



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 12:43 pm BST

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

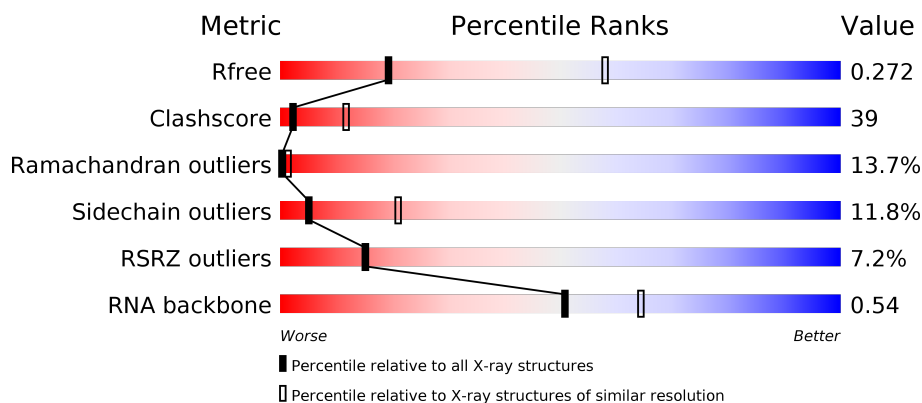
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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>27%</div> <div>61%</div> <div>10%</div> <div>..</div> </div>
1	CA	1522	<div> <div>26%</div> <div>61%</div> <div>10%</div> <div>..</div> </div>
2	AB	256	<div> <div>6%</div> <div>20%</div> <div>56%</div> <div>14%</div> <div>8%</div> </div>
2	CB	256	<div> <div>10%</div> <div>18%</div> <div>59%</div> <div>14%</div> <div>8%</div> </div>


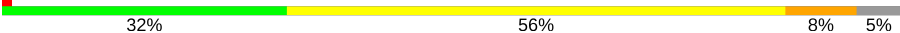
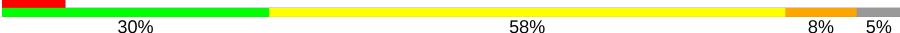


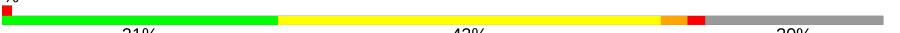
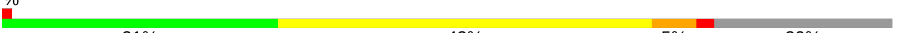




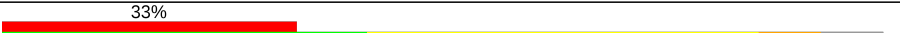


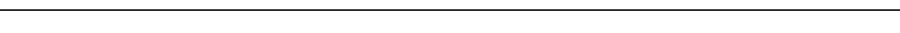
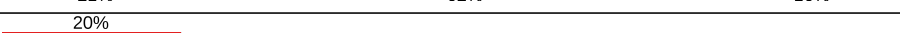
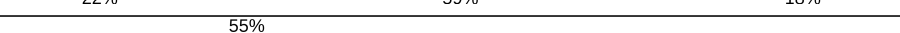


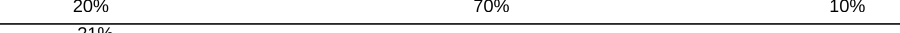




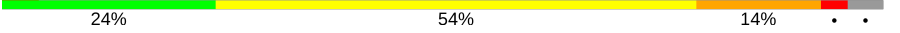
*Continued on next page...*

*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	135	
12	CL	135	
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	CW	76	
24	AX	10	
24	CX	10	
25	AY	77	
25	CY	77	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	

*Continued on next page...*

Continued from previous page...

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

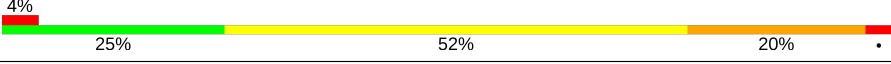
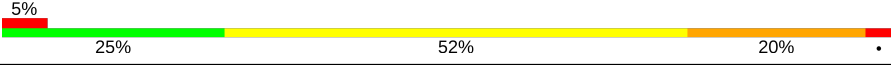
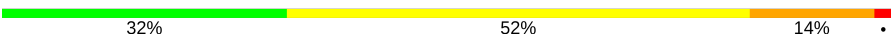
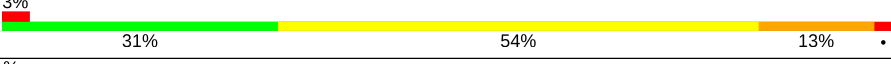


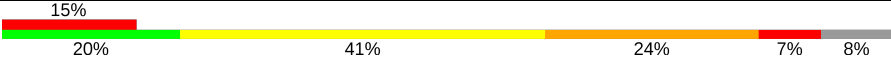
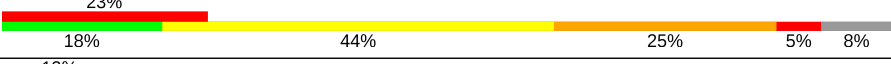
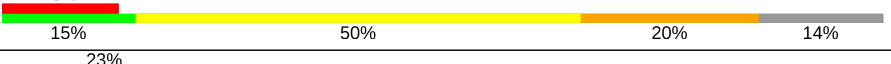

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	1602	-	-	-	X
58	MG	AA	1604	-	-	-	X
58	MG	AA	1608	-	-	-	X
58	MG	AA	1618	-	-	-	X
58	MG	AA	1631	-	-	-	X
58	MG	AA	1635	-	-	-	X
58	MG	AA	1652	-	-	-	X
58	MG	AA	1655	-	-	-	X
58	MG	AA	1666	-	-	-	X
58	MG	AA	1685	-	-	-	X
58	MG	AA	1693	-	-	-	X
58	MG	AA	1694	-	-	-	X
58	MG	AA	1696	-	-	-	X
58	MG	AA	1700	-	-	-	X
58	MG	AA	1730	-	-	-	X
58	MG	AA	1734	-	-	-	X
58	MG	AA	1743	-	-	-	X
58	MG	AA	1745	-	-	-	X
58	MG	AA	1752	-	-	-	X
58	MG	AA	1760	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	1762	-	-	-	X
58	MG	AA	1763	-	-	-	X
58	MG	AA	1765	-	-	-	X
58	MG	AA	1769	-	-	-	X
58	MG	AA	1771	-	-	-	X
58	MG	AA	1772	-	-	-	X
58	MG	AA	1780	-	-	-	X
58	MG	AA	1783	-	-	-	X
58	MG	AA	1788	-	-	-	X
58	MG	AA	1789	-	-	-	X
58	MG	AA	1799	-	-	-	X
58	MG	AA	1808	-	-	-	X
58	MG	AA	1812	-	-	-	X
58	MG	AG	201	-	-	-	X
58	MG	AV	105	-	-	-	X
58	MG	AW	101	-	-	-	X
58	MG	AW	110	-	-	-	X
58	MG	AW	116	-	-	-	X
58	MG	AW	117	-	-	-	X
58	MG	B2	601	-	-	-	X
58	MG	B5	102	-	-	-	X
58	MG	BA	3004	-	-	-	X
58	MG	BA	3009	-	-	-	X
58	MG	BA	3013	-	-	-	X
58	MG	BA	3034	-	-	-	X
58	MG	BA	3050	-	-	-	X
58	MG	BA	3070	-	-	-	X
58	MG	BA	3104	-	-	-	X
58	MG	BA	3130	-	-	-	X
58	MG	BA	3150	-	-	-	X
58	MG	BA	3158	-	-	-	X
58	MG	BA	3163	-	-	-	X
58	MG	BA	3164	-	-	-	X
58	MG	BA	3213	-	-	-	X
58	MG	BA	3221	-	-	-	X
58	MG	BA	3223	-	-	-	X
58	MG	BA	3228	-	-	-	X
58	MG	BA	3232	-	-	-	X
58	MG	BA	3234	-	-	-	X
58	MG	BA	3235	-	-	-	X
58	MG	BA	3238	-	-	-	X
58	MG	BA	3242	-	-	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	BA	3259	-	-	-	X
58	MG	BA	3260	-	-	-	X
58	MG	BA	3269	-	-	-	X
58	MG	BA	3272	-	-	-	X
58	MG	BA	3278	-	-	-	X
58	MG	BA	3284	-	-	-	X
58	MG	BA	3285	-	-	-	X
58	MG	BA	3287	-	-	-	X
58	MG	BA	3288	-	-	-	X
58	MG	BA	3295	-	-	-	X
58	MG	BA	3305	-	-	-	X
58	MG	BA	3308	-	-	-	X
58	MG	BA	3316	-	-	-	X
58	MG	BA	3321	-	-	-	X
58	MG	BA	3336	-	-	-	X
58	MG	BA	3339	-	-	-	X
58	MG	BA	3341	-	-	-	X
58	MG	BA	3345	-	-	-	X
58	MG	BA	3347	-	-	-	X
58	MG	BA	3349	-	-	-	X
58	MG	BA	3351	-	-	-	X
58	MG	BA	3355	-	-	-	X
58	MG	BA	3375	-	-	-	X
58	MG	BA	3377	-	-	-	X
58	MG	BA	3394	-	-	-	X
58	MG	BA	3401	-	-	-	X
58	MG	BA	3404	-	-	-	X
58	MG	BA	3424	-	-	-	X
58	MG	BA	3428	-	-	-	X
58	MG	BA	3429	-	-	-	X
58	MG	BA	3453	-	-	-	X
58	MG	BB	201	-	-	-	X
58	MG	BB	202	-	-	-	X
58	MG	BB	213	-	-	-	X
58	MG	BB	214	-	-	-	X
58	MG	BB	217	-	-	-	X
58	MG	BB	218	-	-	-	X
58	MG	BX	102	-	-	-	X
58	MG	CA	1612	-	-	-	X
58	MG	CA	1617	-	-	-	X
58	MG	CA	1618	-	-	-	X
58	MG	CA	1619	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	CA	1626	-	-	-	X
58	MG	CA	1627	-	-	-	X
58	MG	CA	1638	-	-	-	X
58	MG	CA	1639	-	-	-	X
58	MG	CA	1643	-	-	-	X
58	MG	CA	1647	-	-	-	X
58	MG	CA	1649	-	-	-	X
58	MG	CA	1650	-	-	-	X
58	MG	CA	1651	-	-	-	X
58	MG	CA	1661	-	-	-	X
58	MG	CA	1672	-	-	-	X
58	MG	CA	1675	-	-	-	X
58	MG	CA	1680	-	-	-	X
58	MG	CA	1682	-	-	-	X
58	MG	CA	1687	-	-	-	X
58	MG	CA	1688	-	-	-	X
58	MG	CA	1701	-	-	-	X
58	MG	CA	1710	-	-	-	X
58	MG	CA	1716	-	-	-	X
58	MG	CA	1724	-	-	-	X
58	MG	CA	1730	-	-	-	X
58	MG	CA	1731	-	-	-	X
58	MG	CA	1737	-	-	-	X
58	MG	CA	1739	-	-	-	X
58	MG	CA	1742	-	-	-	X
58	MG	CA	1743	-	-	-	X
58	MG	CA	1751	-	-	-	X
58	MG	CA	1762	-	-	-	X
58	MG	CA	1763	-	-	-	X
58	MG	CA	1767	-	-	-	X
58	MG	CA	1770	-	-	-	X
58	MG	CA	1772	-	-	-	X
58	MG	CA	1773	-	-	-	X
58	MG	CA	1780	-	-	-	X
58	MG	CA	1783	-	-	-	X
58	MG	CA	1810	-	-	-	X
58	MG	CA	1816	-	-	-	X
58	MG	CK	201	-	-	-	X
58	MG	CV	105	-	-	-	X
58	MG	CV	108	-	-	-	X
58	MG	CW	103	-	-	-	X
58	MG	CW	108	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	D1	101	-	-	-	X
58	MG	D7	102	-	-	-	X
58	MG	DA	3005	-	-	-	X
58	MG	DA	3035	-	-	-	X
58	MG	DA	3043	-	-	-	X
58	MG	DA	3088	-	-	-	X
58	MG	DA	3102	-	-	-	X
58	MG	DA	3103	-	-	-	X
58	MG	DA	3141	-	-	-	X
58	MG	DA	3144	-	-	-	X
58	MG	DA	3151	-	-	-	X
58	MG	DA	3156	-	-	-	X
58	MG	DA	3161	-	-	-	X
58	MG	DA	3166	-	-	-	X
58	MG	DA	3171	-	-	-	X
58	MG	DA	3178	-	-	-	X
58	MG	DA	3196	-	-	-	X
58	MG	DA	3198	-	-	-	X
58	MG	DA	3205	-	-	-	X
58	MG	DA	3209	-	-	-	X
58	MG	DA	3213	-	-	-	X
58	MG	DA	3219	-	-	-	X
58	MG	DA	3220	-	-	-	X
58	MG	DA	3224	-	-	-	X
58	MG	DA	3234	-	-	-	X
58	MG	DA	3241	-	-	-	X
58	MG	DA	3245	-	-	-	X
58	MG	DA	3246	-	-	-	X
58	MG	DA	3253	-	-	-	X
58	MG	DA	3255	-	-	-	X
58	MG	DA	3262	-	-	-	X
58	MG	DA	3264	-	-	-	X
58	MG	DA	3265	-	-	-	X
58	MG	DA	3273	-	-	-	X
58	MG	DA	3279	-	-	-	X
58	MG	DA	3283	-	-	-	X
58	MG	DA	3301	-	-	-	X
58	MG	DA	3303	-	-	-	X
58	MG	DA	3304	-	-	-	X
58	MG	DA	3311	-	-	-	X
58	MG	DA	3313	-	-	-	X
58	MG	DA	3327	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	DA	3330	-	-	-	X
58	MG	DA	3331	-	-	-	X
58	MG	DA	3334	-	-	-	X
58	MG	DA	3335	-	-	-	X
58	MG	DA	3336	-	-	-	X
58	MG	DA	3344	-	-	-	X
58	MG	DA	3346	-	-	-	X
58	MG	DA	3348	-	-	-	X
58	MG	DA	3351	-	-	-	X
58	MG	DA	3360	-	-	-	X
58	MG	DA	3364	-	-	-	X
58	MG	DA	3370	-	-	-	X
58	MG	DA	3380	-	-	-	X
58	MG	DA	3391	-	-	-	X
58	MG	DA	3399	-	-	-	X
58	MG	DA	3410	-	-	-	X
58	MG	DA	3414	-	-	-	X
58	MG	DA	3423	-	-	-	X
58	MG	DA	3426	-	-	-	X
58	MG	DA	3434	-	-	-	X
58	MG	DA	3447	-	-	-	X
58	MG	DB	202	-	-	-	X
58	MG	DB	213	-	-	-	X
58	MG	DB	214	-	-	-	X
58	MG	DB	216	-	-	-	X
58	MG	DB	217	-	-	-	X
58	MG	DN	201	-	-	-	X
58	MG	DN	202	-	-	-	X

## 2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

- Molecule 24 is a RNA chain called MRNA.

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

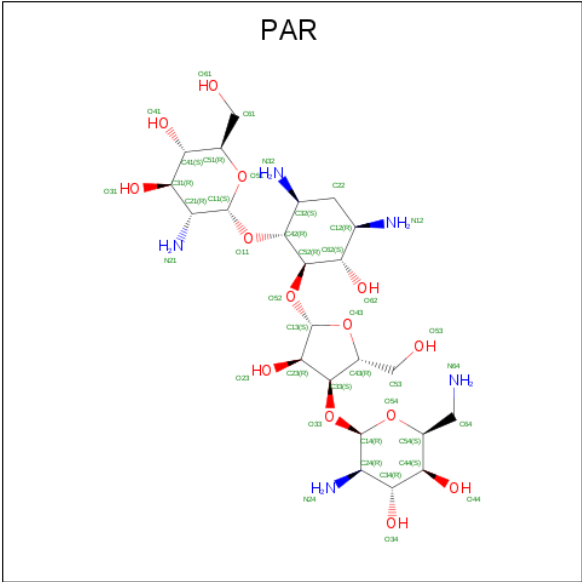
*Continued on next page...*



*Continued from previous page...*

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

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



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

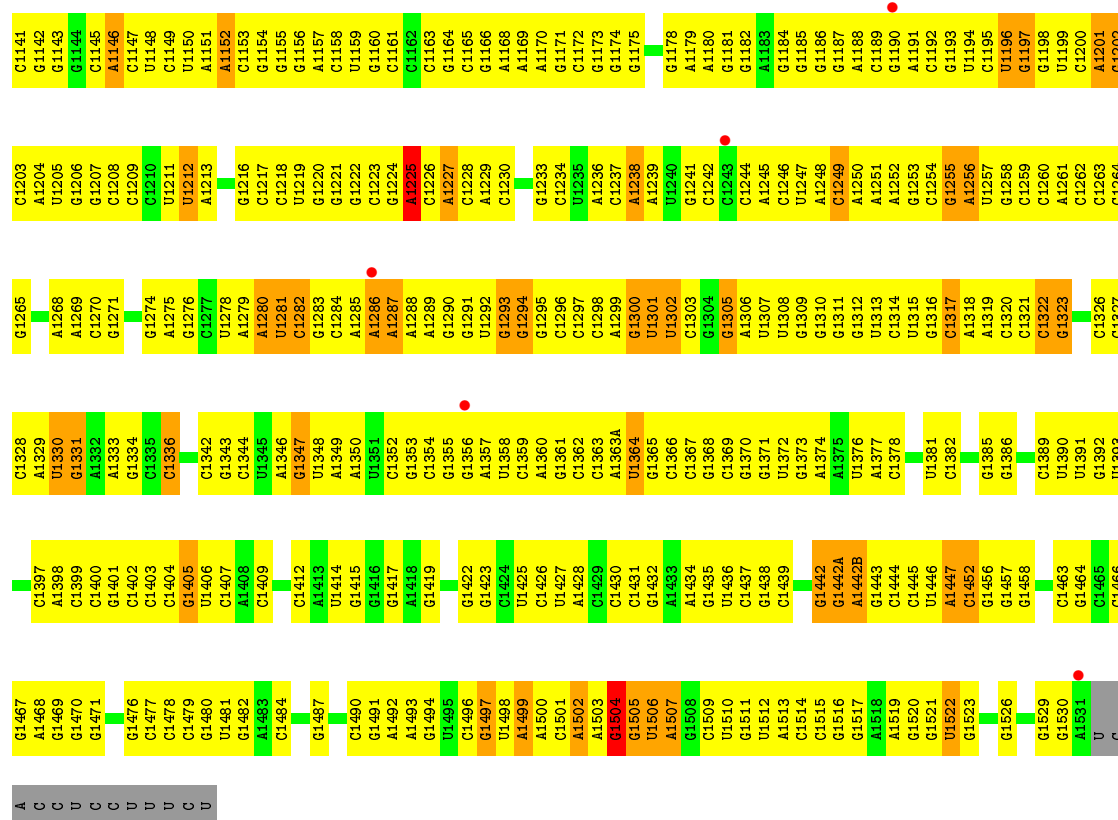
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

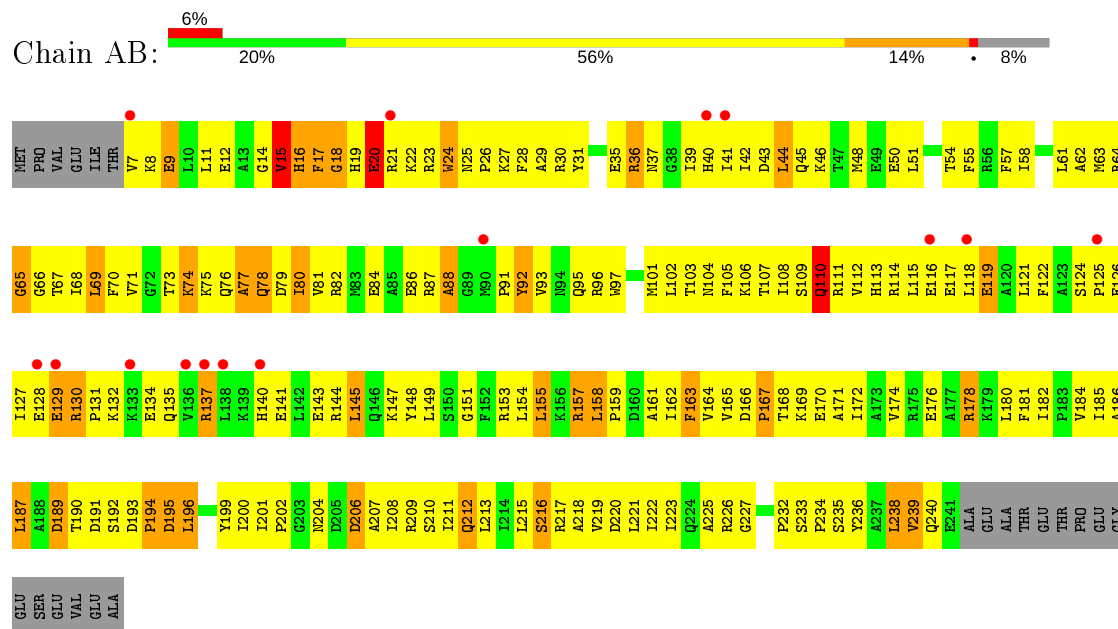




A1080	G1024	U957	C880	C811	U740	G657	G600	U534	C449	U387	C312	A228	G159	U83
G1081	U1025	A958	G881	A814	G741	G668	C601	A535	A452	G388	G319	A231	A160	U94
G1082	C882	A959	C882	A815	G742	G669	A602	G537	A453	A389	G320	G232	A161	A88
U1083	C1027	U960	C883	A816	U743	G671	U603	G538	A454	C390	C321	G233	A162	C89
U1084	U884	U961	U884	C817	C744	G672	U604	A539	C455	G391	A322	C237	U164	U90
U1085	C1029	C962	G885	C818	A745	G673	U605	A540	C456	G392	U823	G238	C165	C91
U1086	C1030	G963	C886	A819	A746	G674	G606	G541	C457	A393	G324	U239	C166	C92
G1087	G1030A	A964	U890	A820	G747	G675	A607	G542	C458	G394	A325	G240	G167	U96
U1088	C1030B	A965	U891	C748	A748	A676	C612	C543	G460	G395	A326	A243	G168	G97
G1089	G1030C	G966	A892	C749	G749	U677	C613	C544	A461	G396	A327	U244	C169	C98
U1090	A1030D	C967	C893	C822	G750	U678	G617	C545	C470	G397	C328	C245	U170	U99
U1091	G1031	A968	G893	C823	C751	C679	C618	G546	C471	G398	G331	C246	A171	C100
A1092	A1092	A969	G894	C824	G752	G680	C619	A547	A472	C400	G332	G247	A172	A101
A1093	C895	C970	G895	G825	G753	G681	U619	U551	G473	C401	G333	G250	U173	G102
G1094	G1034	G971	C896	C826	U757	G682	C620	U552	G474	G402	G334	A251	C174	C103
U1095	U1095	C972	A901	U827	G758	A684	U621	U553	G475	C403	C335	G252	C175	G104
C1096	G902	G973	G902	A828	A759	G685	A622	A554	G476	C404	C336	U253	C176	G105
U1097	G903	A974	G903	G829	G760	G686	C623	C554	G477	U405	C337	G254	C177	C106
A1098	C1038	A975	U831	G830	G761	A687	C624	C555	A478	G406	C338	G255	C178	G107
G1099	C1039	G976	C912	U832	G762	G688	G625	C556	G479	A407	A339	G256	C179	G108
U1100	U1040	A977	C913	U833	G763	C689	U626	G557	G480	A408	C340	U257	U180	A109
A1101	A1041	A978	A913	U834	C764	G691	G627	G558	G481	G409	U340	G258	U181	C110
A1102	G1042	C979	A914	U835	G765	G692	G628	A559	G482	G410	C341	G259	G181	C111
G1103	C1043	C980	A915	G836	A766	U693	G629	U560	C483	A411	C342	G260	G182	G112
G1104	A1044	U981	A916	G837	A767	G694	G630	U561	C484	A412	U343	U261	A185	G113
A1105	C1045	U982	U920	G838	A768	A694	G631	C562	G485	A413	U344	A262	C186	U114
G1106	A1046	C983	U921	U839	G769	G695	A632	A563	G486	G414	C345	A263	C187	G115
C1107	G1047	C984	C924	C840	C770	A706	G633	U564	G487	A415	C346	A264	C188	A116
G1108	U1048	C985	C925	U841	G771	C708	G634	U565	G488	G416	G347	G265	C189	
C1109	U1049	A986	G926	C849	G772	G709	G635	U566	U494	C417	G348	G266	C189A	A119
A1110	G1050	C987	G927	U850	G773	G710	U636	G568	A495	C418	A349	C267	C189B	A120
C1111	C1051	C988	C928	G851	G774	G711	G637	C569	A496	C419	G350	C268	C189C	C121
U1112	U1052	U991	G929	G852	G775	A712	G638	U572	U498	U420	G351	C269	C189D	G122
C1113	G1053	C992	C930	U853	G776	G713	G639	A573	G501	U421	C352	A270	U189E	C123
G1114	C1054	C993	C931	G854	A777	G714	G640	U574	G502	G422	A353	C271	G124	G124
U1115	A1055	A994	C932	G855	G778	A715	U641	A575	G503	G423	G354	C272	U125	U125
C1116	U1056	C995	C933	G856	C779	A716	U642	G576	G504	G424	C355	A273	G126	G126
G1117	G1057	C996	C934	C857	A780	G717	G644	G577	G505	G425	U359	A274	G189F	G127
C1118	U1058	U1000	A935	G858	A781	G718	C645	C578	G506	G426	A360	G275	G189G	C131
U1121	C1059	A1001	C936	U859	A782	G719	U646	G579	A509	U427	G371	G276	G189L	
U1122	G1060	G1001A	C937	A860	C783	C720	C647	U580	A510	G428	U190	C277	U190	C137
A1123	U1062	G1002	A938	G861	C784	G721	A648	G581	C511	U429	C366	G278	G191	G137
G1124	C1063	A1004	G939	C862	U788	A722	G649	U582	U512	U430	U367	A279	U192	G138
U1125	U1064	A1005	C940	U863	U789	U723	G650	A583	C513	A431	C370	C283	C193	G139
U1126	C1065	C1006	G941	A864	G793	G724	C651	G584	C518	A432	G371	G284	C194	A140
G1127	G1066	C1007	U943	C866	A794	G725	U652	C586	C519	C433	G372	G285	A195	G146
C1128	A1067	C1008	U943	C867	C795	G726	A653	G587	A520	U434	A373	G286	A197	G147
G1129	G1068	U1009	A946	G868	G796	A728	C656	G588	G521	C436	A374	U287	G148	G148
A1130	C1069	G1010	G947	G869	C797	G729	G657	C589	C522	U437	U375	A288	A149	A150
C1131	U1070	G1011	C948	U870	G798	G730	G658	C590	A523	G438	G376	G289	U203	C150
G1132	C1071	A1014	C949	U871	U801	G731	G659	U591	G527	A441	G377	G290	U204	A151
U1133	G1072	A1015	A949	U872	A802	G732	G660	G592	C528	A442	C381	G299	C221	A152
G1134	U1073	A1016	U950	A873	G803	A733	G661	G593	G529	C443	A382	U222	U223	G153
U1135	G1074	A1017	G951	G874	G804	G734	G662	G594	G530	C444	A383	U224	C224	C154
C1136	C1075	G1017	U952	G875	G805	G735	G663	G595	U531	G445	G384	C225	C155	C155
G1137	G1076	G1018	G953	G876	C806	G736	A663	G596	A532	G446	C385	G226	G156	G156
G1138	U1077	C1019	G954	G877	A807	G737	A664	U598	A533	A447	C386	A303	G227	G157
G1139	U1078	U1020	G955	G878	C808	G738	A665	C599						G158
C1140	G1079		U956	C879		C739	G666							

