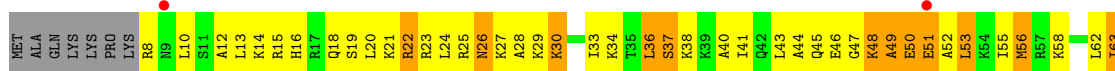
• Molecule 19: 30S ribosomal protein S19



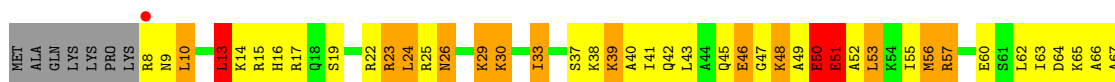
• Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



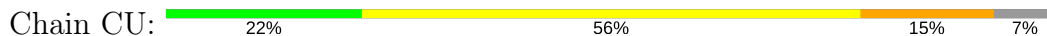
- Molecule 20: 30S ribosomal protein S20



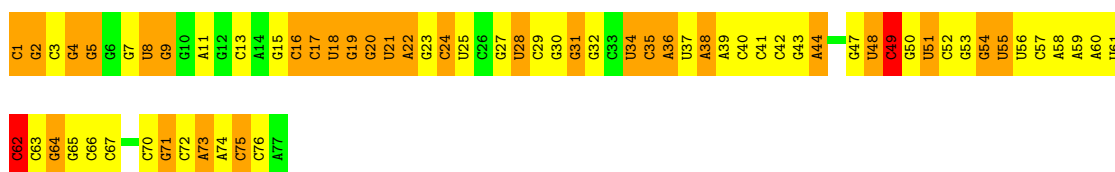
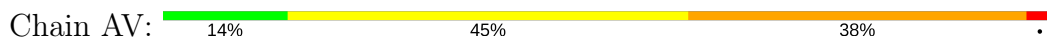
- Molecule 21: 30S ribosomal protein Thx



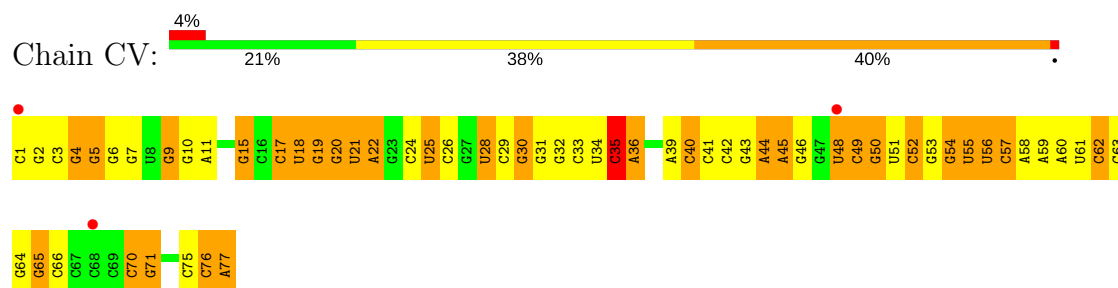
- Molecule 21: 30S ribosomal protein Thx



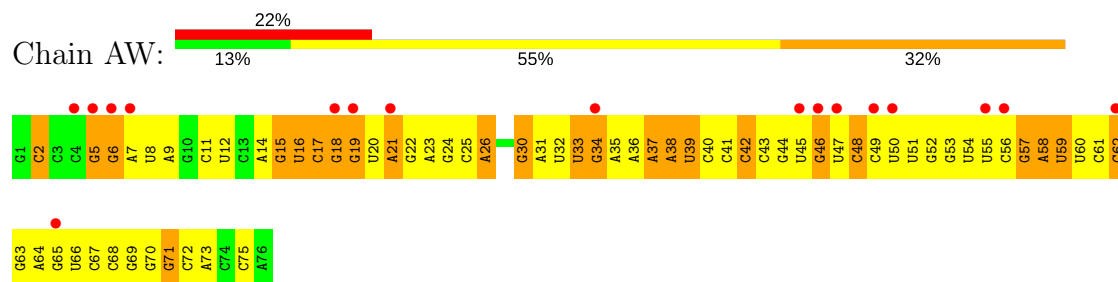
- Molecule 22: P-SITE tRNA fMet



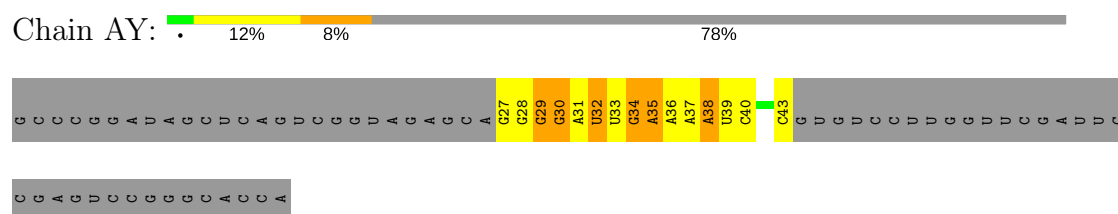
- Molecule 22: P-SITE tRNA fMet



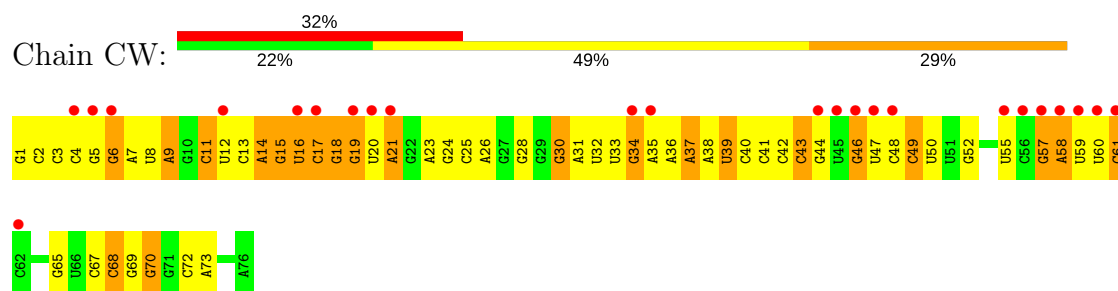
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



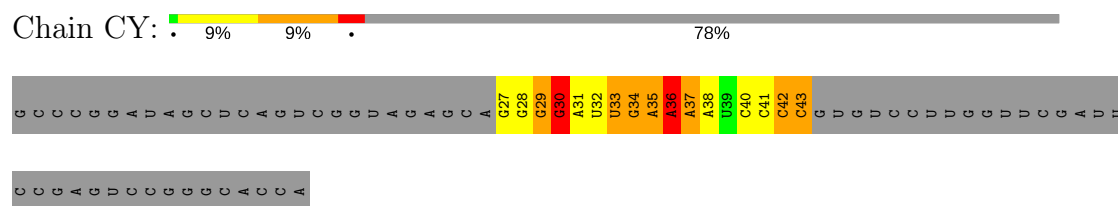
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



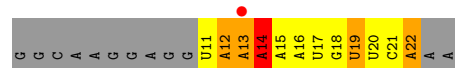
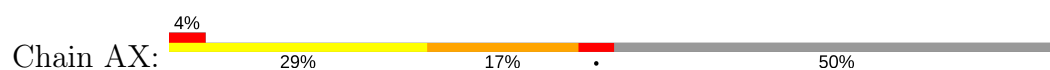
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



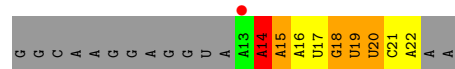
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