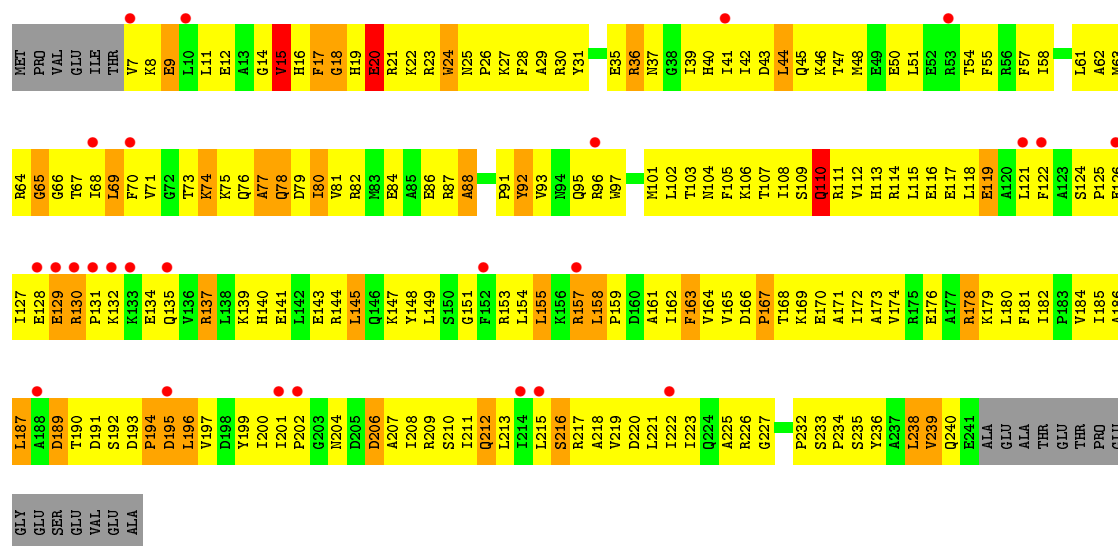


### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

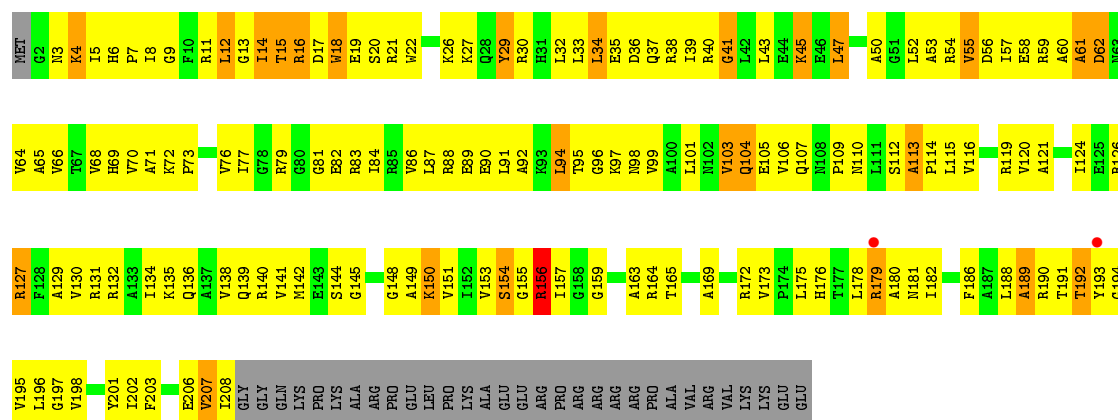


### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

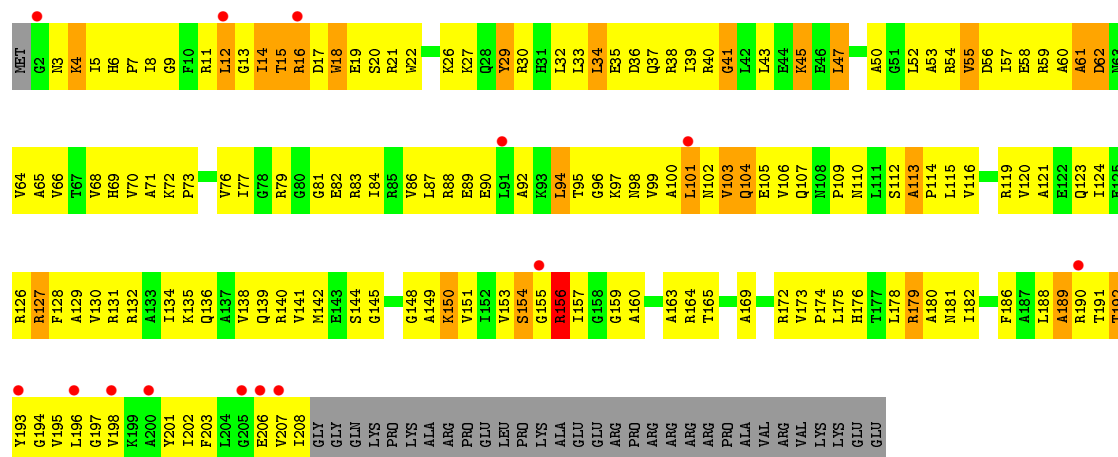




### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



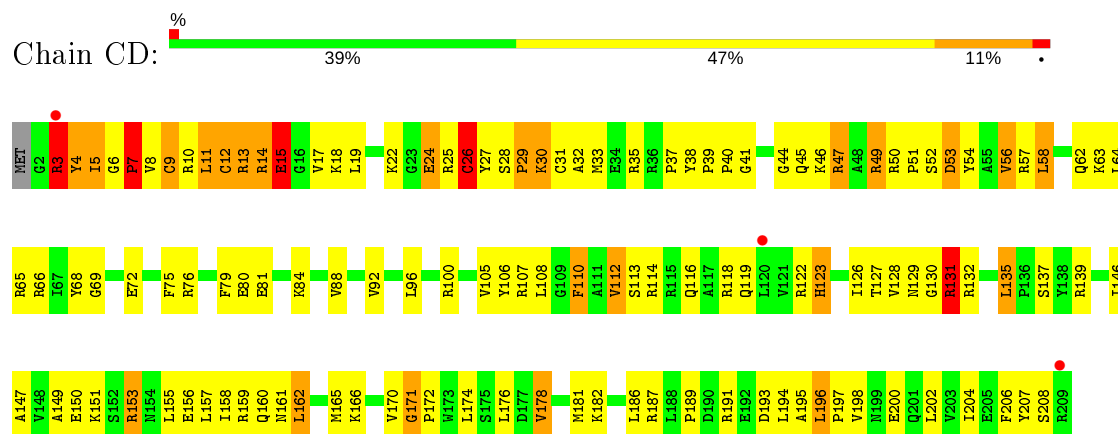
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



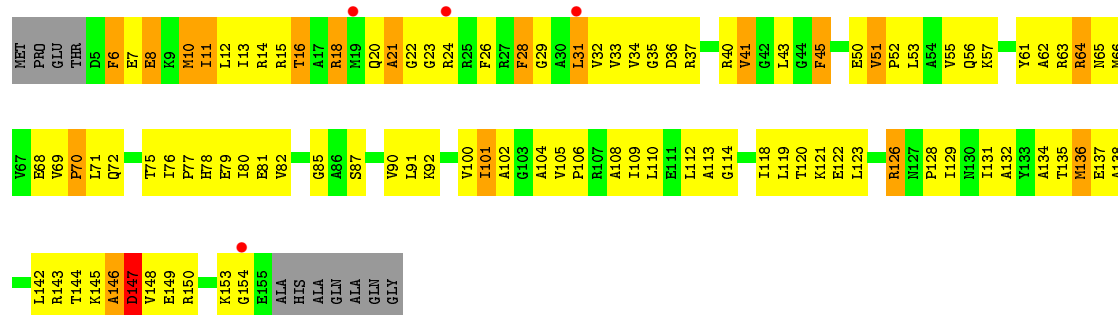
- Molecule 4: 30S RIBOSOMAL PROTEIN S4



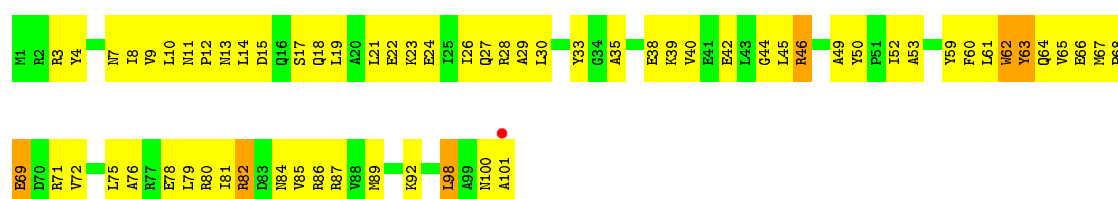
- Molecule 4: 30S RIBOSOMAL PROTEIN S4



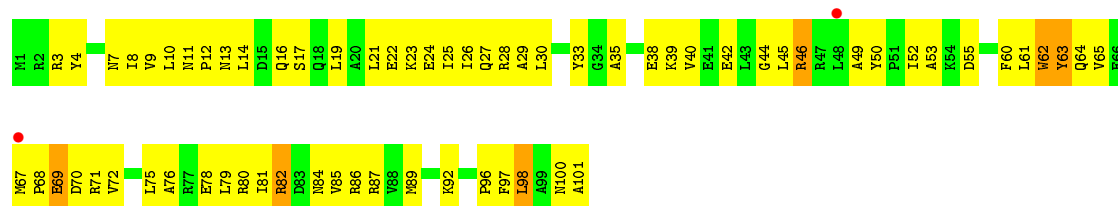




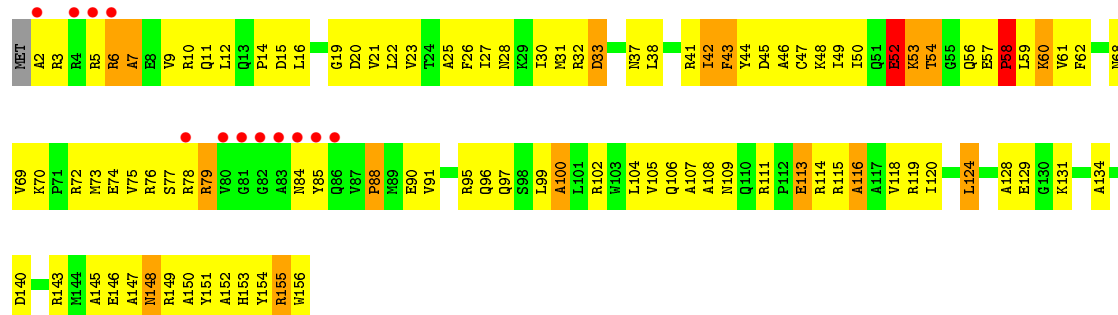
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

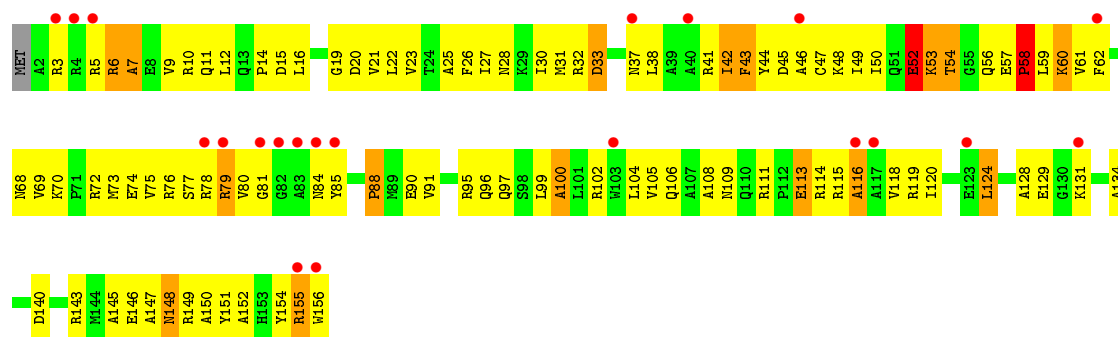


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

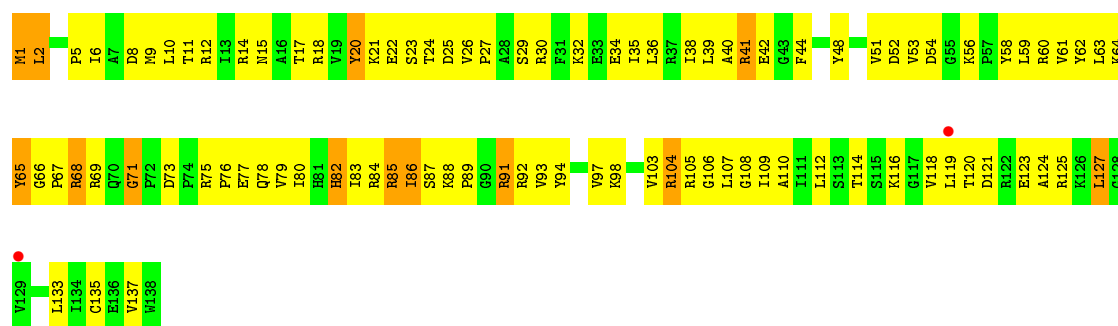


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

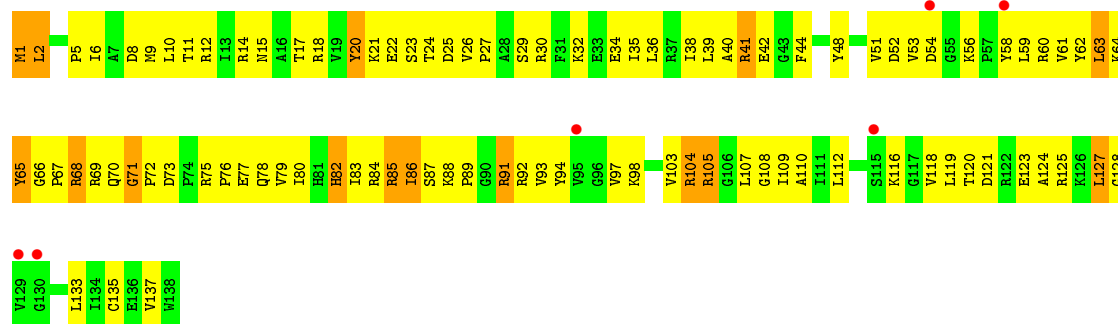




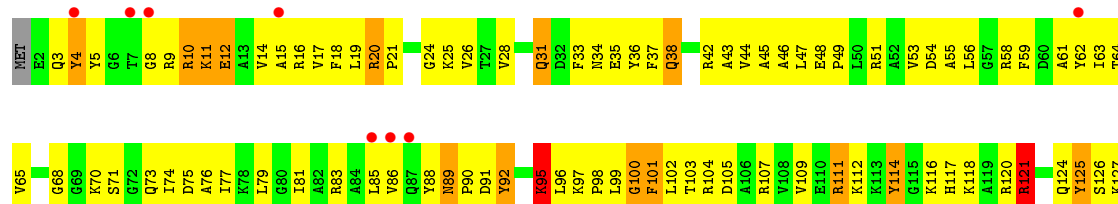
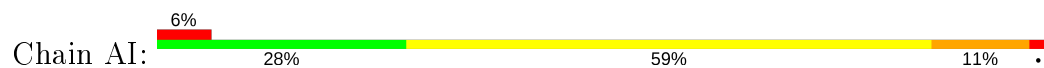
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8



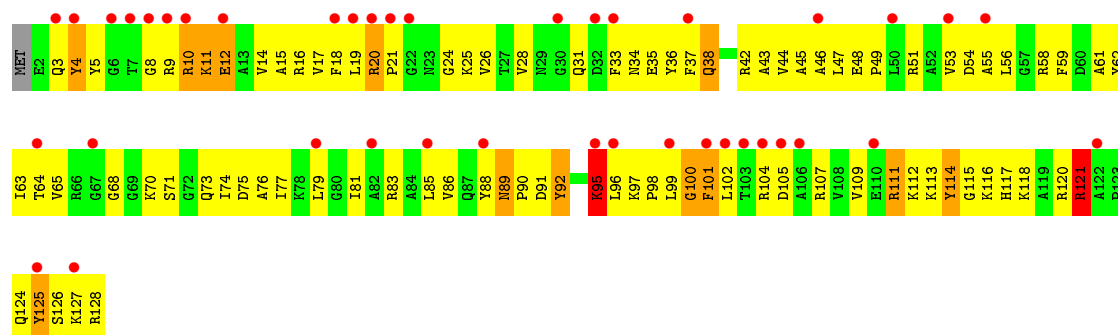
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



R128

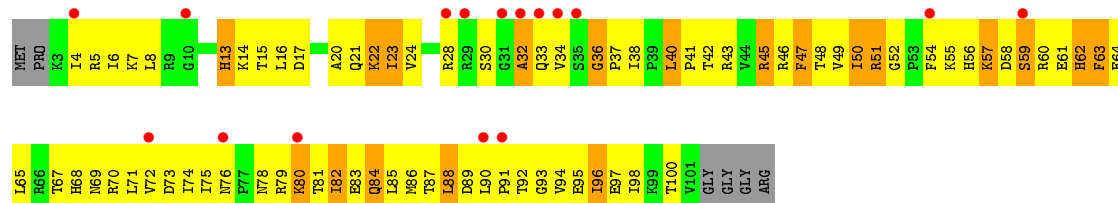
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI: 



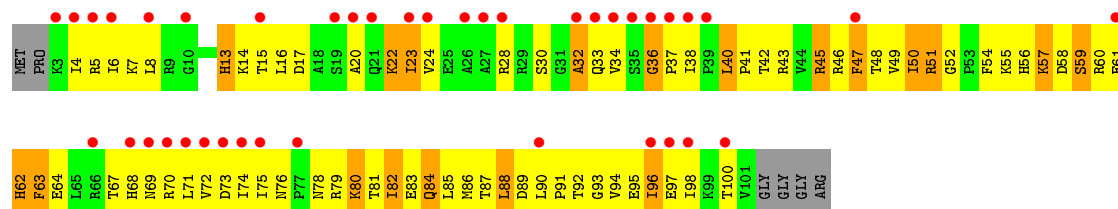
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ: 



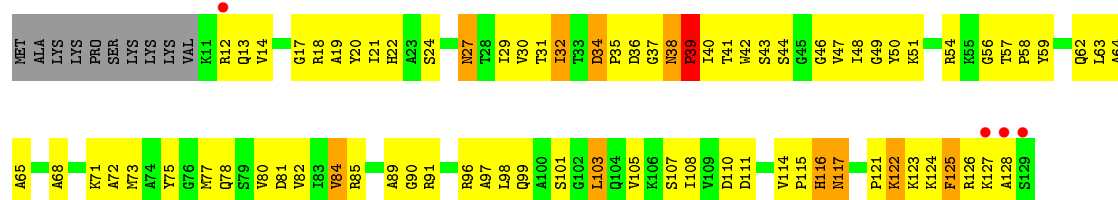
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ: 

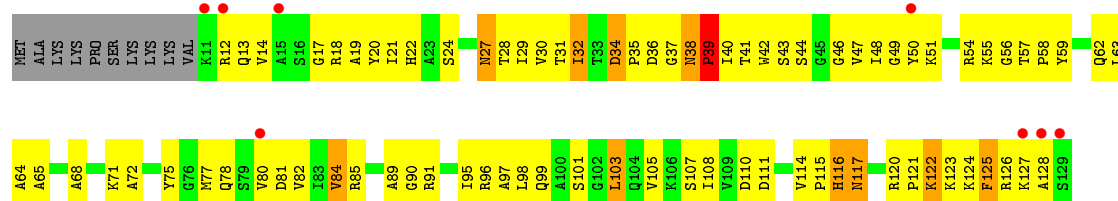


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

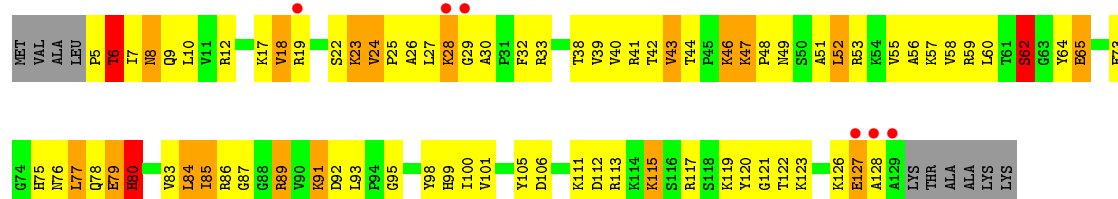
Chain AK: 



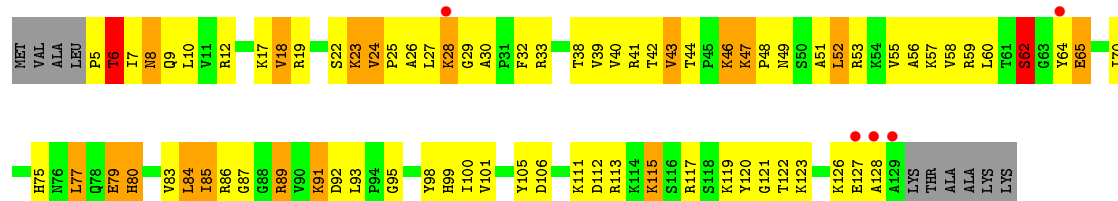
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



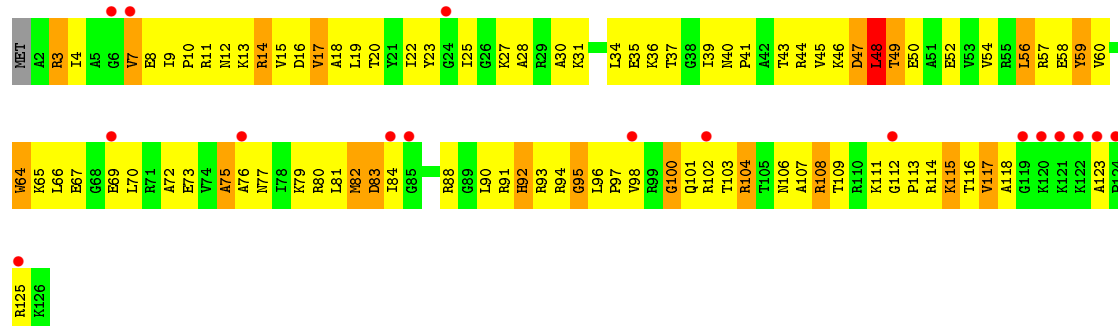
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

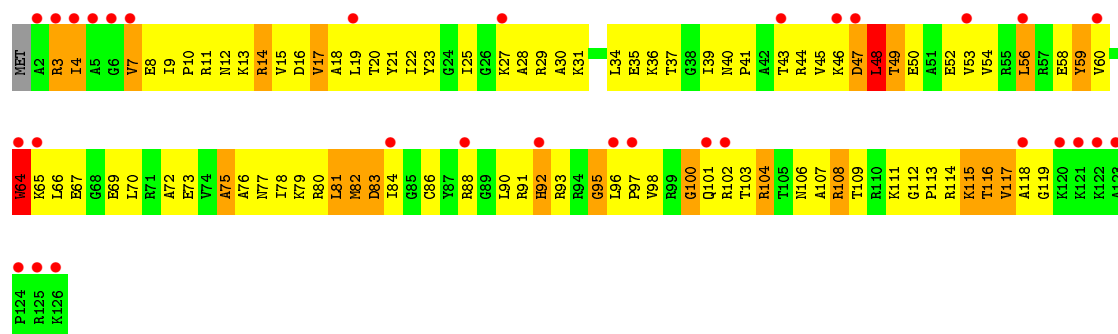


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

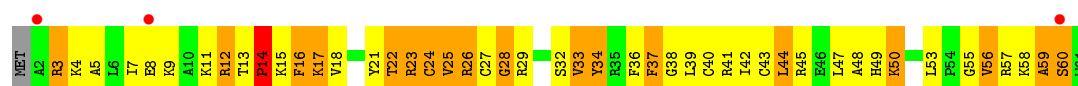
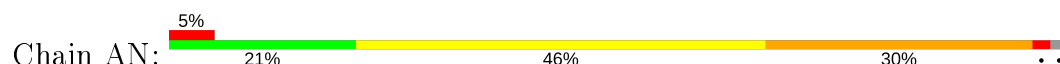


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

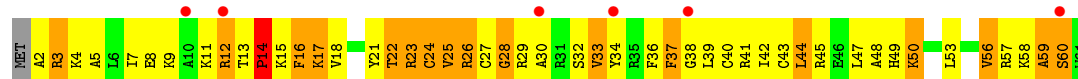
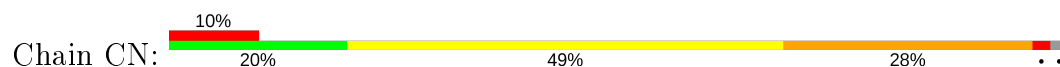




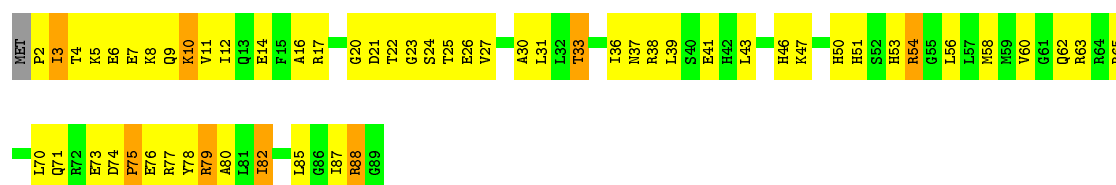
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



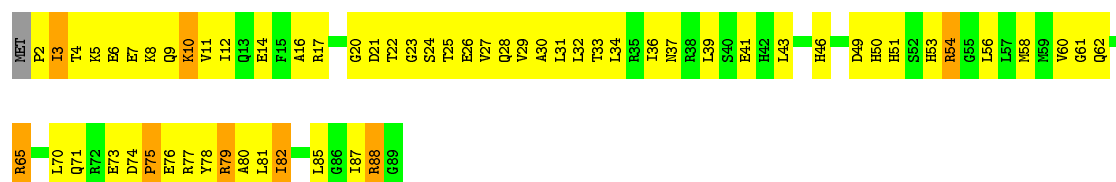
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

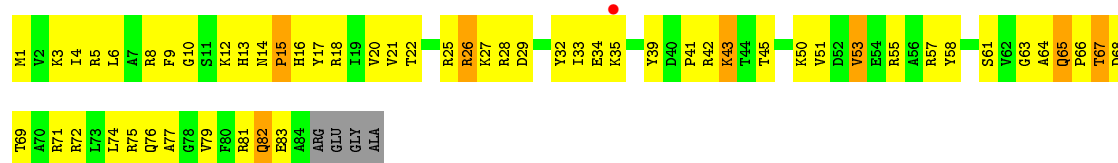


• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

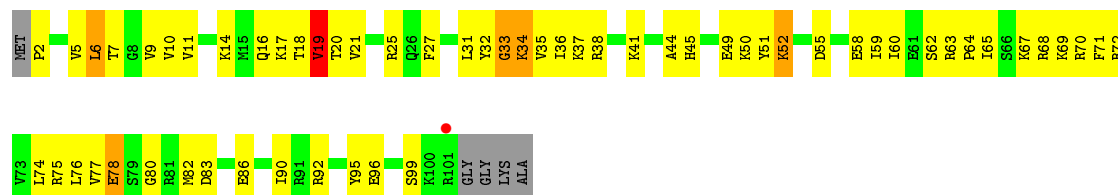




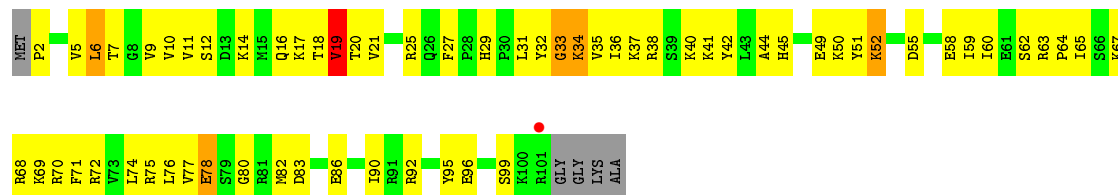
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



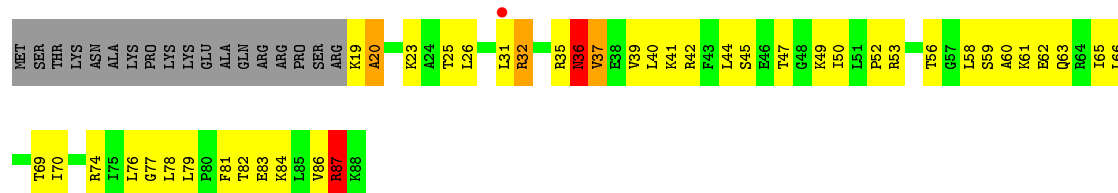
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



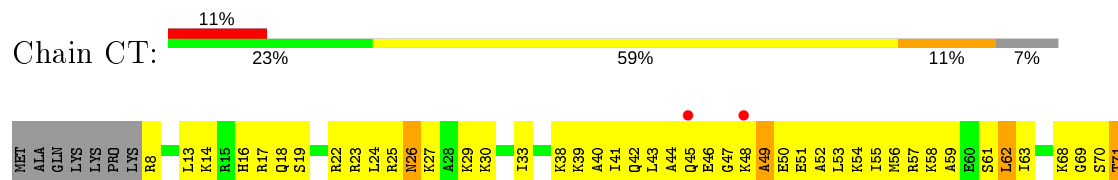
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

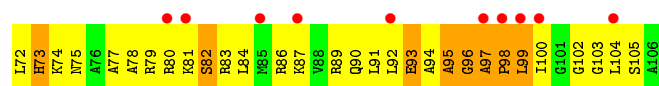


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

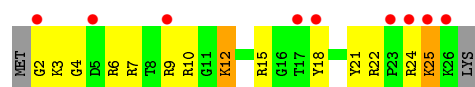


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

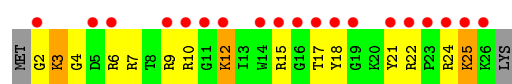
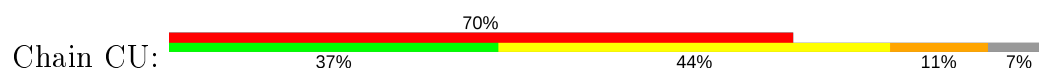




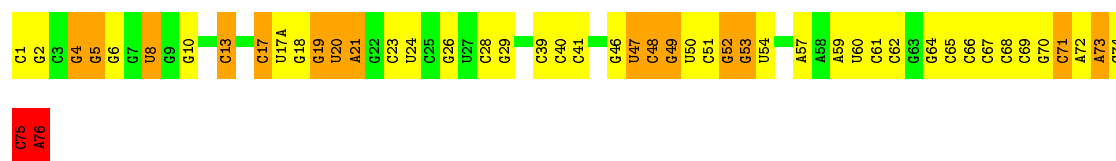
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



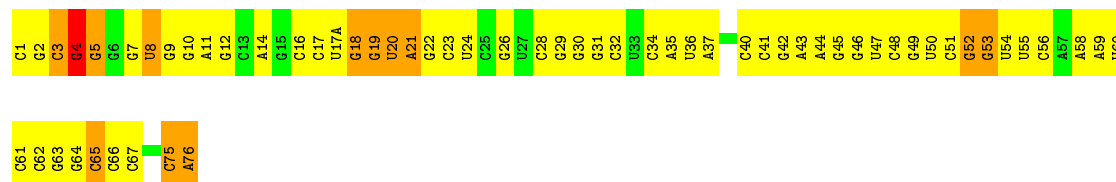
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



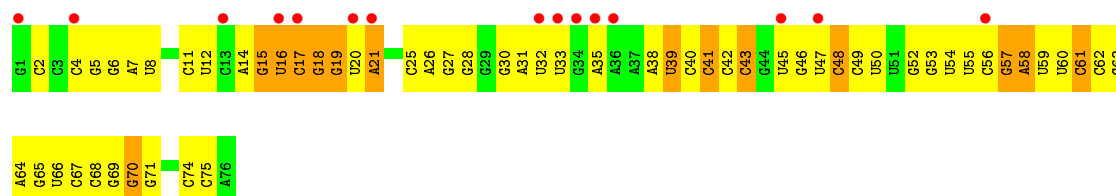
• Molecule 22: P-SITE TRNA FMET



• Molecule 22: P-SITE TRNA FMET



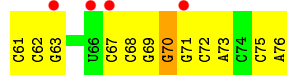
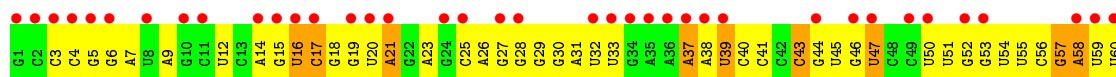
• Molecule 23: E-SITE TRNA PHE



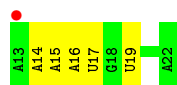
• Molecule 23: E-SITE TRNA PHE







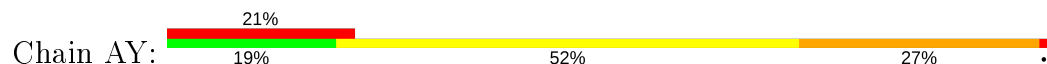
• Molecule 24: MRNA



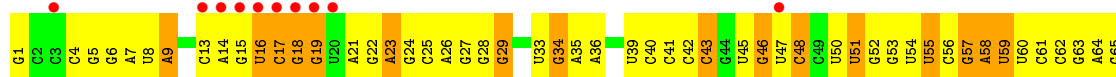
• Molecule 24: MRNA



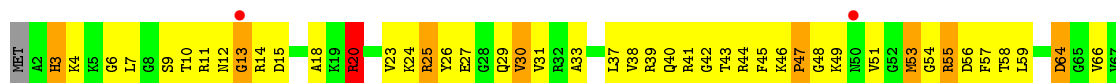
• Molecule 25: A-SITE PHE-TRNA PHE

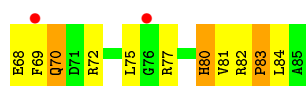


• Molecule 25: A-SITE PHE-TRNA PHE

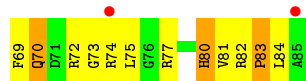


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

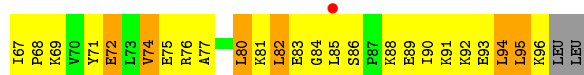




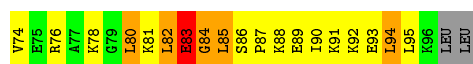
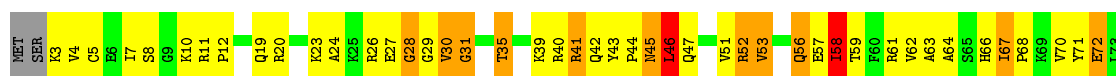
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



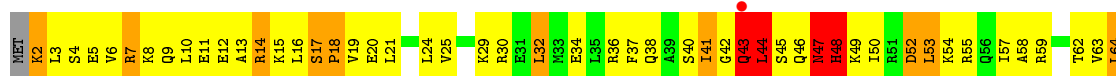
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L28

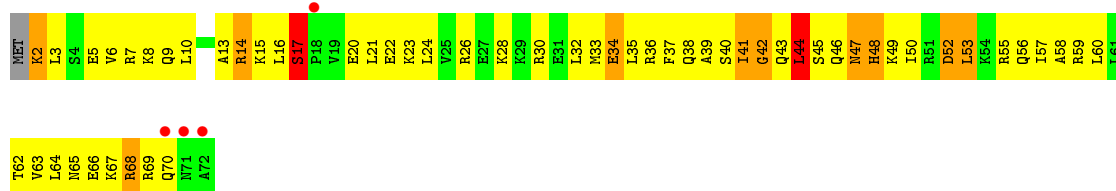


• Molecule 28: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L29

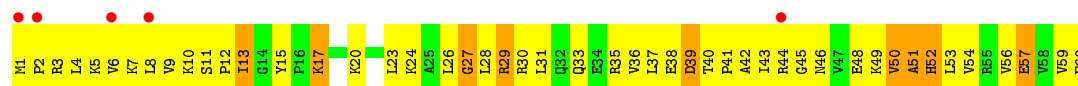




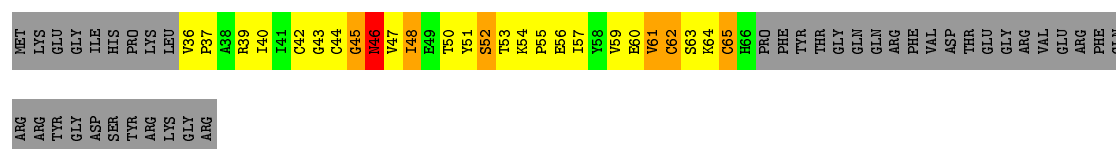
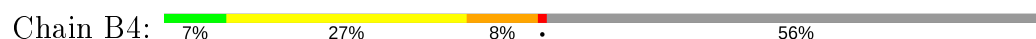
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



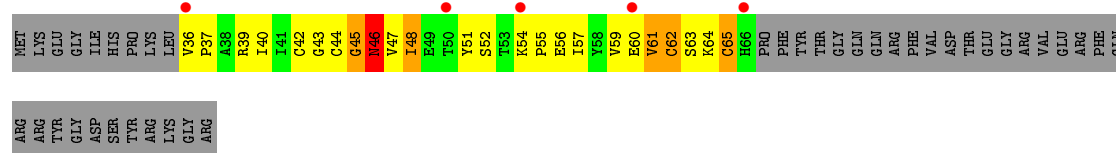
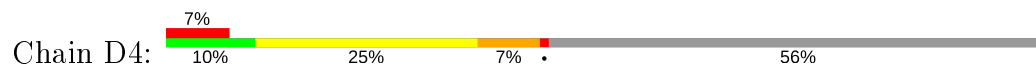
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



• Molecule 30: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L31

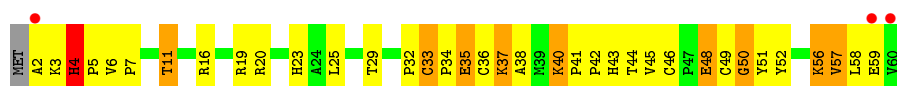


• Molecule 31: 50S RIBOSOMAL PROTEIN L32

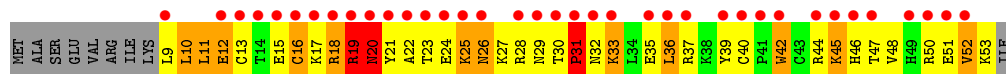


• Molecule 31: 50S RIBOSOMAL PROTEIN L32

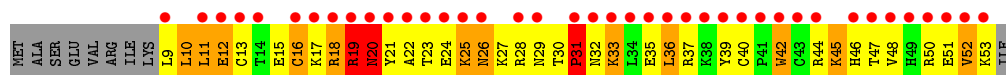
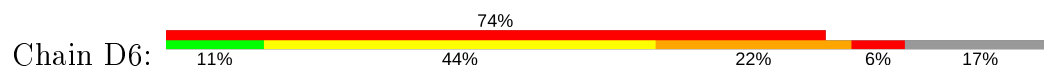




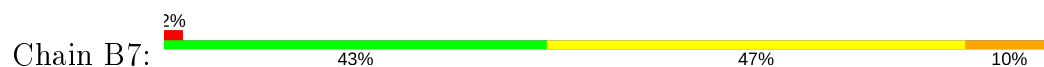
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L33



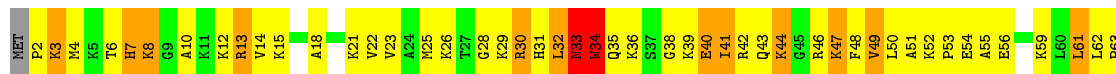
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



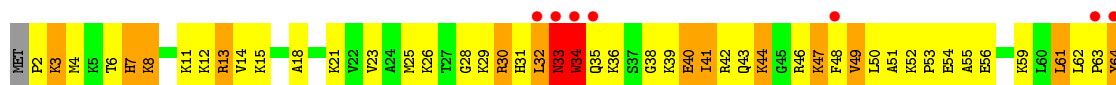
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



• Molecule 34: 50S RIBOSOMAL PROTEIN L35

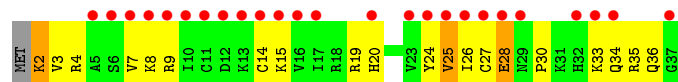
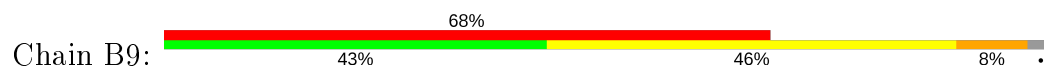


• Molecule 34: 50S RIBOSOMAL PROTEIN L35

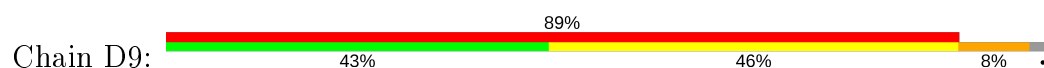


E65

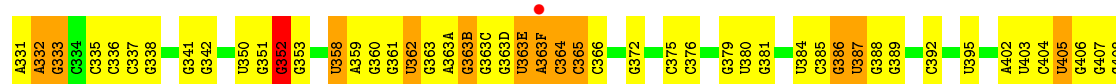
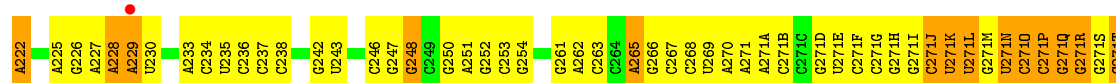
- Molecule 35: 50S RIBOSOMAL PROTEIN L36



- Molecule 35: 50S RIBOSOMAL PROTEIN L36

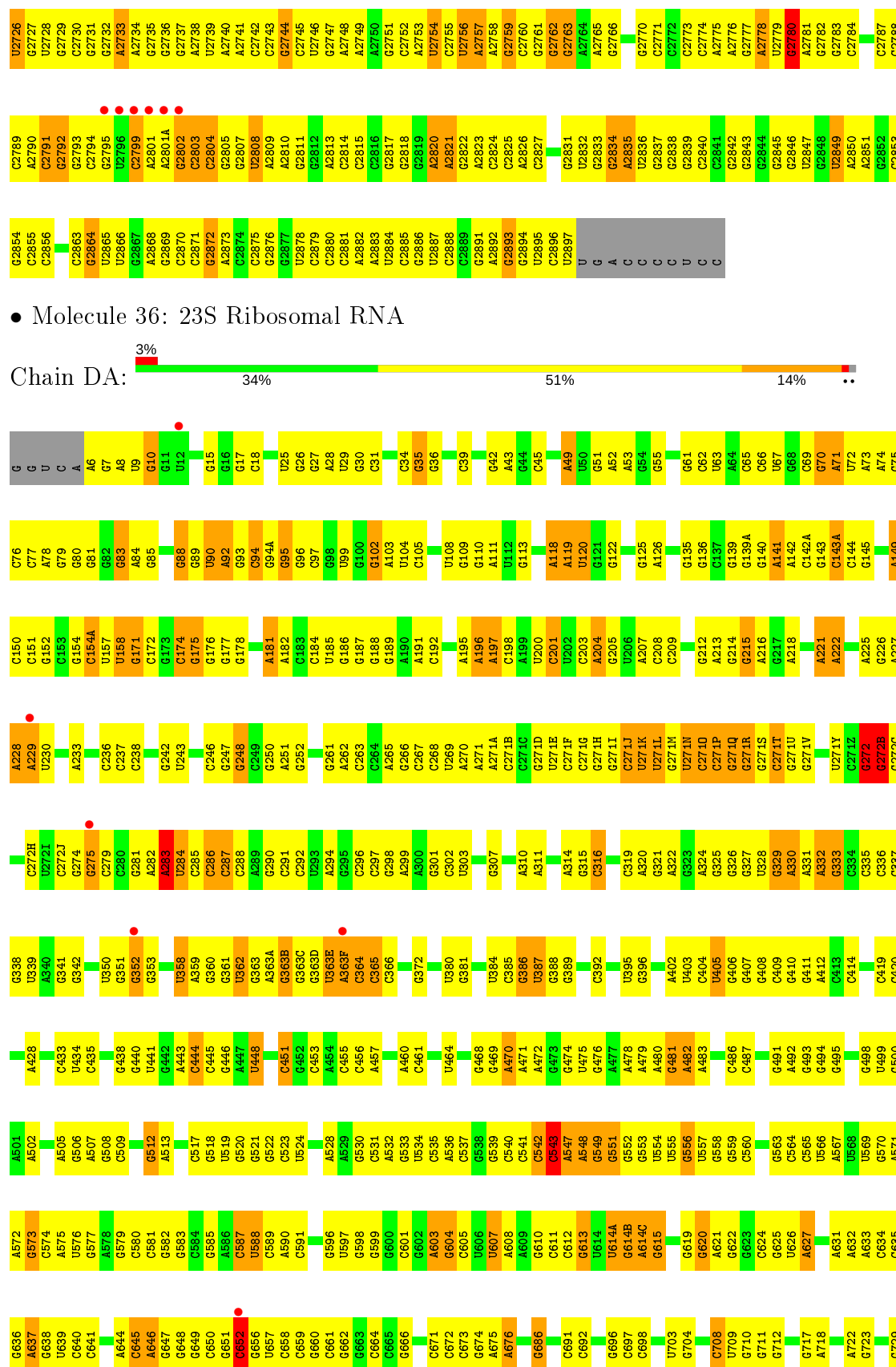


- Molecule 36: 23S Ribosomal RNA



A1580	G1500	C1363	G1293	G1222	G1149	G1025	A959	C885	A718	A631	U566
G1581	C1501	G1364	C1297	G1223	C1150	U1026	A960	C886	A719	A632	A567
A1582	C1502	A1365	C1300	C1224	G1151	U1027	C961	A887	A720	A633	U568
A1583	U1503	G1366	U1301	G1227	G1154	A1029	U962	C888	A721	C634	U569
A1584	C1504	G1367	A1302	G1230	A1155	A1032	U963	C889	A722	C635	G570
A1585	C1505	A1368	U1303	G1231	A1156	U1035	C965	A890	A723	G636	A571
C1506	A1507	G1374	A1308	G1232	G1157	U1036	U969	C892	C730	A637	A572
C1508	A1508	G1375	G1309	G1233	U1158	G1038	U970	C893	A724	U639	G573
C1509	U1509	A1378	G1310	U1234	U1159	U1039	C971	U895	G744	U639	C574
A1509B	A1509A	A1379	G1311	G1235	C1161	G1040	C972	U896	U747	C641	A575
G1510	G1445	G1380	U1312	A1236	G1162	A1041	G973	C897	A752	G642	G577
C1511	C1446A	U1381	U1313	A1237	G1163	C1042	G974	C898	C753	A644	A578
C1512	G1447	G1382	C1314	G1238	G1164	U1043	C975	C899	C754	C645	G579
C1513	G1448	G1383	U1315	G1239	U1165	C1044	C976	C894	G760	C646	C580
U1514	A1449	C1386	U1316	A1240	U1166	A1045	G978	U895	G761	A647	C581
G1515	G1450	G1388	C1318	A1241	U1167	A1046	G979	U896	A762	G648	G582
U1518	C1450A	G1389	G1319	G1242	G1168	U1047	A980	G906	G763	C650	G583
G1519	C1451	U1390	C1320	G1244	U1169	U1048	U907	U907	A764	G651	G584
U1520	U1452	A1393	A1321	G1245	G1170	C1049	U908	C908	C755	C652	A585
U1523	U1453	U1394	A1322	A1246	G1171	A1050	A909	A909	G769	G656	A586
G1524	G1455	U1395	G1323	A1247	A1174	G1051	A984	A910	G770	U657	U588
U1528	G1459	U1396	G1324	G1248	U1175	C1052	C986	C985	U773	C658	C589
A1528A	A1460	U1397	G1325	U1249	G1176	C1053	G987	U847	A774	C660	C590
G1530	A1461	C1398	U1326	G1250	A1177	A1106	A988	C914	G775	C661	G596
C1531	G1467	C1399	G1327	G1251	U1178	G1107	C991	C915	G776	U658	U597
G1532	C1468	G1400	G1328	G1252	U1179	U1108	C992	A917	A777	G663	A598
G1533	A1469	G1401	U1329	A1253	C1109	G1109	C993	A918	G778	C664	G599
C1543	A1470	C1402	G1330	G1256	G1110	A1111	C994	G920	U779	G670	C601
A1544	A1471	U1405	G1331	G1259	G1111	G1112	C995	C921	A781	C671	G602
G1550	A1472	U1406	U1335	G1260	U1113	U1114	A996	C925	A782	C672	A603
C1551	G1473	C1407	A1336	G1264	G1190	G1115	U999	A926	A783	C673	G604
A1554	G1474	C1408	G1337	A1265	G1191	C1116	A1000	U927	A784	C674	C605
C1557	G1475	C1409	G1338	A1266	G1192	G1117	A1001	G931	G785	A675	U606
A1559	G1478	G1410	G1339	U1267	G1193	C1118	G1002	A932	C786	U607	A608
G1563	A1481	C1411	U1340	U1268	A1194	C1119	G1003	A933	A789	C683	A609
C1564	G1482	G1412	U1341	A1269	G1195	G1120	C1004	C934	C791	C686	C610
G1565	G1483	G1413	G1344	C1270	U1198	C1121	C1005	G934	C792	C612	C611
A1566	G1484	G1414	G1345	G1271	U1199	G1122	C1006	A941	G793	C613	C612
A1567	G1485	G1415	G1346	A1272	C1200	C1123	C1007	G942	A793	C691	A614
G1568	A1486	C1417	G1347	U1273	C1201	G1124	A1010	U943	C796	C692	U614A
U1569	G1487	G1418	G1348	A1274	C1202	A1125	G1011	G944	C797	G696	A614B
A1569	G1488	A1419	A1349	A1275	G1203	A1126	U1012	A945	C798	C697	A614C
A1570	U1489	U1420	C1350	A1276	A1204	U1130	G1013	G946	C799	C698	G615
A1571	A1490	G1421	C1351	A1278	U1205	C1135	U1014	G947	A802	U703	G619
A1572	G1491	G1424	U1352	G1281	C1208	G1136	G1015	G950	U803	G704	G620
A1573	G1492	G1425	A1353	A1286	G1209	C1137	G1016	C951	A804	G705	A621
C1574	A1493	G1426	G1354	U1287	A1210	C1140	U1017	G952	C806	C708	G622
C1577	A1494	A1427	G1355	U1288	U1211	U1141	U1018	A953	U807	G709	G623
U1578	A1495	C1428	U1357	U1289	G1216	U1142	A1020	G954	G808	G710	G624
A1579	A1496	G1429	G1358	C1290	C1221	A1142A	A1021	C955	U811	G712	G625
C1587	U1497	U1431	A1359	C1291	C1222	U1022	G956	A957	C812	G713	U627
U1559	C1499	C1432	C1362	U1292	C1221A	G1144	U1023	U958	U813	G717	

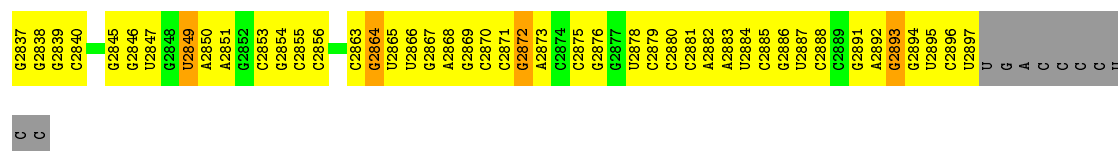
A2662	A2663	G2664	A2665	C2666	C2667	G2672	G2673	A2678	A2679	C2680	C2681	A2600	C2683	A2602	C2606	G2667	G2668	C2689	C2690	C2610	C2611	C2612	C2613	C2638	C2695	C2696	C2697	C2698	C2650	C2656	C2657	C2658	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655	C2656	C2657	C2658	C2659	C2660	C2661	C2662	C2663	C2664	C2665	C2666	C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689	C2690	C2691	C2692	C2693	C2694	C2695	C2696	C2697	C2698	C2699	C2700	C2701	C2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	C2711	C2712	C2713	C2714	C2715	C2716	C2717	C2718	C2719	C2720	C2721	C2722	C2723	C2724	C2725																																							
U2580	G2581	G2582	G2583	U2584	C2585	A2586	A2587	A2590	C2591	U2592	U2593	C2594	A2600	C2601	A2602	C2606	G2607	G2608	C2609	C2610	C2611	C2612	C2613	C2638	C2695	C2696	C2697	C2698	C2650	C2656	C2657	C2658	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655	C2656	C2657	C2658	C2659	C2660	C2661	C2662	C2663	C2664	C2665	C2666	C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689	C2690	C2691	C2692	C2693	C2694	C2695	C2696	C2697	C2698	C2699	C2700	C2701	C2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	C2711	C2712	C2713	C2714	C2715	C2716	C2717	C2718	C2719	C2720	C2721	C2722	C2723	C2724	C2725																																							
U2357	G2358	C2359	A2360	C2364	G2365	G2373	C2374	C2375	A2376	C2377	A2378	G2379	C2380	G2383	C2384	C2385	U2387	A2388	C2389	U2390	C2391	A2392	C2393	C2395	C2396	C2397	U2398	G2399	C2400	U2401	C2402	U2406	U2408	C2409	G2410	G2414	G2415	C2416	U2419	A2422	U2423	C2424	A2425	C2426	C2427	G2428	G2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	A2448	A2453	G2454	G2455	G2456	U2457	C2458	C2461	C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	U2473	C2474	C2475	C2476	C2477	A2478	C2479	C2480	C2481	C2482	C2483	G2484	G2485	G2486	C2487	A2488	U2489	C2490	C2491	C2494	A2495	C2496	A2497	C2498	C2499	A2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2512	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	A2533	C2534	C2535	C2536	C2537	C2538	C2539	C2542	C2543	C2544	C2549	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2577	C2578	C2579
U2357	G2358	C2359	A2360	C2364	G2365	G2373	C2374	C2375	A2376	C2377	A2378	G2379	C2380	G2383	C2384	C2385	U2387	A2388	C2389	U2390	C2391	A2392	C2393	C2395	C2396	C2397	U2398	G2399	C2400	U2401	C2402	U2406	U2408	C2409	G2410	G2414	G2415	C2416	U2419	A2422	U2423	C2424	A2425	C2426	C2427	G2428	G2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	A2448	A2453	G2454	G2455	G2456	U2457	C2458	C2461	C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	U2473	C2474	C2475	C2476	C2477	A2478	C2479	C2480	C2481	C2482	C2483	G2484	G2485	G2486	C2487	A2488	U2489	C2490	C2491	C2494	A2495	C2496	A2497	C2498	C2499	A2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2512	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	A2533	C2534	C2535	C2536	C2537	C2538	C2539	C2542	C2543	C2544	C2549	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2577	C2578	C2579
U2357	G2358	C2359	A2360	C2364	G2365	G2373	C2374	C2375	A2376	C2377	A2378	G2379	C2380	G2383	C2384	C2385	U2387	A2388	C2389	U2390	C2391	A2392	C2393	C2395	C2396	C2397	U2398	G2399	C2400	U2401	C2402	U2406	U2408	C2409	G2410	G2414	G2415	C2416	U2419	A2422	U2423	C2424	A2425	C2426	C2427	G2428	G2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	A2448	A2453	G2454	G2455	G2456	U2457	C2458	C2461	C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	U2473	C2474	C2475	C2476	C2477	A2478	C2479	C2480	C2481	C2482	C2483	G2484	G2485	G2486	C2487	A2488	U2489	C2490	C2491	C2494	A2495	C2496	A2497	C2498	C2499	A2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2512	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	A2533	C2534	C2535	C2536	C2537	C2538	C2539	C2542	C2543	C2544	C2549	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2577	C2578	C2579
U2580	G2581	G2582	G2583	U2584	C2585	A2586	A2587	A2590	C2591	U2592	U2593	C2594	A2600	C2601	A2602	C2606	G2607	G2608	C2609	C2610	C2611	C2612	C2613	C2638	C2695	C2696	C2697	C2698	C2650	C2656	C2657	C2658	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655	C2656	C2657	C2658	C2659	C2660	C2661	C2662	C2663	C2664	C2665	C2666	C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689	C2690	C2691	C2692	C2693	C2694	C2695	C2696	C2697	C2698	C2699	C2700	C2701	C2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	C2711	C2712	C2713	C2714	C2715	C2716	C2717	C2718	C2719	C2720	C2721	C2722	C2723	C2724	C2725																																							
A1665	G1666	G1667	A1668	A1669	C1670	G1674	C1675	G1678	G1681	C1685	C1686	G1687	U1688	A1689	U1692	C1693	G1696	G1697	A1698	A1700	A1701	C1708	U1709	C1710	C1711	C1712	U1713	G1714	G1717	G1719	U1720	G1721	A1722	U1739	G1740	A1741	G1742	C1743	C1744	C1745	C1746	G1747	G1747A	G1748	A1749	C1750	C1751	C1752																																																																																																																		
G1753	C1754	A1762	G1763	G1765	U1766	G1767	C1771	G1772	A1773	U1778	A1780	C1781	C1782	A1783	A1784	A1785	A1786	A1789	C1790	A1791	U1794	C1795	U1796	C1797	C1798	G1799	C1800	G1801	A1802	A1803	C1804	U1805	U1808	A1809	A1810	G1811	A1812	G1813	G1814	A1815	C1816	G1817	U1818	U1820	G1826	C1827	C1828	A1829	C1830																																																																																																																	
G1835	C1836	C1837	U1841	G1842	C1843	G1844	G1845	A1847	A1848	U1851	C1852	A1853	A1854	G1855	G1856	G1857	G1858	U1863	U1864	G1865	C1866	A1876	G1877	C1878	C1879	C1880	C1881	C1882	G1883	A1884	A1885	C1886	C1887	C1888	A1889	G1899	A1900	A1901	C1902	G1906	G1907	C1908	C1909	C1914	U1915	U1923	C1924	C1925	U1926	A1927																																																																																																																
A1928	G1929	G1930	G1935	A1936	A1937	A1938	U1939	U1946	C1947	G1948	A1952	A1953	G1954	U1955	C1958	G1959	A1960	C1961	C1962	U1963	G1964	C1965	A1966	G1967	C1968	A1969	A1970	C1971	G1972	G1973	C1974	G1975	G1980	C1981	C1982	C1983	A1986	G1987	C1988	G1989	C1990	G1991	C1992	U1993	G1997	G1998	C1999	C2000	A2001	G2002	C2006																																																																																																															
G2009	U2010	G2011	A2012	A2013	A2014	A2015	U2016	U2022	G2023	G2024	C2025	C2026	G2029	A2030	A2031	G2032	A2033	U2034	G2035	C2036	C2039	C2040	U2041	A2042	C2043	C2052	C2055	C2056	C2063	C2064	C2065	A2066	G2061	A2062	C2063	C2064	C2065	C2066	U2068	G2069	G2070	C2073	U2074	U2075	C2078	U2079	C2080	C2081	A2082	G2083																																																																																																																
U2086	G2087	G2088	U2091	G2094	U2095	C2096	U2098	U2099	G2100	C2103	C2104	C2105	U2109	G2110	G2111	G2112	U2113	A2114	G2115	G2116	U2117	C2118	A2119	C2120	G2121	U2122	U2123	C2124	G2125	A2126	G2127	C2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	C2136	U2137	C2138	C2139	C2140	G2141	C2142	C2143	U2144	C2145	C2146	G2147	G2148	U2150																																																																																																													
G2151	G2152	G2153	G2154	G2155	G2156	G2157	A2158	G2159	G2160	U2161	G2162	C2163	C2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	C2175	C2176	C2177	C2178	C2179	U2180	C2181	U2182	C2183	G2184	C2185	C2186	G2187	C2188	U2189	C2190	G2191	C2192	C2193	C2194	C2195	C2196	U2197	A2198	C2199	C2200	C2201	C2202	U2203	C2205	G2206	G2207	A2208	U2218	G2219	C2220																																																																																																							
G2221	G2222	G2223	G2224	A2225	A2226	A2227	G2228	G2229	C2230	C2231	U2232	U2233	G2234	G2235	C2236	G2237	G2238	G2239	C2240	A2241	G2242	G2243	U2244	U2245	G2246	A2247	C2248	U2249	G2250	G2251	U2257	C2258	G2259	C2260	C2261	U2262	C2263	C2264	U2272	U2273	A2274	C2275	G2276	G2277	G2282	C2283	G2284	C2285	A2286	C2287	A2288																																																																																																															
G2289	G2290	U2291	C2292	C2293	C2297	A2298	G2299	C2300	C2301	C2302	G2303	G2304	A2305	C2306	G2307	C2308	A2309	A2310	U2312	C2313	C2314	C2315	G2316	C2317	C2318	C2319	C2320	C2321	C2325	C2326	C2327	A2328	C2329	C2330	G2331	C2334	A2335	A2336	C2340	C2341	C2342	C2345	A2346	C2347	U2348	C2349	C2350	C2351	A2352	C2353	C2354	C2356																																																																																																														
U2357	G2358	C2359	A2360	C2364	G2365	G2373	C2374	C2375</																																																																																																																																																										