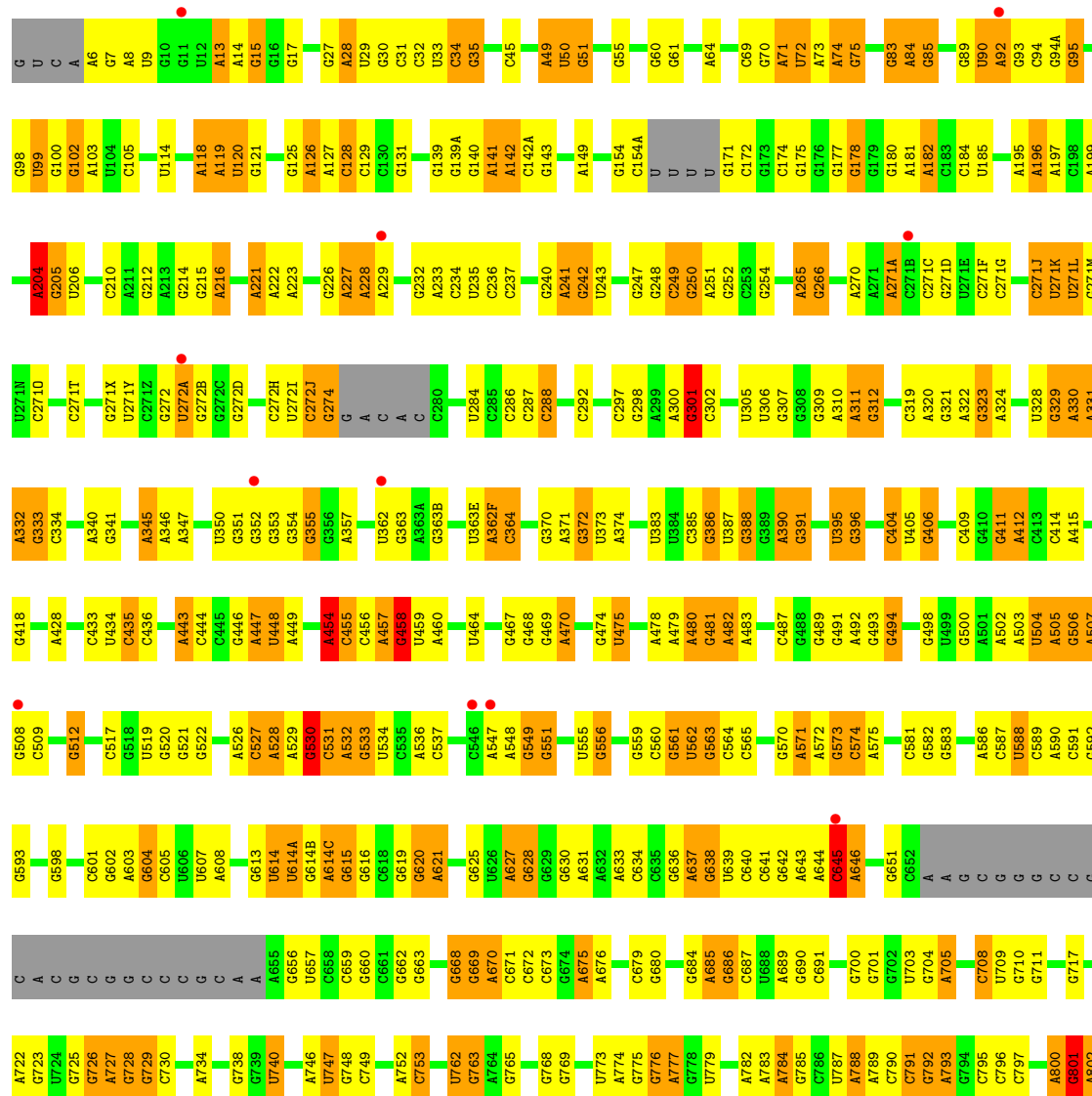
- Molecule 24: mRNA



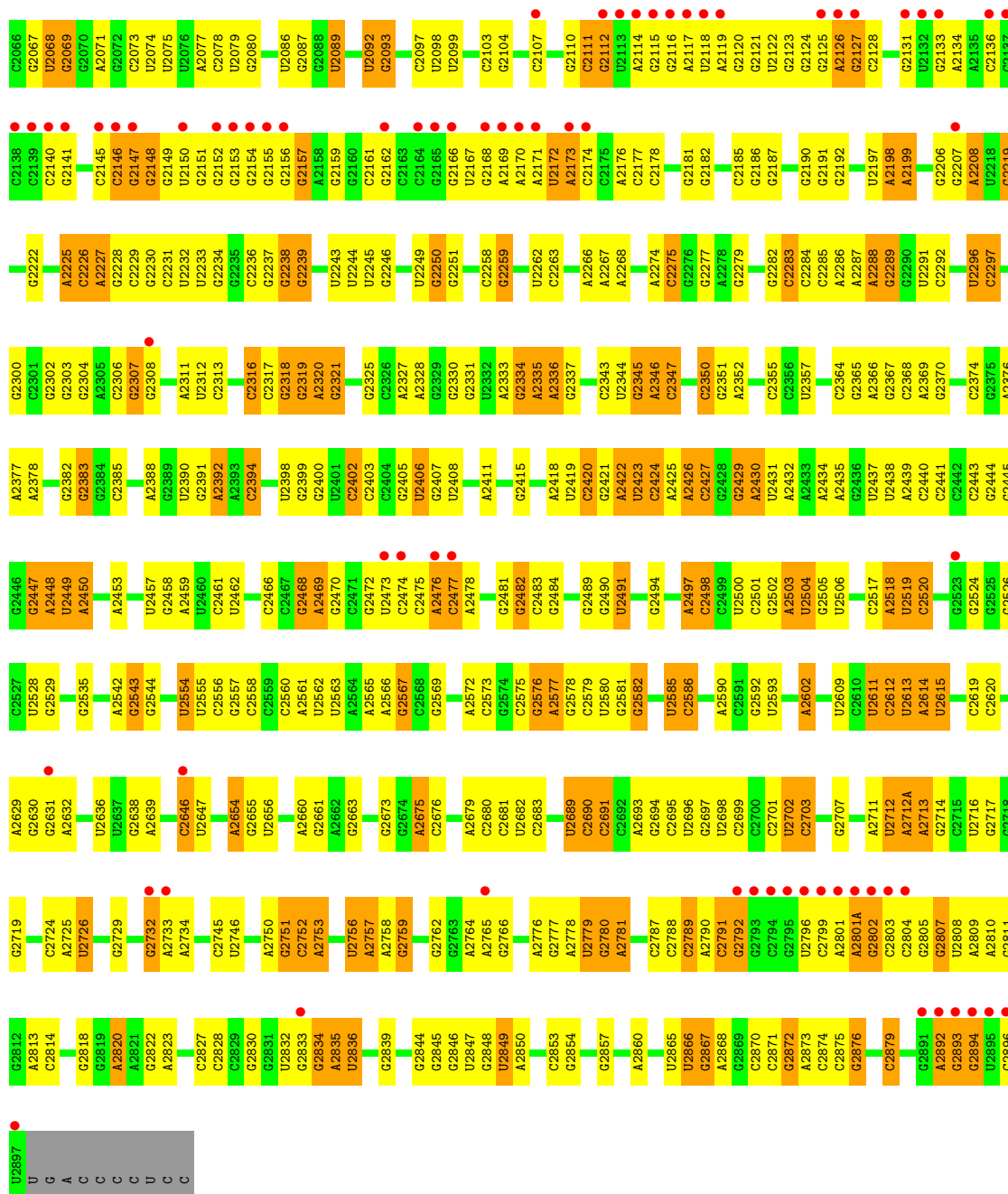
• Molecule 24: mRNA



• Molecule 25: 23S rRNA

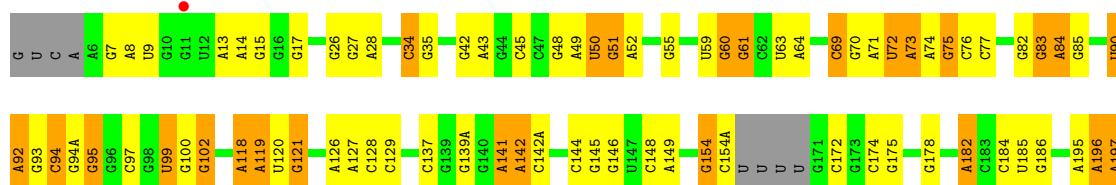


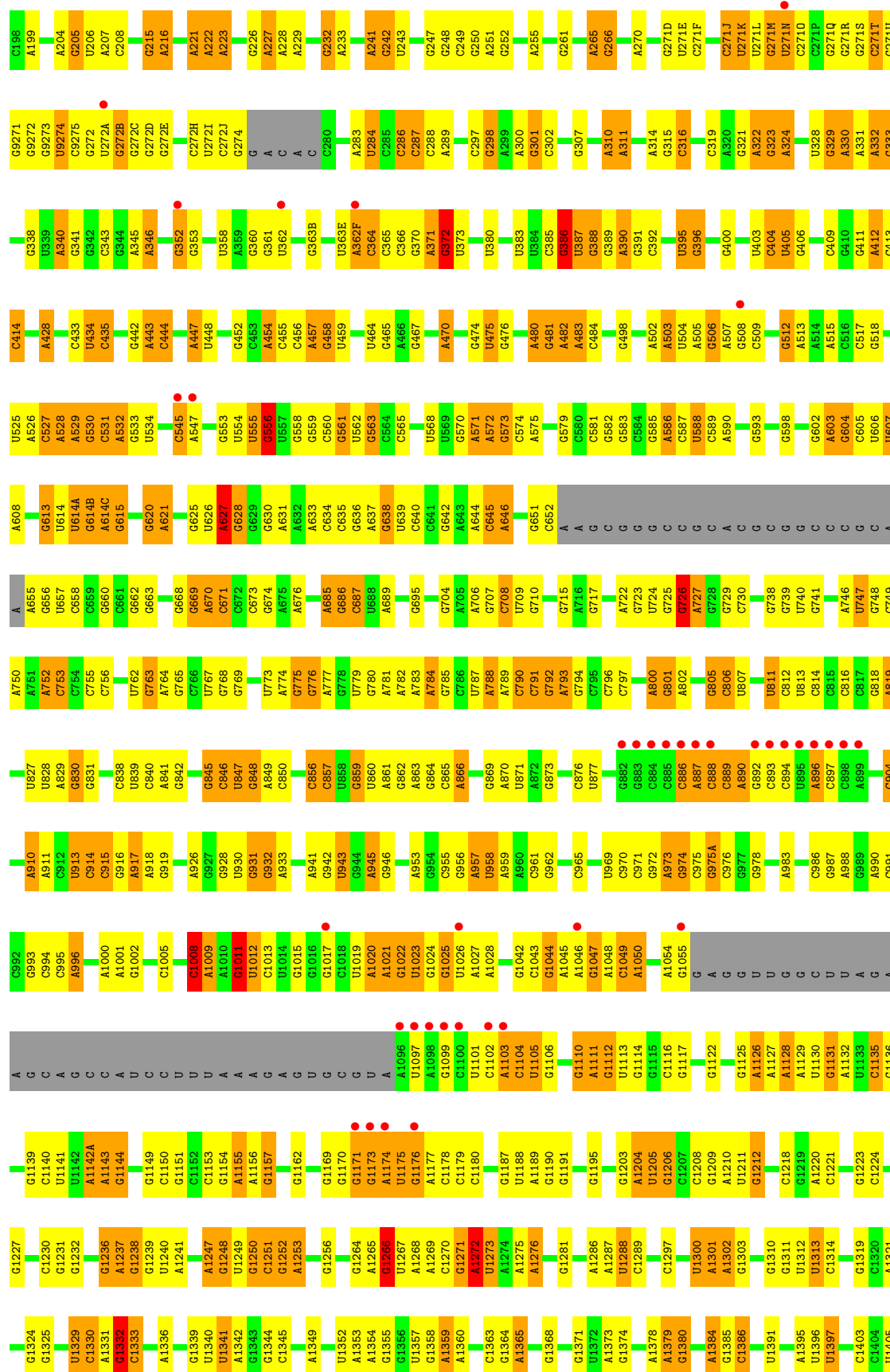




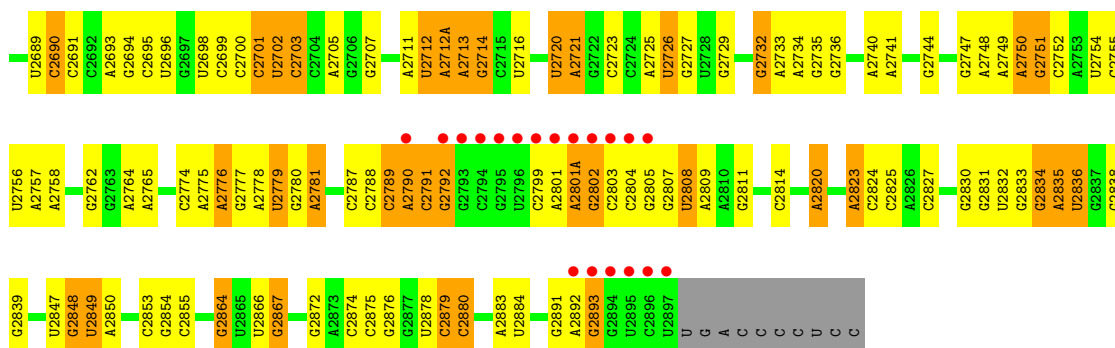
• Molecule 25: 23S rRNA

Chain DA: 4% 48% 31% 17%

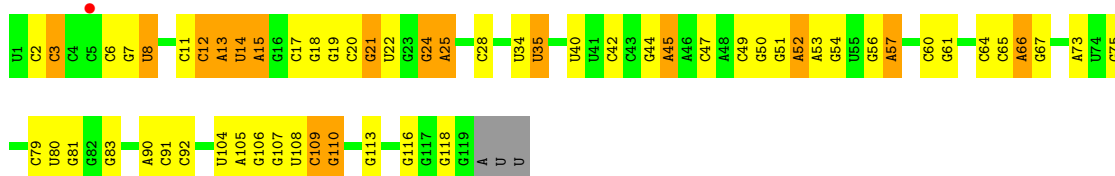




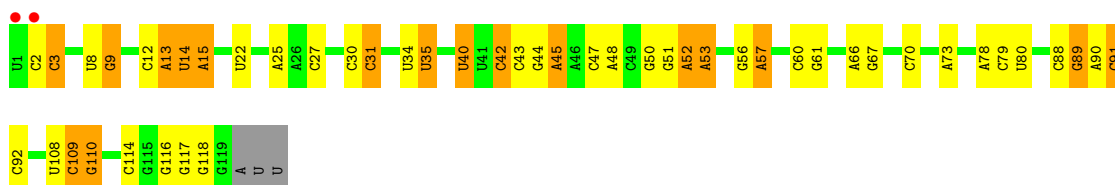
G2576	G2577	C2483	U2398	U2197	G2127	G2046	C1958	A1853	A1762	A1665	G1568	A1490	U1406
A2577	G2399	G2484	G2399	A2196	C2128	G2046	C1962	A1854	G1763	G1566	A1569	G1491	C1407
G2578	G2400	G2485	A2311	A2199	C2129	C2050	U1963	G1858	G1764	A1667	A1570	G1492	C1408
U2580	U2401	G2486	C2317	G2206	G2130	G2051	C1964	A1859	A1765	A1669	C1577	A1494	C1409
G2582	C2402	G2489	G2318	G2207	G2132	G2052	C1965	U1864	G1769	G1674	U1578	A1495	A1412
G2583	G2405	G2490	G2319	A2208	G2133	C2055	A1966	G1865	A1773	A1675	A1579	A1496	G1413
U2584	G2406	U2491	A2320	U2218	A2134	G2056	C1967	C1866	U1778	C1676	C1579	U1497	
U2585	G2407	G2492	G2325	G2219	A2135	C2057	C1968	A1876	A1779	A1677	A1583	U1498	G1416
A2590	G2410	A2411	A2326	A2225	C2136	A2059	C1969	A1877	U1779	C1678	C1584	G1499	G1417
G2497	G2411		A2327	C2226	C2137	A2060	U1970	G1878	U1780	G1678	A1586	G1500	G1418
G2498			G2328	C2227	C2138	A2061	A1971	C1879	C1781	G1681	A1587	C1501	A1419
	G2415		G2329	G2228	C2139	A2062	A1972	C1880	C1782	G1682	U1588	C1502	U1420
			G2330	G2229	C2140			C1881			C1589	U1503	G1421
			G2331	G2230	G2141			C1882	A1783			C1504	
			U2332	U2233	G2142	G2067	A1981	G1883	A1784	U1688	G1594	A1427	A1427
			U2333	G2234	C2145	U2068	C1982	G1884	A1785	A1689	G1595	C1428	G1429
			A2334	G2235	G2146	G2069		A1884	A1786	C1509	A1508	C1509	G1430
			A2335	G2236	G2147	G2070	G1987	A1885	A1787	C1598	A1509A	A1509A	U1431
			A2336	G2237	G2148	A2071	C1988	G1888		U1602		C1513	A1434
			A2337	G2238	G2149	C2072	C1989	A1889	A1791	A1603		G1520	C1437
			A2338	G2239	G2150	C2073	U1991	U1898	U1796	C1607	G1523	G1524	
			A2339	G2240	G2151	U2074	U1992	G1899	C1797	A1608	G1524	G1525	
			U2340	G2241	G2152	U2075	U1993	A1900	U1798	A1609	G1525	G1526	
			G2341	G2242	G2153	U2076	U1994	A1901	U1799	A1700	G1527	G1527	A1445
			A2342	G2243	G2154	U2077	U1995	G1902	C1800	A1701	C1445A	C1445A	
			A2343	G2244	G2155	U2078	C1996	G1903	U1801	U1706	A1449	G1450	
			A2344	G2245	G2156	U2079	U1997	G1904	G1802	G1707	A1451	C1450A	
			A2345	G2246	G2157	U2080	U1998	G1905	A1803	C1708	C1451	C1451	
			A2346	G2247	G2158	U2081	C1999	G1906	U1804	C1711	A1462	A1462	
			A2347	G2248	G2159	U2082	G2000	G1907	C1805	C1712	U1463	U1463	
			A2348	G2249	G2160	U2083	A2001	G1908	A1806	G1718	G1456	G1456	
			A2349	G2250	G2161	U2084	G2002	A1912	A1815	G1622	A1457	A1457	
			A2350	G2251	G2162	U2085	G2003	A1913	G1816	G1458	C1458	C1458	
			A2351	G2252	G2163	U2086	G2004	U1914	G1817	G1489	G1489	G1489	
			A2352	G2253	G2164	U2087	G2005	U1915	U1818	G1490	G1490	G1490	
			A2353	G2254	G2165	U2088	G2006	A1916	U1819	A1634	G1491	G1491	
			A2354	G2255	G2166	U2089	G2007	A1917	A1820	G1635	C1543	C1543	
			A2355	G2256	G2167	U2090	G2008	A1918	A1821	C1636	G1465	G1465	
			A2356	G2257	G2168	U2091	G2009	A1919	G1822	A1637	G1466	G1466	
			A2357	G2258	G2169	U2092	G2010	A1920	G1823	G1467	C1467	C1467	
			A2358	G2259	G2170	U2093	G2011	A1921	U1824	C1547	A1471	A1471	
			A2359	G2260	G2171	U2094	G2012	A1922	U1825	C1548	A1472	A1472	
			A2360	G2261	G2172	U2095	G2013	A1923	A1826	C1549	G1473	G1473	
			A2361	G2262	G2173	U2096	A2014	G1924	G1827	A1544	C1551	C1551	
			A2362	G2263	G2174	U2097	G2015	U1935	A1828	C1640	U1481	U1481	
			A2363	G2264	G2175	U2098	G2016	A1936	G1829	A1641	G1482	G1482	
			A2364	G2265	G2176	U2099	G2017	A1937	U1830	A1642	G1483	G1483	
			A2365	G2266	G2177	U2100	G2018	U1938	A1831	G1643	G1484	G1484	
			A2366	G2267	G2178	U2101	G2019	U1939	G1832	G1644	G1485	G1485	
			A2367	G2268	G2179	U2102	G2020	U1940	A1833	G1645	G1486	G1486	
			A2368	G2269	G2180	U2103	G2021	C1941	G1834	G1646	U1487	U1487	
			A2369	G2270	G2181	U2104	G2022	U1942	G1835	G1647	A1564	A1564	
			A2370	G2271	G2182	U2105	G2023	U1943	U1836	C1648	A1568	A1568	
			A2371	G2272	G2183	U2106	G2024	U1944	G1837	G1649	G1559	G1559	
			A2372	G2273	G2184	U2107	G2025	U1945	G1838	G1650	G1560	G1560	
			A2373	G2274	G2185	U2108	G2026	A1952	G1839	G1651	G1487	G1487	
			A2374	G2275	G2186	U2109	G2027	A1953	G1840	G1652	G1488	G1488	
			A2375	G2276	G2187	U2110	G2028	U1954	G1841	G1653	A1486	A1486	
			A2376	G2277	G2188	U2111	G2029	U1955	G1842	G1654	G1487	G1487	
			A2377	G2278	G2189	U2112	G2030	A1956	G1843	G1655	G1565	G1565	
			A2378	G2279	G2190	U2113	G2031	A1957	U1844	G1656	A1566	A1566	
			A2379	G2280	G2191	U2114	G2032	G1958	G1845	G1657	G1567	G1567	
			A2380	G2281	G2192	U2115	G2033	A1959	G1846	G1658	G1568	G1568	
			A2381	G2282	G2193	U2116	G2034	G1960	G1847	G1659	G1569	G1569	
			A2382	G2283	G2194	U2117	G2035	A1961	G1848	G1660	G1570	G1570	
			A2383	G2284	G2195	U2118	G2036	A1962	G1849	G1661	G1571	G1571	
			A2384	G2285	G2196	U2119	G2037	A1963	G1850	G1662	G1572	G1572	
			A2385	G2286	G2197	U2120	G2038	A1964	G1851	G1663	G1573	G1573	
			A2386	G2287	G2198	U2121	G2039	A1965	G1852	G1664	G1574	G1574	
			A2387	G2288	G2199	U2122	G2040	A1966	G1853	G1665	G1575	G1575	
			A2388	G2289	G2200	U2123	G2041	A1967	G1854	G1666	G1576	G1576	
			A2389	G2290	G2201	U2124	G2042	A1968	G1855	G1667	G1577	G1577	
			A2390	G2291	G2202	U2125	G2043	A1969	G1856	G1668	G1578	G1578	
			A2391	G2292	G2203	U2126	G2044	A1970	G1857	G1669	G1579	G1579	
			A2392	G2293	G2204	U2127	G2045	A1971	G1858	G1670	G1580	G1580	
			A2393	G2294	G2205	U2128	G2046	A1972	G1859	G1671	G1581	G1581	
			A2394	G2295	G2206	U2129	G2047	A1973	G1860	G1672	G1582	G1582	
			A2395	G2296	G2207	U2130	G2048	A1974	G1861	G1673	G1583	G1583	
			A2396	G2297	G2208	U2131	G2049	A1975	G1862	G1674	G1584	G1584	
			A2397	G2298	G2209	U2132	G2050	A1976	G1863	G1675	G1585	G1585	
			A2398	G2299	G2210	U2133	G2051	A1977	G1864	G1676	G1586	G1586	
			A2399	G2300	G2211	U2134	G2052	A1978	G1865	G1677	G1587	G1587	
			A2400	G2301	G2212	U2135	G2053	A1979	G1866	G1678	G1588	G1588	
			A2401	G2302	G2213	U2136	G2054	A1980	G1867	G1679	G1589	G1589	
			A2402	G2303	G2214	U2137	G2055	A1981	G1868	G1680	G1590	G1590	
			A2403	G2304	G2215	U2138	G2056	A1982	G1869	G1681	G1591	G1591	
			A2404	G2305	G2216	U2139	G2057	A1983	G1870	G1682	G1592	G1592	
			A2405	G2306	G2217	U2140	G2058	A1984	G1871	G1683	G1593	G1593	
			A2406	G2307	G2218	U2141	G2059	A1985	G1872	G1684	G1594	G1594	
			A2407	G2308	G2219	U2142	G2060	A1986	G1873	G1685	G1595	G1595	
			A2408	G2309	G2220	U2143	G2061	A1987	G1874	G1686	G1596	G1596	
			A2409	G2310	G2221	U2144	G2062	A1988	G1875	G1687	G1597	G1597	
			A2410	G2311	G2222	U2145	G2063	A1989	G1876	G1688	G1598	G1598	
			A2411	G2312	G2223	U2146	G2064	A1990	G1877	G1689	G1599	G1599	
			A2412	G2313	G2224	U2147	G2065	A1991	G1878	G1690	G1600	G1600	
			A2413	G2314	G2225	U2148	G2066	A1992	G1879	G1691	G1601	G1601	
			A2414	G2315	G2226	U2149	G2067	A1993	G1880	G1692	G1602	G1602	
			A2415	G2316	G2227	U2150	G2068	A1994	G1881	G1693	G1603	G1603	
			A2416	G2317	G2228	U2151	G2069	A1995	G1882	G1694	G1604	G1604	
			A2417	G2318	G2229	U2152	G2070	A1996	G1883	G1695	G1605	G1605	
			A2418	G2319	G2230	U2153	G2071	A1997	G1884	G1696	G1606	G1606	
			A2419	G2320	G2231	U2154	G2072	A1998	G1885	G1697	G1607	G1607	
			A2420	G2321	G2232	U2155	G2073	A1999	G1886	G1698	G1608	G1608	
			A2421	G2322	G2233	U2156	G2074	A2000	G1887	G1699	G1609	G1609	
			A2422	G2323	G2234	U2157	G2075	A2001	G1888	G1700	G1610	G1610	
			A2423	G2324	G2235	U2158	U2076	A2002	G1889	A1701	G1611	G1611	
			A2424	G2325	G2236	U2159	U2077	A2003	G1890	A1702	G1612	G1612	
			A2425	G2326	G2237	U2160	U2078	A2004	G1891	A1703	G1613	G1613	
			A2426										



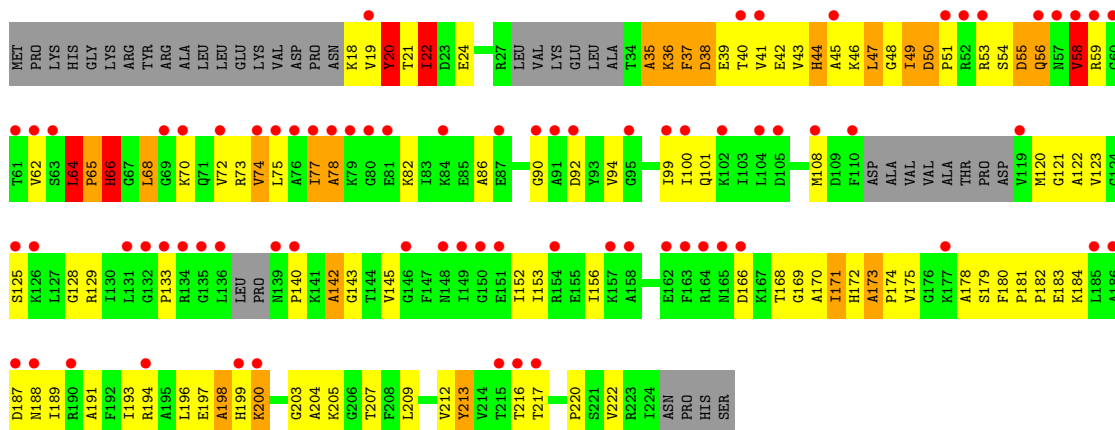
• Molecule 26: 5S rRNA



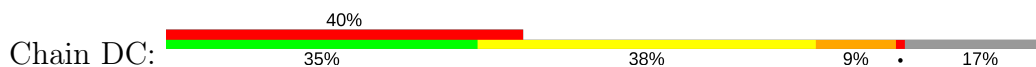
• Molecule 26: 5S rRNA

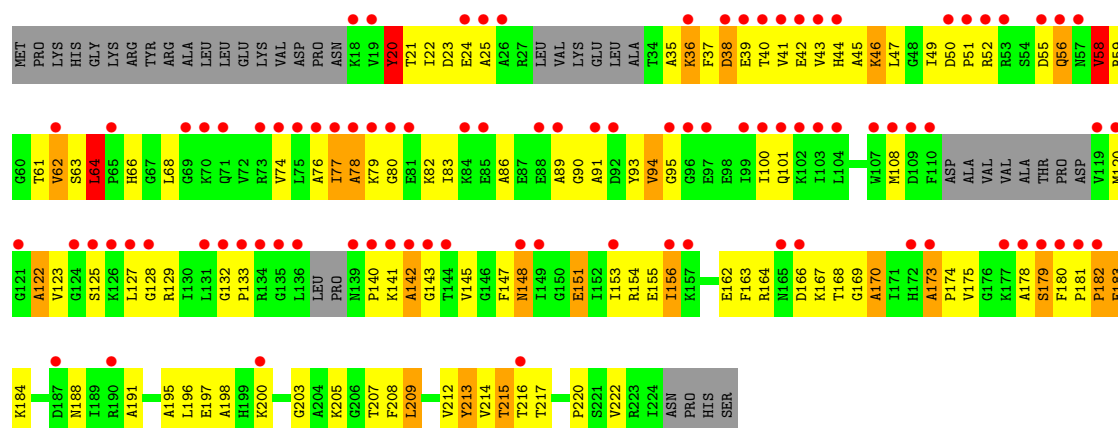


• Molecule 27: 50S RIBOSOMAL PROTEIN L1



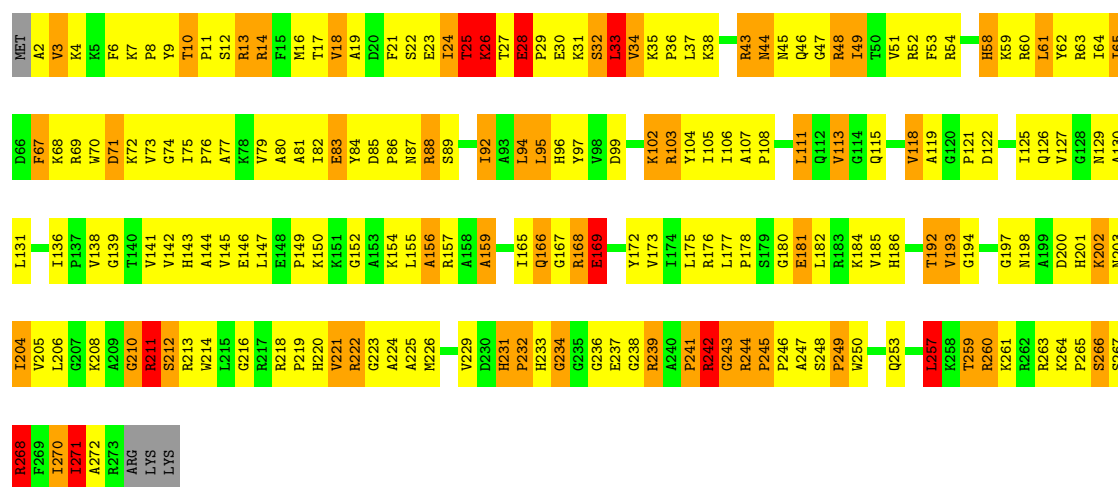
• Molecule 27: 50S RIBOSOMAL PROTEIN L1





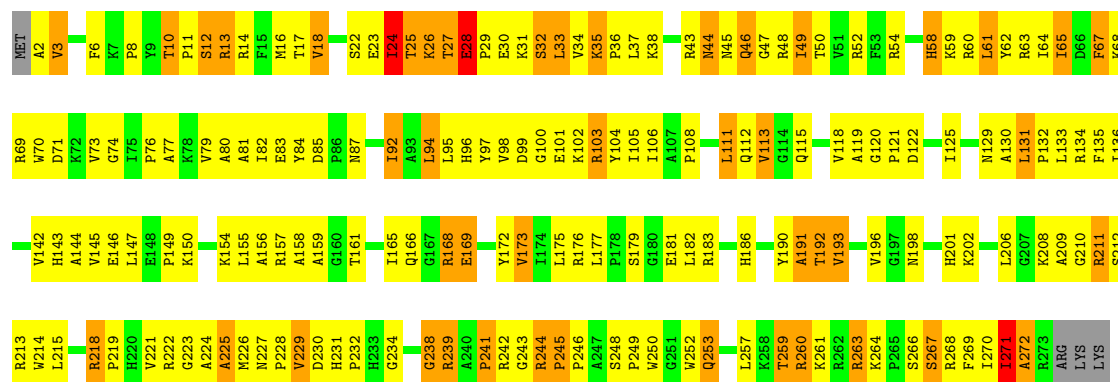
• Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain BD: 27% 49% 19%



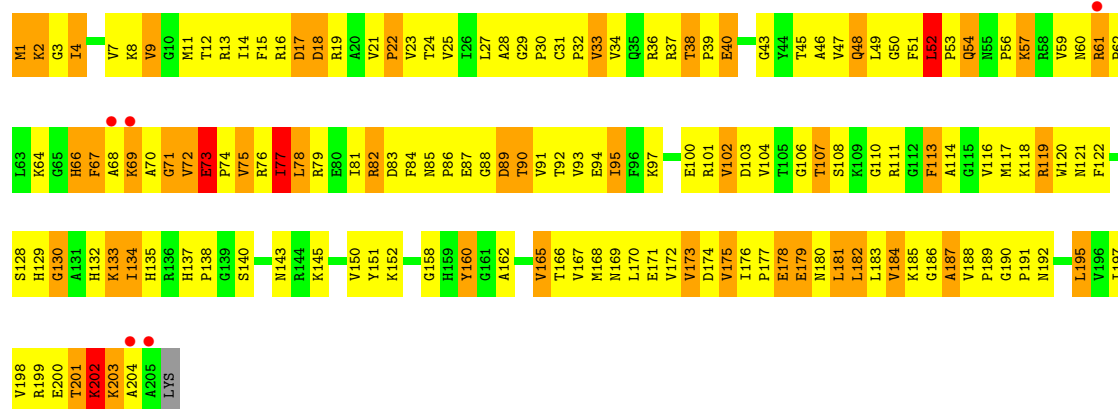
• Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain DD: 32% 49% 16%

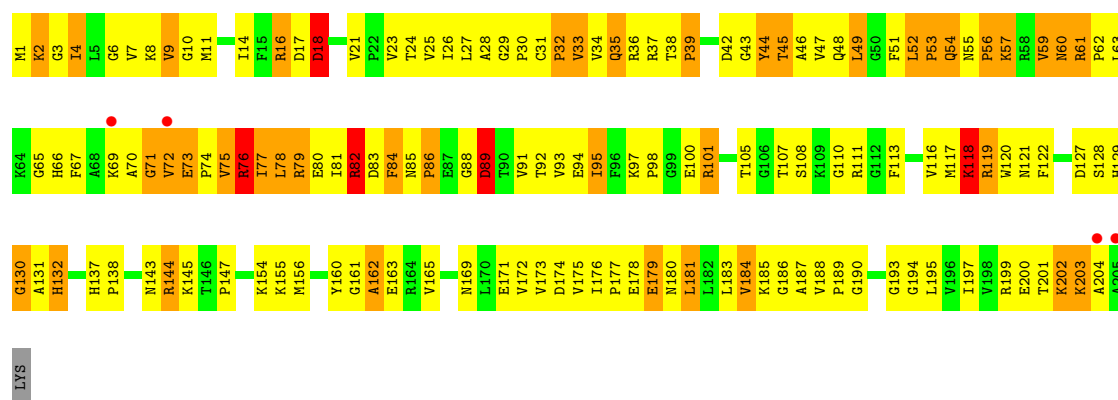


• Molecule 29: 50S RIBOSOMAL PROTEIN L3

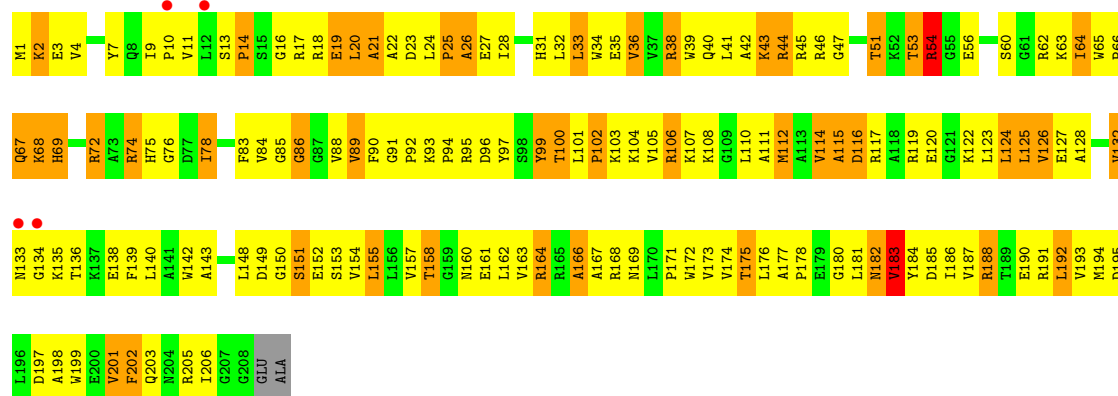
Chain BE: 2% 24% 52% 22%



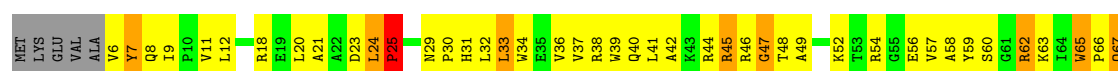
• Molecule 29: 50S RIBOSOMAL PROTEIN L3



• Molecule 30: 50S RIBOSOMAL PROTEIN L4

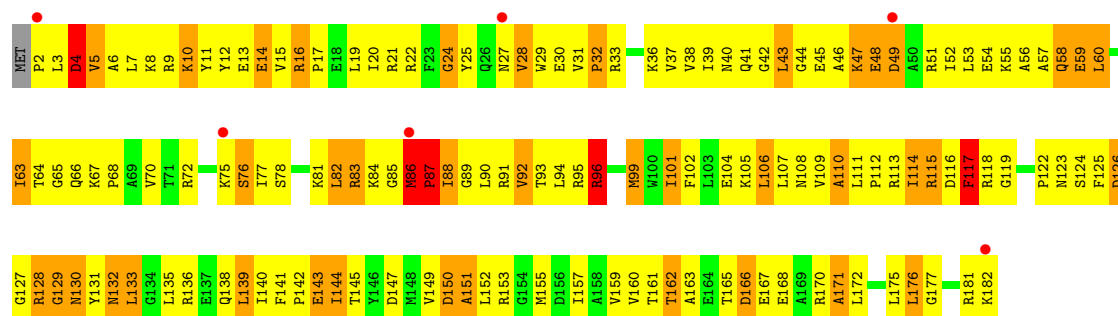


• Molecule 30: 50S RIBOSOMAL PROTEIN L4

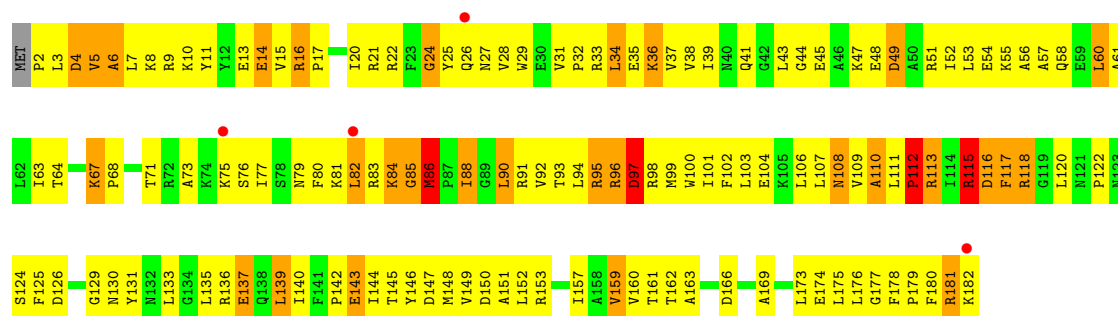




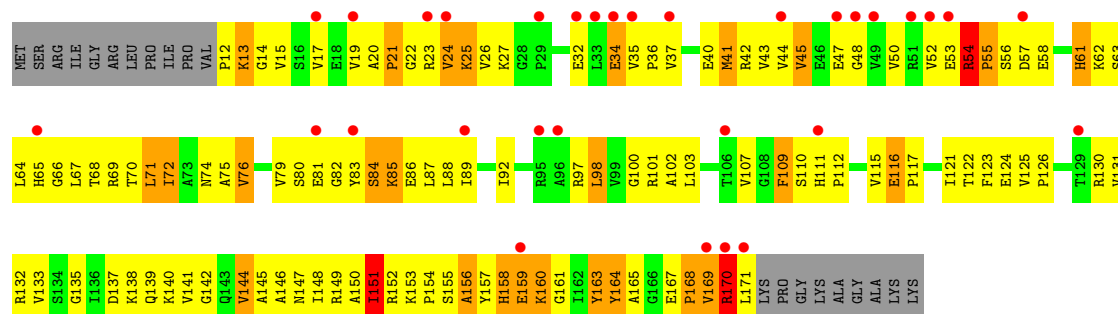
• Molecule 31: 50S RIBOSOMAL PROTEIN L5



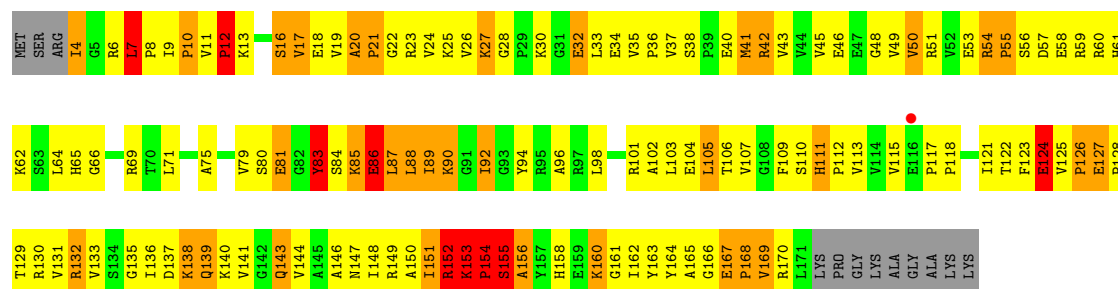
• Molecule 31: 50S RIBOSOMAL PROTEIN L5



• Molecule 32: 50S RIBOSOMAL PROTEIN L6



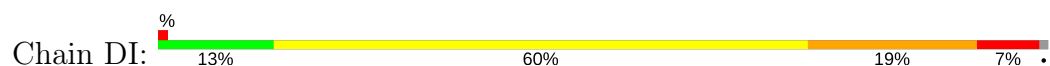
• Molecule 32: 50S RIBOSOMAL PROTEIN L6



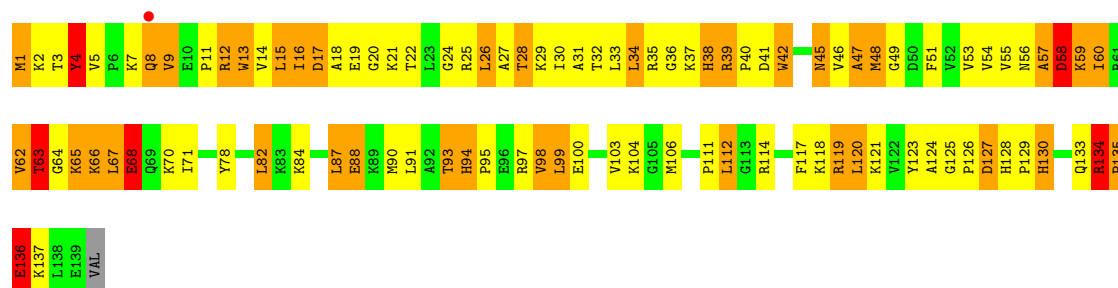
• Molecule 33: 50S RIBOSOMAL PROTEIN L9



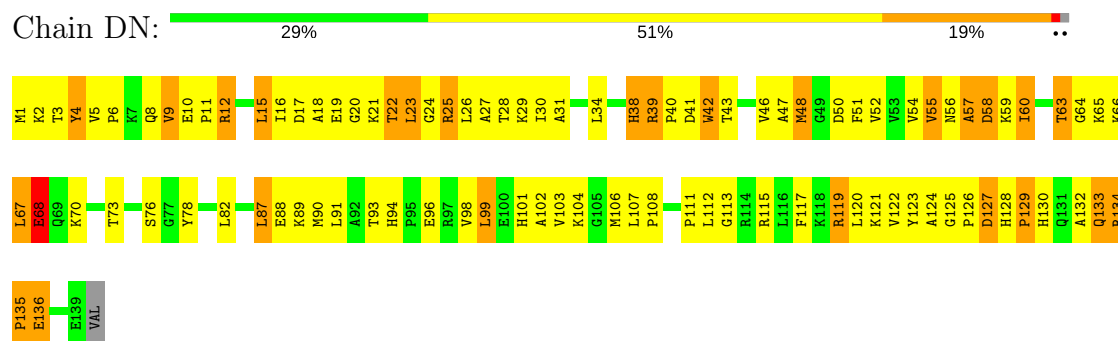
• Molecule 33: 50S RIBOSOMAL PROTEIN L9



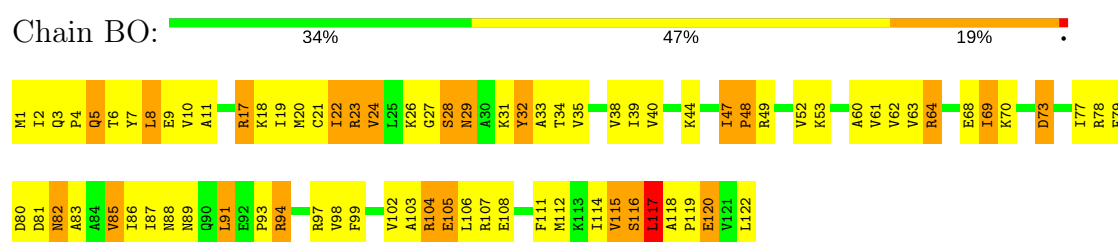
• Molecule 34: 50S RIBOSOMAL PROTEIN L13



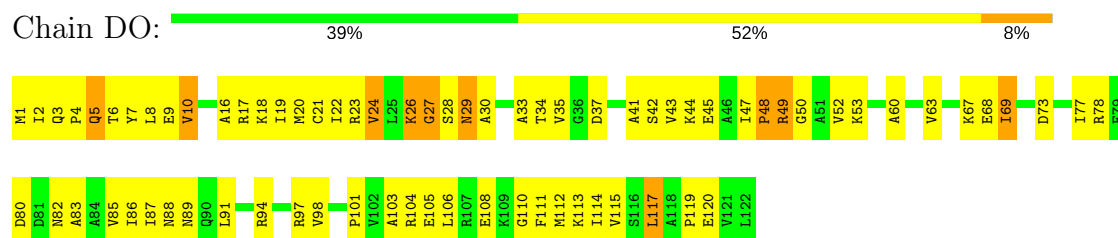
● Molecule 34: 50S RIBOSOMAL PROTEIN L13



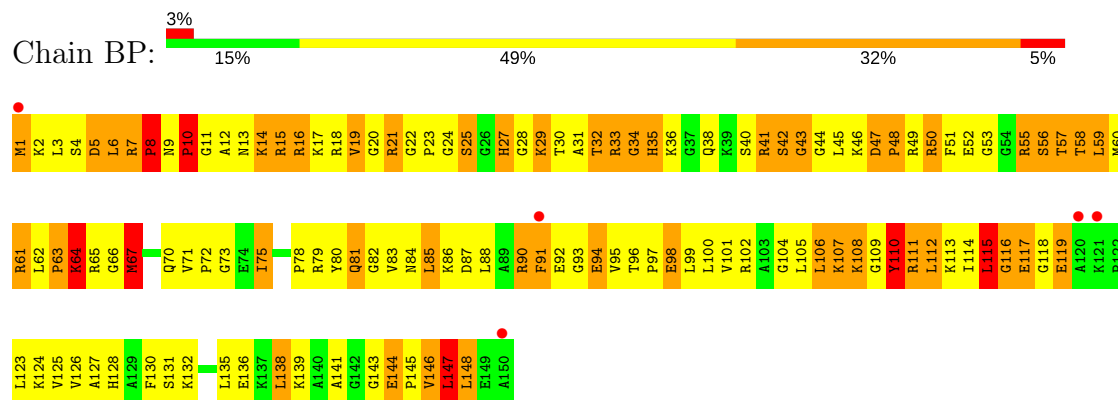
● Molecule 35: 50S RIBOSOMAL PROTEIN L14



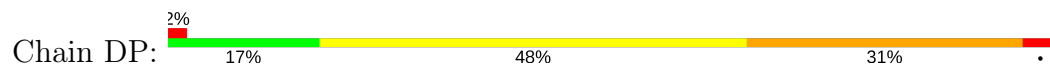
● Molecule 35: 50S RIBOSOMAL PROTEIN L14

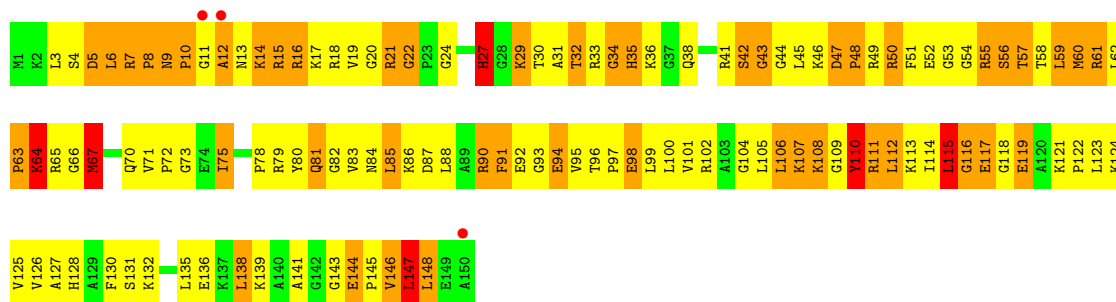


● Molecule 36: 50S RIBOSOMAL PROTEIN L15

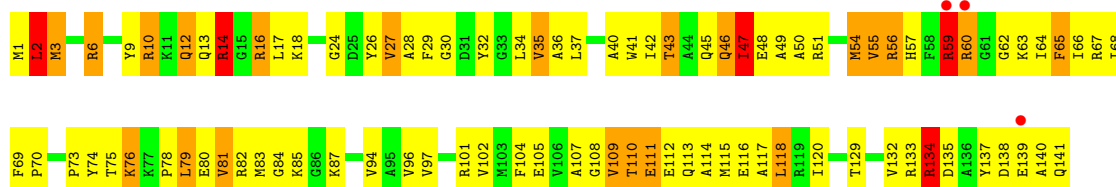


● Molecule 36: 50S RIBOSOMAL PROTEIN L15

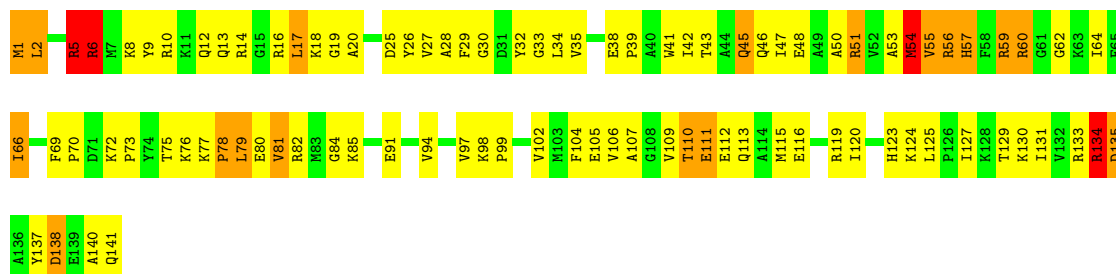




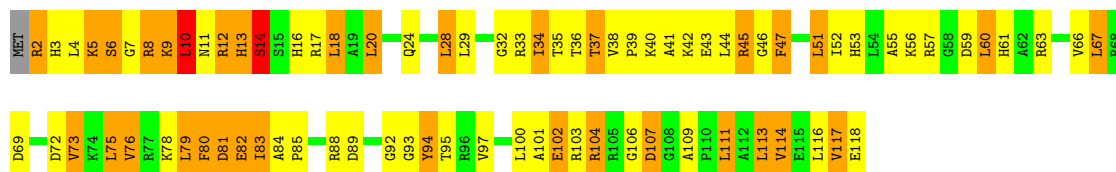
• Molecule 37: 50S RIBOSOMAL PROTEIN L16



• Molecule 37: 50S RIBOSOMAL PROTEIN L16



• Molecule 38: 50S RIBOSOMAL PROTEIN L17

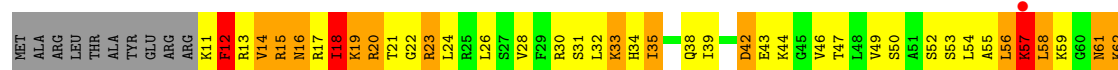
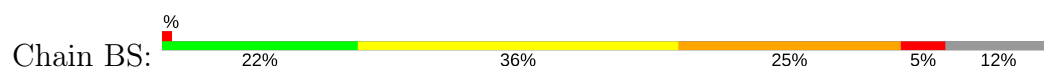


• Molecule 38: 50S RIBOSOMAL PROTEIN L17

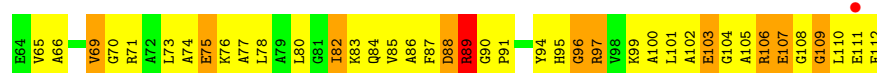




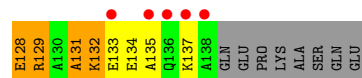
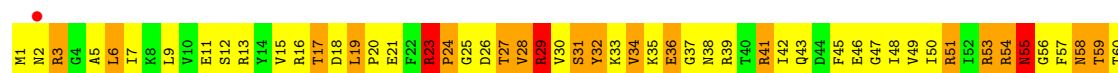
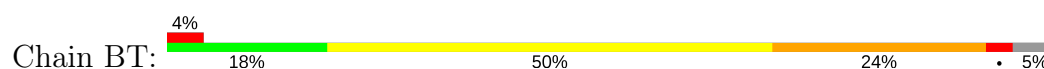
• Molecule 39: 50S RIBOSOMAL PROTEIN L18



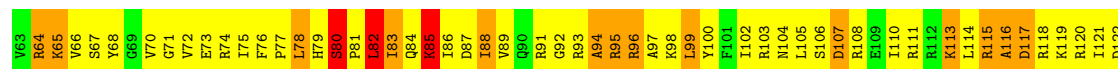
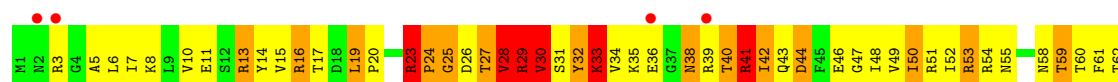
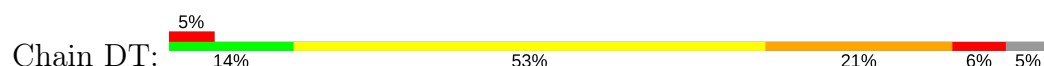
• Molecule 39: 50S RIBOSOMAL PROTEIN L18



• Molecule 40: 50S RIBOSOMAL PROTEIN L19



• Molecule 40: 50S RIBOSOMAL PROTEIN L19



• Molecule 41: 50S RIBOSOMAL PROTEIN L20



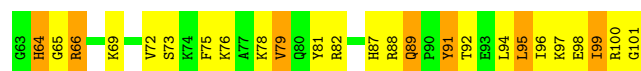
- Molecule 41: 50S RIBOSOMAL PROTEIN L20



• Molecule 42: 50S RIBOSOMAL PROTEIN L21



● Molecule 42: 50S RIBOSOMAL PROTEIN L21

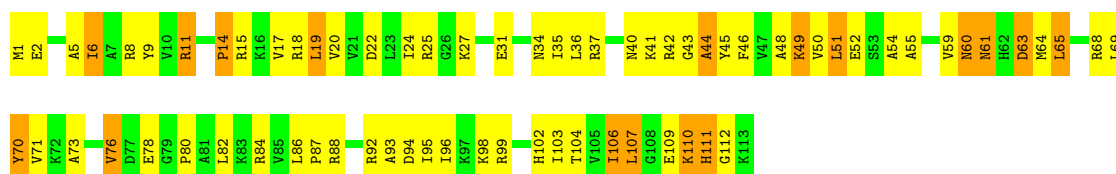


● Molecule 43: 50S RIBOSOMAL PROTEIN L22



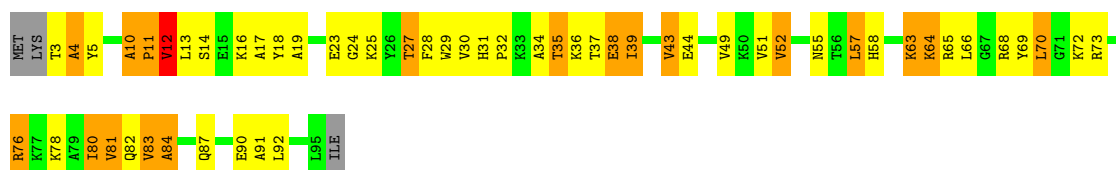
● Molecule 43: 50S RIBOSOMAL PROTEIN L22





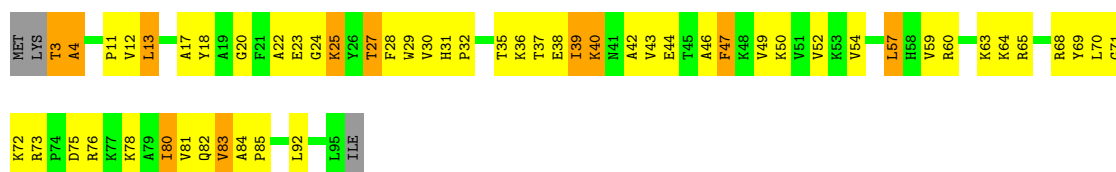
• Molecule 44: 50S RIBOSOMAL PROTEIN L23

Chain BX: 40% 38% 19% . .



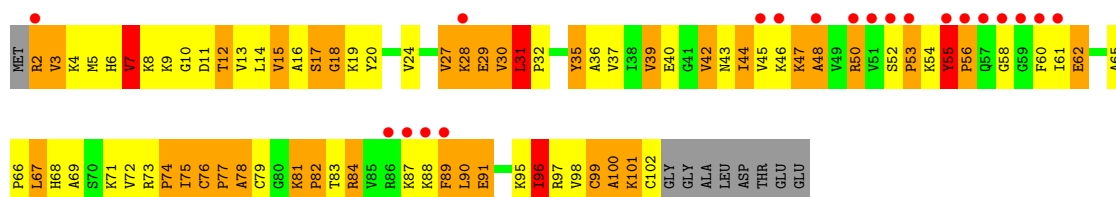
• Molecule 44: 50S RIBOSOMAL PROTEIN L23

Chain DX: 40% 46% 11% .



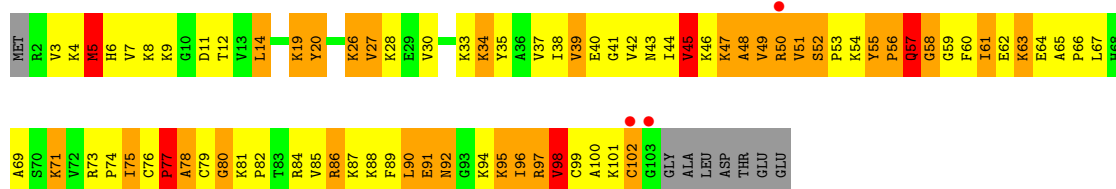
• Molecule 45: 50S RIBOSOMAL PROTEIN L24

Chain BY: 18% 20% 36% 32% 8%



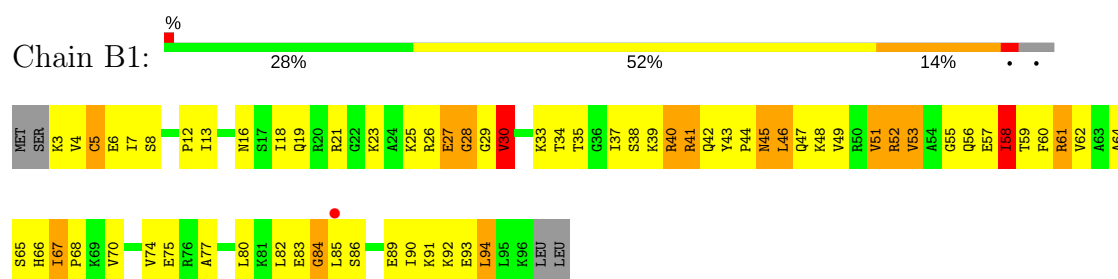
• Molecule 45: 50S RIBOSOMAL PROTEIN L24

Chain DY: 3% 20% 41% 27% 5% 7%

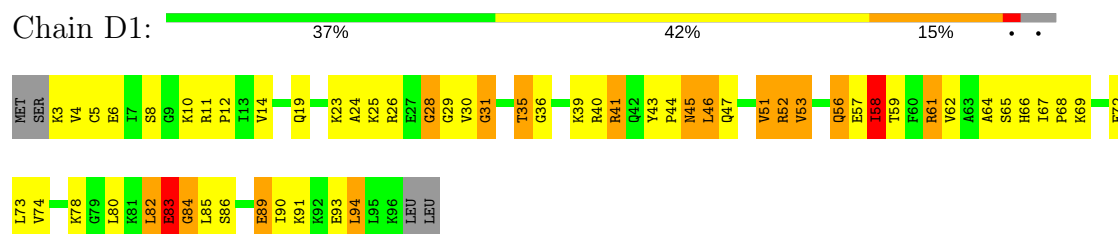


• Molecule 46: 50S RIBOSOMAL PROTEIN L25

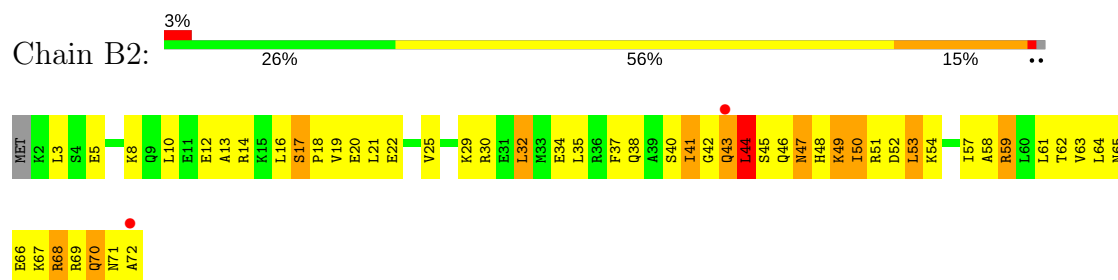
Chain BZ: 8% 23% 47% 13% 14%



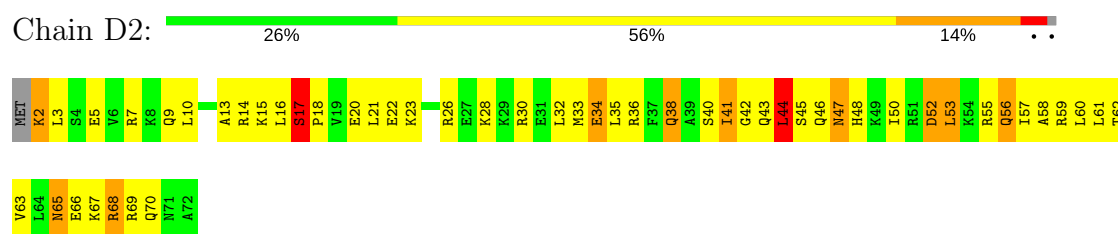
• Molecule 48: 50S RIBOSOMAL PROTEIN L28



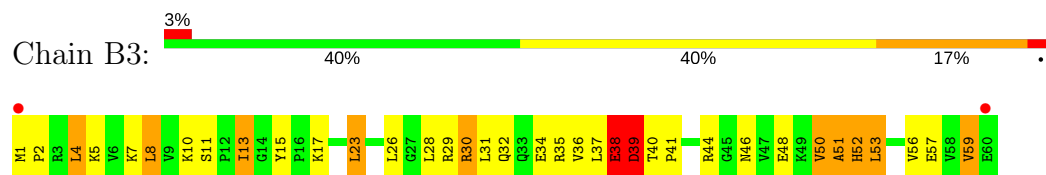
• Molecule 49: 50S RIBOSOMAL PROTEIN L29



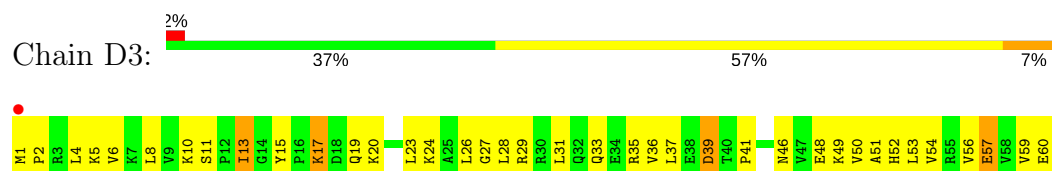
• Molecule 49: 50S RIBOSOMAL PROTEIN L29



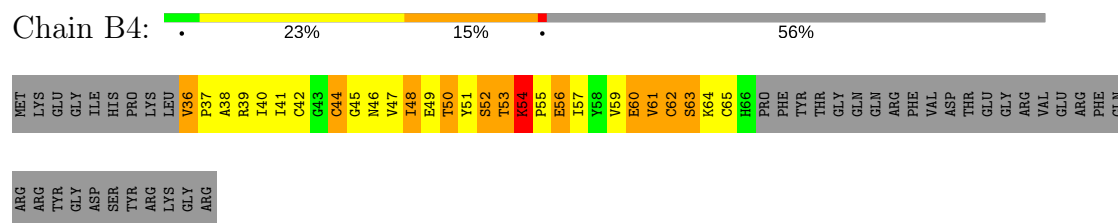
• Molecule 50: 50S RIBOSOMAL PROTEIN L30



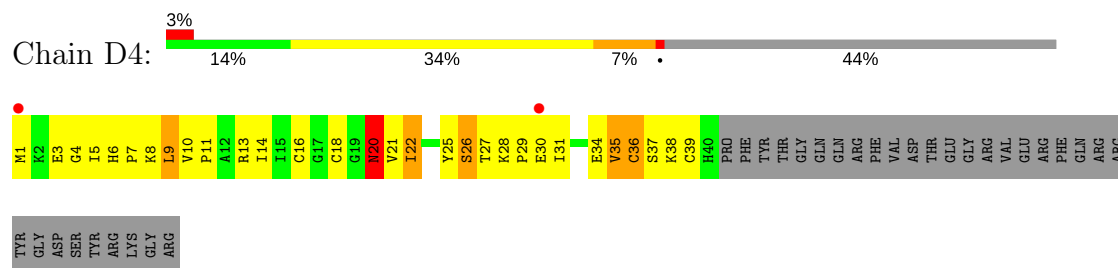
• Molecule 50: 50S RIBOSOMAL PROTEIN L30



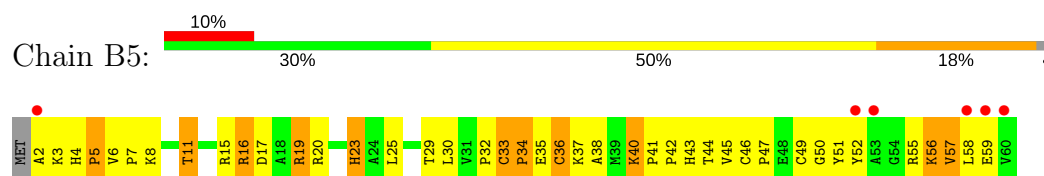
• Molecule 51: 50S RIBOSOMAL PROTEIN L31



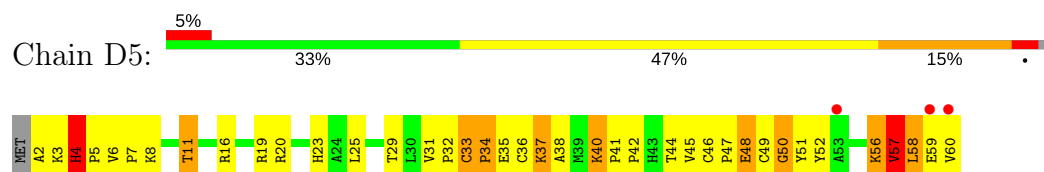
• Molecule 51: 50S RIBOSOMAL PROTEIN L31



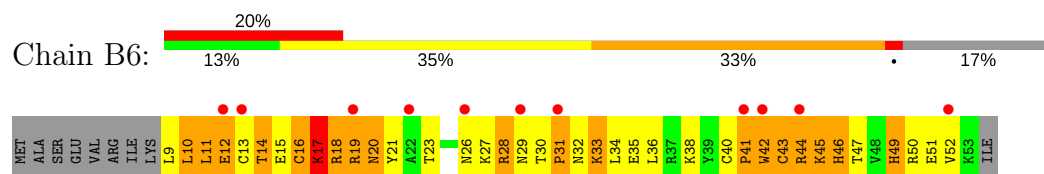
• Molecule 52: 50S RIBOSOMAL PROTEIN L32



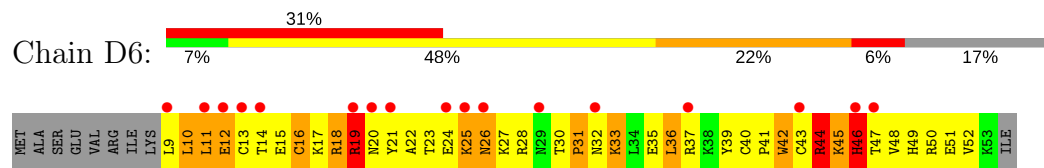
• Molecule 52: 50S RIBOSOMAL PROTEIN L32



• Molecule 53: 50S RIBOSOMAL PROTEIN L33

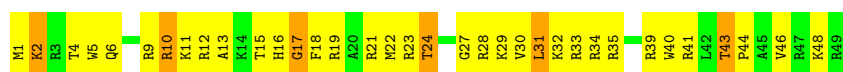


• Molecule 53: 50S RIBOSOMAL PROTEIN L33



• Molecule 54: 50S RIBOSOMAL PROTEIN L34

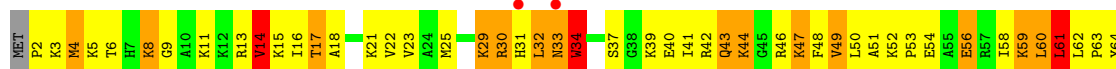




• Molecule 54: 50S RIBOSOMAL PROTEIN L34



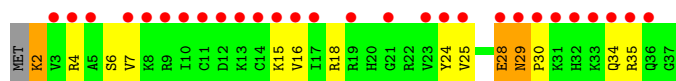
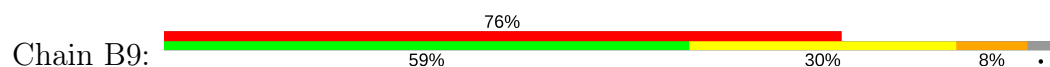
• Molecule 55: 50S RIBOSOMAL PROTEIN L35



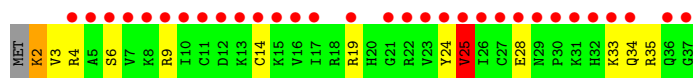
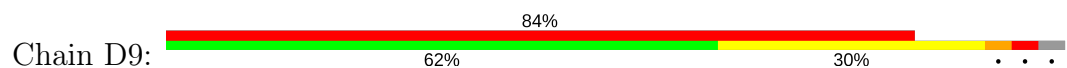
• Molecule 55: 50S RIBOSOMAL PROTEIN L35