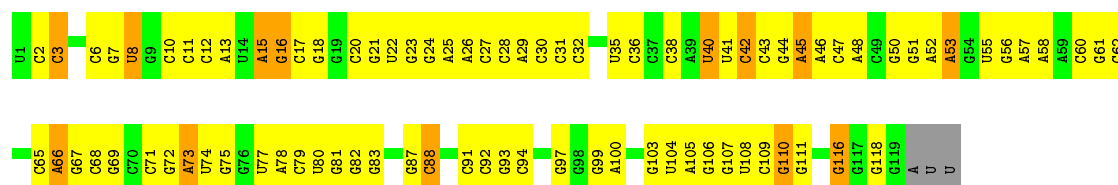




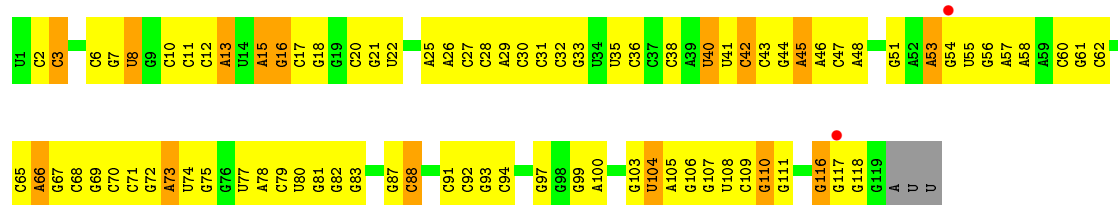
G2770	G2771	A2711	U2637	G2485	G2340	G2271	U2197	G2137	G2065	A1981	C1892	G1804
G2772	G2773	A2712	U2638	G2486	G2341	U2272	A2198	C2138	C2066	C1982	C1893	U1805
G2774	G2775	A2713	G2638	G2487	G2342	A2273	A2199	C2139	G2067	G1898	G1899	A1810
A2776	A2777	C2714	G2645	A2488	G2343	A2274	C2201	C2140	G2069	A1886	A1887	A1811
A2778	A2779	C2715	G2646	G2489	A2345	G2275	C2202	G2141	G2070	A1890	A1891	A1812
A2780	A2781	C2716	U2647	G2490	C2347	G2276	C2203	C2142	U2074	A1901	A1902	G1813
A2782	A2783	G2717	G2648	U2491	U2348	G2277	C2204	C2143	U2075	G1988	G1989	G1814
G2784	G2785	G2718	G2649	G2494	U2349	G2282	C2205	U2144	G2076	G1990	G1991	G1816
G2787	G2788	G2719	G2650	G2495	C2350	G2283	G2206	C2145	G2080	G1992	G1993	G1817
G2789	G2790	G2720	G2651	A2425	C2351	C2284	A2207	C2146	G2081	G1994	G1995	A1819
G2791	G2792	A2721	C2499	C2498	A2352	C2285	G2218	G2147	A2082	U1992	U1993	U1820
G2793	G2794	G2722	C2499	C2499	A2353	C2286	G2219	G2148	G2083	G1997	G1998	G1826
G2795	G2796	C2723	G2502	G2502	U2431	A2287	G2220	U2150	U2086	G1999	G1999	C1827
G2797	G2798	C2724	A2503	U2504	C2355	A2288	G2221	G2151	G2087	A1916	A1917	G1828
G2800	G2801	G2725	U2504	U2504	C2356	G2289	G2222	G2152	G2088	A1918	A1919	A1829
G2802	G2803	U2726	G2505	G2505	U2357	G2290	G2223	G2153	G2089	G2001	G2002	C1830
G2804	G2805	U2727	U2506	U2506	G2358	U2291	G2224	G2154	G2090	U1923	U1924	U1841
G2807	G2808	G2728	C2507	C2507	C2359	C2292	A2225	G2155	G2100	G1935	G1936	G1842
G2809	G2810	A2733	U2511	U2511	A2360	C2293	G2226	G2156	G2103	A1937	A1938	C1843
G2811	G2812	G2734	C2512	C2512	G2364	G2297	A2227	G2157	G2104	U1939	U1940	G1844
G2813	G2814	G2735	G2513	G2513	C2365	A2298	G2228	A2158	G2105	A1941	A1942	G1845
G2815	G2816	G2736	C2514	C2514	G2366	A2299	G2229	G2159	G2106	A1943	A1944	G1846
G2817	G2818	U2737	C2515	C2515	G2367	G2300	U2232	G2160	G2107	A1945	A1946	G1847
G2819	G2820	A2738	U2516	U2516	C2368	G2301	U2233	G2161	G2108	U1851	U1852	A1848
G2821	G2822	U2739	G2517	G2517	A2375	G2302	U2234	G2162	G2109	C1852	C1853	G1854
G2823	G2824	G2740	U2518	U2518	U2376	G2303	G2235	G2163	G2110	A1952	A1953	G1855
G2825	G2826	A2741	G2519	G2519	C2379	G2304	G2236	G2164	G2111	G1954	G1955	G1856
G2827	G2828	G2742	G2520	G2520	C2380	G2305	G2237	U2167	G2112	U1956	U1957	U1857
G2829	G2830	C2743	U2521	U2521	G2381	G2306	G2238	A2168	G2113	G1958	G1959	U1858
G2831	G2832	G2744	U2522	U2522	C2382	G2307	G2239	A2169	G2114	C1962	C1963	G1859
G2833	G2834	U2745	G2523	G2523	U2383	G2308	U2240	A2170	G2115	U1962	U1963	G1860
G2835	G2836	A2746	U2524	U2524	G2384	G2309	A2241	A2171	G2116	G1964	G1965	C1877
G2837	G2838	G2747	G2525	G2525	C2385	A2310	G2242	A2172	G2117	A1966	A1967	C1878
G2839	G2840	U2748	G2526	G2526	U2386	G2311	U2243	A2173	G2118	G1968	G1969	C1879
G2841	G2842	C2749	U2527	U2527	U2387	G2312	U2244	C2174	G2119	U1969	U1970	C1880
G2843	G2844	G2750	G2528	G2528	A2388	G2313	U2245	C2175	G2120	G1971	G1972	C1881
G2845	G2846	C2751	U2529	U2529	G2389	G2314	U2246	A2176	G2121	A1972	A1973	G1882
G2847	G2848	G2752	G2530	G2530	U2390	G2315	G2247	C2177	G2122	G1974	G1975	G1883
G2849	G2850	C2753	U2531	U2531	G2391	G2316	G2248	C2178	G2123	A1884	A1885	G1884
G2851	G2852	U2754	G2532	G2532	A2392	G2317	U2249	C2179	G2124	A1886	A1887	G1885
G2853	G2854	A2755	U2533	U2533	C2393	G2318	U2250	U2180	G2125	G1888	G1889	G1886
G2855	G2856	G2756	G2534	G2534	U2394	G2319	G2251	G2181	G2126	A1969	A1970	C1887
G2857	G2858	U2757	U2535	U2535	C2395	A2320	G2252	G2182	G2127	G1971	G1972	C1888
G2859	G2860	C2758	A2542	A2542	G2396	G2321	G2253	C2183	G2128	C2055	C2056	G1889
G2861	G2862	G2759	G2543	G2543	U2397	G2322	G2254	G2184	G2129	A2059	A2060	G1890
G2863	G2864	U2760	U2544	U2544	G2398	G2323	G2255	C2185	U2130	G2061	G2062	C1891
G2865	G2866	A2761	G2545	G2545	U2399	G2324	G2256	C2186	G2131	G2063	G2064	G1892
G2867	G2868	C2762	G2546	G2546	G2400	A2327	G2257	G2187	G2132	G1973	G1974	C1893
G2869	G2870	G2763	U2547	U2547	U2401	G2328	G2258	C2188	G2133	G1975	G1976	G1894
G2871	G2872	U2764	G2548	G2548	C2402	G2329	G2259	G2189	G2134	G1980	G1981	G1895
G2873	G2874	A2765	U2549	U2549	G2403	G2330	G2260	C2190	G2135	G1982	G1983	G1896
G2875	G2876	G2766	G2550	G2550	U2406	G2331	G2261	G2191	G2136	G1984	G1985	G1897
G2877	G2878	C2767	U2551	U2551	G2407	G2332	G2262	G2192	G2137	G1986	G1987	G1898
G2879	G2880	U2768	G2552	G2552	U2408	G2333	G2263	G2193	G2138	G1988	G1989	G1899
G2881	G2882	G2769	U2553	U2553	G2409	G2334	G2264	G2194	G2139	G1989	G1990	G1900
G2883	G2884	A2770	G2554	G2554	U2410	G2335	G2265	G2195	G2140	G1991	G1992	G1901
G2885	G2886	C2771	U2555	U2555	G2411	G2336	G2266	G2196	G2141	G1993	G1994	G1902
G2887	G2888	G2772	G2556	G2556	G2412	G2337	G2267	G2197	G2142	G1995	G1996	G1903
G2889	G2890	U2773	U2557	U2557	U2413	G2338	G2268	G2198	G2143	G1997	G1998	G1904
G2891	G2892	A2774	G2558	G2558	G2414	G2339	G2269	G2199	G2144	G1999	G2000	G1905
G2893	G2894	G2775	G2559	G2559	G2415	G2340	G2270	G2200	G2145	G2001	G2002	G1906
G2895	G2896	C2776	U2560	U2560	G2416	G2341	G2271	G2201	G2146	G2003	G2004	G1907
G2897	G2898	U2777	G2561	G2561	G2417	G2342	G2272	G2202	G2147	G2005	G2006	G1908
G2899	G2900	G2778	U2562	U2562	G2418	G2343	G2273	G2203	G2148	G2007	G2008	G1909
G2901	G2902	A2779	G2563	G2563	U2419	G2344	G2274	G2204	G2149	G2009	G2010	G1910
G2903	G2904	U2780	U2564	U2564	G2420	G2345	G2275	G2205	U2076	G2011	G2012	G1911
G2905	G2906	C2781	G2565	G2565	A2421	G2346	G2276	G2206	G2077	G2013	G2014	G1912
G2907	G2908	G2782	G2566	G2566	U2422	G2347	G2277	G2207	G2078	G2015	G2016	G1913
G2909	G2910	A2783	U2567	U2567	A2423	G2348	G2278	G2208	G2079	G2017	G2018	G1914
G2911	G2912	G2784	G2568	G2568	U2424	G2349	G2279	G2209	G2080	G2019	G2020	G1915
G2913	G2914	U2785	G2569	G2569	A2425	G2350	G2280	G2210	G2081	G2021	G2022	G1916
G2915	G2916	G2786	G2570	G2570	G2426	G2351	G2281	G2211	G2082	G2023	G2024	G1917
G2917	G2918	A2787	U2571	U2571	A2427	G2352	G2282	G2212	G2083	G2025	G2026	G1918
G2919	G2920	U2788	G2572	G2572	G2428	G2353	G2283	G2213	G2084	G2027	G2028	G1919
G2921	G2922	G2789	C2573	C2573	A2429	G2354	G2284	G2214	G2085	G2029	G2030	G1920
G2923	G2924	A2789	U2574	U2574	U2430	G2355	G2285	G2215	G2086	G2031	G2032	G1921
G2925	G2926	U2790	G2575	G2575	U2431	G2356	G2286	G2216	G2087	G2033	G2034	G1922
G2927	G2928	G2791	G2576	G2576	A2432	G2357	G2287	G2217	G2088	G2035	G2036	G1923
G2929	G2930	A2791	U2577	U2577	G2433	G2358	G2288	G2218	G2089	G2037	G2038	G1924
G2931	G2932	U2792	G2578	G2578	U2434	G2359	G2289	G2219	G2090	G2039	G2040	G1925
G2933	G2934	G2793	C2579	C2579	G2435	G2360	G2290	G2220	G2091	G2041	G2042	G1926
G2935	G2936	A2794	U2580	U2580	G2436	G2361	G2291	G2221	G2092	G2043	G2044	G1927
G2937	G2938	U2795	G2581	G2581	G2437	G2362	G2292	G2222	G2093	G2045	G2046	G1928
G2939	G2940	G2796	G2582	G2582	U2438	G2363	G2293	G2223	G2094	G2047	G2048	G1929
G2941	G2942	A2797	U2583	U2583	G2439	G2364	G2294	G2224	G2095	G2049	G2050	G1930
G2943	G2944	U2798	G2584	G2584	U2440	G2365	G2295	G2225	G2096	G2051	G2052	G1931
G2945	G2946	G2799	U2585	U2585	G2441	G2366	G2296	G2226	G2097	G2053	G2054	G1932
G2947	G2948	A2799	G2586	G2586	G2442	G2367	G2297	G2227	G2098	G2055	G2056	G1933
G2949	G2950	U2800	U2587	U2587	G2443	G2368	G2298	G2228	G2099	G2057	G2058	G1934
G2951	G2952	C2799	G2588	G2588	U2444	G2369	G2299	G2229	G2100	G2059	G2060	G1935
G2953	G2954	G2800	G2589	G2589	G2445	G2370	G2300	G2230	G2101	G2061	G2062	G1936
G2955	G2956	A2801	U2590	U2590	G2446	G2371	G2301	U2231	G2102	G2063	G2064	G1937
G2957	G2958	U2801	G2591	G2591	U2447	G2372	G2302	U2232	G2103	G2065	G2066	G1938
G2959	G2960	G2802	U2592	U2592	G2448	G2373	G2303	U2233	G2104	G2067	G2068	G1939
G2961	G2962	A2803	U2593	U2593	U2449	G2374	G2304	U2234	G2105	G2069	G2070	G1940
G2963	G2964	U2804	G2594	G2594	G2450	G2375	G2305	U2235	G2106	G2071	G2072	G1941
G2965	G2966	G2805	U2595	U2595	A2451	G2376	G2306	U2236	G2107	G2073	G2074	G1942
G2967	G2968	A2806	G2596	G2596	G2452	G2377	G2307	U2237	G2108	G2075	G2076	G1943
G2969	G2970	U2807	U2597	U2597	A2453	G2378	G2308	U2238	G2109	G2077	G2078	G1944
G2971	G2972	G2808	G2598	G2598	G2454	G2379	G2309	U2239	G2110	G207		



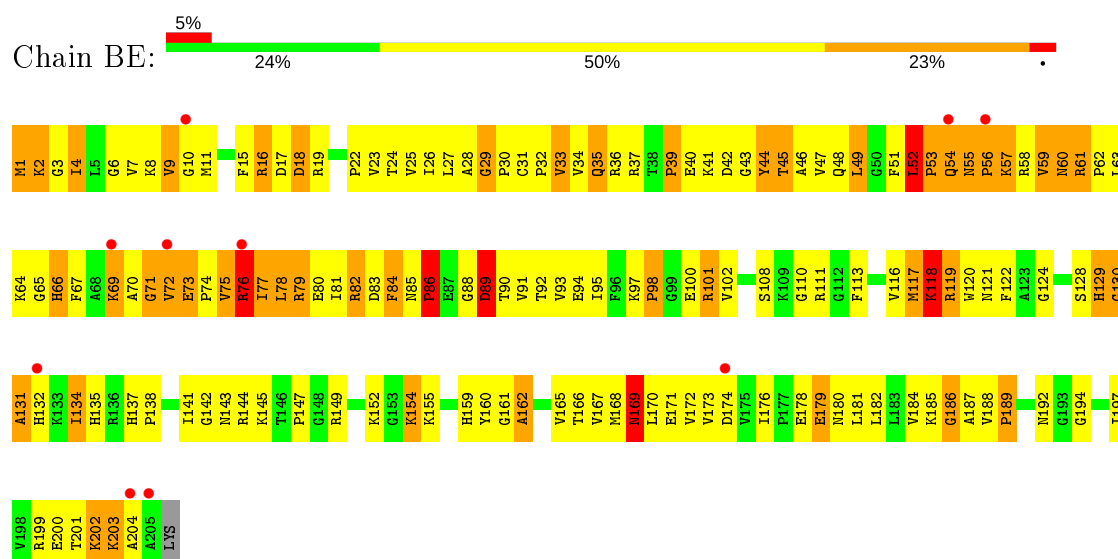
• Molecule 37: 5S RIBOSOMAL RNA



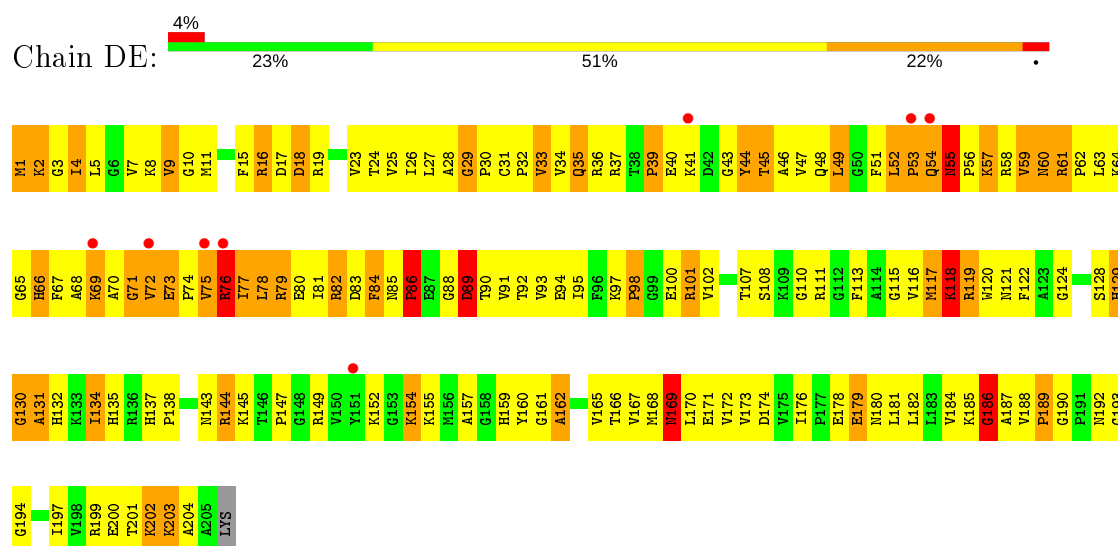
• Molecule 37: 5S RIBOSOMAL RNA



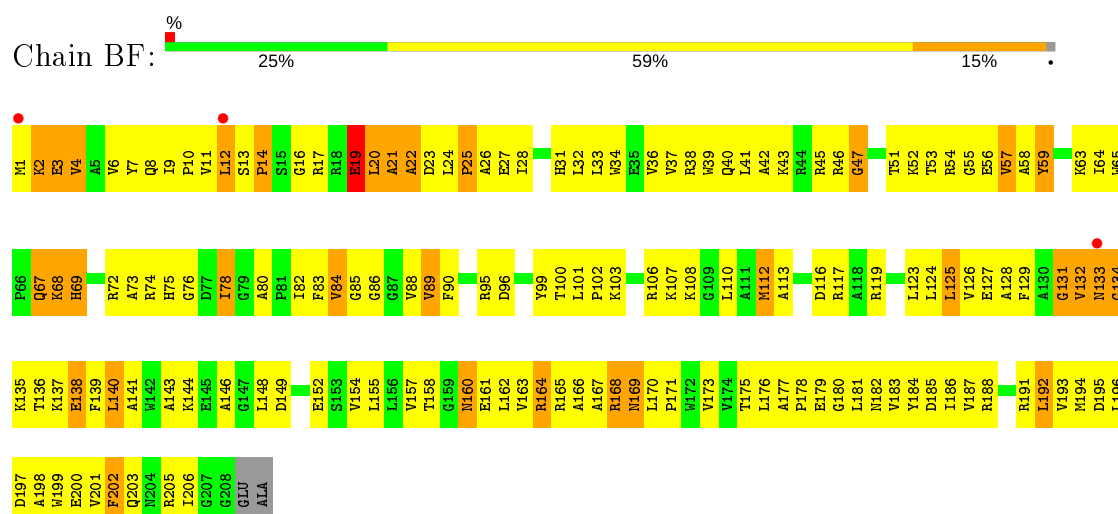




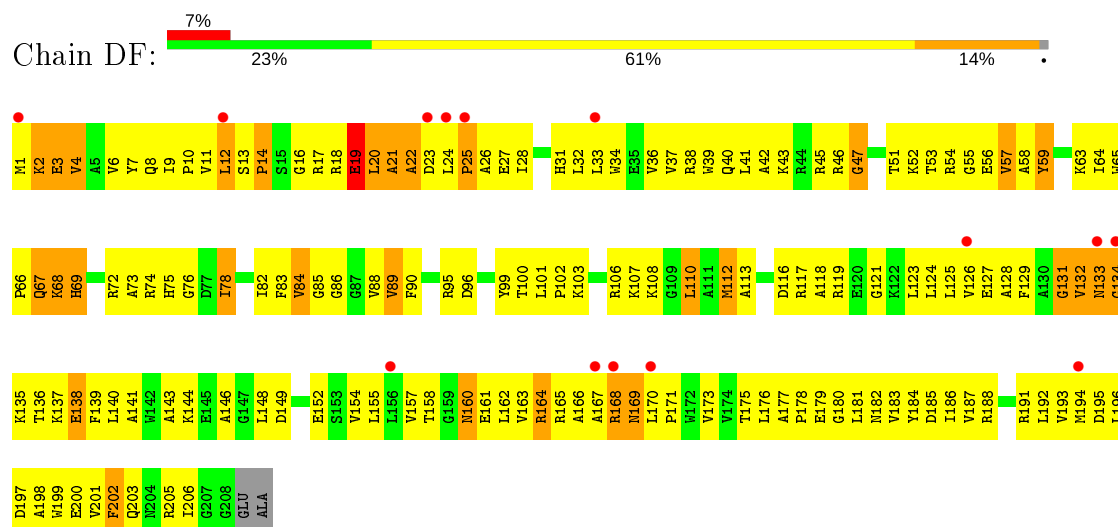
• Molecule 40: 50S RIBOSOMAL PROTEIN L3



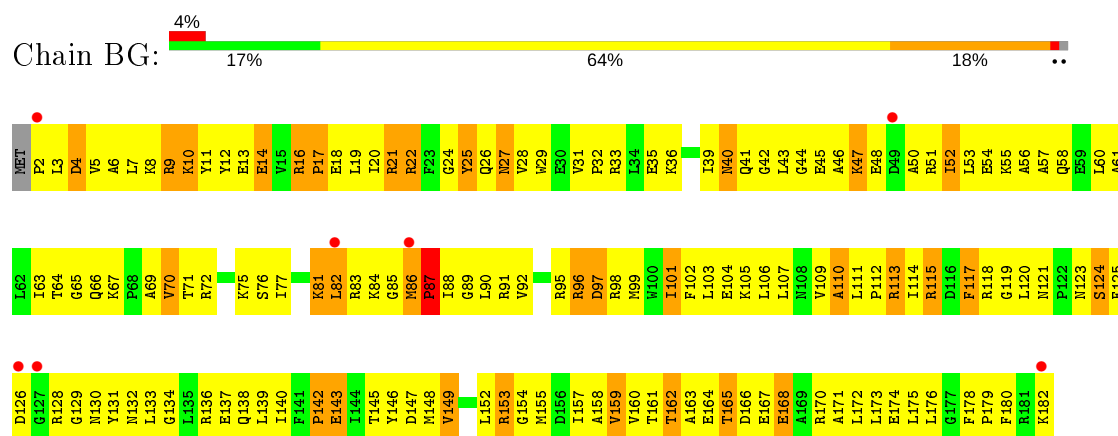
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



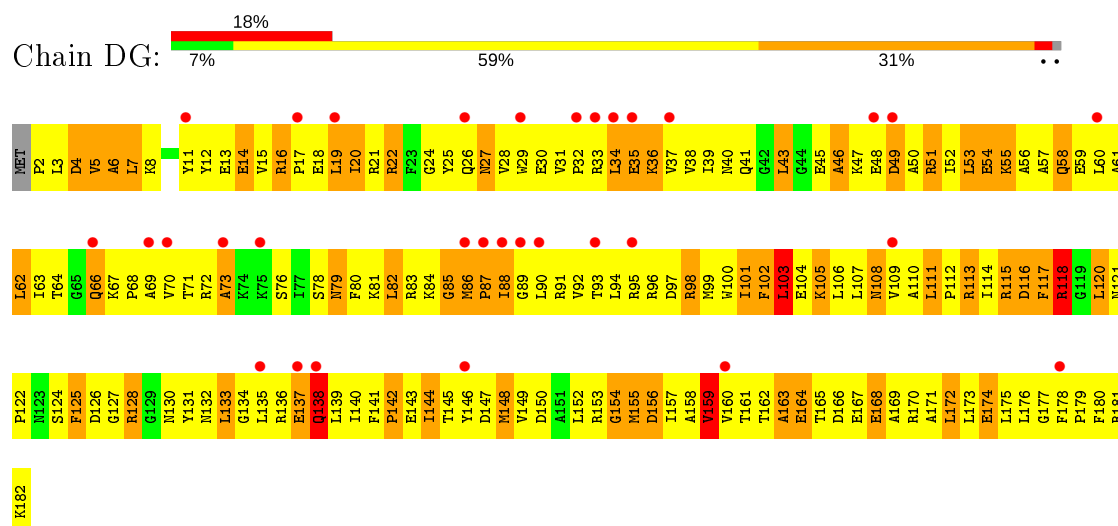
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



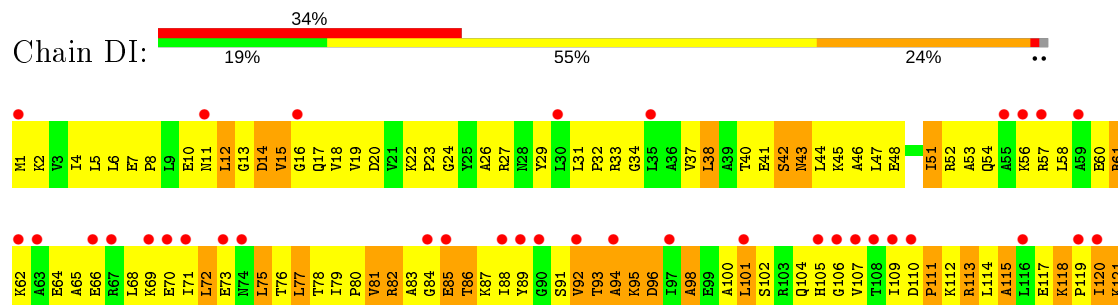
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