• Molecule 56: 50S RIBOSOMAL PROTEIN L36



• Molecule 56: 50S RIBOSOMAL PROTEIN L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.46Å 447.34Å 622.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.07 – 3.52 35.07 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.07-3.52) 99.9 (35.07-3.52)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	0.46	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.47Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.210 , 0.249 0.214 , 0.253	Depositor DCC
R_{free} test set	32826 reflections (4.56%)	DCC
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	293977	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.28	0/36189	0.82	11/56484 (0.0%)
1	CA	0.29	0/36189	0.82	14/56484 (0.0%)
2	AB	0.59	0/1936	0.68	0/2611
2	CB	0.67	0/1936	0.77	0/2611
3	AC	0.70	0/1637	0.76	0/2207
3	CC	0.73	0/1637	0.82	0/2207
4	AD	0.69	0/1733	0.80	0/2318
4	CD	0.77	1/1733 (0.1%)	0.85	0/2318
5	AE	0.71	0/1163	0.88	0/1566
5	CE	0.74	0/1163	0.84	0/1566
6	AF	0.73	0/856	0.89	0/1154
6	CF	0.79	0/856	0.82	0/1154
7	AG	0.72	0/1276	0.79	0/1709
7	CG	0.71	0/1276	0.77	0/1709
8	AH	0.69	1/1136 (0.1%)	0.78	0/1527
8	CH	0.73	0/1136	0.80	1/1527 (0.1%)
9	AI	0.71	0/1029	0.80	0/1379
9	CI	0.70	0/1029	0.81	1/1379 (0.1%)
10	AJ	0.70	0/808	0.79	0/1087
10	CJ	0.65	0/808	0.77	0/1087
11	AK	0.67	0/900	0.81	0/1213
11	CK	0.70	0/900	0.82	0/1213
12	AL	0.86	0/987	0.95	0/1322
12	CL	0.92	1/987 (0.1%)	1.01	0/1322
13	AM	0.67	0/999	0.82	0/1338
13	CM	0.48	1/1008 (0.1%)	0.75	1/1347 (0.1%)
14	AN	0.73	0/501	0.83	1/664 (0.2%)
14	CN	0.77	0/501	0.95	0/664
15	AO	0.72	0/745	0.79	0/992
15	CO	0.71	0/745	0.81	0/992
16	AP	0.72	0/717	0.86	0/965
16	CP	0.79	0/717	0.84	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.69	0/837	0.79	0/1119
17	CQ	0.73	0/837	0.81	0/1119
18	AR	0.69	0/579	0.83	0/768
18	CR	0.76	0/579	0.98	0/768
19	AS	0.66	0/643	0.76	0/867
19	CS	0.80	1/643 (0.2%)	0.86	0/867
20	AT	0.73	0/765	0.77	0/1007
20	CT	0.61	0/765	0.63	0/1007
21	AU	0.73	0/213	0.83	0/279
21	CU	0.75	0/213	0.78	0/279
22	AV	1.13	5/1836 (0.3%)	1.33	13/2859 (0.5%)
22	CV	1.02	0/1835	1.20	13/2859 (0.5%)
23	AW	0.93	3/1809 (0.2%)	1.07	4/2819 (0.1%)
23	AY	1.07	1/408 (0.2%)	1.39	4/634 (0.6%)
23	CW	0.90	0/1809	1.01	0/2819
23	CY	1.15	0/408	1.42	4/634 (0.6%)
24	AX	1.10	1/285 (0.4%)	0.91	2/441 (0.5%)
24	CX	0.96	0/235	1.27	3/364 (0.8%)
25	BA	0.34	1/67788 (0.0%)	0.87	42/105819 (0.0%)
25	DA	0.35	0/68124	0.88	36/106343 (0.0%)
26	BB	0.26	0/2853	0.78	0/4451
26	DB	0.28	0/2853	0.80	0/4451
27	BC	0.65	1/1145 (0.1%)	0.67	0/1556
27	DC	0.24	0/1145	0.46	0/1556
28	BD	0.85	0/2155	0.95	1/2907 (0.0%)
28	DD	0.54	0/2155	0.74	0/2907
29	BE	0.75	0/1597	0.89	0/2155
29	DE	0.49	1/1597 (0.1%)	0.72	0/2155
30	BF	0.80	0/1659	0.87	1/2246 (0.0%)
30	DF	0.49	0/1620	0.76	1/2194 (0.0%)
31	BG	0.70	0/1499	0.78	1/2016 (0.0%)
31	DG	0.42	1/1499 (0.1%)	0.68	1/2016 (0.0%)
32	BH	0.63	0/1246	0.69	0/1684
32	DH	0.40	0/1315	0.79	1/1780 (0.1%)
33	BI	0.67	0/1146	0.81	0/1551
33	DI	0.36	0/1151	0.74	1/1558 (0.1%)
34	BN	0.76	0/1132	0.83	0/1527
34	DN	0.43	0/1132	0.69	0/1527
35	BO	0.76	0/943	0.87	0/1269
35	DO	0.46	0/943	0.68	0/1269
36	BP	0.40	1/1162 (0.1%)	0.78	2/1544 (0.1%)
36	DP	0.39	0/1162	0.76	1/1544 (0.1%)
37	BQ	0.75	0/1143	0.87	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DQ	0.48	0/1143	0.65	0/1527
38	BR	0.80	0/974	0.90	1/1302 (0.1%)
38	DR	0.57	1/982 (0.1%)	0.79	2/1312 (0.2%)
39	BS	0.77	0/779	0.90	0/1038
39	DS	0.40	0/892	0.81	1/1187 (0.1%)
40	BT	0.71	0/1156	0.90	1/1544 (0.1%)
40	DT	0.56	1/1156 (0.1%)	0.84	6/1544 (0.4%)
41	BU	0.81	0/982	0.91	1/1306 (0.1%)
41	DU	0.51	0/975	0.75	0/1297
42	BV	0.72	0/790	0.90	1/1057 (0.1%)
42	DV	0.53	1/790 (0.1%)	0.82	0/1057
43	BW	0.81	0/907	0.89	1/1216 (0.1%)
43	DW	0.48	0/907	0.69	1/1216 (0.1%)
44	BX	0.75	0/740	0.89	1/995 (0.1%)
44	DX	0.52	0/740	0.68	0/995
45	BY	0.74	0/789	0.95	2/1053 (0.2%)
45	DY	0.55	2/798 (0.3%)	0.78	0/1064
46	BZ	0.72	0/1436	0.74	1/1951 (0.1%)
46	DZ	0.35	0/1436	0.57	0/1951
47	B0	0.79	1/671 (0.1%)	0.84	0/892
47	D0	0.44	0/671	0.64	0/892
48	B1	0.87	0/739	0.94	0/983
48	D1	0.48	0/739	0.73	0/983
49	B2	0.72	0/600	0.83	0/793
49	D2	0.54	0/600	0.71	0/793
50	B3	0.73	0/473	0.83	0/636
50	D3	0.43	0/473	0.71	0/636
51	B4	0.72	0/229	0.76	0/311
51	D4	0.40	0/303	0.70	0/409
52	B5	0.82	1/473 (0.2%)	0.83	0/639
52	D5	0.44	0/473	0.65	0/639
53	B6	0.67	0/388	0.92	0/520
53	D6	0.30	0/388	0.58	0/520
54	B7	0.88	0/427	0.99	0/563
54	D7	0.54	0/427	0.75	1/563 (0.2%)
55	B8	0.76	0/516	0.91	0/681
55	D8	0.51	0/516	0.82	0/681
56	B9	0.64	0/302	0.59	0/397
56	D9	0.26	0/302	0.46	0/397
All	All	0.48	27/318178 (0.0%)	0.85	180/475682 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	BD	0	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1453	U	O3'-P	29.98	1.97	1.61
24	AX	14	A	O3'-P	-13.06	1.45	1.61
38	DR	12	ARG	C-N	11.33	1.60	1.34
40	DT	28	VAL	C-N	10.90	1.59	1.34
22	AV	1	C	OP3-P	-9.31	1.50	1.61

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1453	U	P-O3'-C3'	-10.66	106.91	119.70
38	DR	12	ARG	O-C-N	9.52	137.93	122.70
36	BP	1	MET	CG-SD-CE	9.44	115.30	100.20
40	DT	28	VAL	O-C-N	8.73	136.67	122.70
40	DT	28	VAL	CA-C-N	-7.49	100.72	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BD	222	ARG	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	32328	0	16317	795	0
1	CA	32328	0	16317	871	1
2	AB	1901	0	1951	245	0
2	CB	1901	0	1951	232	0
3	AC	1613	0	1677	197	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CC	1613	0	1677	148	0
4	AD	1703	0	1765	191	0
4	CD	1703	0	1764	174	0
5	AE	1147	0	1207	148	0
5	CE	1147	0	1207	159	0
6	AF	843	0	857	87	0
6	CF	843	0	857	63	0
7	AG	1257	0	1296	123	0
7	CG	1257	0	1296	102	0
8	AH	1116	0	1177	111	0
8	CH	1116	0	1177	111	0
9	AI	1010	0	1037	133	0
9	CI	1010	0	1037	144	0
10	AJ	795	0	840	127	0
10	CJ	795	0	840	135	0
11	AK	885	0	904	97	0
11	CK	885	0	904	109	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	123	0
13	AM	988	0	1059	151	0
13	CM	997	0	1072	164	0
14	AN	492	0	529	87	0
14	CN	492	0	531	69	0
15	AO	734	0	771	61	0
15	CO	734	0	771	51	0
16	AP	701	0	720	62	0
16	CP	701	0	720	101	0
17	AQ	824	0	891	68	0
17	CQ	824	0	891	85	0
18	AR	574	0	644	62	0
18	CR	574	0	644	68	0
19	AS	630	0	652	117	0
19	CS	630	0	652	106	0
20	AT	763	0	861	132	0
20	CT	763	0	861	166	0
21	AU	209	0	221	12	0
21	CU	209	0	221	22	0
22	AV	1644	0	836	110	0
22	CV	1643	0	836	143	0
23	AW	1619	0	822	122	0
23	AY	365	0	185	29	0
23	CW	1619	0	822	109	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	CY	365	0	185	37	0
24	AX	255	0	129	49	0
24	CX	210	0	109	23	0
25	BA	60527	0	30515	1623	1
25	DA	60827	0	30663	1373	0
26	BB	2551	0	1295	57	1
26	DB	2551	0	1295	55	0
27	BC	1142	0	865	78	0
27	DC	1142	0	865	70	0
28	BD	2105	0	2182	310	0
28	DD	2105	0	2182	277	0
29	BE	1564	0	1629	216	0
29	DE	1564	0	1629	206	0
30	BF	1624	0	1677	246	0
30	DF	1585	0	1632	188	0
31	BG	1474	0	1535	264	0
31	DG	1474	0	1535	209	0
32	BH	1223	0	1282	136	1
32	DH	1290	0	1364	238	0
33	BI	1131	0	1218	152	0
33	DI	1136	0	1223	229	0
34	BN	1105	0	1180	188	0
34	DN	1105	0	1180	140	0
35	BO	933	0	996	117	0
35	DO	933	0	996	90	0
36	BP	1145	0	1228	279	0
36	DP	1145	0	1228	283	3
37	BQ	1122	0	1179	129	0
37	DQ	1122	0	1179	123	0
38	BR	960	0	1021	146	0
38	DR	968	0	1033	109	0
39	BS	771	0	832	127	0
39	DS	882	0	943	149	0
40	BT	1142	0	1202	240	0
40	DT	1142	0	1202	269	0
41	BU	964	0	1022	160	0
41	DU	958	0	1014	198	0
42	BV	779	0	852	135	0
42	DV	779	0	852	150	3
43	BW	896	0	953	104	0
43	DW	896	0	953	89	0
44	BX	726	0	778	64	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DX	726	0	778	67	0
45	BY	776	0	870	172	0
45	DY	785	0	878	176	0
46	BZ	1404	0	1432	148	0
46	DZ	1404	0	1432	214	0
47	B0	662	0	688	60	0
47	D0	662	0	688	60	0
48	B1	732	0	808	78	0
48	D1	732	0	808	66	0
49	B2	598	0	653	64	0
49	D2	598	0	653	53	0
50	B3	468	0	523	40	3
50	D3	468	0	523	50	0
51	B4	226	0	229	39	0
51	D4	298	0	312	43	0
52	B5	459	0	480	50	0
52	D5	459	0	480	53	3
53	B6	381	0	391	51	0
53	D6	381	0	391	99	0
54	B7	419	0	467	35	0
54	D7	419	0	467	33	0
55	B8	508	0	576	115	0
55	D8	508	0	576	85	0
56	B9	299	0	326	13	0
56	D9	299	0	326	14	0
57	AA	110	0	0	0	0
57	AE	1	0	0	0	0
57	AV	5	0	0	0	0
57	AX	1	0	0	0	0
57	B5	1	0	0	0	0
57	B7	1	0	0	0	0
57	BA	323	0	0	0	0
57	BB	5	0	0	0	0
57	BD	2	0	0	0	0
57	BE	3	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BP	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	141	0	0	0	0
57	CE	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CV	5	0	0	0	0
57	CW	1	0	0	0	0
57	CX	1	0	0	0	0
57	CY	1	0	0	0	0
57	D0	2	0	0	0	0
57	D1	2	0	0	0	0
57	D2	1	0	0	0	0
57	D5	2	0	0	0	0
57	D8	1	0	0	0	0
57	DA	397	0	0	0	0
57	DB	5	0	0	0	0
57	DD	3	0	0	0	0
57	DE	2	0	0	0	0
57	DF	1	0	0	0	0
57	DP	3	0	0	0	0
57	DQ	1	0	0	0	0
57	DU	3	0	0	0	0
57	DW	1	0	0	0	0
57	DX	1	0	0	0	0
58	AA	42	0	45	3	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	1	0
59	CD	1	0	0	0	0
59	CN	1	0	0	3	0
All	All	293977	0	199058	16442	8

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 34.

The worst 5 of 16442 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)
39:BS:34:HIS:CE1	39:BS:54:LEU:HB2	1.32	1.58
42:DV:1:MET:SD	42:DV:1:MET:CG	2.01	1.47
40:BT:28:VAL:CG1	40:BT:46:GLU:HA	1.42	1.44
1:CA:748:C:H1'	1:CA:749:C:C5	1.53	1.44
34:BN:62:VAL:HG22	34:BN:66:LYS:CD	1.49	1.42

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:B3:1:MET:N	36:DP:122:PRO:CG[3_455]	1.46	0.74
50:B3:1:MET:N	36:DP:122:PRO:CD[3_455]	1.64	0.56
42:DV:50:PRO:CG	52:D5:58:LEU:O[4_445]	1.80	0.40
42:DV:48:GLY:O	52:D5:58:LEU:CD1[4_445]	1.84	0.36
25:BA:1593:G:O2'	26:BB:54:G:OP1[1_655]	2.09	0.11

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%)	159 (68%)	53 (23%)	21 (9%)	1	9
2	CB	233/256 (91%)	158 (68%)	45 (19%)	30 (13%)	0	5
3	AC	205/239 (86%)	129 (63%)	54 (26%)	22 (11%)	0	7
3	CC	205/239 (86%)	135 (66%)	52 (25%)	18 (9%)	1	10
4	AD	206/209 (99%)	142 (69%)	43 (21%)	21 (10%)	1	8
4	CD	206/209 (99%)	141 (68%)	47 (23%)	18 (9%)	1	10
5	AE	149/162 (92%)	117 (78%)	20 (13%)	12 (8%)	1	12
5	CE	149/162 (92%)	113 (76%)	22 (15%)	14 (9%)	1	9
6	AF	99/101 (98%)	63 (64%)	29 (29%)	7 (7%)	1	15
6	CF	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	23
7	AG	153/156 (98%)	116 (76%)	26 (17%)	11 (7%)	1	15
7	CG	153/156 (98%)	117 (76%)	29 (19%)	7 (5%)	3	26
8	AH	136/138 (99%)	96 (71%)	35 (26%)	5 (4%)	4	32
8	CH	136/138 (99%)	102 (75%)	28 (21%)	6 (4%)	3	27
9	AI	125/128 (98%)	84 (67%)	32 (26%)	9 (7%)	1	15
9	CI	125/128 (98%)	87 (70%)	23 (18%)	15 (12%)	0	6
10	AJ	97/105 (92%)	59 (61%)	31 (32%)	7 (7%)	1	15
10	CJ	97/105 (92%)	60 (62%)	25 (26%)	12 (12%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	117/129 (91%)	92 (79%)	19 (16%)	6 (5%)	2	23
11	CK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	11	49
12	AL	123/132 (93%)	78 (63%)	25 (20%)	20 (16%)	0	3
12	CL	123/132 (93%)	91 (74%)	20 (16%)	12 (10%)	1	9
13	AM	123/126 (98%)	82 (67%)	23 (19%)	18 (15%)	0	3
13	CM	123/126 (98%)	78 (63%)	22 (18%)	23 (19%)	0	2
14	AN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	6
14	CN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	0	6
15	AO	86/89 (97%)	65 (76%)	20 (23%)	1 (1%)	15	56
15	CO	86/89 (97%)	55 (64%)	25 (29%)	6 (7%)	1	15
16	AP	82/88 (93%)	53 (65%)	25 (30%)	4 (5%)	2	24
16	CP	82/88 (93%)	66 (80%)	13 (16%)	3 (4%)	4	32
17	AQ	98/105 (93%)	79 (81%)	13 (13%)	6 (6%)	2	19
17	CQ	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	2	19
18	AR	68/88 (77%)	49 (72%)	12 (18%)	7 (10%)	0	8
18	CR	68/88 (77%)	49 (72%)	11 (16%)	8 (12%)	0	6
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	12
19	CS	77/93 (83%)	47 (61%)	17 (22%)	13 (17%)	0	2
20	AT	97/106 (92%)	68 (70%)	22 (23%)	7 (7%)	1	15
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	0	5
21	AU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	10
27	BC	183/229 (80%)	85 (46%)	52 (28%)	46 (25%)	0	0
27	DC	183/229 (80%)	87 (48%)	45 (25%)	51 (28%)	0	0
28	BD	270/276 (98%)	200 (74%)	38 (14%)	32 (12%)	0	6
28	DD	270/276 (98%)	202 (75%)	44 (16%)	24 (9%)	1	10
29	BE	203/206 (98%)	145 (71%)	36 (18%)	22 (11%)	0	7
29	DE	203/206 (98%)	134 (66%)	36 (18%)	33 (16%)	0	3
30	BF	206/210 (98%)	142 (69%)	44 (21%)	20 (10%)	1	9
30	DF	200/210 (95%)	160 (80%)	29 (14%)	11 (6%)	2	21
31	BG	179/182 (98%)	121 (68%)	36 (20%)	22 (12%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DG	179/182 (98%)	124 (69%)	30 (17%)	25 (14%)	0	4
32	BH	158/180 (88%)	96 (61%)	37 (23%)	25 (16%)	0	3
32	DH	166/180 (92%)	96 (58%)	42 (25%)	28 (17%)	0	2
33	BI	143/148 (97%)	101 (71%)	26 (18%)	16 (11%)	0	6
33	DI	144/148 (97%)	78 (54%)	39 (27%)	27 (19%)	0	2
34	BN	137/140 (98%)	91 (66%)	24 (18%)	22 (16%)	0	3
34	DN	137/140 (98%)	86 (63%)	39 (28%)	12 (9%)	1	10
35	BO	120/122 (98%)	95 (79%)	17 (14%)	8 (7%)	1	17
35	DO	120/122 (98%)	97 (81%)	18 (15%)	5 (4%)	3	28
36	BP	148/150 (99%)	86 (58%)	26 (18%)	36 (24%)	0	1
36	DP	148/150 (99%)	86 (58%)	23 (16%)	39 (26%)	0	0
37	BQ	139/141 (99%)	104 (75%)	24 (17%)	11 (8%)	1	12
37	DQ	139/141 (99%)	109 (78%)	18 (13%)	12 (9%)	1	11
38	BR	115/118 (98%)	78 (68%)	25 (22%)	12 (10%)	0	7
38	DR	116/118 (98%)	86 (74%)	20 (17%)	10 (9%)	1	11
39	BS	97/112 (87%)	53 (55%)	16 (16%)	28 (29%)	0	0
39	DS	109/112 (97%)	71 (65%)	21 (19%)	17 (16%)	0	3
40	BT	136/146 (93%)	90 (66%)	28 (21%)	18 (13%)	0	4
40	DT	136/146 (93%)	95 (70%)	19 (14%)	22 (16%)	0	3
41	BU	115/118 (98%)	73 (64%)	30 (26%)	12 (10%)	0	7
41	DU	115/118 (98%)	75 (65%)	30 (26%)	10 (9%)	1	10
42	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0	3
42	DV	99/101 (98%)	80 (81%)	9 (9%)	10 (10%)	1	8
43	BW	111/113 (98%)	81 (73%)	22 (20%)	8 (7%)	1	15
43	DW	111/113 (98%)	82 (74%)	19 (17%)	10 (9%)	1	9
44	BX	91/96 (95%)	69 (76%)	16 (18%)	6 (7%)	1	17
44	DX	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	3	27
45	BY	99/110 (90%)	50 (50%)	22 (22%)	27 (27%)	0	0
45	DY	100/110 (91%)	64 (64%)	11 (11%)	25 (25%)	0	0
46	BZ	175/206 (85%)	114 (65%)	40 (23%)	21 (12%)	0	6
46	DZ	175/206 (85%)	101 (58%)	46 (26%)	28 (16%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B0	82/85 (96%)	64 (78%)	13 (16%)	5 (6%)	2	19
47	D0	82/85 (96%)	67 (82%)	8 (10%)	7 (8%)	1	11
48	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	0	6
48	D1	92/98 (94%)	69 (75%)	12 (13%)	11 (12%)	0	6
49	B2	69/72 (96%)	49 (71%)	15 (22%)	5 (7%)	1	15
49	D2	69/72 (96%)	57 (83%)	5 (7%)	7 (10%)	1	8
50	B3	58/60 (97%)	48 (83%)	3 (5%)	7 (12%)	0	6
50	D3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	11
51	B4	29/71 (41%)	17 (59%)	8 (28%)	4 (14%)	0	4
51	D4	38/71 (54%)	21 (55%)	12 (32%)	5 (13%)	0	4
52	B5	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	10
52	D5	57/60 (95%)	46 (81%)	5 (9%)	6 (10%)	0	7
53	B6	43/54 (80%)	17 (40%)	14 (33%)	12 (28%)	0	0
53	D6	43/54 (80%)	18 (42%)	15 (35%)	10 (23%)	0	1
54	B7	47/49 (96%)	38 (81%)	5 (11%)	4 (8%)	1	11
54	D7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	8	45
55	B8	62/65 (95%)	42 (68%)	14 (23%)	6 (10%)	1	9
55	D8	62/65 (95%)	41 (66%)	14 (23%)	7 (11%)	0	6
56	B9	34/37 (92%)	23 (68%)	10 (29%)	1 (3%)	5	37
56	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	5	37
All	All	11730/12586 (93%)	8097 (69%)	2283 (20%)	1350 (12%)	0	6

5 of 1350 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	195	ASP
2	AB	238	LEU
3	AC	18	TRP
3	AC	20	SER

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%)	161 (80%)	41 (20%)	1	8
2	CB	202/220 (92%)	155 (77%)	47 (23%)	1	5
3	AC	160/188 (85%)	127 (79%)	33 (21%)	1	7
3	CC	160/188 (85%)	130 (81%)	30 (19%)	2	10
4	AD	180/181 (99%)	149 (83%)	31 (17%)	2	14
4	CD	180/181 (99%)	151 (84%)	29 (16%)	3	16
5	AE	115/123 (94%)	97 (84%)	18 (16%)	3	18
5	CE	115/123 (94%)	87 (76%)	28 (24%)	1	4
6	AF	90/90 (100%)	76 (84%)	14 (16%)	3	18
6	CF	90/90 (100%)	79 (88%)	11 (12%)	6	27
7	AG	126/127 (99%)	103 (82%)	23 (18%)	2	11
7	CG	126/127 (99%)	106 (84%)	20 (16%)	3	17
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	19
8	CH	119/119 (100%)	87 (73%)	32 (27%)	0	3
9	AI	98/99 (99%)	77 (79%)	21 (21%)	1	6
9	CI	98/99 (99%)	72 (74%)	26 (26%)	0	3
10	AJ	88/92 (96%)	66 (75%)	22 (25%)	1	4
10	CJ	88/92 (96%)	66 (75%)	22 (25%)	1	4
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	12
11	CK	90/99 (91%)	72 (80%)	18 (20%)	1	8
12	AL	104/109 (95%)	85 (82%)	19 (18%)	2	11
12	CL	104/109 (95%)	84 (81%)	20 (19%)	1	9
13	AM	99/101 (98%)	82 (83%)	17 (17%)	2	14
13	CM	100/101 (99%)	83 (83%)	17 (17%)	2	14
14	AN	49/50 (98%)	37 (76%)	12 (24%)	1	4
14	CN	49/50 (98%)	38 (78%)	11 (22%)	1	5
15	AO	79/80 (99%)	64 (81%)	15 (19%)	2	9
15	CO	79/80 (99%)	66 (84%)	13 (16%)	2	15
16	AP	72/74 (97%)	58 (81%)	14 (19%)	1	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/74 (97%)	58 (81%)	14 (19%)	1	9
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	12	45
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	5	26
18	AR	61/77 (79%)	51 (84%)	10 (16%)	2	15
18	CR	61/77 (79%)	50 (82%)	11 (18%)	2	11
19	AS	69/80 (86%)	51 (74%)	18 (26%)	0	4
19	CS	69/80 (86%)	49 (71%)	20 (29%)	0	3
20	AT	76/82 (93%)	56 (74%)	20 (26%)	0	3
20	CT	76/82 (93%)	53 (70%)	23 (30%)	0	3
21	AU	19/22 (86%)	18 (95%)	1 (5%)	26	63
21	CU	19/22 (86%)	14 (74%)	5 (26%)	0	3
27	BC	61/181 (34%)	49 (80%)	12 (20%)	1	8
27	DC	61/181 (34%)	53 (87%)	8 (13%)	5	25
28	BD	213/218 (98%)	164 (77%)	49 (23%)	1	5
28	DD	213/218 (98%)	178 (84%)	35 (16%)	2	15
29	BE	165/166 (99%)	125 (76%)	40 (24%)	1	4
29	DE	165/166 (99%)	141 (86%)	24 (14%)	4	21
30	BF	165/166 (99%)	127 (77%)	38 (23%)	1	5
30	DF	161/166 (97%)	136 (84%)	25 (16%)	3	18
31	BG	155/156 (99%)	118 (76%)	37 (24%)	1	4
31	DG	155/156 (99%)	135 (87%)	20 (13%)	5	25
32	BH	132/148 (89%)	114 (86%)	18 (14%)	4	24
32	DH	140/148 (95%)	114 (81%)	26 (19%)	2	10
33	BI	122/124 (98%)	95 (78%)	27 (22%)	1	6
33	DI	122/124 (98%)	92 (75%)	30 (25%)	1	4
34	BN	117/119 (98%)	88 (75%)	29 (25%)	1	4
34	DN	117/119 (98%)	96 (82%)	21 (18%)	2	12
35	BO	100/100 (100%)	77 (77%)	23 (23%)	1	5
35	DO	100/100 (100%)	90 (90%)	10 (10%)	9	37
36	BP	116/116 (100%)	86 (74%)	30 (26%)	0	4
36	DP	116/116 (100%)	89 (77%)	27 (23%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	3
37	DQ	111/111 (100%)	92 (83%)	19 (17%)	2	14
38	BR	100/101 (99%)	68 (68%)	32 (32%)	0	2
38	DR	101/101 (100%)	86 (85%)	15 (15%)	3	20
39	BS	77/88 (88%)	56 (73%)	21 (27%)	0	3
39	DS	87/88 (99%)	75 (86%)	12 (14%)	4	23
40	BT	120/127 (94%)	90 (75%)	30 (25%)	1	4
40	DT	120/127 (94%)	91 (76%)	29 (24%)	1	4
41	BU	93/94 (99%)	70 (75%)	23 (25%)	1	4
41	DU	92/94 (98%)	80 (87%)	12 (13%)	5	25
42	BV	82/82 (100%)	55 (67%)	27 (33%)	0	2
42	DV	82/82 (100%)	64 (78%)	18 (22%)	1	6
43	BW	91/92 (99%)	69 (76%)	22 (24%)	1	4
43	DW	91/92 (99%)	83 (91%)	8 (9%)	12	44
44	BX	74/78 (95%)	58 (78%)	16 (22%)	1	6
44	DX	74/78 (95%)	61 (82%)	13 (18%)	2	12
45	BY	84/91 (92%)	67 (80%)	17 (20%)	1	8
45	DY	85/91 (93%)	66 (78%)	19 (22%)	1	5
46	BZ	155/179 (87%)	124 (80%)	31 (20%)	1	8
46	DZ	155/179 (87%)	136 (88%)	19 (12%)	5	27
47	B0	66/67 (98%)	57 (86%)	9 (14%)	4	24
47	D0	66/67 (98%)	57 (86%)	9 (14%)	4	24
48	B1	78/83 (94%)	61 (78%)	17 (22%)	1	6
48	D1	78/83 (94%)	61 (78%)	17 (22%)	1	6
49	B2	66/67 (98%)	53 (80%)	13 (20%)	1	8
49	D2	66/67 (98%)	53 (80%)	13 (20%)	1	8
50	B3	51/52 (98%)	40 (78%)	11 (22%)	1	6
50	D3	51/52 (98%)	49 (96%)	2 (4%)	37	72
51	B4	27/63 (43%)	17 (63%)	10 (37%)	0	1
51	D4	35/63 (56%)	31 (89%)	4 (11%)	7	31
52	B5	51/52 (98%)	42 (82%)	9 (18%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	D5	51/52 (98%)	43 (84%)	8 (16%)	3	18
53	B6	43/52 (83%)	31 (72%)	12 (28%)	0	3
53	D6	43/52 (83%)	33 (77%)	10 (23%)	1	5
54	B7	41/42 (98%)	35 (85%)	6 (15%)	3	21
54	D7	41/42 (98%)	37 (90%)	4 (10%)	9	38
55	B8	53/55 (96%)	38 (72%)	15 (28%)	0	3
55	D8	53/55 (96%)	41 (77%)	12 (23%)	1	5
56	B9	33/34 (97%)	29 (88%)	4 (12%)	6	28
56	D9	33/34 (97%)	29 (88%)	4 (12%)	6	28
All	All	9688/10428 (93%)	7777 (80%)	1911 (20%)	1	8

5 of 1911 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BX	43	VAL
2	CB	196	LEU
42	DV	91	TYR
45	BY	89	PHE
50	B3	53	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
2	CB	204	ASN
12	CL	9	GLN
48	D1	45	ASN
5	CE	78	HIS
9	CI	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	366 (24%)	0
1	CA	1503/1522 (98%)	359 (23%)	0
22	AV	76/77 (98%)	26 (34%)	0
22	CV	76/77 (98%)	30 (39%)	0
23	AW	75/76 (98%)	22 (29%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	AY	16/76 (21%)	5 (31%)	0
23	CW	75/76 (98%)	26 (34%)	0
23	CY	16/76 (21%)	8 (50%)	0
24	AX	11/24 (45%)	4 (36%)	0
24	CX	9/24 (37%)	4 (44%)	0
25	BA	2804/2915 (96%)	803 (28%)	0
25	DA	2818/2915 (96%)	804 (28%)	0
26	BB	118/122 (96%)	25 (21%)	0
26	DB	118/122 (96%)	24 (20%)	0
All	All	9218/9624 (95%)	2506 (27%)	0

5 of 2506 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	10	A
1	AA	13	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1039 ligands modelled in this entry, 1037 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	AA	7111	-	45,45,45	1.48	9 (20%)	60,67,67	1.22	5 (8%)
58	PAR	CA	1741	-	45,45,45	1.48	8 (17%)	60,67,67	1.22	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	AA	7111	-	-	0/18/94/94	0/4/4/4
58	PAR	CA	1741	-	-	0/18/94/94	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AA	7111	PAR	O51-C51	2.01	1.49	1.44
58	CA	1741	PAR	O43-C13	2.08	1.45	1.41
58	CA	1741	PAR	O54-C54	2.10	1.49	1.44
58	AA	7111	PAR	O54-C54	2.10	1.49	1.44
58	AA	7111	PAR	C64-C54	2.11	1.57	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	1741	PAR	C22-C12-C62	-2.04	107.11	110.14
58	AA	7111	PAR	C11-O51-C51	2.05	117.57	113.72
58	CA	1741	PAR	C11-O51-C51	2.13	117.72	113.72
58	AA	7111	PAR	O23-C23-C33	2.36	117.88	111.18
58	CA	1741	PAR	O23-C23-C33	2.37	117.93	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AA	7111	PAR	3	0
58	CA	1741	PAR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1453:U	O3'	1455:G	P	1.97

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.18	46 (3%) 49 41	31, 78, 168, 331	0
1	CA	1504/1522 (98%)	0.21	57 (3%) 41 34	24, 68, 165, 363	0
2	AB	235/256 (91%)	-0.08	4 (1%) 70 62	67, 121, 201, 279	0
2	CB	235/256 (91%)	-0.11	9 (3%) 41 34	44, 109, 202, 287	0
3	AC	207/239 (86%)	-0.13	1 (0%) 90 87	44, 104, 173, 240	0
3	CC	207/239 (86%)	-0.21	1 (0%) 90 87	38, 90, 151, 227	0
4	AD	208/209 (99%)	-0.29	3 (1%) 75 68	37, 89, 153, 217	0
4	CD	208/209 (99%)	-0.31	1 (0%) 90 87	30, 77, 129, 209	0
5	AE	151/162 (93%)	-0.24	2 (1%) 77 69	44, 87, 151, 240	0
5	CE	151/162 (93%)	-0.24	2 (1%) 77 69	22, 71, 131, 266	0
6	AF	101/101 (100%)	-0.20	0 100 100	29, 74, 120, 178	0
6	CF	101/101 (100%)	-0.29	0 100 100	25, 68, 134, 192	0
7	AG	155/156 (99%)	-0.15	7 (4%) 34 27	50, 93, 149, 256	0
7	CG	155/156 (99%)	-0.14	5 (3%) 48 40	32, 87, 151, 269	0
8	AH	138/138 (100%)	-0.29	0 100 100	41, 85, 129, 183	0
8	CH	138/138 (100%)	-0.34	1 (0%) 87 82	38, 75, 123, 181	0
9	AI	127/128 (99%)	0.02	3 (2%) 59 50	55, 113, 161, 319	0
9	CI	127/128 (99%)	-0.06	3 (2%) 59 50	45, 97, 170, 245	0
10	AJ	99/105 (94%)	0.29	4 (4%) 39 32	58, 124, 197, 302	0
10	CJ	99/105 (94%)	0.26	5 (5%) 29 23	38, 115, 191, 204	0
11	AK	119/129 (92%)	-0.12	4 (3%) 46 38	41, 77, 147, 249	0
11	CK	119/129 (92%)	-0.06	3 (2%) 58 48	29, 73, 139, 188	0
12	AL	125/132 (94%)	-0.15	3 (2%) 59 50	31, 64, 129, 300	0
12	CL	125/132 (94%)	-0.30	3 (2%) 59 50	9, 47, 127, 252	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.03	4 (3%) 48 40	29, 94, 148, 314	0
13	CM	125/126 (99%)	0.08	6 (4%) 31 25	39, 87, 174, 274	0
14	AN	60/61 (98%)	-0.06	1 (1%) 70 62	53, 92, 138, 207	0
14	CN	60/61 (98%)	-0.12	0 100 100	34, 71, 111, 194	0
15	AO	88/89 (98%)	-0.28	0 100 100	35, 80, 132, 142	0
15	CO	88/89 (98%)	-0.33	0 100 100	23, 69, 122, 147	0
16	AP	84/88 (95%)	-0.43	0 100 100	48, 74, 122, 182	0
16	CP	84/88 (95%)	-0.30	0 100 100	44, 76, 139, 200	0
17	AQ	100/105 (95%)	-0.22	0 100 100	50, 91, 141, 174	0
17	CQ	100/105 (95%)	-0.17	1 (1%) 82 75	38, 87, 144, 192	0
18	AR	70/88 (79%)	-0.21	3 (4%) 36 29	35, 77, 126, 183	0
18	CR	70/88 (79%)	-0.35	1 (1%) 75 68	36, 70, 122, 205	0
19	AS	79/93 (84%)	0.13	1 (1%) 77 69	46, 104, 202, 268	0
19	CS	79/93 (84%)	0.08	1 (1%) 77 69	27, 82, 153, 206	0
20	AT	99/106 (93%)	0.06	5 (5%) 29 23	42, 90, 173, 211	0
20	CT	99/106 (93%)	0.13	3 (3%) 51 42	40, 97, 192, 295	0
21	AU	25/27 (92%)	0.72	5 (20%) 1 1	36, 92, 165, 229	0
21	CU	25/27 (92%)	-0.03	0 100 100	50, 78, 107, 150	0
22	AV	77/77 (100%)	0.10	0 100 100	45, 82, 163, 276	0
22	CV	77/77 (100%)	0.19	3 (3%) 40 33	32, 72, 133, 253	0
23	AW	76/76 (100%)	1.27	17 (22%) 1 1	48, 175, 249, 317	0
23	AY	17/76 (22%)	0.41	0 100 100	64, 94, 167, 176	0
23	CW	76/76 (100%)	1.63	24 (31%) 0 0	34, 184, 271, 295	0
23	CY	17/76 (22%)	0.69	0 100 100	44, 75, 149, 186	0
24	AX	12/24 (50%)	0.73	1 (8%) 12 12	49, 74, 217, 234	0
24	CX	10/24 (41%)	0.56	1 (10%) 8 8	42, 58, 144, 213	0
25	BA	2810/2915 (96%)	0.18	115 (4%) 38 31	17, 58, 187, 375	0
25	DA	2824/2915 (96%)	0.11	106 (3%) 41 34	6, 42, 178, 370	0
26	BB	119/122 (97%)	0.17	1 (0%) 86 79	59, 94, 132, 182	0
26	DB	119/122 (97%)	0.12	2 (1%) 70 62	38, 68, 113, 174	0
27	BC	191/229 (83%)	1.88	75 (39%) 0 0	89, 200, 319, 378	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DC	191/229 (83%)	2.27	92 (48%) 0 0	64, 208, 290, 334	0
28	BD	272/276 (98%)	-0.40	0 100 100	9, 45, 89, 166	0
28	DD	272/276 (98%)	-0.49	0 100 100	3, 33, 80, 197	0
29	BE	205/206 (99%)	-0.23	5 (2%) 59 50	17, 66, 128, 289	0
29	DE	205/206 (99%)	-0.23	4 (1%) 65 57	11, 55, 160, 338	0
30	BF	208/210 (99%)	-0.35	4 (1%) 67 59	14, 64, 164, 286	0
30	DF	202/210 (96%)	-0.32	2 (0%) 82 75	5, 51, 127, 208	0
31	BG	181/182 (99%)	-0.19	6 (3%) 47 39	40, 95, 175, 268	0
31	DG	181/182 (99%)	-0.18	4 (2%) 62 53	25, 76, 143, 219	0
32	BH	160/180 (88%)	0.89	31 (19%) 1 1	85, 179, 331, 429	0
32	DH	168/180 (93%)	0.02	1 (0%) 89 84	29, 81, 155, 234	0
33	BI	145/148 (97%)	-0.13	5 (3%) 46 38	33, 96, 156, 185	0
33	DI	146/148 (98%)	-0.07	1 (0%) 87 82	15, 104, 166, 207	0
34	BN	139/140 (99%)	-0.30	1 (0%) 87 82	36, 79, 147, 305	0
34	DN	139/140 (99%)	-0.34	0 100 100	7, 61, 137, 185	0
35	BO	122/122 (100%)	-0.50	0 100 100	32, 65, 97, 124	0
35	DO	122/122 (100%)	-0.61	0 100 100	10, 41, 84, 112	0
36	BP	150/150 (100%)	0.30	5 (3%) 47 39	27, 87, 179, 250	0
36	DP	150/150 (100%)	0.07	3 (2%) 65 57	23, 71, 151, 264	0
37	BQ	141/141 (100%)	-0.23	3 (2%) 64 56	36, 74, 126, 421	0
37	DQ	141/141 (100%)	-0.40	0 100 100	12, 52, 108, 281	0
38	BR	117/118 (99%)	-0.42	0 100 100	21, 57, 107, 148	0
38	DR	118/118 (100%)	-0.48	0 100 100	15, 50, 92, 126	0
39	BS	99/112 (88%)	-0.17	1 (1%) 82 75	38, 100, 171, 347	0
39	DS	111/112 (99%)	-0.13	2 (1%) 69 60	33, 73, 147, 197	0
40	BT	138/146 (94%)	-0.04	6 (4%) 36 29	29, 80, 225, 351	0
40	DT	138/146 (94%)	-0.05	8 (5%) 24 20	20, 71, 212, 304	0
41	BU	117/118 (99%)	-0.40	1 (0%) 84 77	29, 64, 131, 281	0
41	DU	117/118 (99%)	-0.51	1 (0%) 84 77	17, 52, 114, 180	0
42	BV	101/101 (100%)	-0.28	0 100 100	23, 90, 149, 344	0
42	DV	101/101 (100%)	-0.12	1 (0%) 82 75	9, 70, 131, 303	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BW	113/113 (100%)	-0.23	2 (1%) 69 60	19, 49, 113, 319	0
43	DW	113/113 (100%)	-0.32	0 100 100	14, 42, 128, 204	0
44	BX	93/96 (96%)	-0.34	0 100 100	30, 63, 99, 149	0
44	DX	93/96 (96%)	-0.33	0 100 100	12, 42, 87, 144	0
45	BY	101/110 (91%)	0.88	20 (19%) 1 1	42, 92, 253, 363	0
45	DY	102/110 (92%)	0.06	3 (2%) 52 43	28, 82, 182, 226	0
46	BZ	177/206 (85%)	0.41	17 (9%) 9 9	45, 125, 202, 316	0
46	DZ	177/206 (85%)	0.53	18 (10%) 7 8	29, 116, 254, 322	0
47	B0	84/85 (98%)	-0.03	6 (7%) 17 14	31, 69, 170, 242	0
47	D0	84/85 (98%)	-0.08	6 (7%) 17 14	18, 52, 136, 286	0
48	B1	94/98 (95%)	-0.17	1 (1%) 80 73	17, 53, 113, 219	0
48	D1	94/98 (95%)	-0.31	0 100 100	7, 44, 122, 237	0
49	B2	71/72 (98%)	-0.24	2 (2%) 53 45	35, 77, 128, 195	0
49	D2	71/72 (98%)	-0.23	0 100 100	14, 54, 137, 267	0
50	B3	60/60 (100%)	-0.03	2 (3%) 47 39	35, 75, 125, 382	0
50	D3	60/60 (100%)	-0.25	1 (1%) 70 62	20, 65, 142, 236	0
51	B4	31/71 (43%)	-0.16	0 100 100	67, 121, 152, 204	0
51	D4	40/71 (56%)	0.07	2 (5%) 30 24	55, 116, 173, 266	0
52	B5	59/60 (98%)	0.15	6 (10%) 7 8	17, 72, 180, 340	0
52	D5	59/60 (98%)	0.16	3 (5%) 29 23	12, 63, 214, 299	0
53	B6	45/54 (83%)	1.21	11 (24%) 1 1	44, 138, 207, 343	0
53	D6	45/54 (83%)	1.83	17 (37%) 0 0	59, 139, 235, 285	0
54	B7	49/49 (100%)	-0.42	0 100 100	11, 41, 123, 149	0
54	D7	49/49 (100%)	-0.59	0 100 100	1, 23, 101, 204	0
55	B8	64/65 (98%)	-0.05	2 (3%) 49 41	20, 60, 129, 325	0
55	D8	64/65 (98%)	-0.38	0 100 100	12, 51, 115, 172	0
56	B9	36/37 (97%)	3.54	28 (77%) 0 0	120, 197, 269, 389	0
56	D9	36/37 (97%)	3.45	31 (86%) 0 0	115, 172, 217, 282	0
All	All	21184/22210 (95%)	0.06	908 (4%) 36 29	1, 71, 192, 429	0