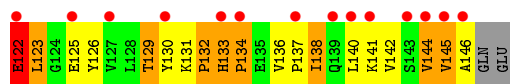


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

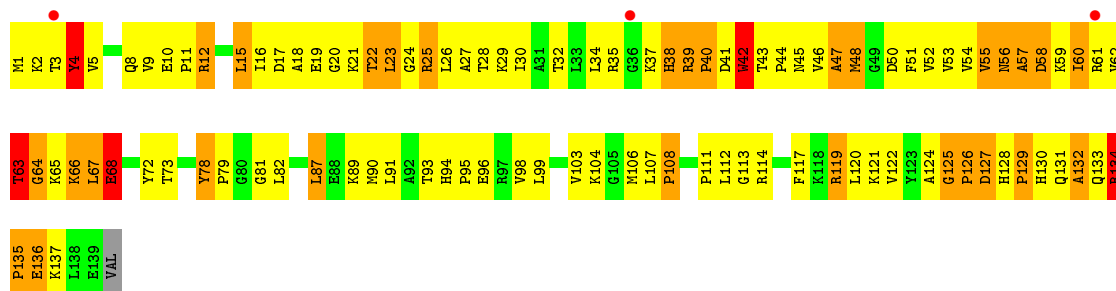


• Molecule 43: 50S RIBOSOMAL PROTEIN L6

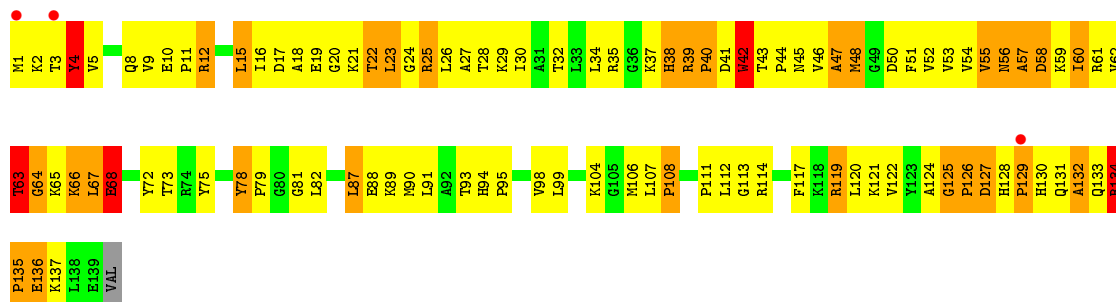




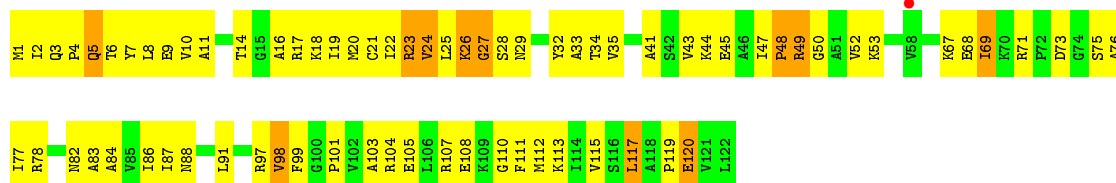
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



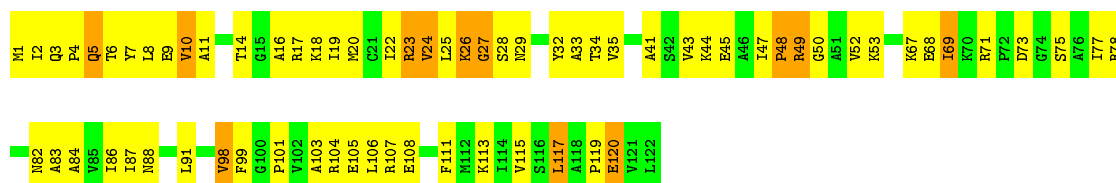
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



• Molecule 46: 50S RIBOSOMAL PROTEIN L14

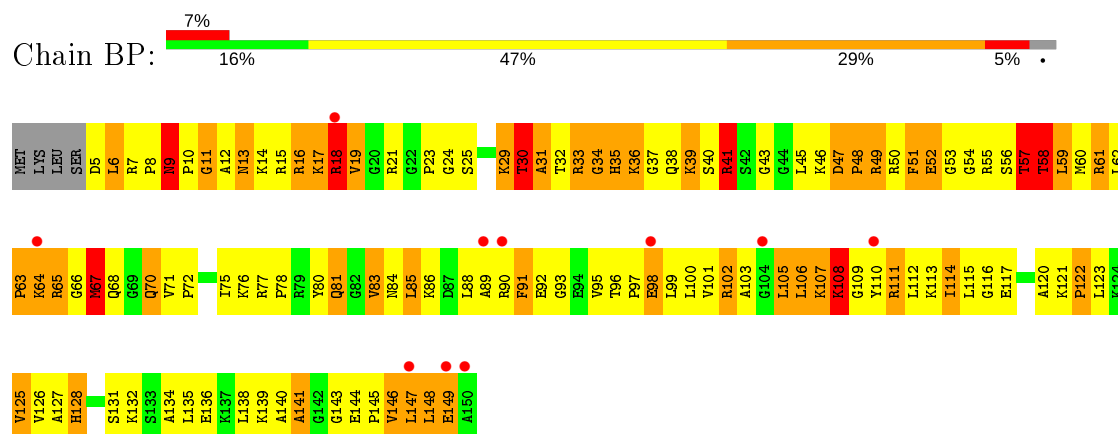


• Molecule 46: 50S RIBOSOMAL PROTEIN L14

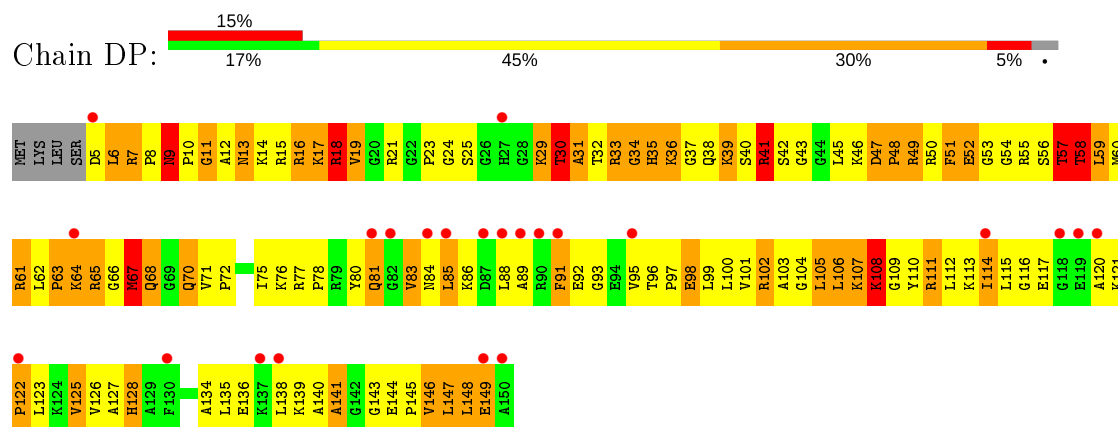




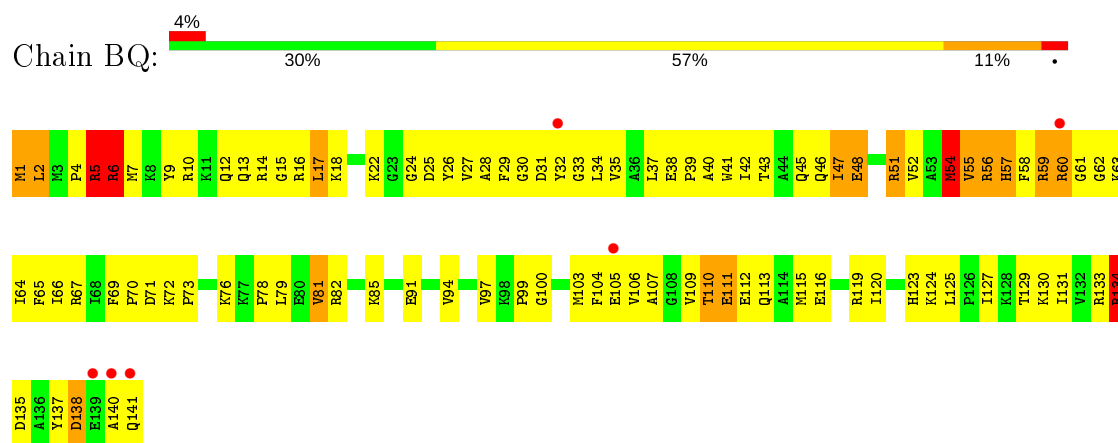
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



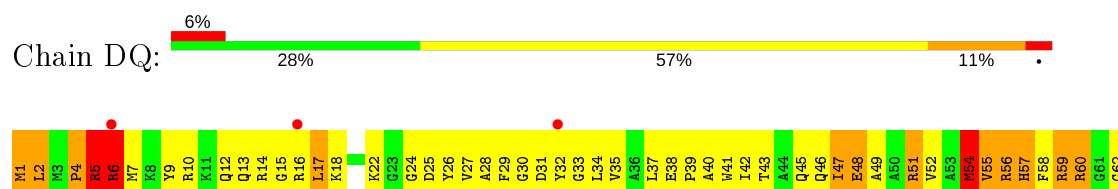
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

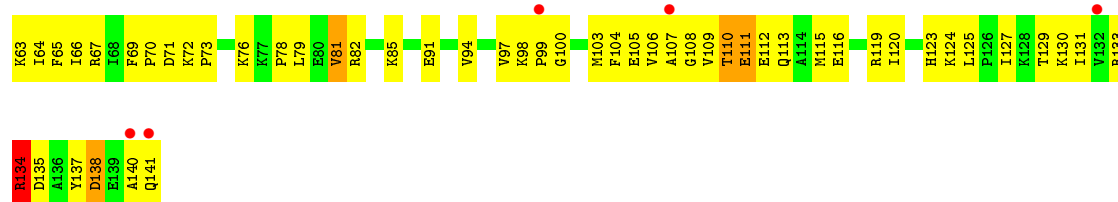


• Molecule 48: 50S RIBOSOMAL PROTEIN L16



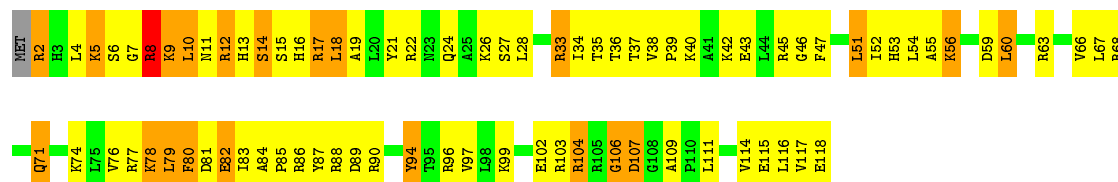
• Molecule 48: 50S RIBOSOMAL PROTEIN L16





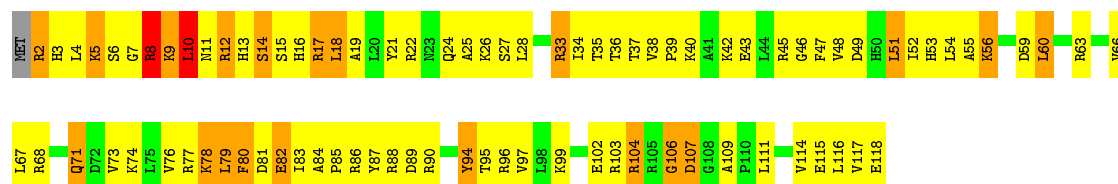
• Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain BR: 31% 50% 18% ..



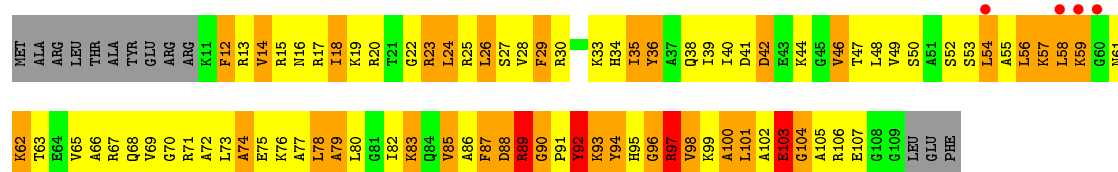
• Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain DR: 25% 55% 17% ..



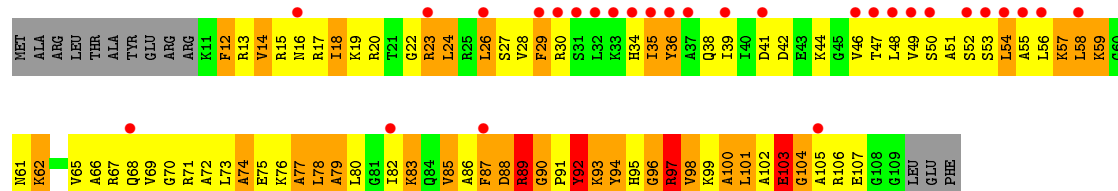
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain BS: 4% 13% 44% 29% 12%



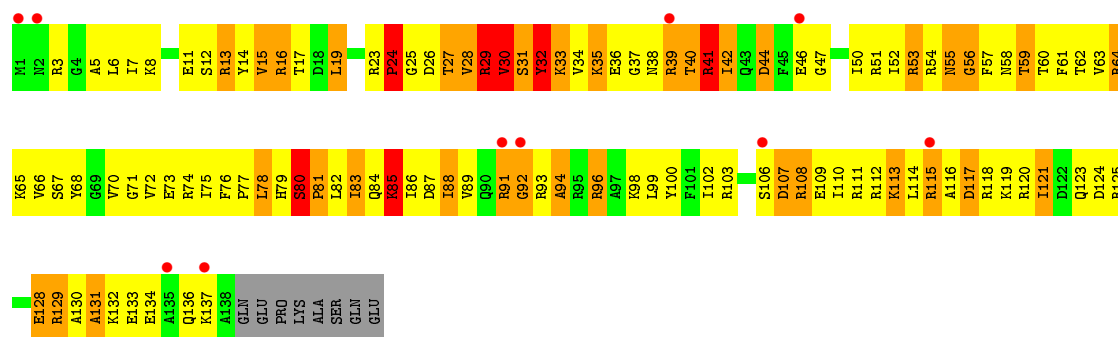
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain DS: 26% 15% 43% 27% 12%

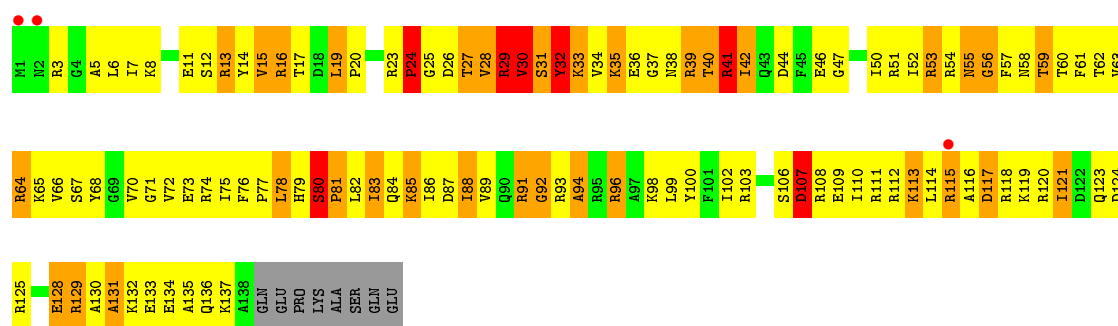
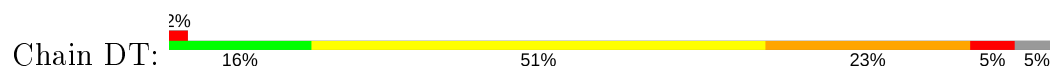


• Molecule 51: 50S RIBOSOMAL PROTEIN L19

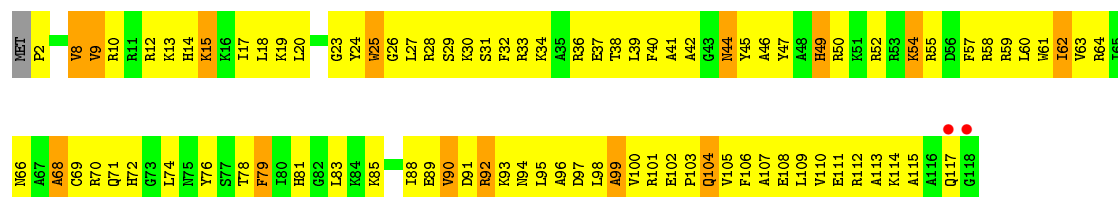
Chain BT: 7% 17% 49% 24% 5% 5%



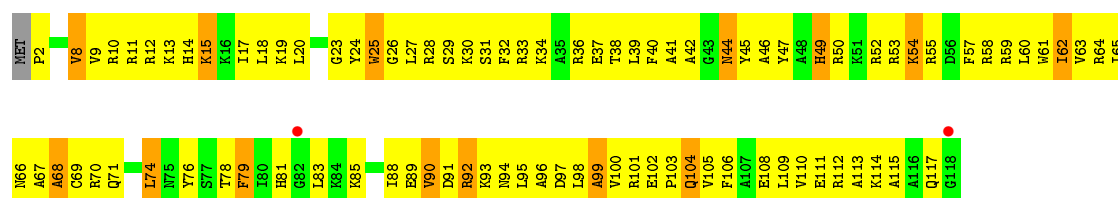
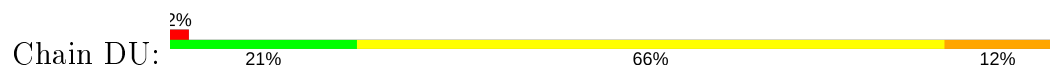
• Molecule 51: 50S RIBOSOMAL PROTEIN L19



• Molecule 52: 50S RIBOSOMAL PROTEIN L20

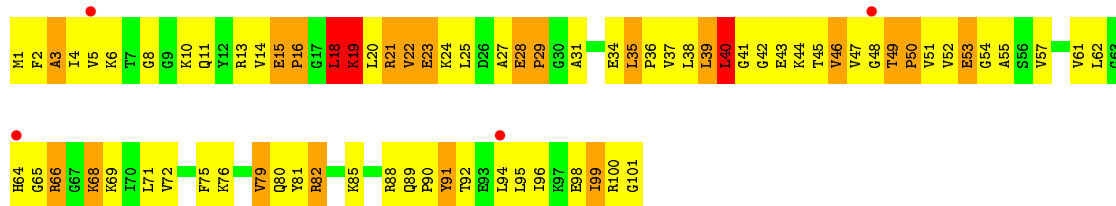


• Molecule 52: 50S RIBOSOMAL PROTEIN L20

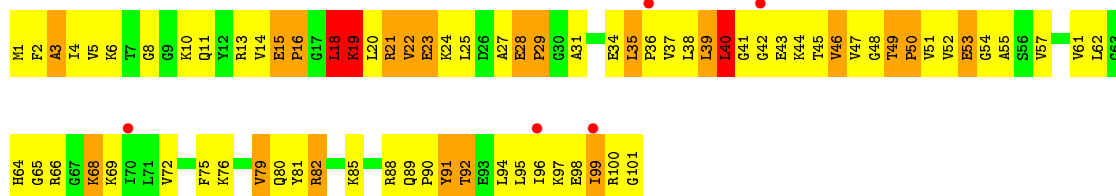


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

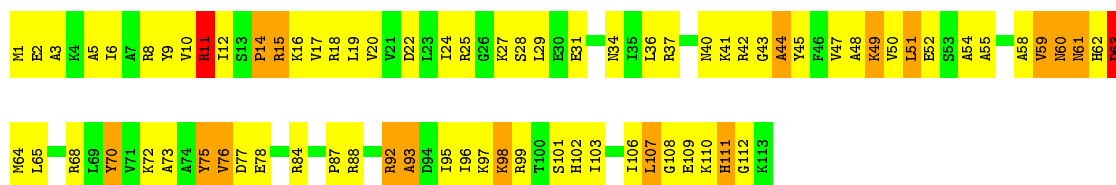




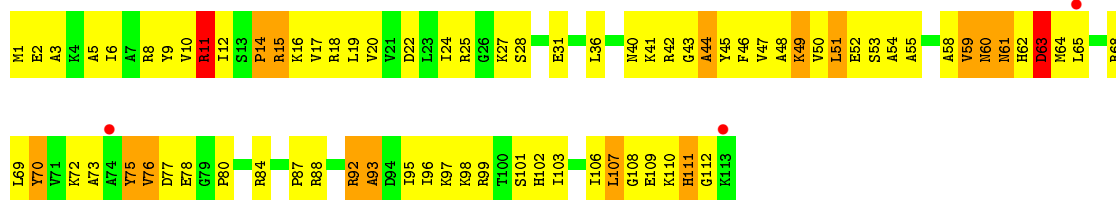
• Molecule 53: 50S RIBOSOMAL PROTEIN L21



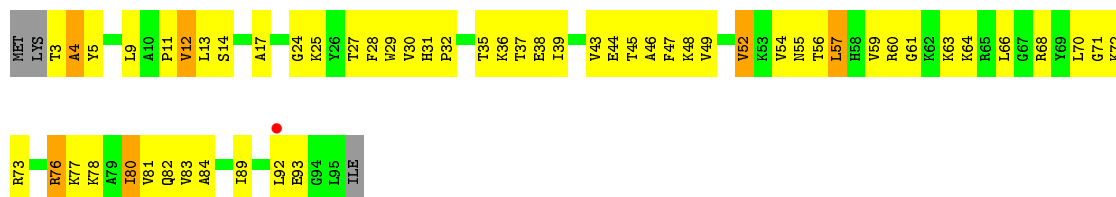
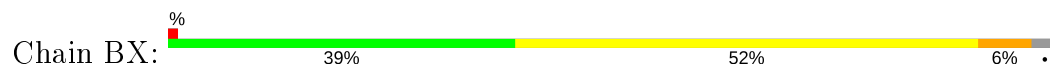
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



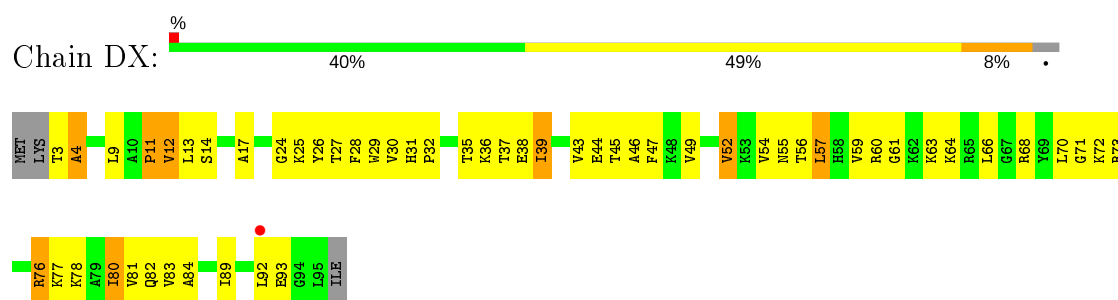
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



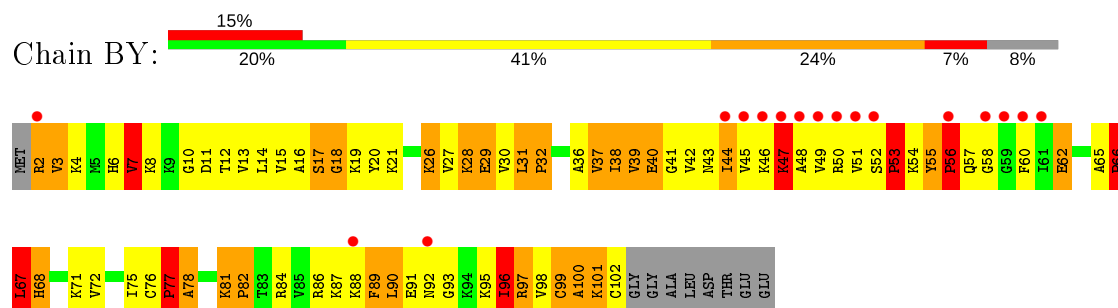
• Molecule 55: 50S RIBOSOMAL PROTEIN L23



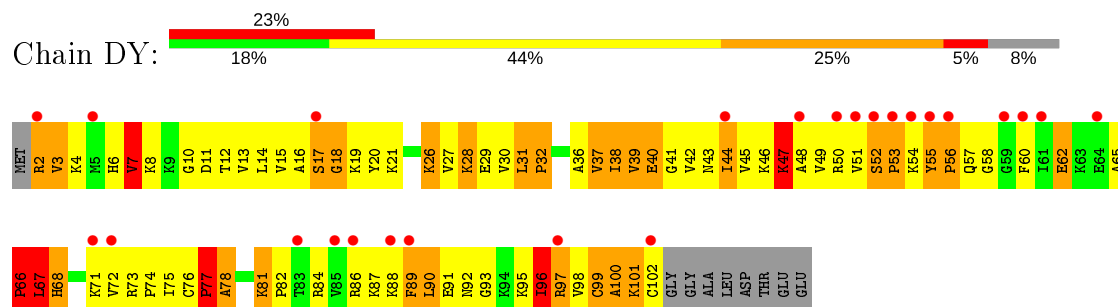
• Molecule 55: 50S RIBOSOMAL PROTEIN L23



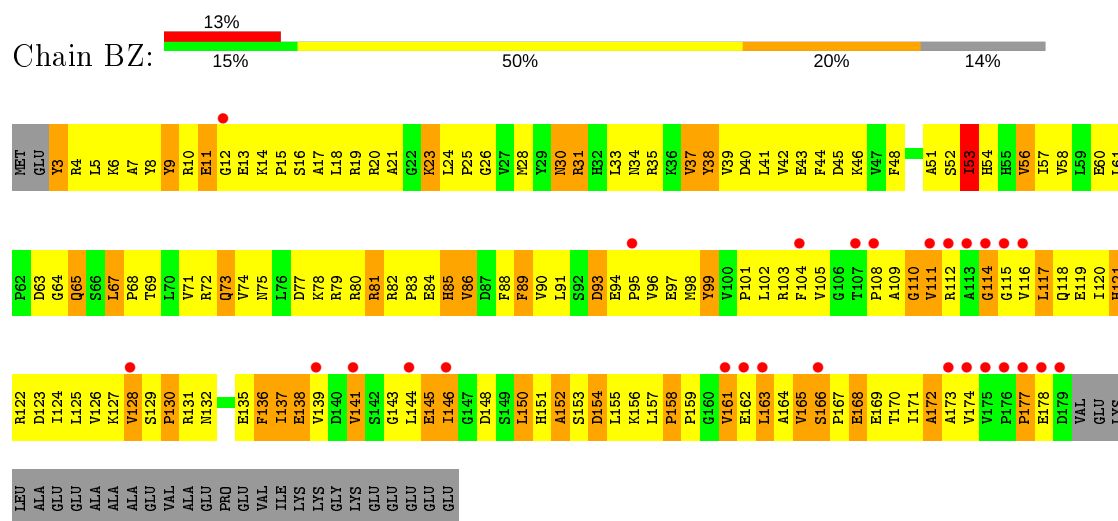
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



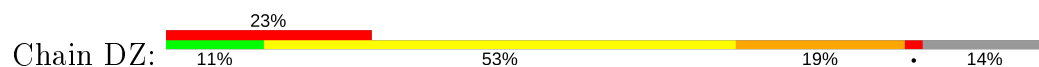
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



• Molecule 57: 50S RIBOSOMAL PROTEIN L25





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.13Å 450.80Å 629.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.99 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.30) 98.2 (49.99-3.01)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.223 , 0.272 0.224 , 0.272	Depositor DCC
$R_{free}$ test set	54674 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 111.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	296168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 5MU, MG, ZN, PHA, PAR, 8AN

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

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



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

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

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

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

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

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

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

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

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

5 of 8 chirality outliers are listed below:

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

5 of 143 planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16314	1190	0
1	CA	32329	0	16315	1198	0
2	AB	1901	0	1951	275	0
2	CB	1901	0	1951	287	0
3	AC	1613	0	1677	212	0
3	CC	1613	0	1677	206	0
4	AD	1703	0	1763	172	0
4	CD	1703	0	1763	167	0
5	AE	1147	0	1207	129	0
5	CE	1147	0	1207	128	0
6	AF	843	0	857	84	0
6	CF	843	0	857	87	0
7	AG	1257	0	1296	145	0
7	CG	1257	0	1296	145	0
8	AH	1116	0	1177	139	0
8	CH	1116	0	1177	150	0
9	AI	1011	0	1041	137	0
9	CI	1011	0	1041	141	0
10	AJ	795	0	840	152	0
10	CJ	795	0	840	148	0
11	AK	885	0	904	103	0
11	CK	885	0	904	115	0
12	AL	971	0	1057	110	0
12	CL	971	0	1057	109	0
13	AM	988	0	1055	130	0
13	CM	988	0	1055	132	0
14	AN	492	0	529	89	0
14	CN	492	0	529	92	0
15	AO	734	0	771	61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	67	0
16	AP	701	0	720	61	0
16	CP	701	0	720	64	0
17	AQ	824	0	891	67	0
17	CQ	824	0	891	70	0
18	AR	574	0	644	60	0
18	CR	574	0	644	62	0
19	AS	630	0	652	110	0
19	CS	630	0	652	115	0
20	AT	763	0	861	100	0
20	CT	763	0	861	102	0
21	AU	209	0	221	16	0
21	CU	209	0	221	18	0
22	AV	1641	0	839	63	0
22	CV	1641	0	839	62	0
23	AW	1619	0	822	93	0
23	CW	1619	0	820	78	0
24	AX	210	0	108	9	0
24	CX	210	0	109	9	0
25	AY	1630	0	831	102	0
25	CY	1630	0	831	101	0
26	B0	662	0	688	74	0
26	D0	662	0	688	80	0
27	B1	732	0	808	96	0
27	D1	732	0	808	92	0
28	B2	598	0	653	72	0
28	D2	598	0	653	75	0
29	B3	468	0	523	67	0
29	D3	468	0	523	69	0
30	B4	226	0	229	34	0
30	D4	226	0	229	32	0
31	B5	459	0	480	51	0
31	D5	459	0	480	51	1
32	B6	381	0	390	63	0
32	D6	381	0	390	64	0
33	B7	419	0	467	46	0
33	D7	419	0	467	44	0
34	B8	508	0	576	100	0
34	D8	508	0	576	95	0
35	B9	299	0	326	22	0
35	D9	299	0	326	24	0
36	BA	60459	0	30476	2031	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DA	60459	0	30472	2077	0
37	BB	2551	0	1295	108	0
37	DB	2551	0	1295	125	0
38	BC	1142	0	865	105	0
38	DC	1142	0	865	100	0
39	BD	2105	0	2182	298	0
39	DD	2105	0	2182	297	0
40	BE	1564	0	1629	259	0
40	DE	1564	0	1629	258	0
41	BF	1624	0	1677	230	0
41	DF	1624	0	1677	229	0
42	BG	1474	0	1534	276	0
42	DG	1474	0	1534	430	0
43	BH	1223	0	1282	197	0
43	DH	1223	0	1282	206	0
44	BI	1132	0	1218	201	0
44	DI	1132	0	1218	209	0
45	BN	1105	0	1180	171	0
45	DN	1105	0	1180	171	0
46	BO	933	0	996	111	0
46	DO	933	0	996	105	0
47	BP	1114	0	1187	300	0
47	DP	1114	0	1187	298	0
48	BQ	1122	0	1179	142	0
48	DQ	1122	0	1179	146	0
49	BR	960	0	1021	145	0
49	DR	960	0	1021	154	0
50	BS	771	0	832	180	0
50	DS	771	0	832	177	0
51	BT	1142	0	1202	260	0
51	DT	1142	0	1202	261	0
52	BU	958	0	1015	179	0
52	DU	958	0	1014	177	0
53	BV	779	0	852	160	0
53	DV	779	0	852	157	1
54	BW	896	0	953	110	0
54	DW	896	0	953	107	0
55	BX	726	0	778	71	0
55	DX	726	0	778	72	0
56	BY	776	0	870	147	0
56	DY	776	0	870	144	0
57	BZ	1404	0	1432	228	0

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DX	3	0	0	0	0
59	AA	42	0	45	1	0
59	CA	42	0	45	3	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	0	0
60	CN	1	0	0	0	0
60	D9	1	0	0	0	0
All	All	296168	0	199731	19126	1

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

The worst 5 of 19126 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BA:1879:C:H2'	36:BA:1880:C:H5"	1.23	1.19
36:DA:1590:U:H2'	36:DA:1591:G:H5"	1.26	1.18
55:BX:27:THR:HG22	55:BX:80:ILE:HB	1.25	1.18
36:DA:271(S):G:H2'	36:DA:271(T):C:H5"	1.25	1.17
13:CM:112:GLY:HA2	13:CM:113:PRO:HD2	1.25	1.16

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D5:59:GLU:N	53:DV:51:VAL:N[4_545]	2.15	0.05

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



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

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BX	91/96 (95%)	66 (72%)	20 (22%)	5 (6%)	2	11
55	DX	91/96 (95%)	65 (71%)	20 (22%)	6 (7%)	1	8
56	BY	99/110 (90%)	47 (48%)	19 (19%)	33 (33%)	0	0
56	DY	99/110 (90%)	47 (48%)	19 (19%)	33 (33%)	0	0
57	BZ	175/206 (85%)	101 (58%)	37 (21%)	37 (21%)	0	0
57	DZ	175/206 (85%)	91 (52%)	48 (27%)	36 (21%)	0	0
All	All	11662/12592 (93%)	7696 (66%)	2368 (20%)	1598 (14%)	0	1

5 of 1598 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	178 (88%)	24 (12%)	5	21
2	CB	202/220 (92%)	179 (89%)	23 (11%)	5	22
3	AC	160/188 (85%)	151 (94%)	9 (6%)	21	52
3	CC	160/188 (85%)	151 (94%)	9 (6%)	21	52
4	AD	180/181 (99%)	161 (89%)	19 (11%)	6	25
4	CD	180/181 (99%)	161 (89%)	19 (11%)	6	25
5	AE	115/123 (94%)	102 (89%)	13 (11%)	6	22
5	CE	115/123 (94%)	103 (90%)	12 (10%)	7	25
6	AF	90/90 (100%)	85 (94%)	5 (6%)	21	52
6	CF	90/90 (100%)	84 (93%)	6 (7%)	16	45

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/127 (99%)	116 (92%)	10 (8%)	12	37
7	CG	126/127 (99%)	116 (92%)	10 (8%)	12	37
8	AH	119/119 (100%)	111 (93%)	8 (7%)	16	45
8	CH	119/119 (100%)	110 (92%)	9 (8%)	13	39
9	AI	98/99 (99%)	87 (89%)	11 (11%)	6	23
9	CI	98/99 (99%)	87 (89%)	11 (11%)	6	23
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	19
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	19
11	AK	90/99 (91%)	81 (90%)	9 (10%)	7	27
11	CK	90/99 (91%)	81 (90%)	9 (10%)	7	27
12	AL	104/111 (94%)	93 (89%)	11 (11%)	6	25
12	CL	104/111 (94%)	93 (89%)	11 (11%)	6	25
13	AM	99/101 (98%)	88 (89%)	11 (11%)	6	23
13	CM	99/101 (98%)	88 (89%)	11 (11%)	6	23
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	10
14	CN	49/50 (98%)	42 (86%)	7 (14%)	3	15
15	AO	79/80 (99%)	72 (91%)	7 (9%)	9	32
15	CO	79/80 (99%)	72 (91%)	7 (9%)	9	32
16	AP	72/74 (97%)	63 (88%)	9 (12%)	4	19
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	29
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	40
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	40
18	AR	61/77 (79%)	57 (93%)	4 (7%)	16	46
18	CR	61/77 (79%)	57 (93%)	4 (7%)	16	46
19	AS	69/80 (86%)	58 (84%)	11 (16%)	2	11
19	CS	69/80 (86%)	58 (84%)	11 (16%)	2	11
20	AT	76/82 (93%)	72 (95%)	4 (5%)	22	53
20	CT	76/82 (93%)	72 (95%)	4 (5%)	22	53
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	53
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	53
26	B0	66/67 (98%)	58 (88%)	8 (12%)	5	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	D0	66/67 (98%)	57 (86%)	9 (14%)	3	16
27	B1	78/83 (94%)	66 (85%)	12 (15%)	2	12
27	D1	78/83 (94%)	62 (80%)	16 (20%)	1	4
28	B2	66/67 (98%)	55 (83%)	11 (17%)	2	10
28	D2	66/67 (98%)	58 (88%)	8 (12%)	5	20
29	B3	51/52 (98%)	49 (96%)	2 (4%)	32	62
29	D3	51/52 (98%)	49 (96%)	2 (4%)	32	62
30	B4	27/63 (43%)	24 (89%)	3 (11%)	6	23
30	D4	27/63 (43%)	24 (89%)	3 (11%)	6	23
31	B5	51/52 (98%)	45 (88%)	6 (12%)	5	21
31	D5	51/52 (98%)	45 (88%)	6 (12%)	5	21
32	B6	43/52 (83%)	34 (79%)	9 (21%)	1	4
32	D6	43/52 (83%)	34 (79%)	9 (21%)	1	4
33	B7	41/42 (98%)	36 (88%)	5 (12%)	5	20
33	D7	41/42 (98%)	35 (85%)	6 (15%)	3	14
34	B8	53/55 (96%)	43 (81%)	10 (19%)	1	6
34	D8	53/55 (96%)	43 (81%)	10 (19%)	1	6
35	B9	33/34 (97%)	30 (91%)	3 (9%)	9	31
35	D9	33/34 (97%)	30 (91%)	3 (9%)	9	31
38	BC	61/181 (34%)	56 (92%)	5 (8%)	11	36
38	DC	61/181 (34%)	55 (90%)	6 (10%)	8	29
39	BD	213/218 (98%)	180 (84%)	33 (16%)	2	12
39	DD	213/218 (98%)	177 (83%)	36 (17%)	2	9
40	BE	165/166 (99%)	140 (85%)	25 (15%)	3	13
40	DE	165/166 (99%)	141 (86%)	24 (14%)	3	14
41	BF	165/166 (99%)	147 (89%)	18 (11%)	6	24
41	DF	165/166 (99%)	149 (90%)	16 (10%)	8	29
42	BG	155/156 (99%)	138 (89%)	17 (11%)	6	24
42	DG	155/156 (99%)	130 (84%)	25 (16%)	2	10
43	BH	132/148 (89%)	119 (90%)	13 (10%)	8	29
43	DH	132/148 (89%)	119 (90%)	13 (10%)	8	29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BI	122/124 (98%)	107 (88%)	15 (12%)	4	20
44	DI	122/124 (98%)	108 (88%)	14 (12%)	5	22
45	BN	117/119 (98%)	96 (82%)	21 (18%)	2	8
45	DN	117/119 (98%)	96 (82%)	21 (18%)	2	8
46	BO	100/100 (100%)	94 (94%)	6 (6%)	19	49
46	DO	100/100 (100%)	93 (93%)	7 (7%)	15	43
47	BP	112/116 (97%)	86 (77%)	26 (23%)	1	3
47	DP	112/116 (97%)	85 (76%)	27 (24%)	0	2
48	BQ	111/111 (100%)	96 (86%)	15 (14%)	4	16
48	DQ	111/111 (100%)	96 (86%)	15 (14%)	4	16
49	BR	100/101 (99%)	86 (86%)	14 (14%)	3	16
49	DR	100/101 (99%)	86 (86%)	14 (14%)	3	16
50	BS	77/88 (88%)	67 (87%)	10 (13%)	4	17
50	DS	77/88 (88%)	68 (88%)	9 (12%)	5	21
51	BT	120/127 (94%)	98 (82%)	22 (18%)	1	7
51	DT	120/127 (94%)	100 (83%)	20 (17%)	2	10
52	BU	92/94 (98%)	85 (92%)	7 (8%)	13	39
52	DU	92/94 (98%)	85 (92%)	7 (8%)	13	39
53	BV	82/82 (100%)	72 (88%)	10 (12%)	5	20
53	DV	82/82 (100%)	71 (87%)	11 (13%)	4	16
54	BW	91/92 (99%)	82 (90%)	9 (10%)	8	28
54	DW	91/92 (99%)	82 (90%)	9 (10%)	8	28
55	BX	74/78 (95%)	67 (90%)	7 (10%)	8	29
55	DX	74/78 (95%)	67 (90%)	7 (10%)	8	29
56	BY	84/91 (92%)	69 (82%)	15 (18%)	2	8
56	DY	84/91 (92%)	70 (83%)	14 (17%)	2	10
57	BZ	155/179 (87%)	138 (89%)	17 (11%)	6	24
57	DZ	155/179 (87%)	136 (88%)	19 (12%)	4	20
All	All	9654/10432 (92%)	8513 (88%)	1141 (12%)	5	21

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

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

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

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

### 5.3.3 RNA ⓘ

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

5 of 1599 RNA backbone outliers are listed below:

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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	AA	47	C

5 of 169 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	5MU	AV	54	22	15,22,23	1.19	2 (13%)	16,32,35	3.68	2 (12%)
25	PHA	CY	77	25	10,11,11	0.53	0	10,13,13	0.71	1 (10%)
25	PHA	AY	77	25	10,11,11	0.59	0	10,13,13	0.90	1 (10%)
25	8AN	CY	76	25,36	19,24,25	1.23	1 (5%)	13,35,38	0.90	1 (7%)
22	5MU	CV	54	22	15,22,23	1.13	2 (13%)	16,32,35	3.73	1 (6%)
25	8AN	AY	76	25,36	19,24,25	1.22	2 (10%)	13,35,38	0.77	0

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

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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8AN	CY	76	25,36	-	0/3/25/26	0/3/3/3
22	5MU	CV	54	22	-	0/5/25/26	0/2/2/2
25	8AN	AY	76	25,36	-	0/3/25/26	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CY	76	8AN	C3'-N3'	-4.42	1.40	1.47
25	AY	76	8AN	C3'-N3'	-4.37	1.40	1.47
22	AV	54	5MU	C4-N3	3.38	1.38	1.33
22	CV	54	5MU	C4-N3	3.22	1.38	1.33
22	AV	54	5MU	C6-C5	-2.10	1.34	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CV	54	5MU	C4-N3-C2	14.56	127.44	115.14
22	AV	54	5MU	C4-N3-C2	14.33	127.24	115.14
25	AY	77	PHA	CB-CA-C	-2.64	106.52	111.47
25	CY	76	8AN	C5-C6-N6	2.25	123.77	120.35
22	AV	54	5MU	C5M-C5-C6	2.10	123.11	118.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	AY	77	PHA	O-C-CA-CB
25	CY	77	PHA	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
59	PAR	AA	1814	-	45,45,45	1.56	9 (20%)	64,67,67	1.26	6 (9%)
59	PAR	CA	1817	-	45,45,45	1.86	11 (24%)	64,67,67	1.38	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PAR	AA	1814	-	-	5/18/94/94	0/4/4/4
59	PAR	CA	1817	-	-	3/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CA	1817	PAR	C34-C24	6.08	1.61	1.53
59	CA	1817	PAR	C64-C54	5.62	1.59	1.52
59	AA	1814	PAR	C64-C54	4.48	1.58	1.52
59	CA	1817	PAR	C52-C42	3.64	1.59	1.52
59	AA	1814	PAR	C34-C24	3.32	1.57	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	CA	1817	PAR	C14-O54-C54	4.49	122.51	113.69

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	CA	1817	PAR	O54-C54-C64	4.19	113.81	106.01
59	AA	1814	PAR	O54-C54-C64	3.89	113.26	106.01
59	CA	1817	PAR	O52-C13-C23	3.84	115.93	107.96
59	AA	1814	PAR	C14-O54-C54	3.67	120.89	113.69

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

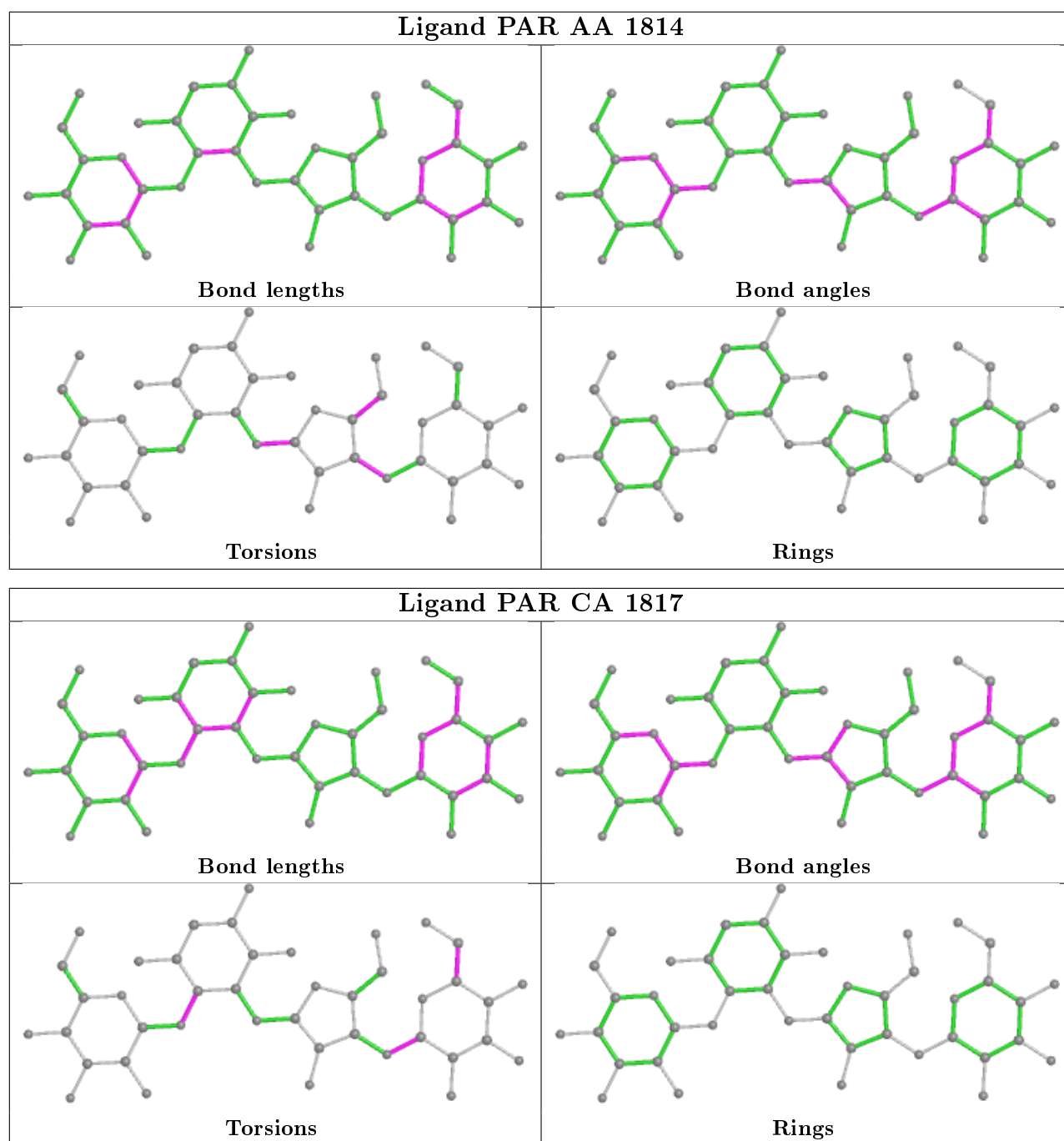
Mol	Chain	Res	Type	Atoms
59	AA	1814	PAR	C23-C13-O52-C52
59	AA	1814	PAR	O43-C43-C53-O53
59	AA	1814	PAR	C33-C43-C53-O53
59	AA	1814	PAR	O43-C13-O52-C52
59	CA	1817	PAR	C44-C54-C64-N64

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

The worst 5 of 18 chain breaks are listed below:

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

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1504/1522 (98%)	-0.21	22 (1%) 73 72	56, 99, 180, 200	0
1	CA	1504/1522 (98%)	-0.06	21 (1%) 75 75	55, 119, 194, 200	0
2	AB	235/256 (91%)	0.18	15 (6%) 19 19	65, 132, 188, 200	0
2	CB	235/256 (91%)	0.69	26 (11%) 5 5	83, 158, 197, 200	0
3	AC	207/239 (86%)	-0.09	2 (0%) 82 82	72, 120, 172, 200	0
3	CC	207/239 (86%)	0.37	14 (6%) 17 17	83, 147, 188, 200	0
4	AD	208/209 (99%)	-0.16	1 (0%) 91 91	59, 97, 139, 199	0
4	CD	208/209 (99%)	0.06	3 (1%) 75 75	70, 115, 158, 194	0
5	AE	151/162 (93%)	-0.20	1 (0%) 87 88	51, 99, 134, 164	0
5	CE	151/162 (93%)	0.23	4 (2%) 56 53	67, 116, 165, 199	0
6	AF	101/101 (100%)	-0.21	1 (0%) 82 82	69, 108, 147, 198	0
6	CF	101/101 (100%)	-0.05	2 (1%) 65 64	67, 107, 154, 167	0
7	AG	155/156 (99%)	0.34	12 (7%) 13 12	73, 120, 164, 188	0
7	CG	155/156 (99%)	0.69	21 (13%) 3 3	90, 155, 196, 200	0
8	AH	138/138 (100%)	-0.01	2 (1%) 75 75	65, 102, 141, 173	0
8	CH	138/138 (100%)	0.22	6 (4%) 35 34	74, 121, 168, 200	0
9	AI	127/128 (99%)	0.42	8 (6%) 20 20	86, 139, 185, 198	0
9	CI	127/128 (99%)	1.63	40 (31%) 0 0	83, 170, 200, 200	0
10	AJ	99/105 (94%)	0.75	16 (16%) 1 2	81, 139, 195, 200	0
10	CJ	99/105 (94%)	1.98	40 (40%) 0 0	92, 170, 195, 200	0
11	AK	119/129 (92%)	0.12	4 (3%) 45 43	65, 100, 162, 200	0
11	CK	119/129 (92%)	0.42	8 (6%) 17 17	68, 118, 177, 200	0
12	AL	125/135 (92%)	0.15	6 (4%) 30 28	56, 93, 136, 200	0
12	CL	125/135 (92%)	0.16	5 (4%) 38 36	60, 90, 157, 200	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	125/126 (99%)	0.63	17 (13%) 3 2	86, 123, 177, 200	0
13	CM	125/126 (99%)	1.10	31 (24%) 0 0	100, 161, 200, 200	0
14	AN	60/61 (98%)	0.39	3 (5%) 28 27	72, 117, 161, 173	0
14	CN	60/61 (98%)	0.71	6 (10%) 7 7	84, 144, 185, 200	0
15	AO	88/89 (98%)	0.03	0 100 100	52, 92, 144, 159	0
15	CO	88/89 (98%)	0.10	0 100 100	63, 107, 147, 155	0
16	AP	84/88 (95%)	0.11	1 (1%) 79 78	67, 87, 142, 154	0
16	CP	84/88 (95%)	0.44	6 (7%) 16 16	76, 113, 167, 192	0
17	AQ	100/105 (95%)	-0.03	1 (1%) 82 82	63, 95, 133, 147	0
17	CQ	100/105 (95%)	0.13	1 (1%) 82 82	73, 118, 154, 200	0
18	AR	70/88 (79%)	-0.04	1 (1%) 75 75	71, 104, 153, 170	0
18	CR	70/88 (79%)	0.13	1 (1%) 75 75	71, 110, 158, 170	0
19	AS	79/93 (84%)	0.82	12 (15%) 2 2	85, 136, 188, 200	0
19	CS	79/93 (84%)	1.05	15 (18%) 1 1	107, 160, 198, 200	0
20	AT	99/106 (93%)	0.36	6 (6%) 21 20	63, 105, 167, 199	0
20	CT	99/106 (93%)	0.77	12 (12%) 4 3	80, 128, 184, 200	0
21	AU	25/27 (92%)	1.72	9 (36%) 0 0	85, 125, 162, 187	0
21	CU	25/27 (92%)	3.98	19 (76%) 0 0	87, 142, 197, 200	0
22	AV	76/77 (98%)	-0.47	0 100 100	68, 102, 144, 189	0
22	CV	76/77 (98%)	-0.35	0 100 100	63, 116, 168, 182	0
23	AW	76/76 (100%)	1.34	15 (19%) 1 1	107, 196, 200, 200	0
23	CW	76/76 (100%)	2.53	42 (55%) 0 0	128, 199, 200, 200	0
24	AX	10/10 (100%)	0.15	1 (10%) 7 7	62, 94, 148, 162	0
24	CX	10/10 (100%)	0.65	1 (10%) 7 7	92, 111, 183, 192	0
25	AY	75/77 (97%)	1.15	16 (21%) 0 1	57, 187, 200, 200	0
25	CY	75/77 (97%)	1.20	11 (14%) 2 2	64, 189, 200, 200	0
26	B0	84/85 (98%)	0.50	4 (4%) 30 28	63, 94, 144, 189	0
26	D0	84/85 (98%)	0.67	7 (8%) 11 11	76, 127, 170, 191	0
27	B1	94/98 (95%)	0.11	4 (4%) 35 34	47, 77, 135, 155	0
27	D1	94/98 (95%)	0.06	0 100 100	49, 80, 138, 157	0
28	B2	71/72 (98%)	-0.09	2 (2%) 53 51	68, 99, 133, 184	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	D2	71/72 (98%)	0.30	4 (5%) 24 23	61, 105, 152, 190	0
29	B3	60/60 (100%)	0.42	4 (6%) 17 17	72, 108, 152, 188	0
29	D3	60/60 (100%)	0.89	5 (8%) 11 11	75, 134, 178, 200	0
30	B4	31/71 (43%)	-0.14	0 100 100	87, 126, 171, 176	0
30	D4	31/71 (43%)	0.95	5 (16%) 1 2	118, 175, 194, 200	0
31	B5	59/60 (98%)	0.35	6 (10%) 6 6	52, 100, 190, 200	0
31	D5	59/60 (98%)	0.09	3 (5%) 28 26	43, 99, 189, 200	0
32	B6	45/54 (83%)	4.65	37 (82%) 0 0	109, 171, 197, 200	0
32	D6	45/54 (83%)	5.02	40 (88%) 0 0	146, 183, 200, 200	0
33	B7	49/49 (100%)	0.13	1 (2%) 65 64	49, 65, 124, 185	0
33	D7	49/49 (100%)	0.29	5 (10%) 6 6	37, 62, 124, 198	0
34	B8	64/65 (98%)	0.28	1 (1%) 72 70	51, 87, 151, 173	0
34	D8	64/65 (98%)	0.83	8 (12%) 3 3	75, 110, 159, 200	0
35	B9	36/37 (97%)	3.01	25 (69%) 0 0	117, 148, 189, 200	0
35	D9	36/37 (97%)	4.10	33 (91%) 0 0	101, 145, 182, 197	0
36	BA	2807/2822 (99%)	-0.12	57 (2%) 65 64	48, 87, 188, 200	0
36	DA	2807/2822 (99%)	-0.05	79 (2%) 53 51	35, 94, 191, 200	0
37	BB	119/122 (97%)	-0.44	0 100 100	88, 121, 165, 179	0
37	DB	119/122 (97%)	0.17	2 (1%) 70 68	114, 168, 197, 200	0
38	BC	191/229 (83%)	2.81	118 (61%) 0 0	119, 183, 200, 200	0
38	DC	191/229 (83%)	3.82	143 (74%) 0 0	149, 184, 200, 200	0
39	BD	272/276 (98%)	-0.23	1 (0%) 92 93	39, 71, 116, 164	0
39	DD	272/276 (98%)	-0.18	1 (0%) 92 93	31, 69, 114, 173	0
40	BE	205/206 (99%)	0.23	10 (4%) 29 27	47, 96, 160, 200	0
40	DE	205/206 (99%)	0.04	8 (3%) 39 37	47, 90, 159, 199	0
41	BF	208/210 (99%)	-0.20	3 (1%) 75 75	43, 89, 164, 200	0
41	DF	208/210 (99%)	0.28	14 (6%) 17 17	44, 120, 179, 200	0
42	BG	181/182 (99%)	-0.04	7 (3%) 39 37	68, 118, 162, 194	0
42	DG	181/182 (99%)	0.88	32 (17%) 1 1	105, 163, 200, 200	0
43	BH	160/180 (88%)	1.32	49 (30%) 0 0	98, 160, 199, 200	0
43	DH	160/180 (88%)	0.51	12 (7%) 14 13	65, 135, 186, 200	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BI	146/148 (98%)	0.41	9 (6%) 20 20	62, 122, 180, 199	0
44	DI	146/148 (98%)	1.95	50 (34%) 0 0	54, 152, 200, 200	0
45	BN	139/140 (99%)	0.19	3 (2%) 62 60	69, 110, 162, 198	0
45	DN	139/140 (99%)	0.08	3 (2%) 62 60	65, 107, 161, 190	0
46	BO	122/122 (100%)	-0.13	1 (0%) 86 86	53, 85, 116, 134	0
46	DO	122/122 (100%)	-0.21	0 100 100	48, 75, 110, 131	0
47	BP	146/150 (97%)	0.47	10 (6%) 17 17	46, 105, 171, 200	0
47	DP	146/150 (97%)	1.02	23 (15%) 2 2	60, 130, 184, 200	0
48	BQ	141/141 (100%)	0.23	6 (4%) 35 34	64, 103, 160, 200	0
48	DQ	141/141 (100%)	0.27	8 (5%) 23 23	55, 109, 156, 200	0
49	BR	117/118 (99%)	-0.09	0 100 100	53, 85, 130, 157	0
49	DR	117/118 (99%)	-0.02	0 100 100	49, 91, 138, 150	0
50	BS	99/112 (88%)	0.31	4 (4%) 38 36	65, 115, 170, 200	0
50	DS	99/112 (88%)	1.45	29 (29%) 0 0	113, 164, 199, 200	0
51	BT	138/146 (94%)	0.06	10 (7%) 15 15	55, 102, 175, 200	0
51	DT	138/146 (94%)	-0.03	3 (2%) 62 60	62, 101, 178, 200	0
52	BU	117/118 (99%)	0.10	2 (1%) 70 68	52, 95, 146, 198	0
52	DU	117/118 (99%)	0.21	2 (1%) 70 68	59, 103, 156, 200	0
53	BV	101/101 (100%)	0.28	4 (3%) 38 36	66, 120, 158, 200	0
53	DV	101/101 (100%)	0.51	5 (4%) 28 27	57, 136, 175, 200	0
54	BW	113/113 (100%)	-0.12	0 100 100	48, 85, 143, 200	0
54	DW	113/113 (100%)	-0.03	3 (2%) 54 52	57, 93, 155, 200	0
55	BX	93/96 (96%)	-0.17	1 (1%) 80 81	56, 86, 120, 156	0
55	DX	93/96 (96%)	0.02	1 (1%) 80 81	57, 95, 135, 152	0
56	BY	101/110 (91%)	1.14	17 (16%) 1 1	67, 115, 183, 200	0
56	DY	101/110 (91%)	1.31	25 (24%) 0 0	62, 134, 192, 200	0
57	BZ	177/206 (85%)	0.82	27 (15%) 2 2	80, 150, 200, 200	0
57	DZ	177/206 (85%)	1.16	47 (26%) 0 0	94, 164, 200, 200	0
All	All	21244/22004 (96%)	0.26	1530 (7%) 15 15	31, 108, 192, 200	0