The worst 5 of 908 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	2802	G	15.5
25	BA	2802	G	13.6
1	AA	81	U	13.4
1	AA	89	C	12.6
23	CW	20	U	12.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9364	1/1	0.98	0.82	64.10	1,1,1,1	0
57	MG	AA	7054	1/1	0.87	0.99	61.11	29,29,29,29	0
57	MG	DA	9435	1/1	0.92	0.98	50.74	30,30,30,30	0
57	MG	BA	3144	1/1	0.89	0.71	49.63	41,41,41,41	0
57	MG	DA	9523	1/1	0.97	0.77	37.34	9,9,9,9	0
57	MG	BA	3281	1/1	0.90	0.62	33.32	53,53,53,53	0
57	MG	DA	9312	1/1	0.98	0.67	32.69	4,4,4,4	0
57	MG	BA	3081	1/1	0.86	0.76	30.47	24,24,24,24	1
57	MG	DA	9549	1/1	0.94	0.74	27.03	44,44,44,44	0
57	MG	CA	1737	1/1	0.89	0.64	26.38	28,28,28,28	0
57	MG	DA	9514	1/1	0.94	0.82	25.36	19,19,19,19	0
57	MG	AA	7034	1/1	0.83	0.75	25.21	43,43,43,43	0
57	MG	AA	7090	1/1	0.89	1.01	24.68	69,69,69,69	0
57	MG	DA	9399	1/1	0.74	0.78	23.48	52,52,52,52	0
57	MG	DA	9655	1/1	0.37	0.92	23.17	35,35,35,35	0
57	MG	DA	9545	1/1	0.96	0.43	22.19	1,1,1,1	0
57	MG	DA	9369	1/1	0.99	0.59	22.14	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9392	1/1	0.98	0.70	21.90	12,12,12,12	0
57	MG	BA	3306	1/1	0.66	0.47	20.98	48,48,48,48	0
57	MG	CA	1631	1/1	0.95	0.89	20.74	22,22,22,22	0
57	MG	DA	9498	1/1	0.96	0.50	20.49	2,2,2,2	0
57	MG	DA	9530	1/1	0.84	0.85	20.42	41,41,41,41	0
57	MG	DA	9696	1/1	0.96	0.43	20.35	34,34,34,34	0
57	MG	DA	9436	1/1	0.94	0.54	20.19	3,3,3,3	0
57	MG	CA	1651	1/1	0.64	0.44	20.14	39,39,39,39	0
57	MG	CA	1640	1/1	0.94	0.84	20.01	49,49,49,49	0
57	MG	BA	3073	1/1	0.98	0.67	19.93	8,8,8,8	0
57	MG	BA	3297	1/1	0.79	0.93	19.92	46,46,46,46	0
57	MG	DA	9324	1/1	0.98	0.48	19.37	2,2,2,2	0
57	MG	BA	3045	1/1	0.92	0.59	19.35	2,2,2,2	0
57	MG	DA	9570	1/1	0.79	0.31	18.79	61,61,61,61	0
57	MG	DA	9618	1/1	0.92	0.79	18.75	28,28,28,28	1
57	MG	BA	3007	1/1	0.95	0.66	18.68	4,4,4,4	0
57	MG	BA	3264	1/1	0.82	0.65	18.53	36,36,36,36	0
57	MG	CA	1720	1/1	0.92	0.41	17.98	2,2,2,2	0
57	MG	CA	1699	1/1	0.61	0.39	17.78	45,45,45,45	1
57	MG	DA	9355	1/1	0.98	0.67	17.63	0,0,0,0	0
57	MG	BA	3028	1/1	0.67	0.55	17.54	44,44,44,44	0
57	MG	DA	9479	1/1	0.98	0.63	17.50	0,0,0,0	0
57	MG	DA	9359	1/1	0.98	0.38	17.15	0,0,0,0	0
57	MG	AA	7066	1/1	0.92	0.54	16.97	36,36,36,36	0
57	MG	DA	9473	1/1	0.94	0.64	16.93	0,0,0,0	0
57	MG	BA	3198	1/1	0.96	0.34	16.87	0,0,0,0	0
57	MG	DA	9398	1/1	0.99	0.44	16.86	0,0,0,0	0
57	MG	DA	9438	1/1	0.78	0.38	16.85	21,21,21,21	0
57	MG	DA	9319	1/1	0.90	0.80	16.75	30,30,30,30	0
57	MG	DA	9528	1/1	0.94	0.36	16.23	6,6,6,6	0
57	MG	BA	3309	1/1	0.95	0.79	16.18	25,25,25,25	0
57	MG	BA	3187	1/1	0.90	0.60	15.99	24,24,24,24	0
57	MG	DA	9521	1/1	0.96	0.57	15.28	2,2,2,2	0
57	MG	DA	9472	1/1	0.98	0.41	15.20	16,16,16,16	0
57	MG	BA	3220	1/1	0.85	0.77	15.07	56,56,56,56	0
57	MG	DA	9366	1/1	0.95	0.46	15.04	1,1,1,1	0
57	MG	BA	3065	1/1	0.97	0.66	14.95	2,2,2,2	0
57	MG	CA	1670	1/1	0.94	0.36	14.77	2,2,2,2	0
57	MG	BA	3227	1/1	0.58	0.71	14.67	40,40,40,40	0
57	MG	BA	3205	1/1	0.91	0.54	14.62	0,0,0,0	0
57	MG	BA	3044	1/1	0.93	0.58	14.61	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9516	1/1	0.96	0.46	14.46	1,1,1,1	0
57	MG	BA	3153	1/1	0.93	0.55	14.40	0,0,0,0	0
57	MG	DA	9383	1/1	0.81	0.41	14.38	18,18,18,18	0
57	MG	BA	3234	1/1	0.98	0.56	14.31	10,10,10,10	0
57	MG	BA	3116	1/1	0.85	0.27	14.30	38,38,38,38	0
57	MG	DA	9402	1/1	0.88	0.38	13.99	25,25,25,25	0
57	MG	DA	9459	1/1	0.95	0.52	13.92	3,3,3,3	0
57	MG	BA	3265	1/1	0.95	0.51	13.90	43,43,43,43	0
57	MG	BA	3276	1/1	0.88	0.56	13.70	31,31,31,31	0
57	MG	DA	9647	1/1	0.95	0.61	13.20	1,1,1,1	0
57	MG	BA	3210	1/1	0.98	0.74	13.18	11,11,11,11	0
57	MG	DA	9358	1/1	0.93	0.47	13.18	5,5,5,5	0
57	MG	DA	9445	1/1	0.84	0.44	13.15	22,22,22,22	0
57	MG	BA	3307	1/1	0.96	0.54	12.93	25,25,25,25	0
57	MG	AA	7026	1/1	0.89	0.40	12.83	30,30,30,30	0
57	MG	DA	9381	1/1	0.85	0.26	12.54	12,12,12,12	0
57	MG	BA	3193	1/1	0.86	0.44	12.46	12,12,12,12	0
57	MG	AA	7053	1/1	0.92	0.49	12.45	32,32,32,32	0
57	MG	DA	9305	1/1	0.96	0.46	12.38	0,0,0,0	0
57	MG	DA	9518	1/1	0.99	0.36	12.31	0,0,0,0	0
57	MG	BA	3203	1/1	0.67	0.45	12.24	37,37,37,37	0
57	MG	DA	9349	1/1	0.96	0.61	12.21	3,3,3,3	0
57	MG	BA	3008	1/1	0.98	0.46	12.18	2,2,2,2	0
57	MG	BA	3146	1/1	0.96	0.71	11.86	0,0,0,0	0
57	MG	BA	3120	1/1	0.68	0.65	11.73	24,24,24,24	0
57	MG	DA	9681	1/1	0.80	0.35	11.72	13,13,13,13	0
57	MG	DA	9370	1/1	0.89	0.39	11.36	0,0,0,0	0
57	MG	BA	3030	1/1	0.93	0.55	11.27	22,22,22,22	0
57	MG	DA	9529	1/1	0.96	0.29	11.26	0,0,0,0	0
57	MG	BA	3196	1/1	0.75	0.76	11.24	30,30,30,30	0
57	MG	BA	3041	1/1	0.96	0.50	11.23	7,7,7,7	0
57	MG	AA	7008	1/1	0.80	0.85	11.18	35,35,35,35	0
57	MG	AA	7094	1/1	0.93	0.54	11.17	8,8,8,8	0
57	MG	BA	3249	1/1	0.83	0.41	11.11	25,25,25,25	0
57	MG	AA	7018	1/1	0.92	0.56	10.96	27,27,27,27	0
57	MG	DA	9536	1/1	0.96	0.44	10.86	0,0,0,0	0
57	MG	AA	7075	1/1	0.82	0.49	10.84	53,53,53,53	0
57	MG	BA	3204	1/1	0.95	0.32	10.68	3,3,3,3	0
57	MG	DA	9425	1/1	0.90	0.41	10.66	37,37,37,37	0
57	MG	DA	9441	1/1	0.79	0.58	10.40	31,31,31,31	1
57	MG	CA	1645	1/1	0.98	0.34	10.23	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9673	1/1	0.87	0.42	10.15	8,8,8,8	0
57	MG	BA	3159	1/1	0.94	0.53	10.15	9,9,9,9	0
57	MG	DA	9587	1/1	0.97	0.28	10.11	2,2,2,2	0
57	MG	AA	7037	1/1	0.98	0.32	10.05	7,7,7,7	0
57	MG	BA	3248	1/1	0.63	0.70	10.01	49,49,49,49	0
57	MG	DA	9340	1/1	0.94	0.33	10.00	1,1,1,1	0
57	MG	BA	3020	1/1	0.97	0.48	9.92	1,1,1,1	0
57	MG	DA	9483	1/1	0.90	0.48	9.68	0,0,0,0	0
57	MG	CA	1626	1/1	0.95	0.55	9.33	28,28,28,28	0
57	MG	AA	7051	1/1	0.93	0.45	9.30	22,22,22,22	0
57	MG	AA	7059	1/1	0.93	0.51	9.26	96,96,96,96	0
57	MG	BA	3188	1/1	0.96	0.34	9.09	0,0,0,0	0
57	MG	DA	9360	1/1	0.98	0.36	8.87	7,7,7,7	0
57	MG	CA	1610	1/1	0.79	0.63	8.83	58,58,58,58	0
57	MG	DA	9653	1/1	0.94	0.41	8.75	5,5,5,5	0
57	MG	DD	7101	1/1	0.97	0.48	8.70	3,3,3,3	0
57	MG	DA	9430	1/1	0.98	0.39	8.67	0,0,0,0	0
57	MG	DA	9546	1/1	0.97	0.34	8.53	2,2,2,2	0
57	MG	BA	3051	1/1	0.98	0.41	8.51	6,6,6,6	0
57	MG	BA	3272	1/1	0.92	0.37	8.49	10,10,10,10	0
57	MG	BD	301	1/1	0.97	0.57	8.45	7,7,7,7	0
57	MG	DA	9356	1/1	0.95	0.32	8.42	1,1,1,1	0
57	MG	AA	7019	1/1	0.99	0.56	8.41	16,16,16,16	0
57	MG	CA	1653	1/1	0.89	0.53	8.37	29,29,29,29	0
57	MG	DA	9526	1/1	0.89	0.50	8.27	12,12,12,12	0
57	MG	AA	7071	1/1	0.70	0.53	8.14	38,38,38,38	0
57	MG	DA	9310	1/1	0.98	0.28	8.09	0,0,0,0	0
57	MG	CA	1629	1/1	0.96	0.34	7.83	37,37,37,37	0
57	MG	BA	3255	1/1	0.97	0.44	7.81	45,45,45,45	0
57	MG	DA	9491	1/1	0.96	0.45	7.77	11,11,11,11	0
57	MG	DA	9421	1/1	0.82	0.36	7.59	28,28,28,28	0
57	MG	CA	1652	1/1	0.97	0.60	7.54	6,6,6,6	0
57	MG	DA	9527	1/1	0.91	0.38	7.46	1,1,1,1	0
57	MG	CA	1710	1/1	0.88	0.50	7.41	19,19,19,19	0
57	MG	DA	9335	1/1	0.82	0.33	7.41	21,21,21,21	0
57	MG	B7	101	1/1	0.94	0.38	7.38	13,13,13,13	0
57	MG	DA	9515	1/1	0.97	0.32	7.20	10,10,10,10	0
57	MG	BA	3270	1/1	0.97	0.50	7.17	0,0,0,0	1
57	MG	BA	3182	1/1	0.98	0.57	7.11	2,2,2,2	0
57	MG	DA	9308	1/1	0.98	0.44	7.10	2,2,2,2	0
57	MG	BA	3027	1/1	0.98	0.34	7.10	4,4,4,4	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9544	1/1	0.84	0.41	7.08	10,10,10,10	0
57	MG	BA	3136	1/1	0.83	0.44	7.02	46,46,46,46	1
57	MG	BA	3243	1/1	0.97	0.45	6.96	5,5,5,5	0
57	MG	CA	1607	1/1	0.93	0.50	6.92	32,32,32,32	0
57	MG	DA	9489	1/1	0.92	0.41	6.86	37,37,37,37	0
57	MG	DA	9533	1/1	0.93	0.30	6.77	0,0,0,0	0
57	MG	BA	3046	1/1	0.98	0.64	6.76	1,1,1,1	0
57	MG	CA	1685	1/1	0.93	0.34	6.71	41,41,41,41	0
57	MG	CA	1674	1/1	0.72	0.40	6.44	89,89,89,89	0
57	MG	CA	1709	1/1	0.83	0.49	6.43	68,68,68,68	0
57	MG	DA	9621	1/1	0.97	0.59	6.35	0,0,0,0	1
57	MG	BA	3111	1/1	0.89	0.32	6.19	35,35,35,35	0
57	MG	DA	9512	1/1	0.93	0.43	6.16	2,2,2,2	0
57	MG	BA	3252	1/1	0.97	0.47	6.11	56,56,56,56	0
57	MG	DA	9581	1/1	0.94	0.42	6.10	4,4,4,4	0
57	MG	DA	9649	1/1	0.97	0.43	6.06	1,1,1,1	0
57	MG	DA	9458	1/1	0.79	0.41	6.05	22,22,22,22	0
57	MG	DA	9418	1/1	0.82	0.28	6.01	61,61,61,61	0
57	MG	BA	3160	1/1	0.93	0.39	5.99	22,22,22,22	0
57	MG	BA	3191	1/1	0.96	0.41	5.90	2,2,2,2	0
57	MG	BA	3004	1/1	0.96	0.59	5.89	1,1,1,1	0
57	MG	AA	7013	1/1	0.91	0.37	5.81	27,27,27,27	0
57	MG	DA	9590	1/1	0.97	0.49	5.76	1,1,1,1	0
57	MG	BA	3235	1/1	0.92	0.36	5.67	25,25,25,25	0
57	MG	DA	9584	1/1	0.98	0.35	5.67	0,0,0,0	0
57	MG	DA	9623	1/1	0.97	0.37	5.59	13,13,13,13	0
57	MG	BA	3142	1/1	0.98	0.44	5.58	10,10,10,10	0
57	MG	BA	3300	1/1	0.93	0.45	5.58	1,1,1,1	0
57	MG	DA	9553	1/1	0.95	0.35	5.54	20,20,20,20	0
57	MG	BA	3222	1/1	0.96	0.39	5.48	5,5,5,5	0
57	MG	DA	9417	1/1	0.93	0.29	5.48	20,20,20,20	0
57	MG	DA	9408	1/1	0.98	0.25	5.47	3,3,3,3	0
57	MG	DA	9409	1/1	0.90	0.31	5.45	4,4,4,4	0
57	MG	AA	7061	1/1	0.89	0.25	5.45	19,19,19,19	0
57	MG	DA	9503	1/1	0.88	0.31	5.37	66,66,66,66	0
57	MG	AA	7006	1/1	0.99	0.37	5.37	20,20,20,20	0
57	MG	DA	9347	1/1	0.82	0.29	5.19	22,22,22,22	0
57	MG	DA	9454	1/1	0.94	0.44	5.15	34,34,34,34	0
57	MG	DA	9428	1/1	0.94	0.41	5.09	15,15,15,15	0
57	MG	DA	9484	1/1	0.92	0.40	5.05	5,5,5,5	0
57	MG	BA	3119	1/1	0.73	0.32	5.03	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3098	1/1	0.93	0.29	4.97	36,36,36,36	0
57	MG	BA	3125	1/1	0.98	0.29	4.75	20,20,20,20	0
57	MG	BA	3241	1/1	0.94	0.45	4.71	4,4,4,4	0
57	MG	CA	1668	1/1	0.94	0.34	4.68	56,56,56,56	0
57	MG	BA	3084	1/1	0.99	0.50	4.66	1,1,1,1	0
57	MG	CA	1683	1/1	0.65	0.26	4.65	29,29,29,29	0
57	MG	AA	7064	1/1	0.94	0.28	4.53	50,50,50,50	0
57	MG	BA	3310	1/1	0.84	0.40	4.45	35,35,35,35	0
57	MG	DA	9404	1/1	0.97	0.31	4.43	12,12,12,12	0
57	MG	DA	9382	1/1	0.90	0.45	4.43	0,0,0,0	0
57	MG	BA	3069	1/1	0.95	0.32	4.41	5,5,5,5	0
57	MG	DA	9672	1/1	0.98	0.37	4.25	5,5,5,5	0
58	PAR	CA	1741	42/42	0.89	0.32	4.25	55,55,55,55	0
57	MG	DA	9614	1/1	0.84	0.25	4.21	12,12,12,12	0
57	MG	DA	9537	1/1	0.98	0.38	4.19	0,0,0,0	0
57	MG	DA	9517	1/1	0.97	0.29	4.18	0,0,0,0	0
57	MG	AA	7043	1/1	0.91	0.35	4.13	16,16,16,16	0
57	MG	BA	3086	1/1	0.96	0.23	4.01	1,1,1,1	0
57	MG	CA	1665	1/1	0.95	0.40	3.98	16,16,16,16	0
57	MG	BA	3047	1/1	0.97	0.29	3.92	0,0,0,0	0
57	MG	AA	7011	1/1	0.83	0.40	3.89	43,43,43,43	0
57	MG	AA	7044	1/1	0.95	0.35	3.79	21,21,21,21	0
57	MG	DA	9613	1/1	0.96	0.22	3.75	5,5,5,5	0
57	MG	AA	7110	1/1	0.96	0.33	3.72	31,31,31,31	0
57	MG	AA	7021	1/1	0.95	0.31	3.70	25,25,25,25	0
57	MG	AA	7091	1/1	0.96	0.23	3.62	22,22,22,22	0
57	MG	DA	9554	1/1	0.98	0.27	3.53	10,10,10,10	0
57	MG	BA	3201	1/1	0.91	0.32	3.49	6,6,6,6	0
57	MG	BA	3218	1/1	0.98	0.30	3.34	24,24,24,24	0
57	MG	DA	9365	1/1	0.90	0.28	3.25	1,1,1,1	0
57	MG	AA	7058	1/1	0.95	0.27	3.24	13,13,13,13	0
57	MG	CA	1667	1/1	0.96	0.28	3.22	12,12,12,12	0
57	MG	BA	3308	1/1	0.90	0.40	3.19	37,37,37,37	0
57	MG	BA	3066	1/1	0.87	0.27	3.15	48,48,48,48	0
57	MG	DA	9439	1/1	0.83	0.23	3.11	32,32,32,32	0
57	MG	BA	3251	1/1	0.86	0.22	3.06	34,34,34,34	0
57	MG	BA	3054	1/1	0.96	0.32	3.00	14,14,14,14	0
57	MG	CA	1705	1/1	0.93	0.27	2.98	15,15,15,15	0
57	MG	CA	1617	1/1	0.92	0.42	2.95	16,16,16,16	0
57	MG	DA	9497	1/1	0.95	0.36	2.93	29,29,29,29	0
57	MG	AA	7056	1/1	0.97	0.34	2.85	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9539	1/1	0.91	0.26	2.81	35,35,35,35	0
57	MG	DA	9675	1/1	0.96	0.29	2.79	11,11,11,11	0
57	MG	DQ	201	1/1	0.92	0.31	2.72	36,36,36,36	0
57	MG	BA	3145	1/1	0.92	0.28	2.72	22,22,22,22	0
57	MG	BA	3229	1/1	0.93	0.19	2.68	19,19,19,19	0
57	MG	DA	9461	1/1	0.83	0.34	2.60	13,13,13,13	0
57	MG	DA	9557	1/1	0.81	0.31	2.56	25,25,25,25	0
57	MG	DA	9460	1/1	0.89	0.25	2.52	40,40,40,40	0
57	MG	DA	9493	1/1	0.98	0.27	2.47	1,1,1,1	0
57	MG	DA	9600	1/1	0.79	0.34	2.47	55,55,55,55	0
57	MG	DA	9508	1/1	0.96	0.25	2.38	0,0,0,0	0
57	MG	BA	3225	1/1	0.94	0.29	2.35	2,2,2,2	0
57	MG	DA	9363	1/1	0.96	0.23	2.31	1,1,1,1	0
57	MG	BA	3090	1/1	0.94	0.41	2.28	2,2,2,2	0
57	MG	DA	9437	1/1	0.98	0.19	2.26	14,14,14,14	0
57	MG	DD	7103	1/1	0.97	0.42	2.24	0,0,0,0	0
57	MG	CA	1630	1/1	0.91	0.23	2.23	34,34,34,34	0
57	MG	CA	1727	1/1	0.92	0.34	2.22	27,27,27,27	0
57	MG	BA	3099	1/1	0.93	0.23	2.20	30,30,30,30	0
57	MG	DA	9597	1/1	0.93	0.23	2.15	12,12,12,12	0
57	MG	BE	302	1/1	0.89	0.28	2.12	74,74,74,74	0
57	MG	DA	9443	1/1	0.89	0.24	2.10	37,37,37,37	0
57	MG	BA	3279	1/1	0.98	0.25	2.10	31,31,31,31	0
57	MG	CA	1624	1/1	0.97	0.33	2.08	18,18,18,18	0
57	MG	AA	7016	1/1	0.94	0.32	2.07	45,45,45,45	0
57	MG	DA	9605	1/1	0.91	0.20	2.06	19,19,19,19	0
57	MG	BA	3238	1/1	0.98	0.33	2.03	9,9,9,9	0
58	PAR	AA	7111	42/42	0.92	0.26	2.03	58,58,58,58	0
57	MG	BA	3071	1/1	0.96	0.31	2.00	0,0,0,0	0
57	MG	BA	3149	1/1	0.47	0.34	1.96	27,27,27,27	0
57	MG	AA	7067	1/1	0.86	0.45	1.93	28,28,28,28	0
57	MG	BA	3178	1/1	0.95	0.24	1.93	28,28,28,28	0
57	MG	BA	3022	1/1	0.89	0.23	1.92	40,40,40,40	0
57	MG	BA	3058	1/1	0.91	0.33	1.87	1,1,1,1	0
57	MG	BU	201	1/1	0.94	0.30	1.82	170,170,170,170	1
57	MG	BA	3108	1/1	0.80	0.25	1.80	27,27,27,27	0
57	MG	DA	9431	1/1	0.83	0.30	1.80	12,12,12,12	0
57	MG	CA	1633	1/1	0.88	0.27	1.72	9,9,9,9	0
57	MG	BA	3076	1/1	0.70	0.22	1.70	18,18,18,18	0
57	MG	BA	3053	1/1	0.89	0.29	1.64	17,17,17,17	0
57	MG	BA	3185	1/1	0.94	0.26	1.60	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1666	1/1	0.77	0.36	1.58	66,66,66,66	0
57	MG	BA	3056	1/1	0.96	0.24	1.55	5,5,5,5	0
57	MG	CA	1719	1/1	0.95	0.35	1.40	10,10,10,10	0
57	MG	BA	3109	1/1	0.90	0.22	1.37	66,66,66,66	0
57	MG	DA	9561	1/1	0.93	0.27	1.34	10,10,10,10	0
57	MG	BA	3043	1/1	0.95	0.21	1.21	8,8,8,8	0
57	MG	BA	3085	1/1	0.97	0.26	1.18	29,29,29,29	0
57	MG	DA	9410	1/1	0.94	0.25	1.15	4,4,4,4	0
57	MG	DA	9388	1/1	0.72	0.18	1.06	28,28,28,28	0
57	MG	DA	9316	1/1	0.97	0.23	1.02	0,0,0,0	0
57	MG	BA	3208	1/1	0.92	0.22	1.01	8,8,8,8	0
57	MG	DB	202	1/1	0.83	0.22	1.01	28,28,28,28	0
57	MG	AA	7029	1/1	0.90	0.27	1.00	41,41,41,41	0
57	MG	DU	201	1/1	0.95	0.34	0.98	30,30,30,30	1
57	MG	DA	9433	1/1	0.93	0.22	0.95	13,13,13,13	0
57	MG	CA	1726	1/1	0.92	0.21	0.91	38,38,38,38	0
57	MG	BA	3061	1/1	0.92	0.25	0.87	32,32,32,32	0
57	MG	D0	101	1/1	0.95	0.45	0.85	27,27,27,27	0
57	MG	BA	3161	1/1	0.95	0.26	0.84	11,11,11,11	0
57	MG	DD	7102	1/1	0.94	0.28	0.82	0,0,0,0	0
57	MG	BA	3015	1/1	0.98	0.20	0.82	3,3,3,3	0
57	MG	DA	9506	1/1	0.96	0.23	0.77	0,0,0,0	0
57	MG	DA	9395	1/1	0.70	0.24	0.76	29,29,29,29	0
57	MG	DA	9482	1/1	0.93	0.21	0.66	12,12,12,12	0
57	MG	CA	1679	1/1	0.96	0.28	0.59	9,9,9,9	0
57	MG	DA	9339	1/1	0.90	0.20	0.55	13,13,13,13	0
57	MG	AA	7030	1/1	0.95	0.23	0.48	2,2,2,2	0
57	MG	BD	302	1/1	0.96	0.27	0.47	4,4,4,4	0
57	MG	BA	3031	1/1	0.88	0.23	0.47	44,44,44,44	0
57	MG	CA	1677	1/1	0.90	0.18	0.45	22,22,22,22	0
59	ZN	AD	301	1/1	0.93	0.32	0.41	41,41,41,41	0
57	MG	DP	203	1/1	0.90	0.24	0.40	11,11,11,11	0
57	MG	DA	9697	1/1	0.97	0.23	0.39	41,41,41,41	0
59	ZN	CD	301	1/1	0.98	0.32	0.39	44,44,44,44	0
57	MG	DA	9586	1/1	0.97	0.20	0.37	3,3,3,3	0
57	MG	BA	3115	1/1	0.84	0.24	0.32	33,33,33,33	0
57	MG	BA	3089	1/1	0.97	0.23	0.23	18,18,18,18	0
57	MG	DA	9487	1/1	0.93	0.25	0.19	71,71,71,71	0
57	MG	CA	1678	1/1	0.92	0.22	0.16	17,17,17,17	0
57	MG	CA	1671	1/1	0.89	0.23	0.15	38,38,38,38	0
57	MG	BA	3237	1/1	0.98	0.24	0.08	43,43,43,43	0
57	MG	BN	201	1/1	0.91	0.30	0.05	125,125,125,125	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3033	1/1	0.84	0.19	0.05	6,6,6,6	0
57	MG	DA	9302	1/1	0.87	0.18	-0.10	34,34,34,34	0
57	MG	DA	9547	1/1	0.96	0.21	-0.12	3,3,3,3	0
57	MG	DA	9499	1/1	0.96	0.15	-0.26	29,29,29,29	0
57	MG	CA	1656	1/1	0.91	0.21	-0.31	22,22,22,22	0
57	MG	BA	3293	1/1	0.95	0.21	-0.51	1,1,1,1	0
57	MG	CA	1605	1/1	0.87	0.21	-0.59	32,32,32,32	0
57	MG	CV	102	1/1	0.92	0.21	-0.60	1,1,1,1	0
59	ZN	CN	101	1/1	0.79	0.19	-0.61	171,171,171,171	0
57	MG	AA	7040	1/1	0.92	0.17	-0.64	36,36,36,36	0
57	MG	DA	9592	1/1	0.96	0.17	-0.64	36,36,36,36	0
57	MG	BA	3091	1/1	0.98	0.19	-0.66	0,0,0,0	0
57	MG	BA	3072	1/1	0.98	0.17	-0.68	25,25,25,25	0
57	MG	AA	7057	1/1	0.96	0.18	-0.68	44,44,44,44	0
57	MG	BA	3167	1/1	0.96	0.17	-0.70	30,30,30,30	0
57	MG	BA	3174	1/1	0.93	0.14	-0.73	31,31,31,31	0
57	MG	DA	9678	1/1	0.97	0.19	-0.75	33,33,33,33	0
57	MG	DA	9583	1/1	0.94	0.18	-0.76	1,1,1,1	0
57	MG	BF	301	1/1	0.86	0.22	-0.77	39,39,39,39	0
57	MG	BA	3224	1/1	0.99	0.17	-0.78	5,5,5,5	0
57	MG	BA	3256	1/1	0.92	0.15	-0.79	13,13,13,13	0
57	MG	DA	9629	1/1	0.93	0.15	-0.83	52,52,52,52	0
59	ZN	AN	101	1/1	0.97	0.10	-0.90	147,147,147,147	0
57	MG	BE	303	1/1	0.99	0.15	-1.02	1,1,1,1	0
57	MG	DA	9619	1/1	0.98	0.15	-1.08	0,0,0,0	0