The worst 5 of 1530 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	BQ	140	ALA	20.5
25	CY	17	C	19.2
38	DC	172	HIS	18.4
13	AM	123	ALA	17.9
29	D3	1	MET	14.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
22	5MU	CV	54	21/22	0.82	0.27	173,181,194,194	0
22	5MU	AV	54	21/22	0.91	0.14	104,135,151,151	0
25	PHA	AY	77	11/11	0.94	0.34	60,62,65,66	0
25	PHA	CY	77	11/11	0.94	0.46	60,62,65,66	0
25	8AN	CY	76	22/23	0.95	0.22	37,58,79,189	0
25	8AN	AY	76	22/23	0.95	0.18	37,58,79,189	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	BA	3288	1/1	-0.16	2.52	88,88,88,88	1
58	MG	CW	114	1/1	-0.08	0.33	108,108,108,108	1
58	MG	AA	1688	1/1	-0.01	0.33	118,118,118,118	0
58	MG	DA	3443	1/1	0.01	0.22	111,111,111,111	0
58	MG	DB	201	1/1	0.01	0.30	135,135,135,135	0
58	MG	CA	1719	1/1	0.08	0.26	112,112,112,112	0
58	MG	AA	1666	1/1	0.08	0.92	122,122,122,122	0
58	MG	DA	3327	1/1	0.11	0.73	106,106,106,106	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3424	1/1	0.15	0.55	107,107,107,107	0
58	MG	BA	3450	1/1	0.16	0.25	125,125,125,125	0
58	MG	DA	3213	1/1	0.18	0.49	124,124,124,124	0
58	MG	BA	3336	1/1	0.18	0.74	105,105,105,105	1
58	MG	DA	3360	1/1	0.21	1.08	97,97,97,97	1
58	MG	CA	1626	1/1	0.24	0.87	119,119,119,119	0
58	MG	DA	3103	1/1	0.24	1.05	102,102,102,102	1
58	MG	DA	3273	1/1	0.26	0.76	155,155,155,155	0
58	MG	BA	3009	1/1	0.26	1.95	109,109,109,109	0
58	MG	BA	3305	1/1	0.30	1.07	112,112,112,112	0
58	MG	BA	3285	1/1	0.31	0.97	112,112,112,112	0
58	MG	BA	3050	1/1	0.31	0.76	84,84,84,84	0
58	MG	AA	1725	1/1	0.32	0.31	77,77,77,77	0
58	MG	BB	213	1/1	0.32	0.97	148,148,148,148	0
58	MG	AA	1763	1/1	0.32	1.06	114,114,114,114	1
58	MG	CA	1722	1/1	0.32	0.16	106,106,106,106	0
58	MG	CW	103	1/1	0.33	0.48	119,119,119,119	0
58	MG	DA	3448	1/1	0.33	0.12	97,97,97,97	0
58	MG	CA	1783	1/1	0.34	1.21	100,100,100,100	0
58	MG	AA	1789	1/1	0.34	0.56	152,152,152,152	0
58	MG	CE	201	1/1	0.35	0.28	132,132,132,132	0
58	MG	DA	3434	1/1	0.35	0.76	107,107,107,107	1
58	MG	BA	3213	1/1	0.36	0.56	109,109,109,109	0
58	MG	DA	3166	1/1	0.36	0.96	104,104,104,104	0
58	MG	CA	1663	1/1	0.36	0.32	127,127,127,127	0
58	MG	DA	3357	1/1	0.36	0.24	111,111,111,111	0
58	MG	CA	1801	1/1	0.36	0.40	128,128,128,128	0
58	MG	BA	3104	1/1	0.38	0.63	65,65,65,65	1
58	MG	DA	3358	1/1	0.38	0.36	102,102,102,102	0
58	MG	AA	1762	1/1	0.38	1.01	76,76,76,76	1
58	MG	BA	3242	1/1	0.39	1.09	115,115,115,115	0
58	MG	CA	1688	1/1	0.39	1.02	115,115,115,115	0
58	MG	DA	3345	1/1	0.40	0.28	110,110,110,110	1
58	MG	CA	1739	1/1	0.41	0.73	109,109,109,109	0
58	MG	AW	117	1/1	0.41	1.09	134,134,134,134	0
58	MG	CA	1636	1/1	0.42	0.19	103,103,103,103	1
58	MG	CA	1680	1/1	0.42	0.77	83,83,83,83	1
58	MG	CA	1751	1/1	0.43	0.89	128,128,128,128	0
58	MG	CA	1772	1/1	0.44	0.67	101,101,101,101	0
58	MG	AA	1670	1/1	0.44	0.32	95,95,95,95	0
58	MG	BA	3234	1/1	0.44	0.67	115,115,115,115	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	1731	1/1	0.45	0.42	142,142,142,142	0
58	MG	DA	3264	1/1	0.45	1.03	98,98,98,98	0
58	MG	BA	3130	1/1	0.45	0.87	92,92,92,92	1
58	MG	BA	3446	1/1	0.45	0.19	92,92,92,92	0
58	MG	DA	3346	1/1	0.46	1.11	109,109,109,109	0
58	MG	CA	1724	1/1	0.46	0.67	91,91,91,91	1
58	MG	CW	115	1/1	0.46	0.36	139,139,139,139	0
58	MG	CA	1810	1/1	0.46	0.76	95,95,95,95	0
58	MG	DA	3411	1/1	0.47	0.29	115,115,115,115	1
58	MG	DA	3447	1/1	0.47	1.49	87,87,87,87	1
58	MG	CA	1726	1/1	0.47	0.26	65,65,65,65	0
58	MG	AA	1676	1/1	0.47	0.32	95,95,95,95	0
58	MG	DA	3227	1/1	0.47	0.40	91,91,91,91	0
58	MG	AA	1773	1/1	0.47	0.22	71,71,71,71	0
58	MG	CW	105	1/1	0.48	0.20	123,123,123,123	0
58	MG	AA	1772	1/1	0.48	0.46	100,100,100,100	1
58	MG	BA	3340	1/1	0.48	0.38	97,97,97,97	1
58	MG	CA	1649	1/1	0.48	0.48	82,82,82,82	0
58	MG	AW	110	1/1	0.49	0.59	77,77,77,77	1
58	MG	BA	3223	1/1	0.49	0.48	82,82,82,82	0
58	MG	DA	3262	1/1	0.49	0.89	96,96,96,96	0
58	MG	CA	1682	1/1	0.49	0.54	83,83,83,83	0
58	MG	DA	3219	1/1	0.49	0.44	102,102,102,102	0
58	MG	AA	1652	1/1	0.50	0.43	107,107,107,107	0
58	MG	BA	3187	1/1	0.50	0.16	98,98,98,98	0
58	MG	B2	601	1/1	0.51	0.53	68,68,68,68	1
58	MG	DA	3151	1/1	0.51	0.54	94,94,94,94	0
58	MG	AA	1696	1/1	0.51	0.83	103,103,103,103	0
58	MG	DA	3395	1/1	0.51	0.34	73,73,73,73	1
58	MG	AA	1700	1/1	0.52	0.53	90,90,90,90	0
58	MG	DB	213	1/1	0.52	0.60	102,102,102,102	0
58	MG	DA	3344	1/1	0.52	0.49	72,72,72,72	1
58	MG	AA	1608	1/1	0.52	0.96	110,110,110,110	0
58	MG	DA	3420	1/1	0.53	0.38	66,66,66,66	0
58	MG	DN	202	1/1	0.53	0.76	97,97,97,97	0
58	MG	DA	3223	1/1	0.53	0.38	82,82,82,82	0
58	MG	AA	1602	1/1	0.53	0.52	91,91,91,91	0
58	MG	BA	3309	1/1	0.53	0.31	94,94,94,94	0
58	MG	BA	3259	1/1	0.54	0.48	91,91,91,91	0
58	MG	CA	1627	1/1	0.54	0.87	97,97,97,97	0
58	MG	DB	214	1/1	0.54	0.66	94,94,94,94	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CW	108	1/1	0.54	0.48	130,130,130,130	0
58	MG	CA	1716	1/1	0.54	0.74	83,83,83,83	0
58	MG	BA	3389	1/1	0.55	0.33	107,107,107,107	0
58	MG	DA	3209	1/1	0.55	0.64	105,105,105,105	0
58	MG	DA	3351	1/1	0.55	0.52	79,79,79,79	1
58	MG	BA	3221	1/1	0.55	0.47	72,72,72,72	0
58	MG	BA	3345	1/1	0.55	0.60	93,93,93,93	1
58	MG	CA	1678	1/1	0.55	0.28	109,109,109,109	0
58	MG	DA	3255	1/1	0.56	0.41	96,96,96,96	0
58	MG	DA	3304	1/1	0.56	0.59	88,88,88,88	0
58	MG	AD	301	1/1	0.56	0.23	84,84,84,84	0
58	MG	DA	3161	1/1	0.56	0.62	131,131,131,131	0
58	MG	BA	3291	1/1	0.56	0.16	90,90,90,90	0
58	MG	CV	105	1/1	0.56	0.81	110,110,110,110	0
58	MG	DA	3156	1/1	0.56	0.52	94,94,94,94	0
58	MG	DA	3224	1/1	0.56	0.97	99,99,99,99	1
58	MG	AA	1745	1/1	0.56	1.51	121,121,121,121	0
58	MG	BA	3347	1/1	0.56	0.54	85,85,85,85	1
58	MG	AA	1661	1/1	0.56	0.18	83,83,83,83	0
58	MG	CA	1639	1/1	0.57	0.46	140,140,140,140	0
58	MG	BB	202	1/1	0.57	0.50	97,97,97,97	1
58	MG	DA	3102	1/1	0.57	0.80	107,107,107,107	0
58	MG	CA	1730	1/1	0.57	1.30	111,111,111,111	0
58	MG	DA	3265	1/1	0.57	0.51	69,69,69,69	0
58	MG	CA	1661	1/1	0.58	0.50	98,98,98,98	0
58	MG	BA	3422	1/1	0.58	0.28	67,67,67,67	0
58	MG	AA	1743	1/1	0.58	0.73	86,86,86,86	0
58	MG	BA	3249	1/1	0.59	0.36	57,57,57,57	0
58	MG	AA	1685	1/1	0.59	0.49	101,101,101,101	0
58	MG	DA	3183	1/1	0.59	0.30	68,68,68,68	0
58	MG	AW	112	1/1	0.59	0.18	107,107,107,107	1
58	MG	DA	3178	1/1	0.59	0.55	125,125,125,125	0
58	MG	BA	3260	1/1	0.59	0.60	102,102,102,102	1
58	MG	DA	3445	1/1	0.59	0.08	98,98,98,98	0
58	MG	CA	1635	1/1	0.59	0.31	81,81,81,81	0
58	MG	BA	3164	1/1	0.60	0.47	84,84,84,84	0
58	MG	CA	1701	1/1	0.60	0.58	113,113,113,113	0
58	MG	DA	3234	1/1	0.60	1.45	91,91,91,91	0
58	MG	DA	3301	1/1	0.60	0.76	91,91,91,91	0
58	MG	AA	1662	1/1	0.60	0.22	95,95,95,95	0
58	MG	DA	3191	1/1	0.60	0.25	75,75,75,75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3196	1/1	0.60	0.56	82,82,82,82	0
58	MG	CA	1774	1/1	0.60	0.23	63,63,63,63	0
58	MG	AA	1655	1/1	0.60	0.87	89,89,89,89	0
58	MG	DA	3005	1/1	0.61	1.01	138,138,138,138	0
58	MG	DA	3231	1/1	0.61	0.38	85,85,85,85	0
58	MG	CA	1643	1/1	0.61	0.41	95,95,95,95	0
58	MG	DA	3159	1/1	0.61	0.35	74,74,74,74	0
58	MG	BX	102	1/1	0.61	0.46	97,97,97,97	0
58	MG	DA	3374	1/1	0.61	0.21	72,72,72,72	0
58	MG	CA	1770	1/1	0.61	0.50	121,121,121,121	0
58	MG	BA	3394	1/1	0.61	1.27	105,105,105,105	0
58	MG	BA	3423	1/1	0.62	0.11	125,125,125,125	1
58	MG	AA	1796	1/1	0.62	0.13	106,106,106,106	1
58	MG	DA	3291	1/1	0.62	0.22	105,105,105,105	0
58	MG	BA	3163	1/1	0.62	1.05	132,132,132,132	0
58	MG	BA	3278	1/1	0.62	0.49	119,119,119,119	0
58	MG	BA	3298	1/1	0.62	0.35	91,91,91,91	0
58	MG	CA	1816	1/1	0.62	1.29	102,102,102,102	0
58	MG	AA	1780	1/1	0.62	0.52	84,84,84,84	0
58	MG	BA	3295	1/1	0.62	0.65	89,89,89,89	0
58	MG	DA	3311	1/1	0.62	0.64	93,93,93,93	0
58	MG	AA	1730	1/1	0.62	0.49	93,93,93,93	0
58	MG	BA	3428	1/1	0.62	0.80	90,90,90,90	0
58	MG	DA	3250	1/1	0.62	0.18	82,82,82,82	0
58	MG	CA	1762	1/1	0.63	0.53	60,60,60,60	1
58	MG	DA	3440	1/1	0.63	0.10	77,77,77,77	0
58	MG	CA	1647	1/1	0.63	0.51	94,94,94,94	0
58	MG	AA	1765	1/1	0.63	0.67	116,116,116,116	0
58	MG	BA	3436	1/1	0.64	0.21	60,60,60,60	1
58	MG	BA	3034	1/1	0.64	0.47	73,73,73,73	0
58	MG	DA	3334	1/1	0.64	0.48	107,107,107,107	1
58	MG	BA	3089	1/1	0.64	0.21	61,61,61,61	0
58	MG	BA	3431	1/1	0.64	0.32	124,124,124,124	0
58	MG	DA	3364	1/1	0.64	0.45	95,95,95,95	0
58	MG	DA	3317	1/1	0.64	0.22	88,88,88,88	1
58	MG	DA	3426	1/1	0.64	0.51	88,88,88,88	0
58	MG	AV	105	1/1	0.64	0.52	86,86,86,86	0
58	MG	CA	1743	1/1	0.65	0.48	128,128,128,128	0
58	MG	BA	3355	1/1	0.65	0.49	63,63,63,63	1
58	MG	DA	3325	1/1	0.65	0.21	90,90,90,90	0
58	MG	AA	1704	1/1	0.65	0.14	87,87,87,87	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	1734	1/1	0.65	0.41	92,92,92,92	0
58	MG	DA	3197	1/1	0.65	0.15	89,89,89,89	1
58	MG	D1	101	1/1	0.65	0.61	113,113,113,113	0
58	MG	DA	3179	1/1	0.66	0.22	109,109,109,109	0
58	MG	BB	219	1/1	0.66	0.26	89,89,89,89	1
58	MG	CA	1710	1/1	0.66	1.36	127,127,127,127	0
58	MG	DA	3309	1/1	0.66	0.34	89,89,89,89	0
58	MG	BA	3351	1/1	0.66	1.07	125,125,125,125	0
58	MG	BA	3214	1/1	0.66	0.29	97,97,97,97	0
58	MG	CA	1677	1/1	0.66	0.21	88,88,88,88	0
58	MG	CA	1697	1/1	0.66	0.23	87,87,87,87	0
58	MG	BA	3013	1/1	0.66	0.60	80,80,80,80	0
58	MG	AA	1606	1/1	0.66	0.24	76,76,76,76	0
58	MG	BA	3160	1/1	0.66	0.21	61,61,61,61	0
58	MG	BA	3270	1/1	0.66	0.27	74,74,74,74	0
58	MG	DA	3449	1/1	0.66	0.10	92,92,92,92	0
58	MG	AA	1629	1/1	0.66	0.21	87,87,87,87	0
58	MG	AA	1601	1/1	0.67	0.24	92,92,92,92	0
58	MG	DA	3375	1/1	0.67	0.22	106,106,106,106	0
58	MG	BA	3220	1/1	0.67	0.13	80,80,80,80	1
58	MG	DA	3251	1/1	0.67	0.18	95,95,95,95	0
58	MG	CA	1773	1/1	0.67	0.47	82,82,82,82	1
58	MG	BA	3158	1/1	0.67	0.57	97,97,97,97	0
58	MG	BA	3074	1/1	0.67	0.28	75,75,75,75	0
58	MG	BB	204	1/1	0.67	0.23	103,103,103,103	0
58	MG	DA	3380	1/1	0.67	0.44	85,85,85,85	1
58	MG	AA	1693	1/1	0.67	1.61	109,109,109,109	1
58	MG	BA	3070	1/1	0.67	0.87	116,116,116,116	0
58	MG	DA	3043	1/1	0.67	0.41	111,111,111,111	0
58	MG	CA	1808	1/1	0.67	0.10	107,107,107,107	0
58	MG	AA	1635	1/1	0.67	0.48	94,94,94,94	0
58	MG	DB	202	1/1	0.68	1.14	113,113,113,113	1
58	MG	DA	3348	1/1	0.68	0.52	94,94,94,94	0
58	MG	DA	3175	1/1	0.68	0.33	87,87,87,87	0
58	MG	DA	3409	1/1	0.68	0.27	141,141,141,141	0
58	MG	DA	3171	1/1	0.68	1.84	88,88,88,88	0
58	MG	AG	201	1/1	0.68	1.31	127,127,127,127	0
58	MG	AA	1672	1/1	0.68	0.31	87,87,87,87	0
58	MG	BA	3404	1/1	0.68	0.50	97,97,97,97	0
58	MG	BA	3276	1/1	0.68	0.22	68,68,68,68	0
58	MG	CW	116	1/1	0.68	0.22	103,103,103,103	1
58	MG	AA	1808	1/1	0.68	0.50	101,101,101,101	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	1705	1/1	0.68	0.21	76,76,76,76	0
58	MG	AA	1711	1/1	0.68	0.22	85,85,85,85	0
58	MG	DA	3410	1/1	0.68	0.96	99,99,99,99	0
58	MG	AA	1799	1/1	0.69	0.46	117,117,117,117	0
58	MG	BA	3200	1/1	0.69	0.20	52,52,52,52	0
58	MG	BB	208	1/1	0.69	0.10	103,103,103,103	0
58	MG	BA	3296	1/1	0.69	0.33	83,83,83,83	0
58	MG	BA	3363	1/1	0.69	0.37	116,116,116,116	0
58	MG	DA	3277	1/1	0.69	0.16	104,104,104,104	0
58	MG	DA	3148	1/1	0.69	0.39	88,88,88,88	0
58	MG	BA	3339	1/1	0.69	0.48	120,120,120,120	1
58	MG	BA	3287	1/1	0.69	0.74	92,92,92,92	1
58	MG	AA	1769	1/1	0.69	0.46	74,74,74,74	0
58	MG	BA	3316	1/1	0.69	0.49	81,81,81,81	0
58	MG	CA	1621	1/1	0.70	0.20	91,91,91,91	0
58	MG	DN	201	1/1	0.70	1.46	95,95,95,95	0
58	MG	AA	1812	1/1	0.70	0.46	93,93,93,93	0
58	MG	BA	3148	1/1	0.70	0.24	59,59,59,59	1
58	MG	DA	3279	1/1	0.70	0.78	92,92,92,92	0
58	MG	BB	214	1/1	0.70	0.48	92,92,92,92	0
58	MG	AA	1747	1/1	0.70	0.39	85,85,85,85	1
58	MG	BA	3233	1/1	0.70	0.11	98,98,98,98	0
58	MG	CA	1629	1/1	0.70	0.22	89,89,89,89	0
58	MG	AA	1650	1/1	0.70	0.24	66,66,66,66	0
58	MG	AA	1742	1/1	0.70	0.25	96,96,96,96	0
58	MG	BA	3199	1/1	0.70	0.23	73,73,73,73	0
58	MG	CA	1673	1/1	0.70	0.28	92,92,92,92	0
58	MG	BA	3228	1/1	0.70	0.62	107,107,107,107	1
58	MG	DA	3335	1/1	0.70	0.42	87,87,87,87	1
58	MG	DA	3414	1/1	0.71	0.79	130,130,130,130	0
58	MG	CA	1672	1/1	0.71	0.46	86,86,86,86	0
58	MG	BA	3453	1/1	0.71	0.40	114,114,114,114	0
58	MG	DA	3141	1/1	0.71	1.03	102,102,102,102	0
58	MG	AA	1783	1/1	0.71	0.52	144,144,144,144	0
58	MG	BA	3403	1/1	0.71	0.38	58,58,58,58	0
58	MG	DB	216	1/1	0.71	0.59	108,108,108,108	0
58	MG	BA	3141	1/1	0.71	0.22	60,60,60,60	0
58	MG	DA	3331	1/1	0.71	0.97	116,116,116,116	1
58	MG	D7	102	1/1	0.71	0.64	73,73,73,73	1
58	MG	AA	1631	1/1	0.71	0.49	109,109,109,109	0
58	MG	DA	3071	1/1	0.71	0.23	73,73,73,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	DA	3198	1/1	0.71	0.54	106,106,106,106	0
58	MG	DA	3323	1/1	0.71	0.23	105,105,105,105	1
58	MG	DA	3377	1/1	0.71	0.12	89,89,89,89	0
58	MG	CA	1618	1/1	0.72	1.10	109,109,109,109	0
58	MG	DA	3035	1/1	0.72	0.50	78,78,78,78	0
58	MG	AA	1618	1/1	0.72	0.69	106,106,106,106	0
58	MG	BA	3202	1/1	0.72	0.28	80,80,80,80	1
58	MG	CV	108	1/1	0.72	0.54	67,67,67,67	1
58	MG	DA	3298	1/1	0.72	0.27	50,50,50,50	0
58	MG	CA	1651	1/1	0.72	0.43	85,85,85,85	0
58	MG	DA	3252	1/1	0.72	0.27	65,65,65,65	0
58	MG	CW	106	1/1	0.72	0.24	106,106,106,106	0
58	MG	BA	3447	1/1	0.72	0.39	104,104,104,104	0
58	MG	DA	3144	1/1	0.72	0.40	68,68,68,68	0
58	MG	BA	3341	1/1	0.72	0.46	112,112,112,112	0
58	MG	BA	3401	1/1	0.72	0.65	119,119,119,119	0
58	MG	CA	1665	1/1	0.72	0.33	64,64,64,64	0
58	MG	DA	3070	1/1	0.73	0.12	54,54,54,54	0
58	MG	BA	3331	1/1	0.73	0.20	119,119,119,119	0
58	MG	CA	1609	1/1	0.73	0.37	109,109,109,109	0
58	MG	AA	1760	1/1	0.73	0.44	66,66,66,66	0
58	MG	BA	3279	1/1	0.73	0.36	105,105,105,105	0
58	MG	AA	1779	1/1	0.73	0.34	72,72,72,72	1
58	MG	DA	3399	1/1	0.73	0.74	131,131,131,131	0
58	MG	DA	3107	1/1	0.73	0.32	95,95,95,95	0
58	MG	AA	1647	1/1	0.73	0.14	94,94,94,94	0
58	MG	DA	3088	1/1	0.73	0.44	83,83,83,83	0
58	MG	BA	3362	1/1	0.73	0.29	90,90,90,90	0
58	MG	DA	3423	1/1	0.73	0.57	117,117,117,117	0
58	MG	CA	1675	1/1	0.73	0.68	116,116,116,116	0
58	MG	AA	1695	1/1	0.73	0.26	62,62,62,62	0
58	MG	BA	3329	1/1	0.74	0.13	88,88,88,88	1
58	MG	CK	201	1/1	0.74	0.61	95,95,95,95	1
58	MG	BA	3170	1/1	0.74	0.12	65,65,65,65	0
58	MG	AW	103	1/1	0.74	0.22	100,100,100,100	0
58	MG	BB	209	1/1	0.74	0.23	114,114,114,114	0
58	MG	BA	3227	1/1	0.74	0.35	73,73,73,73	0
58	MG	AW	104	1/1	0.74	0.25	98,98,98,98	1
58	MG	CA	1687	1/1	0.74	0.63	84,84,84,84	0
58	MG	AA	1668	1/1	0.74	0.34	66,66,66,66	0
58	MG	BA	3238	1/1	0.74	0.58	67,67,67,67	0
58	MG	BA	3232	1/1	0.74	0.67	101,101,101,101	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	1788	1/1	0.74	0.45	81,81,81,81	0
58	MG	AA	1813	1/1	0.74	0.39	101,101,101,101	0
58	MG	DA	3332	1/1	0.74	0.18	100,100,100,100	0
58	MG	CX	101	1/1	0.75	0.20	83,83,83,83	0
58	MG	BA	3183	1/1	0.75	0.22	122,122,122,122	0
58	MG	DA	3249	1/1	0.75	0.33	83,83,83,83	0
58	MG	BA	3429	1/1	0.75	0.67	87,87,87,87	0
58	MG	BA	3230	1/1	0.75	0.32	82,82,82,82	0
58	MG	BA	3269	1/1	0.75	0.54	85,85,85,85	0
58	MG	CA	1617	1/1	0.75	0.71	73,73,73,73	0
58	MG	DA	3195	1/1	0.75	0.31	96,96,96,96	0
58	MG	CA	1619	1/1	0.75	0.78	119,119,119,119	0
58	MG	DA	3330	1/1	0.75	0.46	97,97,97,97	0
58	MG	CA	1613	1/1	0.75	0.28	68,68,68,68	0
58	MG	BA	3409	1/1	0.75	0.10	95,95,95,95	0
58	MG	DA	3220	1/1	0.75	1.42	97,97,97,97	0
58	MG	DA	3435	1/1	0.75	0.20	59,59,59,59	0
58	MG	AW	101	1/1	0.76	0.52	73,73,73,73	1
58	MG	DA	3303	1/1	0.76	1.03	97,97,97,97	0
58	MG	DA	3391	1/1	0.76	0.65	86,86,86,86	1
58	MG	BA	3209	1/1	0.76	0.23	49,49,49,49	0
58	MG	BA	3176	1/1	0.76	0.21	62,62,62,62	0
58	MG	DA	3287	1/1	0.76	0.36	77,77,77,77	0
58	MG	DA	3241	1/1	0.76	0.57	60,60,60,60	0
58	MG	CA	1638	1/1	0.76	0.46	82,82,82,82	0
58	MG	DA	3205	1/1	0.76	0.57	81,81,81,81	0
58	MG	DA	3283	1/1	0.76	0.49	66,66,66,66	1
58	MG	BA	3235	1/1	0.76	0.53	82,82,82,82	0
58	MG	BA	3377	1/1	0.76	0.55	94,94,94,94	0
58	MG	DA	3379	1/1	0.76	0.37	66,66,66,66	0
58	MG	BA	3308	1/1	0.76	0.86	97,97,97,97	0
58	MG	DA	3387	1/1	0.76	0.23	63,63,63,63	0
58	MG	CA	1742	1/1	0.76	0.61	94,94,94,94	0
58	MG	BA	3272	1/1	0.76	0.52	92,92,92,92	0
58	MG	BB	217	1/1	0.76	0.43	121,121,121,121	0
58	MG	AV	103	1/1	0.76	0.17	102,102,102,102	0
58	MG	BA	3262	1/1	0.76	0.17	81,81,81,81	0
58	MG	CA	1780	1/1	0.77	0.86	81,81,81,81	1
58	MG	BA	3236	1/1	0.77	0.38	67,67,67,67	0
58	MG	CA	1612	1/1	0.77	0.43	116,116,116,116	0
58	MG	AA	1624	1/1	0.77	0.12	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3206	1/1	0.77	0.23	63,63,63,63	0