57	MG	DA	9464	1/1	0.91	0.14	-1.13	25,25,25,25	0
57	MG	CA	1711	1/1	0.95	0.12	-1.19	26,26,26,26	0
57	MG	DU	202	1/1	0.98	0.14	-1.26	6,6,6,6	0
57	MG	DA	9504	1/1	0.84	0.15	-1.27	27,27,27,27	0
57	MG	AV	101	1/1	0.96	0.14	-1.35	2,2,2,2	0
57	MG	AA	7062	1/1	0.94	0.11	-1.37	31,31,31,31	0
57	MG	BP	201	1/1	0.75	0.20	-1.40	166,166,166,166	0
57	MG	DA	9558	1/1	0.99	0.15	-1.49	6,6,6,6	0
57	MG	BA	3092	1/1	0.96	0.17	-1.51	1,1,1,1	0
57	MG	DB	205	1/1	0.81	0.17	-1.52	6,6,6,6	1
57	MG	CA	1662	1/1	0.92	0.17	-1.56	29,29,29,29	0
57	MG	CA	1649	1/1	0.96	0.10	-1.63	33,33,33,33	0
57	MG	DA	9389	1/1	0.92	0.15	-1.73	11,11,11,11	0
57	MG	CA	1602	1/1	0.96	0.17	-1.77	14,14,14,14	0
57	MG	AA	7007	1/1	0.97	0.13	-1.77	1,1,1,1	0
57	MG	DA	9575	1/1	0.96	0.12	-1.79	35,35,35,35	0
57	MG	DA	9342	1/1	0.96	0.10	-1.80	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3029	1/1	0.93	0.15	-1.80	24,24,24,24	0
57	MG	DA	9373	1/1	0.88	0.16	-1.82	0,0,0,0	0
57	MG	BA	3038	1/1	0.83	0.16	-1.83	31,31,31,31	0
57	MG	AA	7087	1/1	0.96	0.13	-1.90	24,24,24,24	0
57	MG	BA	3059	1/1	0.86	0.16	-1.92	0,0,0,0	0
57	MG	BB	202	1/1	0.88	0.17	-1.95	62,62,62,62	0
57	MG	DA	9391	1/1	0.96	0.17	-1.99	1,1,1,1	0
57	MG	AA	7092	1/1	0.74	0.13	-2.07	37,37,37,37	0
57	MG	BA	3062	1/1	0.92	0.14	-2.20	27,27,27,27	0
57	MG	AA	7104	1/1	0.93	0.13	-2.22	33,33,33,33	0
57	MG	DU	203	1/1	0.99	0.14	-2.43	0,0,0,0	1
57	MG	DA	9377	1/1	0.85	0.19	-2.54	19,19,19,19	0
57	MG	CA	1632	1/1	0.93	0.15	-2.62	18,18,18,18	0
57	MG	BB	205	1/1	0.61	0.11	-3.12	19,19,19,19	1
57	MG	DA	9690	1/1	0.88	0.11	-3.15	5,5,5,5	0
57	MG	BA	3240	1/1	0.97	0.13	-3.20	21,21,21,21	0
57	MG	DF	301	1/1	0.87	0.14	-3.23	20,20,20,20	0
57	MG	DA	9446	1/1	0.93	0.08	-3.51	13,13,13,13	0
57	MG	CA	1622	1/1	0.97	0.09	-4.22	37,37,37,37	0
57	MG	BA	3068	1/1	0.95	0.11	-4.57	11,11,11,11	0
57	MG	AA	7042	1/1	0.97	0.08	-5.18	31,31,31,31	0
57	MG	AA	7095	1/1	0.95	0.08	-5.77	17,17,17,17	0
57	MG	AA	7003	1/1	0.97	0.10	-5.90	27,27,27,27	0
57	MG	DA	9481	1/1	0.98	0.09	-8.28	0,0,0,0	0
57	MG	AA	7027	1/1	0.79	0.41	-	28,28,28,28	0
57	MG	BA	3275	1/1	0.97	0.27	-	1,1,1,1	1
57	MG	DA	9563	1/1	0.76	0.26	-	3,3,3,3	0
57	MG	BA	3282	1/1	0.84	0.47	-	24,24,24,24	0
57	MG	BA	3133	1/1	0.92	0.21	-	43,43,43,43	0
57	MG	BA	3287	1/1	0.91	0.36	-	30,30,30,30	0
57	MG	AA	7068	1/1	0.97	0.09	-	34,34,34,34	0
57	MG	BA	3127	1/1	0.95	0.39	-	8,8,8,8	0
57	MG	BA	3312	1/1	0.95	0.30	-	45,45,45,45	0
57	MG	DA	9303	1/1	0.92	0.31	-	42,42,42,42	0
57	MG	DA	9434	1/1	0.70	0.45	-	4,4,4,4	0
57	MG	BA	3164	1/1	0.78	0.44	-	39,39,39,39	0
57	MG	AA	7085	1/1	0.94	0.17	-	15,15,15,15	0
57	MG	BA	3034	1/1	0.98	0.22	-	7,7,7,7	0
57	MG	DA	9354	1/1	0.99	0.49	-	2,2,2,2	0
57	MG	BA	3173	1/1	0.73	0.62	-	27,27,27,27	0
57	MG	DA	9593	1/1	0.84	0.62	-	25,25,25,25	0
57	MG	DA	9679	1/1	0.90	0.31	-	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7014	1/1	0.83	0.96	-	20,20,20,20	0
57	MG	BA	3050	1/1	0.91	0.58	-	4,4,4,4	0
57	MG	BA	3253	1/1	0.94	0.60	-	34,34,34,34	0
57	MG	BA	3039	1/1	0.69	0.39	-	30,30,30,30	0
57	MG	DA	9680	1/1	0.89	0.39	-	24,24,24,24	0
57	MG	D2	101	1/1	0.90	0.24	-	34,34,34,34	0
57	MG	DB	203	1/1	0.89	0.90	-	1,1,1,1	1
57	MG	AA	7035	1/1	0.98	0.11	-	42,42,42,42	0
57	MG	DA	9574	1/1	0.82	0.38	-	14,14,14,14	1
57	MG	CA	1707	1/1	0.96	0.83	-	1,1,1,1	1
57	MG	BA	3102	1/1	0.87	0.48	-	1,1,1,1	0
57	MG	CA	1614	1/1	0.81	1.22	-	38,38,38,38	0
57	MG	CA	1738	1/1	0.88	0.42	-	49,49,49,49	0
57	MG	BA	3088	1/1	0.92	0.39	-	43,43,43,43	0
57	MG	BA	3131	1/1	0.85	0.40	-	38,38,38,38	0
57	MG	DA	9486	1/1	0.92	0.34	-	21,21,21,21	0
57	MG	DA	9659	1/1	0.83	0.27	-	52,52,52,52	0
57	MG	BA	3126	1/1	0.49	0.61	-	44,44,44,44	0
57	MG	CA	1657	1/1	0.85	0.26	-	30,30,30,30	0
57	MG	BA	3083	1/1	0.95	0.32	-	27,27,27,27	1
57	MG	AV	104	1/1	0.81	0.41	-	16,16,16,16	0
57	MG	CA	1730	1/1	0.93	0.15	-	49,49,49,49	0
57	MG	BA	3319	1/1	0.87	0.29	-	27,27,27,27	0
57	MG	CA	1606	1/1	0.94	0.20	-	8,8,8,8	0
57	MG	CA	1643	1/1	0.92	0.58	-	40,40,40,40	1
57	MG	BA	3158	1/1	0.90	0.37	-	29,29,29,29	0
57	MG	DA	9329	1/1	0.72	0.50	-	21,21,21,21	0
57	MG	DA	9644	1/1	0.97	0.16	-	25,25,25,25	0
57	MG	DA	9551	1/1	0.90	0.21	-	48,48,48,48	0
57	MG	DA	9684	1/1	0.93	0.21	-	8,8,8,8	0
57	MG	BA	3245	1/1	0.71	0.72	-	45,45,45,45	0
57	MG	CA	1639	1/1	0.59	0.69	-	55,55,55,55	0
57	MG	CA	1619	1/1	0.98	0.52	-	11,11,11,11	0
57	MG	DA	9307	1/1	0.97	0.37	-	12,12,12,12	0
57	MG	DA	9452	1/1	0.95	0.37	-	10,10,10,10	0
57	MG	DA	9555	1/1	0.93	0.32	-	39,39,39,39	0
57	MG	DA	9683	1/1	0.92	0.52	-	19,19,19,19	0
57	MG	DA	9610	1/1	0.95	0.64	-	19,19,19,19	0
57	MG	BA	3005	1/1	0.95	0.26	-	22,22,22,22	0
57	MG	BA	3097	1/1	0.86	0.26	-	43,43,43,43	0
57	MG	AA	7096	1/1	0.80	0.55	-	31,31,31,31	0
57	MG	BA	3316	1/1	0.98	0.42	-	7,7,7,7	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3087	1/1	0.89	0.24	-	21,21,21,21	0
57	MG	CE	201	1/1	0.95	0.67	-	16,16,16,16	0
57	MG	CA	1713	1/1	0.73	0.54	-	31,31,31,31	0
57	MG	AX	101	1/1	0.80	0.28	-	43,43,43,43	0
57	MG	BA	3016	1/1	0.96	0.35	-	8,8,8,8	0
57	MG	CA	1694	1/1	0.79	0.73	-	51,51,51,51	0
57	MG	BA	3244	1/1	0.96	0.20	-	1,1,1,1	0
57	MG	AA	7041	1/1	0.91	0.58	-	20,20,20,20	0
57	MG	BA	3217	1/1	0.84	0.16	-	28,28,28,28	0
57	MG	BA	3166	1/1	0.93	0.63	-	40,40,40,40	0
57	MG	BA	3018	1/1	0.95	0.17	-	37,37,37,37	0
57	MG	DA	9652	1/1	0.93	0.23	-	44,44,44,44	0
57	MG	CA	1655	1/1	0.82	0.47	-	24,24,24,24	0
57	MG	BA	3219	1/1	0.96	0.18	-	19,19,19,19	0
57	MG	DA	9320	1/1	0.93	0.25	-	10,10,10,10	0
57	MG	BA	3055	1/1	0.97	0.21	-	11,11,11,11	0
57	MG	DA	9687	1/1	0.68	0.28	-	12,12,12,12	0
57	MG	DA	9313	1/1	0.93	0.22	-	18,18,18,18	0
57	MG	BA	3094	1/1	0.87	0.35	-	7,7,7,7	0
57	MG	CA	1611	1/1	0.97	0.55	-	0,0,0,0	0
57	MG	AA	7023	1/1	0.90	0.26	-	56,56,56,56	0
57	MG	BA	3154	1/1	0.92	0.43	-	17,17,17,17	0
57	MG	DA	9641	1/1	0.98	0.07	-	11,11,11,11	0
57	MG	DA	9416	1/1	0.71	0.33	-	38,38,38,38	0
57	MG	BA	3157	1/1	0.89	0.22	-	6,6,6,6	0
57	MG	CA	1697	1/1	0.91	0.18	-	49,49,49,49	0
57	MG	BA	3323	1/1	0.91	0.48	-	26,26,26,26	0
57	MG	DA	9560	1/1	0.96	0.26	-	4,4,4,4	0
57	MG	BA	3048	1/1	0.97	0.29	-	17,17,17,17	0
57	MG	CA	1708	1/1	0.70	0.67	-	34,34,34,34	0
57	MG	AA	7069	1/1	0.77	0.76	-	11,11,11,11	1
57	MG	AA	7052	1/1	0.91	0.19	-	74,74,74,74	0
57	MG	DA	9361	1/1	0.86	0.34	-	5,5,5,5	0
57	MG	CA	1701	1/1	0.91	0.51	-	1,1,1,1	0
57	MG	DA	9676	1/1	0.79	0.23	-	13,13,13,13	0
57	MG	DA	9585	1/1	0.91	0.18	-	18,18,18,18	0
57	MG	DA	9379	1/1	0.80	0.32	-	41,41,41,41	0
57	MG	DA	9405	1/1	0.71	0.29	-	5,5,5,5	0
57	MG	BA	3318	1/1	0.74	0.41	-	37,37,37,37	0
57	MG	DA	9631	1/1	0.92	0.32	-	21,21,21,21	0
57	MG	DA	9668	1/1	0.97	0.51	-	4,4,4,4	0
57	MG	CA	1693	1/1	0.96	0.39	-	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9566	1/1	0.97	0.29	-	18,18,18,18	0
57	MG	DA	9427	1/1	0.97	0.20	-	91,91,91,91	0
57	MG	CA	1654	1/1	0.90	0.35	-	31,31,31,31	0
57	MG	BA	3194	1/1	0.96	0.28	-	1,1,1,1	0
57	MG	DA	9674	1/1	0.74	0.81	-	17,17,17,17	0
57	MG	BA	3180	1/1	0.97	0.60	-	2,2,2,2	0
57	MG	CA	1716	1/1	0.72	0.46	-	26,26,26,26	0
57	MG	DA	9390	1/1	0.98	0.28	-	0,0,0,0	0
57	MG	DA	9559	1/1	0.71	0.55	-	58,58,58,58	0
57	MG	DA	9686	1/1	0.88	0.20	-	11,11,11,11	0
57	MG	BA	3283	1/1	0.93	0.20	-	22,22,22,22	0
57	MG	BA	3063	1/1	0.63	0.47	-	55,55,55,55	0
57	MG	DA	9346	1/1	0.98	0.30	-	0,0,0,0	0
57	MG	BA	3280	1/1	0.97	0.28	-	19,19,19,19	1
57	MG	DA	9625	1/1	0.93	0.36	-	26,26,26,26	0
57	MG	CA	1660	1/1	0.85	0.37	-	9,9,9,9	0
57	MG	BA	3215	1/1	0.97	0.41	-	1,1,1,1	0
57	MG	DA	9456	1/1	0.88	0.62	-	19,19,19,19	0
57	MG	DA	9304	1/1	0.94	0.45	-	27,27,27,27	0
57	MG	AA	7070	1/1	0.93	0.15	-	61,61,61,61	0
57	MG	DA	9376	1/1	0.89	0.27	-	26,26,26,26	0
57	MG	DA	9323	1/1	0.94	0.56	-	33,33,33,33	0
57	MG	BA	3231	1/1	0.82	0.38	-	90,90,90,90	0
57	MG	CA	1736	1/1	0.92	0.31	-	6,6,6,6	0
57	MG	CA	1689	1/1	0.90	0.25	-	15,15,15,15	0
57	MG	BA	3132	1/1	0.92	0.32	-	51,51,51,51	0
57	MG	DA	9371	1/1	0.87	0.38	-	29,29,29,29	0
57	MG	DA	9415	1/1	0.93	0.49	-	0,0,0,0	0
57	MG	BA	3269	1/1	0.90	0.50	-	20,20,20,20	0
57	MG	DA	9509	1/1	0.97	0.44	-	17,17,17,17	0
57	MG	DA	9401	1/1	0.96	0.55	-	21,21,21,21	1
57	MG	AV	102	1/1	0.84	0.43	-	25,25,25,25	1
57	MG	BA	3095	1/1	0.77	1.01	-	35,35,35,35	0
57	MG	DA	9396	1/1	0.90	0.24	-	26,26,26,26	0
57	MG	DA	9535	1/1	0.88	0.42	-	14,14,14,14	0
57	MG	DA	9689	1/1	0.93	0.80	-	25,25,25,25	0
57	MG	CA	1733	1/1	0.98	0.46	-	11,11,11,11	0
57	MG	DA	9397	1/1	0.90	0.41	-	25,25,25,25	1
57	MG	BA	3320	1/1	0.76	0.42	-	54,54,54,54	0
57	MG	BA	3295	1/1	0.79	0.37	-	27,27,27,27	0
57	MG	DA	9608	1/1	0.90	0.46	-	19,19,19,19	0
57	MG	DA	9467	1/1	0.74	0.40	-	53,53,53,53	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CV	103	1/1	0.77	0.33	-	43,43,43,43	1
57	MG	CA	1729	1/1	0.98	0.43	-	35,35,35,35	0
57	MG	BA	3321	1/1	0.83	0.35	-	35,35,35,35	0
57	MG	BA	3021	1/1	0.80	0.48	-	49,49,49,49	0
57	MG	BA	3003	1/1	0.77	0.33	-	33,33,33,33	0
57	MG	DA	9630	1/1	0.91	0.27	-	16,16,16,16	1
57	MG	DA	9496	1/1	0.92	0.35	-	26,26,26,26	0
57	MG	BA	3035	1/1	0.95	0.39	-	0,0,0,0	0
57	MG	BA	3143	1/1	0.91	0.20	-	7,7,7,7	0
57	MG	CA	1650	1/1	0.93	0.52	-	34,34,34,34	0
57	MG	DA	9429	1/1	0.60	0.97	-	51,51,51,51	0
57	MG	CA	1625	1/1	0.94	0.43	-	26,26,26,26	0
57	MG	BA	3301	1/1	0.79	0.27	-	20,20,20,20	0
57	MG	AA	7074	1/1	0.75	0.76	-	26,26,26,26	0
57	MG	BA	3103	1/1	0.80	0.19	-	31,31,31,31	0
57	MG	DA	9400	1/1	0.98	0.41	-	0,0,0,0	0
57	MG	CA	1608	1/1	0.91	0.39	-	16,16,16,16	0
57	MG	CA	1703	1/1	0.94	0.46	-	9,9,9,9	0
57	MG	DA	9318	1/1	0.96	0.40	-	2,2,2,2	0
57	MG	DA	9353	1/1	0.96	0.55	-	24,24,24,24	0
57	MG	BA	3200	1/1	0.97	0.51	-	5,5,5,5	0
57	MG	D1	101	1/1	0.66	0.60	-	55,55,55,55	0
57	MG	AA	7073	1/1	0.90	0.23	-	29,29,29,29	0
57	MG	BA	3074	1/1	0.71	0.63	-	34,34,34,34	0
57	MG	BA	3246	1/1	0.74	0.65	-	33,33,33,33	0
57	MG	BA	3278	1/1	0.71	0.40	-	22,22,22,22	0
57	MG	BA	3226	1/1	0.91	0.65	-	36,36,36,36	0
57	MG	CA	1635	1/1	0.88	0.24	-	4,4,4,4	0
57	MG	CA	1682	1/1	0.76	0.27	-	60,60,60,60	0
57	MG	DA	9519	1/1	0.93	0.43	-	1,1,1,1	0
57	MG	AA	7098	1/1	0.93	0.34	-	28,28,28,28	0
57	MG	AA	7080	1/1	0.72	0.43	-	8,8,8,8	1
57	MG	DA	9651	1/1	0.89	0.14	-	81,81,81,81	0
57	MG	CA	1628	1/1	0.79	0.22	-	9,9,9,9	0
57	MG	BA	3209	1/1	0.89	0.34	-	1,1,1,1	0
57	MG	BA	3114	1/1	0.95	0.32	-	41,41,41,41	0
57	MG	BA	3186	1/1	0.92	0.36	-	2,2,2,2	0
57	MG	CA	1680	1/1	0.88	0.15	-	49,49,49,49	0
57	MG	CA	1641	1/1	0.86	0.21	-	40,40,40,40	0
57	MG	BA	3117	1/1	0.79	0.68	-	11,11,11,11	1
57	MG	DA	9643	1/1	0.76	0.72	-	34,34,34,34	1
57	MG	DA	9471	1/1	0.94	0.56	-	50,50,50,50	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	D8	101	1/1	0.95	0.23	-	3,3,3,3	0
57	MG	DA	9341	1/1	0.92	0.56	-	11,11,11,11	0
57	MG	DA	9685	1/1	0.65	0.64	-	22,22,22,22	0
57	MG	CA	1658	1/1	0.68	0.34	-	44,44,44,44	0
57	MG	BA	3267	1/1	0.88	0.39	-	41,41,41,41	0
57	MG	BA	3019	1/1	0.87	0.35	-	44,44,44,44	0
57	MG	DA	9543	1/1	0.96	0.30	-	5,5,5,5	0
57	MG	BA	3129	1/1	0.94	0.53	-	1,1,1,1	0
57	MG	AA	7086	1/1	0.56	1.00	-	30,30,30,30	0
57	MG	BA	3314	1/1	0.93	0.04	-	42,42,42,42	0
57	MG	DA	9495	1/1	0.97	0.74	-	3,3,3,3	0
57	MG	BA	3213	1/1	0.94	0.40	-	8,8,8,8	0
57	MG	AA	7022	1/1	0.92	0.26	-	32,32,32,32	0
57	MG	BA	3260	1/1	0.98	0.57	-	8,8,8,8	0
57	MG	DA	9576	1/1	0.88	0.42	-	22,22,22,22	0
57	MG	CA	1725	1/1	0.84	0.29	-	29,29,29,29	0
57	MG	CA	1698	1/1	0.96	0.14	-	1,1,1,1	1
57	MG	CA	1715	1/1	0.96	0.51	-	12,12,12,12	0
57	MG	BA	3172	1/1	0.97	0.28	-	58,58,58,58	0
57	MG	BA	3296	1/1	0.94	0.38	-	0,0,0,0	1
57	MG	DA	9656	1/1	0.89	0.29	-	58,58,58,58	0
57	MG	DA	9606	1/1	0.93	0.94	-	4,4,4,4	0
57	MG	BA	3292	1/1	0.83	0.29	-	28,28,28,28	0
57	MG	AA	7063	1/1	0.90	0.25	-	31,31,31,31	0
57	MG	DA	9591	1/1	0.92	0.25	-	52,52,52,52	0
57	MG	AA	7032	1/1	0.94	0.47	-	24,24,24,24	0
57	MG	CX	101	1/1	0.82	0.23	-	25,25,25,25	0
57	MG	DA	9474	1/1	0.96	0.30	-	28,28,28,28	0
57	MG	CA	1742	1/1	0.96	0.45	-	10,10,10,10	0
57	MG	DA	9594	1/1	0.91	0.78	-	19,19,19,19	0
57	MG	DA	9494	1/1	0.95	0.38	-	39,39,39,39	0
57	MG	DA	9635	1/1	0.81	0.59	-	24,24,24,24	0
57	MG	DA	9351	1/1	0.89	0.45	-	2,2,2,2	0
57	MG	BA	3266	1/1	0.79	0.39	-	33,33,33,33	0
57	MG	BA	3100	1/1	0.97	0.15	-	21,21,21,21	0
57	MG	DA	9598	1/1	0.92	0.50	-	14,14,14,14	0
57	MG	DA	9599	1/1	0.96	0.34	-	20,20,20,20	0
57	MG	BA	3163	1/1	0.93	0.32	-	28,28,28,28	0
57	MG	BA	3257	1/1	0.77	0.31	-	21,21,21,21	0
57	MG	DA	9660	1/1	0.79	0.27	-	176,176,176,176	0
57	MG	BA	3012	1/1	0.90	0.60	-	29,29,29,29	0
57	MG	BA	3118	1/1	0.93	0.61	-	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9322	1/1	0.97	0.25	-	8,8,8,8	0
57	MG	AA	7082	1/1	0.80	0.27	-	24,24,24,24	0
57	MG	BA	3273	1/1	0.63	0.26	-	71,71,71,71	0
57	MG	BA	3112	1/1	0.91	0.57	-	14,14,14,14	0
57	MG	DA	9548	1/1	0.95	0.72	-	26,26,26,26	0
57	MG	DA	9321	1/1	0.94	0.50	-	35,35,35,35	0
57	MG	D1	102	1/1	0.95	0.18	-	9,9,9,9	1
57	MG	DA	9432	1/1	0.74	0.63	-	38,38,38,38	0
57	MG	DA	9449	1/1	0.98	0.43	-	0,0,0,0	0
57	MG	BA	3305	1/1	0.96	0.25	-	24,24,24,24	0
57	MG	CA	1691	1/1	0.71	0.70	-	91,91,91,91	0
57	MG	DA	9542	1/1	0.98	0.35	-	6,6,6,6	0
57	MG	BA	3170	1/1	0.94	0.79	-	1,1,1,1	0
57	MG	DA	9567	1/1	0.93	0.43	-	31,31,31,31	0
57	MG	BA	3184	1/1	0.92	0.95	-	22,22,22,22	0
57	MG	BA	3223	1/1	0.95	0.19	-	9,9,9,9	0
57	MG	DA	9588	1/1	0.92	0.14	-	16,16,16,16	0
57	MG	CA	1681	1/1	0.84	0.86	-	18,18,18,18	1
57	MG	CA	1704	1/1	0.67	0.99	-	28,28,28,28	0
57	MG	DA	9637	1/1	0.97	0.37	-	18,18,18,18	0
57	MG	DA	9457	1/1	0.90	0.59	-	13,13,13,13	0
57	MG	BA	3002	1/1	0.92	0.27	-	53,53,53,53	0
57	MG	BA	3148	1/1	0.94	0.38	-	16,16,16,16	0
57	MG	CA	1603	1/1	0.96	0.17	-	0,0,0,0	0
57	MG	DA	9615	1/1	0.77	0.70	-	45,45,45,45	0
57	MG	DA	9344	1/1	0.97	0.44	-	33,33,33,33	0
57	MG	DA	9552	1/1	0.79	0.53	-	58,58,58,58	0
57	MG	BA	3075	1/1	0.93	0.70	-	12,12,12,12	0
57	MG	CA	1637	1/1	0.72	0.35	-	57,57,57,57	0
57	MG	DA	9667	1/1	0.85	0.36	-	10,10,10,10	0
57	MG	AA	7097	1/1	0.71	0.46	-	20,20,20,20	0
57	MG	BA	3151	1/1	0.97	0.13	-	12,12,12,12	0
57	MG	BA	3040	1/1	0.97	0.27	-	0,0,0,0	0
57	MG	AA	7106	1/1	0.95	0.25	-	12,12,12,12	0
57	MG	DA	9669	1/1	0.94	0.23	-	5,5,5,5	0
57	MG	CA	1723	1/1	0.68	0.34	-	15,15,15,15	0
57	MG	BA	3290	1/1	0.76	0.76	-	19,19,19,19	1
57	MG	BO	201	1/1	0.87	0.42	-	45,45,45,45	0
57	MG	D0	102	1/1	0.93	0.54	-	15,15,15,15	0
57	MG	BA	3070	1/1	0.82	0.43	-	34,34,34,34	0
57	MG	DA	9387	1/1	0.96	0.76	-	1,1,1,1	0
57	MG	CA	1673	1/1	0.86	0.24	-	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9465	1/1	0.89	0.39	-	34,34,34,34	0
57	MG	BA	3288	1/1	0.98	0.14	-	18,18,18,18	0
57	MG	BA	3214	1/1	0.85	0.31	-	39,39,39,39	0
57	MG	CA	1627	1/1	0.95	0.62	-	22,22,22,22	0
57	MG	DA	9573	1/1	0.77	0.40	-	45,45,45,45	0
57	MG	BA	3171	1/1	0.91	0.45	-	7,7,7,7	0
57	MG	AA	7031	1/1	0.81	0.20	-	44,44,44,44	0
57	MG	BA	3134	1/1	0.84	0.48	-	21,21,21,21	0
57	MG	DA	9357	1/1	0.96	0.37	-	0,0,0,0	0
57	MG	DA	9478	1/1	0.96	0.40	-	13,13,13,13	0
57	MG	AA	7048	1/1	0.91	0.27	-	27,27,27,27	0
57	MG	BA	3299	1/1	0.99	0.47	-	10,10,10,10	0
57	MG	BA	3271	1/1	0.57	0.72	-	52,52,52,52	0
57	MG	CA	1717	1/1	0.89	0.30	-	11,11,11,11	0
57	MG	CA	1687	1/1	0.52	0.36	-	47,47,47,47	0
57	MG	BA	3285	1/1	0.85	1.73	-	32,32,32,32	1
57	MG	BA	3011	1/1	0.97	0.52	-	36,36,36,36	0
57	MG	DA	9492	1/1	0.96	0.11	-	76,76,76,76	0
57	MG	BA	3211	1/1	0.96	0.17	-	2,2,2,2	0
57	MG	BA	3274	1/1	0.80	0.26	-	8,8,8,8	1
57	MG	DA	9330	1/1	0.95	0.35	-	0,0,0,0	0
57	MG	AA	7033	1/1	0.97	0.18	-	35,35,35,35	0
57	MG	DA	9677	1/1	0.77	0.50	-	27,27,27,27	0
57	MG	BA	3026	1/1	0.78	0.50	-	29,29,29,29	0
57	MG	AA	7105	1/1	0.84	0.74	-	42,42,42,42	0
57	MG	DA	9520	1/1	0.97	0.47	-	2,2,2,2	0
57	MG	BB	203	1/1	0.66	0.70	-	16,16,16,16	1
57	MG	DA	9477	1/1	0.90	0.56	-	36,36,36,36	0
57	MG	AA	7089	1/1	0.94	0.24	-	21,21,21,21	0
57	MG	DA	9695	1/1	0.83	0.39	-	63,63,63,63	0
57	MG	BA	3032	1/1	0.93	0.19	-	18,18,18,18	0
57	MG	AA	7025	1/1	0.97	0.21	-	1,1,1,1	0
57	MG	DA	9315	1/1	0.97	0.10	-	26,26,26,26	0
57	MG	DA	9607	1/1	0.91	0.34	-	49,49,49,49	0
57	MG	BA	3189	1/1	0.96	0.46	-	1,1,1,1	0
57	MG	B5	101	1/1	0.92	0.30	-	2,2,2,2	0
57	MG	AA	7107	1/1	0.87	0.45	-	24,24,24,24	0
57	MG	DA	9534	1/1	0.97	0.51	-	1,1,1,1	0
57	MG	BA	3199	1/1	0.92	0.48	-	1,1,1,1	0
57	MG	DA	9577	1/1	0.90	0.91	-	102,102,102,102	0
57	MG	DA	9476	1/1	0.94	0.47	-	2,2,2,2	0
57	MG	DA	9617	1/1	0.97	0.29	-	11,11,11,11	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3138	1/1	0.95	0.32	-	15,15,15,15	0
57	MG	AV	103	1/1	0.89	0.26	-	7,7,7,7	1
57	MG	CA	1621	1/1	0.66	0.39	-	52,52,52,52	0
57	MG	BA	3277	1/1	0.65	0.56	-	2,2,2,2	1
57	MG	AA	7039	1/1	0.93	0.34	-	11,11,11,11	0
57	MG	DA	9350	1/1	0.44	0.18	-	48,48,48,48	1
57	MG	BA	3197	1/1	0.98	0.22	-	1,1,1,1	0
57	MG	DA	9424	1/1	0.95	0.52	-	5,5,5,5	0
57	MG	BA	3302	1/1	0.94	0.48	-	8,8,8,8	0
57	MG	AA	7102	1/1	0.95	0.48	-	38,38,38,38	0
57	MG	CV	104	1/1	0.92	0.28	-	22,22,22,22	1
57	MG	DA	9507	1/1	0.95	0.55	-	2,2,2,2	0
57	MG	CA	1732	1/1	0.88	0.53	-	27,27,27,27	0
57	MG	BA	3124	1/1	0.98	0.20	-	17,17,17,17	0
57	MG	DA	9326	1/1	0.95	0.24	-	1,1,1,1	0
57	MG	BA	3181	1/1	0.95	0.49	-	1,1,1,1	0
57	MG	AA	7093	1/1	0.93	0.34	-	30,30,30,30	0
57	MG	CA	1672	1/1	0.75	0.39	-	62,62,62,62	0
57	MG	BA	3049	1/1	0.92	0.51	-	30,30,30,30	0
57	MG	DA	9616	1/1	0.87	0.54	-	54,54,54,54	0
57	MG	BA	3023	1/1	0.94	0.28	-	4,4,4,4	0
57	MG	DA	9501	1/1	0.90	0.48	-	42,42,42,42	0
57	MG	BA	3232	1/1	0.93	0.18	-	44,44,44,44	0
57	MG	BA	3303	1/1	0.96	0.29	-	19,19,19,19	0
57	MG	DA	9485	1/1	0.95	0.41	-	15,15,15,15	0
57	MG	BA	3155	1/1	0.76	0.56	-	33,33,33,33	0
57	MG	CA	1731	1/1	0.70	0.15	-	30,30,30,30	0
57	MG	BA	3104	1/1	0.90	0.24	-	16,16,16,16	0
57	MG	BA	3152	1/1	0.96	0.32	-	18,18,18,18	0
57	MG	DA	9654	1/1	0.95	0.29	-	15,15,15,15	0
57	MG	BA	3284	1/1	0.86	0.33	-	21,21,21,21	0
57	MG	BA	3101	1/1	0.87	1.28	-	27,27,27,27	1
57	MG	AA	7109	1/1	0.95	0.36	-	33,33,33,33	0
57	MG	CA	1706	1/1	0.79	0.36	-	32,32,32,32	0
57	MG	BA	3230	1/1	0.93	0.61	-	22,22,22,22	0
57	MG	CA	1663	1/1	0.90	0.66	-	11,11,11,11	0
57	MG	DA	9306	1/1	0.93	0.35	-	4,4,4,4	0
57	MG	CA	1675	1/1	0.87	0.42	-	55,55,55,55	0
57	MG	DA	9657	1/1	0.69	0.32	-	29,29,29,29	0
57	MG	DA	9693	1/1	0.83	0.97	-	47,47,47,47	0
57	MG	DA	9531	1/1	0.94	0.37	-	1,1,1,1	0
57	MG	CA	1616	1/1	0.91	0.41	-	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7072	1/1	0.93	0.15	-	23,23,23,23	0
57	MG	DA	9571	1/1	0.97	0.44	-	0,0,0,0	0
57	MG	DA	9671	1/1	0.77	0.19	-	45,45,45,45	0
57	MG	DA	9627	1/1	0.98	0.30	-	0,0,0,0	1
57	MG	AA	7049	1/1	0.82	0.25	-	41,41,41,41	0
57	MG	BA	3014	1/1	0.93	0.25	-	33,33,33,33	0
57	MG	BA	3216	1/1	0.66	0.50	-	48,48,48,48	0
57	MG	CA	1601	1/1	0.88	0.39	-	39,39,39,39	0
57	MG	CA	1690	1/1	0.89	0.54	-	17,17,17,17	0
57	MG	BA	3258	1/1	0.87	1.06	-	19,19,19,19	0
57	MG	CA	1636	1/1	0.94	0.32	-	19,19,19,19	0
57	MG	DA	9568	1/1	0.89	0.37	-	3,3,3,3	0
57	MG	BA	3147	1/1	0.95	0.58	-	48,48,48,48	0
57	MG	BA	3042	1/1	0.94	0.67	-	8,8,8,8	0
57	MG	BA	3289	1/1	0.95	0.51	-	21,21,21,21	0
57	MG	CA	1721	1/1	0.94	0.20	-	1,1,1,1	0
57	MG	DA	9604	1/1	0.91	0.33	-	21,21,21,21	0
57	MG	BA	3141	1/1	0.91	0.26	-	18,18,18,18	0
57	MG	CA	1612	1/1	0.73	0.30	-	31,31,31,31	0
57	MG	DA	9311	1/1	0.95	0.47	-	29,29,29,29	0
57	MG	CA	1647	1/1	0.97	0.36	-	6,6,6,6	0
57	MG	BA	3082	1/1	0.78	0.32	-	23,23,23,23	0
57	MG	BA	3162	1/1	0.81	0.73	-	4,4,4,4	0
57	MG	DA	9336	1/1	0.79	0.33	-	52,52,52,52	0
57	MG	DA	9569	1/1	0.73	0.81	-	54,54,54,54	0
57	MG	CV	105	1/1	0.94	0.15	-	69,69,69,69	0
57	MG	DA	9692	1/1	0.83	0.42	-	30,30,30,30	0
57	MG	BB	204	1/1	0.95	0.30	-	23,23,23,23	0
57	MG	DA	9510	1/1	0.95	0.51	-	1,1,1,1	0
57	MG	BA	3202	1/1	0.89	0.50	-	7,7,7,7	0
57	MG	DE	302	1/1	0.90	0.22	-	35,35,35,35	0
57	MG	DE	301	1/1	0.95	0.32	-	1,1,1,1	0
57	MG	DA	9469	1/1	0.92	0.58	-	17,17,17,17	0
57	MG	DA	9579	1/1	0.82	0.67	-	38,38,38,38	0
57	MG	AA	7045	1/1	0.87	0.75	-	38,38,38,38	0
57	MG	AA	7065	1/1	0.76	0.38	-	23,23,23,23	0
57	MG	BA	3179	1/1	0.98	0.31	-	10,10,10,10	0
57	MG	CA	1642	1/1	0.78	0.37	-	54,54,54,54	0
57	MG	DA	9691	1/1	0.92	0.41	-	12,12,12,12	0
57	MG	DA	9648	1/1	0.74	0.31	-	34,34,34,34	0
57	MG	CA	1684	1/1	0.89	0.21	-	41,41,41,41	0
57	MG	DA	9375	1/1	0.95	0.54	-	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9622	1/1	0.70	0.56	-	36,36,36,36	0
57	MG	AA	7084	1/1	0.88	0.12	-	49,49,49,49	0
57	MG	DA	9448	1/1	0.94	0.38	-	18,18,18,18	0
57	MG	DA	9343	1/1	0.97	0.27	-	2,2,2,2	0
57	MG	DA	9620	1/1	0.79	0.41	-	26,26,26,26	0
57	MG	DA	9511	1/1	0.94	0.80	-	7,7,7,7	0
57	MG	DA	9378	1/1	0.78	0.34	-	29,29,29,29	0
57	MG	DA	9642	1/1	0.96	0.30	-	1,1,1,1	0
57	MG	DA	9661	1/1	0.57	0.38	-	57,57,57,57	0
57	MG	DA	9601	1/1	0.97	0.35	-	31,31,31,31	0
57	MG	DA	9420	1/1	0.91	0.52	-	6,6,6,6	0
57	MG	BA	3291	1/1	0.93	0.16	-	22,22,22,22	0
57	MG	DA	9386	1/1	0.98	0.47	-	2,2,2,2	0
57	MG	DA	9463	1/1	0.95	0.26	-	12,12,12,12	0
57	MG	DA	9480	1/1	0.90	0.28	-	30,30,30,30	0
57	MG	DA	9524	1/1	0.98	0.36	-	2,2,2,2	0
57	MG	AA	7004	1/1	0.88	0.29	-	30,30,30,30	0
57	MG	BA	3206	1/1	0.98	0.45	-	29,29,29,29	0
57	MG	DA	9406	1/1	0.98	0.19	-	32,32,32,32	0
57	MG	DA	9645	1/1	0.77	0.72	-	4,4,4,4	0
57	MG	CA	1648	1/1	0.96	0.42	-	23,23,23,23	0
57	MG	CA	1734	1/1	0.93	0.24	-	22,22,22,22	0
57	MG	DA	9500	1/1	0.97	0.22	-	1,1,1,1	0
57	MG	DP	202	1/1	0.87	0.26	-	173,173,173,173	0
57	MG	AA	7083	1/1	0.85	0.55	-	18,18,18,18	0
57	MG	DB	201	1/1	0.95	0.41	-	22,22,22,22	0
57	MG	BA	3268	1/1	0.84	0.33	-	13,13,13,13	1
57	MG	AA	7028	1/1	0.96	0.85	-	30,30,30,30	0
57	MG	DA	9367	1/1	0.89	0.41	-	35,35,35,35	0
57	MG	DA	9462	1/1	0.85	0.40	-	30,30,30,30	0
57	MG	BA	3036	1/1	0.47	0.19	-	78,78,78,78	1
57	MG	AA	7050	1/1	0.92	1.06	-	29,29,29,29	0
57	MG	BA	3052	1/1	0.70	0.45	-	40,40,40,40	0
57	MG	DA	9380	1/1	0.87	1.55	-	23,23,23,23	1
57	MG	BA	3192	1/1	0.93	0.38	-	2,2,2,2	0
57	MG	BA	3001	1/1	0.90	0.38	-	38,38,38,38	0
57	MG	BA	3123	1/1	0.92	0.20	-	14,14,14,14	0
57	MG	AA	7077	1/1	0.98	0.16	-	22,22,22,22	0
57	MG	DA	9532	1/1	0.94	0.43	-	9,9,9,9	0
57	MG	DA	9301	1/1	0.83	0.36	-	32,32,32,32	0
57	MG	AA	7024	1/1	0.95	0.50	-	27,27,27,27	0
57	MG	BA	3113	1/1	0.83	0.87	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9411	1/1	0.97	0.27	-	2,2,2,2	0
57	MG	DA	9646	1/1	0.96	0.22	-	31,31,31,31	0
57	MG	DA	9440	1/1	0.68	0.49	-	25,25,25,25	0
57	MG	AA	7002	1/1	0.64	0.48	-	35,35,35,35	0
57	MG	DA	9670	1/1	0.88	0.47	-	11,11,11,11	0
57	MG	DA	9314	1/1	0.93	0.32	-	1,1,1,1	0
57	MG	DA	9325	1/1	0.82	0.48	-	32,32,32,32	0
57	MG	CA	1735	1/1	0.87	0.47	-	29,29,29,29	0
57	MG	DA	9423	1/1	0.88	0.29	-	1,1,1,1	0
57	MG	BA	3169	1/1	0.95	0.51	-	3,3,3,3	0
57	MG	BA	3298	1/1	0.87	0.80	-	18,18,18,18	0
57	MG	AE	201	1/1	0.84	0.40	-	45,45,45,45	0
57	MG	DA	9550	1/1	0.73	0.44	-	55,55,55,55	0
57	MG	DA	9419	1/1	0.80	0.95	-	10,10,10,10	1
57	MG	BA	3122	1/1	0.55	0.30	-	13,13,13,13	0
57	MG	CA	1613	1/1	0.97	0.95	-	31,31,31,31	0
57	MG	DA	9468	1/1	0.88	0.72	-	2,2,2,2	1
57	MG	BA	3263	1/1	0.92	0.64	-	16,16,16,16	1
57	MG	BA	3259	1/1	0.99	0.32	-	18,18,18,18	0
57	MG	BA	3177	1/1	0.89	0.20	-	0,0,0,0	0
57	MG	BA	3107	1/1	0.78	0.45	-	36,36,36,36	0
57	MG	CA	1686	1/1	0.93	0.22	-	77,77,77,77	0
57	MG	BA	3137	1/1	0.86	0.61	-	1,1,1,1	1
57	MG	DA	9345	1/1	0.95	0.52	-	19,19,19,19	0
57	MG	DB	204	1/1	0.91	0.70	-	0,0,0,0	1
57	MG	AA	7079	1/1	0.90	0.41	-	35,35,35,35	0
57	MG	AA	7015	1/1	0.95	0.29	-	4,4,4,4	0
57	MG	DA	9538	1/1	0.96	0.46	-	1,1,1,1	0
57	MG	DA	9562	1/1	0.97	0.60	-	2,2,2,2	0
57	MG	BA	3080	1/1	0.97	0.56	-	0,0,0,0	0
57	MG	DA	9374	1/1	0.82	0.40	-	28,28,28,28	0
57	MG	AA	7012	1/1	0.89	0.78	-	12,12,12,12	0
57	MG	CA	1739	1/1	0.75	0.66	-	36,36,36,36	0
57	MG	DA	9407	1/1	0.91	0.22	-	2,2,2,2	0
57	MG	BA	3261	1/1	0.96	0.32	-	10,10,10,10	0
57	MG	DA	9662	1/1	0.93	0.54	-	2,2,2,2	0
57	MG	DW	201	1/1	0.84	0.47	-	27,27,27,27	0
57	MG	BA	3221	1/1	0.85	0.69	-	17,17,17,17	0
57	MG	BA	3006	1/1	0.91	0.33	-	38,38,38,38	0
57	MG	DA	9332	1/1	0.91	0.37	-	34,34,34,34	0
57	MG	CA	1700	1/1	0.91	0.28	-	20,20,20,20	0
57	MG	BA	3078	1/1	0.98	0.43	-	2,2,2,2	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7046	1/1	0.69	0.42	-	35,35,35,35	0
57	MG	BA	3195	1/1	0.85	0.32	-	3,3,3,3	0
57	MG	AA	7020	1/1	0.90	0.36	-	33,33,33,33	0
57	MG	DA	9475	1/1	0.86	0.65	-	26,26,26,26	0
57	MG	DA	9596	1/1	0.95	0.14	-	27,27,27,27	0
57	MG	CW	101	1/1	0.82	0.47	-	29,29,29,29	1
57	MG	DA	9513	1/1	0.90	0.48	-	22,22,22,22	0
57	MG	DA	9694	1/1	0.74	0.85	-	25,25,25,25	0
57	MG	CY	101	1/1	0.90	0.58	-	33,33,33,33	0
57	MG	CA	1618	1/1	0.94	0.22	-	31,31,31,31	0
57	MG	BA	3017	1/1	0.92	0.55	-	22,22,22,22	0
57	MG	BA	3313	1/1	0.69	0.26	-	42,42,42,42	0
57	MG	DA	9633	1/1	0.91	0.73	-	30,30,30,30	0
57	MG	DA	9666	1/1	0.91	0.36	-	7,7,7,7	0
57	MG	BA	3037	1/1	0.49	0.27	-	83,83,83,83	0
57	MG	D5	102	1/1	0.95	0.33	-	32,32,32,32	1
57	MG	DA	9611	1/1	0.89	0.46	-	8,8,8,8	0
57	MG	DA	9522	1/1	0.97	0.48	-	2,2,2,2	0
57	MG	BA	3079	1/1	0.94	0.34	-	29,29,29,29	1
57	MG	DA	9639	1/1	0.88	0.49	-	57,57,57,57	0
57	MG	DA	9455	1/1	0.95	0.45	-	0,0,0,0	0
57	MG	BA	3139	1/1	0.96	0.46	-	0,0,0,0	0
57	MG	DA	9578	1/1	0.81	0.43	-	44,44,44,44	0
57	MG	BA	3156	1/1	0.96	0.33	-	19,19,19,19	0
57	MG	AA	7038	1/1	0.96	0.64	-	10,10,10,10	0
57	MG	BA	3067	1/1	0.92	0.79	-	2,2,2,2	0
57	MG	DA	9609	1/1	0.87	0.45	-	2,2,2,2	0
57	MG	BA	3150	1/1	0.88	0.30	-	1,1,1,1	0
57	MG	BA	3247	1/1	0.97	0.80	-	55,55,55,55	0
57	MG	DA	9540	1/1	0.95	0.34	-	0,0,0,0	0
57	MG	BA	3207	1/1	0.97	0.38	-	1,1,1,1	0
57	MG	BA	3212	1/1	0.94	0.24	-	8,8,8,8	0
57	MG	BA	3236	1/1	0.91	0.56	-	17,17,17,17	0
57	MG	BA	3250	1/1	0.97	0.31	-	18,18,18,18	0
57	MG	DA	9580	1/1	0.95	0.46	-	0,0,0,0	0
57	MG	CA	1714	1/1	0.74	0.45	-	53,53,53,53	0
57	MG	BA	3025	1/1	0.96	0.16	-	37,37,37,37	0
57	MG	BA	3009	1/1	0.98	0.15	-	2,2,2,2	0
57	MG	CA	1718	1/1	0.98	0.27	-	27,27,27,27	0
57	MG	BA	3239	1/1	0.99	0.35	-	1,1,1,1	0
57	MG	DA	9502	1/1	0.87	0.41	-	3,3,3,3	0
57	MG	AA	7017	1/1	0.96	0.08	-	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CE	202	1/1	0.90	0.38	-	34,34,34,34	0
57	MG	BA	3228	1/1	0.95	0.61	-	13,13,13,13	0
57	MG	DA	9682	1/1	0.95	0.42	-	20,20,20,20	0
57	MG	BA	3190	1/1	0.97	0.47	-	8,8,8,8	0
57	MG	DA	9368	1/1	0.94	0.19	-	1,1,1,1	0
57	MG	CA	1695	1/1	0.93	0.37	-	15,15,15,15	0
57	MG	BA	3121	1/1	0.97	0.60	-	1,1,1,1	0
57	MG	DA	9470	1/1	0.93	0.27	-	0,0,0,0	0
57	MG	DA	9664	1/1	0.96	0.54	-	1,1,1,1	0
57	MG	DA	9556	1/1	0.90	0.23	-	23,23,23,23	0
57	MG	AA	7088	1/1	0.90	0.13	-	60,60,60,60	0
57	MG	DA	9688	1/1	0.83	0.40	-	78,78,78,78	0
57	MG	CA	1692	1/1	0.80	0.37	-	28,28,28,28	0
57	MG	DP	201	1/1	0.96	0.12	-	7,7,7,7	0
57	MG	AA	7009	1/1	0.91	0.27	-	18,18,18,18	0
57	MG	DA	9442	1/1	0.94	0.54	-	36,36,36,36	0
57	MG	CA	1615	1/1	0.98	0.27	-	0,0,0,0	0
57	MG	DA	9422	1/1	0.88	0.96	-	56,56,56,56	0
57	MG	AA	7036	1/1	0.88	0.38	-	42,42,42,42	0
57	MG	AA	7108	1/1	0.87	0.42	-	27,27,27,27	0
57	MG	CA	1634	1/1	0.92	0.32	-	43,43,43,43	0
57	MG	AA	7100	1/1	0.84	0.82	-	21,21,21,21	0
57	MG	CA	1609	1/1	0.67	0.42	-	30,30,30,30	0
57	MG	BA	3254	1/1	0.84	0.90	-	54,54,54,54	0
57	MG	AA	7103	1/1	0.94	0.53	-	13,13,13,13	0
57	MG	DA	9334	1/1	0.92	0.44	-	27,27,27,27	0
57	MG	DA	9603	1/1	0.78	0.88	-	33,33,33,33	0
57	MG	CA	1644	1/1	0.94	0.14	-	45,45,45,45	0
57	MG	AA	7001	1/1	0.93	0.28	-	26,26,26,26	0
57	MG	DA	9393	1/1	0.91	0.30	-	24,24,24,24	0
57	MG	BB	201	1/1	0.84	0.15	-	34,34,34,34	0
57	MG	DA	9348	1/1	0.81	0.72	-	47,47,47,47	0
57	MG	CA	1712	1/1	0.95	0.21	-	34,34,34,34	1
57	MG	CA	1646	1/1	0.91	0.42	-	7,7,7,7	0
57	MG	AA	7078	1/1	0.93	0.25	-	30,30,30,30	0
57	MG	CA	1638	1/1	0.83	0.42	-	24,24,24,24	0
57	MG	CA	1604	1/1	0.96	0.43	-	15,15,15,15	0
57	MG	BA	3183	1/1	0.91	0.65	-	56,56,56,56	0
57	MG	DA	9333	1/1	0.90	0.11	-	31,31,31,31	0
57	MG	DA	9663	1/1	0.91	0.59	-	7,7,7,7	0
57	MG	CA	1620	1/1	0.98	0.27	-	1,1,1,1	0
57	MG	D5	101	1/1	0.96	0.36	-	7,7,7,7	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3057	1/1	0.93	0.54	-	2,2,2,2	0
57	MG	DA	9412	1/1	0.75	0.34	-	27,27,27,27	0
57	MG	DA	9384	1/1	0.95	0.29	-	16,16,16,16	0
57	MG	BA	3013	1/1	0.99	0.30	-	16,16,16,16	0
57	MG	BA	3315	1/1	0.17	0.44	-	84,84,84,84	0
57	MG	CA	1676	1/1	0.83	0.60	-	88,88,88,88	0
57	MG	DA	9327	1/1	0.86	0.17	-	20,20,20,20	0
57	MG	DA	9394	1/1	0.92	0.47	-	16,16,16,16	0
57	MG	DA	9450	1/1	0.79	0.53	-	2,2,2,2	1
57	MG	DA	9403	1/1	0.94	0.26	-	0,0,0,0	0
57	MG	DA	9650	1/1	0.97	0.26	-	7,7,7,7	0
57	MG	DA	9372	1/1	0.88	0.43	-	8,8,8,8	0
57	MG	CA	1669	1/1	0.94	0.10	-	10,10,10,10	0
57	MG	DA	9309	1/1	0.98	0.35	-	6,6,6,6	0
57	MG	DA	9352	1/1	0.85	0.22	-	89,89,89,89	0
57	MG	DA	9612	1/1	0.96	0.70	-	1,1,1,1	1
57	MG	BA	3168	1/1	0.92	0.71	-	36,36,36,36	0
57	MG	BA	3294	1/1	0.87	0.50	-	15,15,15,15	1
57	MG	DA	9640	1/1	0.85	0.41	-	42,42,42,42	0
57	MG	AA	7101	1/1	0.88	0.65	-	22,22,22,22	0
57	MG	DA	9466	1/1	0.87	0.45	-	36,36,36,36	0
57	MG	DA	9602	1/1	0.77	0.52	-	37,37,37,37	0
57	MG	AA	7060	1/1	0.95	0.13	-	8,8,8,8	0
57	MG	AA	7047	1/1	0.86	0.35	-	41,41,41,41	0
57	MG	BA	3311	1/1	0.95	0.43	-	13,13,13,13	0
57	MG	DA	9632	1/1	0.94	0.48	-	12,12,12,12	1
57	MG	DA	9636	1/1	0.92	0.28	-	16,16,16,16	0
57	MG	DA	9634	1/1	0.85	0.41	-	44,44,44,44	0
57	MG	BA	3024	1/1	0.93	0.61	-	22,22,22,22	0
57	MG	DA	9490	1/1	0.88	0.22	-	39,39,39,39	0
57	MG	CA	1659	1/1	0.95	0.28	-	28,28,28,28	0
57	MG	BA	3304	1/1	0.94	0.43	-	13,13,13,13	0
57	MG	DA	9338	1/1	0.91	0.56	-	58,58,58,58	0
57	MG	DA	9624	1/1	0.70	0.23	-	18,18,18,18	1
57	MG	BA	3093	1/1	0.87	0.29	-	49,49,49,49	0
57	MG	AA	7099	1/1	0.97	0.36	-	6,6,6,6	0
57	MG	DX	101	1/1	0.86	0.35	-	6,6,6,6	0
57	MG	BA	3060	1/1	0.98	0.57	-	1,1,1,1	0
57	MG	CA	1661	1/1	0.86	0.35	-	50,50,50,50	0
57	MG	CV	101	1/1	0.87	0.37	-	12,12,12,12	1
57	MG	AA	7081	1/1	0.94	0.46	-	44,44,44,44	0
57	MG	DA	9595	1/1	0.68	0.58	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1623	1/1	0.97	0.27	-	19,19,19,19	0
57	MG	DA	9328	1/1	0.89	0.33	-	1,1,1,1	0
57	MG	DA	9628	1/1	0.75	0.28	-	35,35,35,35	1
57	MG	CA	1728	1/1	0.78	0.35	-	59,59,59,59	0
57	MG	DA	9337	1/1	0.86	0.61	-	45,45,45,45	0
57	MG	DA	9658	1/1	0.74	0.19	-	36,36,36,36	0
57	MG	BA	3077	1/1	0.86	0.43	-	21,21,21,21	0
57	MG	BA	3242	1/1	0.74	0.59	-	44,44,44,44	0
57	MG	AV	105	1/1	0.90	0.34	-	54,54,54,54	0
57	MG	DA	9331	1/1	0.80	0.21	-	8,8,8,8	0
57	MG	DA	9444	1/1	0.88	0.51	-	42,42,42,42	0
57	MG	BA	3322	1/1	0.81	0.35	-	54,54,54,54	0
57	MG	AA	7055	1/1	0.68	0.46	-	29,29,29,29	0
57	MG	DA	9414	1/1	0.97	0.81	-	16,16,16,16	0
57	MG	AA	7010	1/1	0.73	0.26	-	30,30,30,30	0
57	MG	BA	3286	1/1	0.78	0.25	-	22,22,22,22	0
57	MG	BA	3010	1/1	0.96	0.89	-	28,28,28,28	0
57	MG	DA	9385	1/1	0.83	0.24	-	5,5,5,5	0
57	MG	AA	7076	1/1	0.66	0.57	-	60,60,60,60	0
57	MG	AA	7005	1/1	0.91	0.28	-	45,45,45,45	0
57	MG	DA	9317	1/1	0.90	0.26	-	18,18,18,18	0
57	MG	DA	9572	1/1	0.83	0.42	-	4,4,4,4	0
57	MG	CA	1722	1/1	0.79	0.34	-	27,27,27,27	0
57	MG	BA	3140	1/1	0.92	0.24	-	40,40,40,40	0
57	MG	DA	9488	1/1	0.98	0.56	-	0,0,0,0	0
57	MG	DA	9451	1/1	0.92	0.56	-	35,35,35,35	0
57	MG	BA	3175	1/1	0.96	0.28	-	4,4,4,4	0
57	MG	DA	9541	1/1	0.89	0.39	-	2,2,2,2	0
57	MG	BA	3176	1/1	0.98	0.33	-	0,0,0,0	0
57	MG	BA	3105	1/1	0.98	0.69	-	26,26,26,26	0
57	MG	DA	9426	1/1	0.95	0.43	-	9,9,9,9	1
57	MG	BA	3128	1/1	0.94	0.26	-	57,57,57,57	0
57	MG	DA	9626	1/1	0.58	0.19	-	8,8,8,8	1
57	MG	DA	9362	1/1	0.98	0.34	-	5,5,5,5	0
57	MG	CA	1740	1/1	0.87	0.61	-	48,48,48,48	0
57	MG	DA	9564	1/1	0.98	0.58	-	17,17,17,17	0
57	MG	DA	9525	1/1	0.93	0.30	-	4,4,4,4	0
57	MG	BA	3262	1/1	0.71	0.62	-	39,39,39,39	0
57	MG	DA	9413	1/1	0.91	0.38	-	3,3,3,3	0
57	MG	BA	3064	1/1	0.95	0.25	-	29,29,29,29	1
57	MG	DA	9665	1/1	0.70	0.99	-	9,9,9,9	0
57	MG	CA	1724	1/1	0.95	0.44	-	5,5,5,5	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9453	1/1	0.91	0.44	-	4,4,4,4	1
57	MG	DA	9565	1/1	0.86	0.38	-	11,11,11,11	0
57	MG	DA	9589	1/1	0.88	0.18	-	32,32,32,32	0
57	MG	CA	1688	1/1	0.90	0.15	-	16,16,16,16	0
57	MG	BA	3165	1/1	0.97	0.57	-	0,0,0,0	0
57	MG	BA	3130	1/1	0.86	0.19	-	3,3,3,3	0
57	MG	BA	3096	1/1	0.94	0.42	-	12,12,12,12	0
57	MG	DA	9582	1/1	0.94	0.88	-	21,21,21,21	0
57	MG	CA	1664	1/1	0.93	0.45	-	24,24,24,24	0
57	MG	BA	3233	1/1	0.91	0.45	-	19,19,19,19	0
57	MG	BA	3317	1/1	0.79	0.73	-	21,21,21,21	0
57	MG	DA	9505	1/1	0.95	0.29	-	0,0,0,0	0
57	MG	BE	301	1/1	0.82	0.24	-	0,0,0,0	0
57	MG	CA	1702	1/1	0.61	0.14	-	49,49,49,49	0
57	MG	BA	3110	1/1	0.73	0.59	-	23,23,23,23	1
57	MG	DA	9638	1/1	0.95	0.27	-	8,8,8,8	1
57	MG	BA	3106	1/1	0.83	0.49	-	34,34,34,34	0
57	MG	CA	1696	1/1	0.95	0.34	-	49,49,49,49	0
57	MG	DA	9447	1/1	0.95	0.23	-	68,68,68,68	0
57	MG	BA	3135	1/1	0.93	0.58	-	43,43,43,43	0

6.5 Other polymers

There are no such residues in this entry.