58	MG	CA	1784	1/1	0.77	0.35	78,78,78,78	0
58	MG	BA	3307	1/1	0.77	0.19	104,104,104,104	0
58	MG	DA	3313	1/1	0.77	0.63	73,73,73,73	0
58	MG	AE	201	1/1	0.77	0.13	110,110,110,110	0
58	MG	AA	1616	1/1	0.77	0.34	74,74,74,74	0
58	MG	DB	217	1/1	0.77	0.66	110,110,110,110	1
58	MG	DA	3370	1/1	0.77	1.79	74,74,74,74	1
58	MG	BA	3346	1/1	0.77	0.23	76,76,76,76	1
58	MG	AA	1694	1/1	0.77	0.42	22,22,22,22	1
58	MG	DA	3146	1/1	0.77	0.28	58,58,58,58	1
58	MG	AA	1697	1/1	0.77	0.18	92,92,92,92	0
58	MG	AA	1689	1/1	0.77	0.21	106,106,106,106	0
58	MG	BA	3192	1/1	0.77	0.36	124,124,124,124	0
58	MG	BA	3284	1/1	0.77	0.40	77,77,77,77	0
58	MG	BA	3231	1/1	0.77	0.30	114,114,114,114	0
58	MG	B5	102	1/1	0.77	0.90	73,73,73,73	1
58	MG	AA	1764	1/1	0.77	0.08	94,94,94,94	0
58	MG	DA	3336	1/1	0.77	0.42	75,75,75,75	1
58	MG	CA	1737	1/1	0.77	0.45	95,95,95,95	1
58	MG	DA	3428	1/1	0.77	0.13	91,91,91,91	0
58	MG	DA	3388	1/1	0.77	0.36	94,94,94,94	0
58	MG	DA	3036	1/1	0.78	0.18	94,94,94,94	0
58	MG	BB	218	1/1	0.78	0.44	78,78,78,78	1
58	MG	DA	3253	1/1	0.78	0.42	72,72,72,72	1
58	MG	AA	1626	1/1	0.78	0.31	99,99,99,99	0
58	MG	BB	201	1/1	0.78	0.81	94,94,94,94	0
58	MG	BA	3381	1/1	0.78	0.10	108,108,108,108	0
58	MG	AA	1683	1/1	0.78	0.35	72,72,72,72	0
58	MG	AA	1731	1/1	0.78	0.12	64,64,64,64	0
58	MG	BA	3001	1/1	0.78	0.32	71,71,71,71	0
58	MG	BA	3321	1/1	0.78	0.42	102,102,102,102	0
58	MG	DA	3245	1/1	0.78	0.55	64,64,64,64	0
58	MG	BA	3375	1/1	0.78	0.76	58,58,58,58	1
58	MG	DA	3398	1/1	0.78	0.23	57,57,57,57	0
58	MG	CA	1799	1/1	0.78	0.17	89,89,89,89	0
58	MG	BA	3150	1/1	0.78	0.45	73,73,73,73	0
58	MG	AA	1785	1/1	0.78	0.27	70,70,70,70	0
58	MG	BA	3004	1/1	0.78	0.47	109,109,109,109	0
58	MG	AA	1723	1/1	0.78	0.39	85,85,85,85	1
58	MG	CA	1644	1/1	0.78	0.24	72,72,72,72	0
58	MG	DA	3376	1/1	0.78	0.34	128,128,128,128	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3290	1/1	0.78	0.29	51,51,51,51	0
58	MG	CA	1650	1/1	0.78	0.42	98,98,98,98	0
58	MG	BA	3445	1/1	0.79	0.25	84,84,84,84	0
58	MG	CA	1660	1/1	0.79	0.29	91,91,91,91	0
58	MG	AA	1658	1/1	0.79	0.37	58,58,58,58	1
58	MG	BA	3327	1/1	0.79	0.14	123,123,123,123	0
58	MG	AA	1604	1/1	0.79	0.42	99,99,99,99	0
58	MG	CA	1763	1/1	0.79	0.67	93,93,93,93	1
58	MG	DA	3421	1/1	0.79	0.24	107,107,107,107	1
58	MG	AW	116	1/1	0.79	0.58	129,129,129,129	1
58	MG	CA	1747	1/1	0.79	0.16	67,67,67,67	0
58	MG	DA	3246	1/1	0.79	0.51	53,53,53,53	0
58	MG	AA	1753	1/1	0.79	0.38	81,81,81,81	0
58	MG	DA	3390	1/1	0.79	0.30	112,112,112,112	0
58	MG	DA	3259	1/1	0.79	0.16	70,70,70,70	0
58	MG	AW	119	1/1	0.79	0.15	98,98,98,98	0
58	MG	BA	3267	1/1	0.80	0.23	66,66,66,66	0
58	MG	CA	1603	1/1	0.80	0.37	88,88,88,88	0
58	MG	BA	3328	1/1	0.80	0.47	116,116,116,116	1
58	MG	DA	3333	1/1	0.80	0.20	130,130,130,130	0
58	MG	AA	1691	1/1	0.80	0.30	54,54,54,54	0
58	MG	BA	3108	1/1	0.80	0.24	87,87,87,87	0
58	MG	BA	3113	1/1	0.80	0.89	82,82,82,82	0
58	MG	CA	1745	1/1	0.80	0.55	96,96,96,96	0
58	MG	AA	1686	1/1	0.80	0.33	75,75,75,75	0
58	MG	BA	3071	1/1	0.80	0.33	70,70,70,70	0
58	MG	AA	1718	1/1	0.80	0.17	150,150,150,150	0
58	MG	BA	3289	1/1	0.80	0.21	93,93,93,93	0
58	MG	DA	3282	1/1	0.80	0.36	73,73,73,73	1
58	MG	BA	3253	1/1	0.80	0.37	85,85,85,85	0
58	MG	DA	3319	1/1	0.80	0.44	105,105,105,105	1
58	MG	CA	1767	1/1	0.80	0.43	76,76,76,76	0
58	MG	CA	1725	1/1	0.80	0.49	131,131,131,131	0
58	MG	AA	1752	1/1	0.80	0.47	104,104,104,104	0
58	MG	BA	3349	1/1	0.80	0.46	76,76,76,76	1
58	MG	BA	3002	1/1	0.80	0.28	71,71,71,71	0
58	MG	AA	1632	1/1	0.80	0.14	64,64,64,64	0
58	MG	AA	1771	1/1	0.80	0.41	73,73,73,73	0
58	MG	CA	1755	1/1	0.80	0.23	105,105,105,105	0
58	MG	DX	103	1/1	0.81	0.24	112,112,112,112	0
58	MG	CA	1686	1/1	0.81	0.37	80,80,80,80	0
58	MG	BA	3142	1/1	0.81	0.41	77,77,77,77	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	1813	1/1	0.81	0.56	96,96,96,96	0
58	MG	DA	3117	1/1	0.81	0.63	69,69,69,69	0
58	MG	CA	1658	1/1	0.81	1.44	103,103,103,103	0
58	MG	AA	1719	1/1	0.81	0.27	91,91,91,91	0
58	MG	CW	119	1/1	0.81	0.37	108,108,108,108	0
58	MG	AA	1802	1/1	0.81	0.21	110,110,110,110	0
58	MG	DA	3314	1/1	0.81	0.39	72,72,72,72	0
58	MG	DA	3181	1/1	0.81	0.61	74,74,74,74	0
58	MG	AA	1612	1/1	0.81	0.33	80,80,80,80	0
58	MG	CA	1709	1/1	0.81	0.73	96,96,96,96	0
58	MG	CV	102	1/1	0.81	0.12	89,89,89,89	1
58	MG	CA	1656	1/1	0.81	0.63	74,74,74,74	0
58	MG	AA	1740	1/1	0.81	0.43	81,81,81,81	1
58	MG	CA	1750	1/1	0.81	0.28	109,109,109,109	0
58	MG	CA	1653	1/1	0.81	0.52	110,110,110,110	0
58	MG	BA	3177	1/1	0.81	0.14	55,55,55,55	0
58	MG	BN	201	1/1	0.81	0.93	79,79,79,79	0
58	MG	BA	3451	1/1	0.81	0.11	85,85,85,85	0
58	MG	AA	1643	1/1	0.81	0.22	65,65,65,65	0
58	MG	BA	3419	1/1	0.81	0.77	93,93,93,93	0
58	MG	CA	1815	1/1	0.81	0.53	68,68,68,68	0
58	MG	DA	3201	1/1	0.81	0.65	55,55,55,55	0
58	MG	BP	202	1/1	0.81	0.29	14,14,14,14	1
58	MG	DA	3297	1/1	0.81	0.15	84,84,84,84	0
58	MG	CA	1690	1/1	0.81	0.12	122,122,122,122	0
58	MG	BA	3292	1/1	0.81	0.24	65,65,65,65	0
58	MG	AA	1728	1/1	0.81	0.26	69,69,69,69	0
58	MG	AV	108	1/1	0.81	0.18	67,67,67,67	1
58	MG	BA	3365	1/1	0.81	0.61	76,76,76,76	1
58	MG	BA	3191	1/1	0.81	0.27	71,71,71,71	0
58	MG	BA	3123	1/1	0.81	0.21	46,46,46,46	0
58	MG	DA	3401	1/1	0.82	0.34	68,68,68,68	0
58	MG	DA	3296	1/1	0.82	1.24	66,66,66,66	1
58	MG	DA	3189	1/1	0.82	0.39	77,77,77,77	0
58	MG	AA	1791	1/1	0.82	0.48	60,60,60,60	1
58	MG	DA	3293	1/1	0.82	0.51	52,52,52,52	0
58	MG	AX	104	1/1	0.82	0.64	71,71,71,71	1
58	MG	DA	3009	1/1	0.82	0.29	44,44,44,44	0
58	MG	DA	3049	1/1	0.82	0.89	83,83,83,83	0
58	MG	DA	3430	1/1	0.82	0.22	106,106,106,106	0
58	MG	BA	3275	1/1	0.82	0.13	61,61,61,61	0
58	MG	CA	1659	1/1	0.82	0.39	64,64,64,64	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	1729	1/1	0.82	0.35	81,81,81,81	0
58	MG	DA	3258	1/1	0.82	0.28	66,66,66,66	0
58	MG	CA	1732	1/1	0.82	0.11	66,66,66,66	0
58	MG	DA	3318	1/1	0.82	0.35	122,122,122,122	0
58	MG	DA	3269	1/1	0.82	0.18	65,65,65,65	0
58	MG	DA	3216	1/1	0.82	0.16	78,78,78,78	1
58	MG	DA	3389	1/1	0.82	0.28	42,42,42,42	1
58	MG	CW	117	1/1	0.82	0.73	125,125,125,125	0
58	MG	CA	1601	1/1	0.82	0.29	49,49,49,49	0
58	MG	AA	1790	1/1	0.82	0.98	28,28,28,28	1
58	MG	AA	1755	1/1	0.82	0.42	83,83,83,83	0
58	MG	BA	3060	1/1	0.83	0.27	72,72,72,72	0
58	MG	BA	3386	1/1	0.83	0.09	63,63,63,63	0
58	MG	BA	3273	1/1	0.83	0.32	76,76,76,76	0
58	MG	DA	3128	1/1	0.83	0.27	65,65,65,65	0
58	MG	BA	3181	1/1	0.83	0.47	67,67,67,67	0
58	MG	DD	302	1/1	0.83	0.37	64,64,64,64	0
58	MG	DA	3093	1/1	0.83	0.38	50,50,50,50	0
58	MG	BA	3255	1/1	0.83	0.19	102,102,102,102	0
58	MG	CA	1775	1/1	0.83	0.14	69,69,69,69	0
58	MG	AA	1638	1/1	0.83	0.54	115,115,115,115	0
58	MG	BA	3350	1/1	0.83	0.34	105,105,105,105	0
58	MG	BA	3157	1/1	0.83	0.45	78,78,78,78	1
58	MG	BA	3313	1/1	0.83	0.24	38,38,38,38	0
58	MG	AA	1778	1/1	0.83	0.23	84,84,84,84	0
58	MG	BA	3393	1/1	0.83	0.34	101,101,101,101	1
58	MG	DA	3254	1/1	0.83	0.28	123,123,123,123	0
58	MG	BA	3271	1/1	0.83	0.08	114,114,114,114	0
58	MG	BA	3378	1/1	0.83	0.49	65,65,65,65	1
58	MG	BA	3149	1/1	0.83	0.42	116,116,116,116	0
58	MG	CA	1756	1/1	0.83	0.22	59,59,59,59	0
58	MG	DA	3289	1/1	0.83	0.19	73,73,73,73	0
58	MG	CA	1606	1/1	0.83	0.35	66,66,66,66	0
58	MG	BA	3256	1/1	0.83	0.39	61,61,61,61	0
58	MG	DA	3018	1/1	0.83	0.53	51,51,51,51	0
58	MG	CA	1615	1/1	0.83	0.17	81,81,81,81	0
58	MG	AW	114	1/1	0.84	0.67	91,91,91,91	1
58	MG	DA	3059	1/1	0.84	0.76	84,84,84,84	0
58	MG	DA	3408	1/1	0.84	1.02	106,106,106,106	0
58	MG	BA	3300	1/1	0.84	0.11	80,80,80,80	0
58	MG	DB	215	1/1	0.84	0.14	64,64,64,64	1
58	MG	CA	1764	1/1	0.84	0.14	87,87,87,87	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3180	1/1	0.84	0.14	79,79,79,79	0
58	MG	BA	3006	1/1	0.84	0.37	104,104,104,104	0
58	MG	BA	3055	1/1	0.84	0.16	33,33,33,33	0
58	MG	DA	3135	1/1	0.84	0.36	52,52,52,52	0
58	MG	CA	1727	1/1	0.84	0.45	80,80,80,80	0
58	MG	DA	3363	1/1	0.84	0.08	114,114,114,114	0
58	MG	BA	3304	1/1	0.84	0.34	95,95,95,95	0
58	MG	DA	3154	1/1	0.84	0.29	101,101,101,101	0
58	MG	BA	3061	1/1	0.84	0.28	38,38,38,38	0
58	MG	AA	1776	1/1	0.84	0.14	94,94,94,94	0
58	MG	AA	1761	1/1	0.84	0.64	83,83,83,83	1
58	MG	DA	3404	1/1	0.84	0.21	51,51,51,51	0
58	MG	CA	1805	1/1	0.84	0.18	59,59,59,59	1
58	MG	CA	1645	1/1	0.84	0.41	78,78,78,78	0
58	MG	DA	3372	1/1	0.84	0.26	106,106,106,106	0
58	MG	BA	3302	1/1	0.84	0.17	56,56,56,56	0
58	MG	DA	3167	1/1	0.84	0.12	79,79,79,79	0
58	MG	BA	3153	1/1	0.84	0.62	118,118,118,118	0
58	MG	BA	3257	1/1	0.84	0.28	46,46,46,46	1
58	MG	DA	3040	1/1	0.84	0.13	78,78,78,78	0
58	MG	CA	1691	1/1	0.84	0.15	67,67,67,67	0
58	MG	AA	1774	1/1	0.84	0.15	70,70,70,70	0
58	MG	DB	205	1/1	0.84	0.32	58,58,58,58	1
58	MG	BA	3314	1/1	0.84	0.33	74,74,74,74	0
58	MG	BA	3432	1/1	0.84	0.13	57,57,57,57	0
58	MG	DA	3362	1/1	0.84	0.17	111,111,111,111	0
58	MG	CA	1602	1/1	0.84	0.15	64,64,64,64	0
58	MG	DA	3341	1/1	0.84	0.48	78,78,78,78	1
58	MG	AW	118	1/1	0.85	0.44	103,103,103,103	1
58	MG	AA	1758	1/1	0.85	0.35	70,70,70,70	1
58	MG	CW	107	1/1	0.85	0.13	91,91,91,91	1
58	MG	CA	1614	1/1	0.85	0.31	71,71,71,71	0
58	MG	CV	104	1/1	0.85	0.24	85,85,85,85	1
58	MG	DA	3299	1/1	0.85	0.20	119,119,119,119	0
58	MG	BA	3325	1/1	0.85	0.38	104,104,104,104	1
58	MG	AA	1807	1/1	0.85	0.37	71,71,71,71	1
58	MG	DA	3321	1/1	0.85	0.28	100,100,100,100	0
58	MG	CA	1708	1/1	0.85	0.52	81,81,81,81	0
58	MG	BA	3065	1/1	0.85	0.35	59,59,59,59	0
58	MG	BA	3174	1/1	0.85	1.34	77,77,77,77	0
58	MG	BA	3005	1/1	0.85	0.48	85,85,85,85	0
58	MG	BB	205	1/1	0.85	1.13	45,45,45,45	1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BF	301	1/1	0.85	0.19	70,70,70,70	0
58	MG	BA	3121	1/1	0.85	0.20	82,82,82,82	0
58	MG	AA	1675	1/1	0.85	0.30	69,69,69,69	0
58	MG	BA	3128	1/1	0.85	0.24	37,37,37,37	0
58	MG	CA	1753	1/1	0.85	0.13	74,74,74,74	0
58	MG	CW	104	1/1	0.85	0.44	108,108,108,108	1
58	MG	BA	3186	1/1	0.85	0.20	63,63,63,63	0
58	MG	DA	3199	1/1	0.85	0.31	68,68,68,68	0
58	MG	CA	1684	1/1	0.85	0.26	67,67,67,67	0
58	MG	DA	3033	1/1	0.85	0.30	91,91,91,91	0
58	MG	DX	102	1/1	0.85	0.73	68,68,68,68	0
58	MG	AA	1709	1/1	0.85	1.05	119,119,119,119	0
58	MG	BA	3373	1/1	0.85	0.68	56,56,56,56	1
58	MG	BA	3411	1/1	0.85	0.63	95,95,95,95	0
58	MG	AA	1712	1/1	0.85	0.46	67,67,67,67	0
58	MG	CA	1804	1/1	0.85	0.12	85,85,85,85	0
58	MG	BA	3323	1/1	0.85	0.16	83,83,83,83	1
58	MG	BA	3261	1/1	0.85	0.19	79,79,79,79	0
58	MG	AA	1748	1/1	0.86	0.12	76,76,76,76	0
58	MG	DA	3431	1/1	0.86	0.22	137,137,137,137	0
58	MG	DA	3320	1/1	0.86	0.15	101,101,101,101	1
58	MG	CA	1789	1/1	0.86	0.31	61,61,61,61	0
58	MG	BA	3319	1/1	0.86	0.39	75,75,75,75	0
58	MG	AA	1660	1/1	0.86	0.49	90,90,90,90	0
58	MG	BA	3299	1/1	0.86	0.26	68,68,68,68	0
58	MG	DA	3140	1/1	0.86	0.26	64,64,64,64	0
58	MG	CW	121	1/1	0.86	0.53	125,125,125,125	0
58	MG	DV	202	1/1	0.86	0.39	63,63,63,63	1
58	MG	DA	3069	1/1	0.86	0.20	79,79,79,79	0
58	MG	BA	3293	1/1	0.86	0.30	75,75,75,75	0
58	MG	BA	3396	1/1	0.86	0.34	78,78,78,78	1
58	MG	CW	109	1/1	0.86	0.16	57,57,57,57	1
58	MG	BA	3161	1/1	0.86	0.42	68,68,68,68	0
58	MG	CA	1797	1/1	0.86	0.54	111,111,111,111	0
58	MG	DA	3275	1/1	0.86	0.29	57,57,57,57	0
58	MG	DA	3163	1/1	0.86	0.36	84,84,84,84	0
58	MG	AA	1803	1/1	0.86	0.15	33,33,33,33	1
58	MG	AA	1805	1/1	0.86	0.60	88,88,88,88	1
58	MG	DB	211	1/1	0.86	0.62	69,69,69,69	1
58	MG	CA	1671	1/1	0.86	0.35	79,79,79,79	0
58	MG	DB	208	1/1	0.86	0.15	87,87,87,87	0
58	MG	BA	3371	1/1	0.86	0.27	81,81,81,81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	1620	1/1	0.86	1.10	91,91,91,91	0
58	MG	BA	3337	1/1	0.86	0.08	116,116,116,116	0
58	MG	BA	3166	1/1	0.86	0.27	71,71,71,71	0
58	MG	DA	3170	1/1	0.86	0.14	46,46,46,46	1
58	MG	BA	3367	1/1	0.86	0.59	107,107,107,107	0
58	MG	BA	3437	1/1	0.86	0.15	75,75,75,75	0
58	MG	BA	3317	1/1	0.86	0.25	117,117,117,117	0
58	MG	DA	3048	1/1	0.86	0.35	44,44,44,44	0
58	MG	DA	3230	1/1	0.86	0.52	119,119,119,119	0
58	MG	CA	1744	1/1	0.86	0.72	75,75,75,75	0
58	MG	CA	1634	1/1	0.86	0.14	97,97,97,97	0
58	MG	AA	1609	1/1	0.86	0.24	58,58,58,58	0
58	MG	DA	3120	1/1	0.87	0.32	81,81,81,81	0
58	MG	AA	1615	1/1	0.87	0.15	63,63,63,63	0
58	MG	BA	3154	1/1	0.87	0.36	106,106,106,106	1
58	MG	DA	3032	1/1	0.87	0.28	69,69,69,69	0
58	MG	D2	101	1/1	0.87	0.27	73,73,73,73	0
58	MG	BA	3410	1/1	0.87	0.28	113,113,113,113	0
58	MG	CA	1749	1/1	0.87	0.52	87,87,87,87	0
58	MG	AA	1687	1/1	0.87	0.33	105,105,105,105	0
58	MG	DA	3393	1/1	0.87	0.56	89,89,89,89	0
58	MG	BA	3237	1/1	0.87	0.43	78,78,78,78	0
58	MG	CW	110	1/1	0.87	0.30	85,85,85,85	1
58	MG	AA	1645	1/1	0.87	0.44	59,59,59,59	0
58	MG	BA	3151	1/1	0.87	0.38	64,64,64,64	0
58	MG	AA	1692	1/1	0.87	0.59	61,61,61,61	0
58	MG	CA	1779	1/1	0.87	0.28	121,121,121,121	0
58	MG	BA	3244	1/1	0.87	0.36	75,75,75,75	0
58	MG	AA	1707	1/1	0.87	0.45	66,66,66,66	0
58	MG	BA	3201	1/1	0.87	0.31	59,59,59,59	0
58	MG	DA	3218	1/1	0.87	0.19	75,75,75,75	0
58	MG	DA	3127	1/1	0.87	0.20	65,65,65,65	0
58	MG	AA	1744	1/1	0.87	0.27	84,84,84,84	0
58	MG	BA	3344	1/1	0.87	0.21	46,46,46,46	1
58	MG	AA	1619	1/1	0.87	0.47	78,78,78,78	0
58	MG	AA	1669	1/1	0.87	0.42	82,82,82,82	0
58	MG	BA	3217	1/1	0.87	0.46	79,79,79,79	0
58	MG	BA	3398	1/1	0.87	0.12	113,113,113,113	0
58	MG	BA	3023	1/1	0.87	0.26	71,71,71,71	0
58	MG	CA	1712	1/1	0.87	0.16	128,128,128,128	0
58	MG	DA	3194	1/1	0.87	0.30	84,84,84,84	0
58	MG	AW	120	1/1	0.87	0.22	92,92,92,92	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	1807	1/1	0.87	0.50	62,62,62,62	1
58	MG	CA	1679	1/1	0.87	0.23	86,86,86,86	1
58	MG	BA	3353	1/1	0.87	0.32	89,89,89,89	0
58	MG	DA	3203	1/1	0.87	0.30	50,50,50,50	0
58	MG	BB	211	1/1	0.87	0.99	75,75,75,75	1
58	MG	AA	1633	1/1	0.87	0.14	75,75,75,75	0
58	MG	DA	3187	1/1	0.87	0.28	71,71,71,71	0
58	MG	CX	102	1/1	0.87	0.09	95,95,95,95	0
58	MG	DA	3302	1/1	0.87	0.10	86,86,86,86	0
58	MG	DA	3013	1/1	0.87	0.25	67,67,67,67	0
58	MG	BA	3198	1/1	0.87	0.24	61,61,61,61	0
58	MG	DA	3268	1/1	0.87	0.20	79,79,79,79	0
58	MG	BA	3007	1/1	0.87	0.53	66,66,66,66	0
58	MG	CA	1785	1/1	0.88	0.42	85,85,85,85	0
58	MG	BB	203	1/1	0.88	0.13	134,134,134,134	0
58	MG	CA	1769	1/1	0.88	0.21	122,122,122,122	0
58	MG	DA	3100	1/1	0.88	0.61	71,71,71,71	0
58	MG	BA	3118	1/1	0.88	0.38	53,53,53,53	0
60	ZN	D9	101	1/1	0.88	0.24	196,196,196,196	0
58	MG	DA	3056	1/1	0.88	0.18	48,48,48,48	0
58	MG	DA	3124	1/1	0.88	0.20	63,63,63,63	0
58	MG	AA	1797	1/1	0.88	0.33	137,137,137,137	0
58	MG	DA	3042	1/1	0.88	0.56	76,76,76,76	0
58	MG	CA	1791	1/1	0.88	0.86	27,27,27,27	1
58	MG	DA	3347	1/1	0.88	0.09	71,71,71,71	0
58	MG	AA	1656	1/1	0.88	0.10	68,68,68,68	0
58	MG	CW	112	1/1	0.88	0.17	81,81,81,81	1
58	MG	AA	1729	1/1	0.88	0.48	104,104,104,104	0
58	MG	BA	3144	1/1	0.88	0.44	68,68,68,68	0
58	MG	CA	1616	1/1	0.88	0.09	75,75,75,75	0
58	MG	BA	3136	1/1	0.88	0.17	64,64,64,64	0
58	MG	AA	1678	1/1	0.88	0.32	93,93,93,93	1
58	MG	DA	3115	1/1	0.88	0.15	36,36,36,36	0
58	MG	DA	3343	1/1	0.88	0.40	89,89,89,89	1
58	MG	BA	3294	1/1	0.88	0.16	85,85,85,85	0
58	MG	AA	1702	1/1	0.88	0.24	57,57,57,57	0
58	MG	AA	1766	1/1	0.88	0.33	74,74,74,74	0
58	MG	AA	1677	1/1	0.88	0.44	96,96,96,96	0
58	MG	DA	3206	1/1	0.88	0.29	55,55,55,55	0
58	MG	CV	107	1/1	0.88	0.20	66,66,66,66	0
58	MG	BA	3263	1/1	0.88	0.10	77,77,77,77	0
58	MG	AA	1703	1/1	0.88	0.10	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3006	1/1	0.88	0.27	87,87,87,87	0
58	MG	BA	3173	1/1	0.88	0.32	72,72,72,72	1
58	MG	AA	1681	1/1	0.88	0.37	69,69,69,69	0
58	MG	DA	3162	1/1	0.88	0.22	65,65,65,65	0
58	MG	DA	3361	1/1	0.88	0.36	71,71,71,71	0
58	MG	AA	1682	1/1	0.88	0.16	75,75,75,75	0
58	MG	BB	210	1/1	0.88	0.28	50,50,50,50	1
58	MG	BA	3380	1/1	0.88	0.07	66,66,66,66	0
58	MG	BA	3178	1/1	0.88	0.30	67,67,67,67	0
58	MG	AA	1767	1/1	0.88	0.28	44,44,44,44	1
58	MG	AA	1679	1/1	0.88	0.15	49,49,49,49	1
58	MG	DA	3003	1/1	0.88	0.41	79,79,79,79	0
58	MG	DA	3286	1/1	0.88	0.19	53,53,53,53	0
58	MG	DA	3300	1/1	0.88	0.34	63,63,63,63	0
58	MG	BA	3400	1/1	0.88	0.14	67,67,67,67	0
58	MG	BA	3100	1/1	0.88	0.54	43,43,43,43	0
58	MG	DA	3290	1/1	0.88	0.59	64,64,64,64	0
58	MG	DA	3165	1/1	0.88	0.08	100,100,100,100	0
58	MG	CA	1787	1/1	0.88	0.09	56,56,56,56	0
58	MG	DA	3322	1/1	0.88	0.35	100,100,100,100	1
58	MG	AW	108	1/1	0.88	0.16	143,143,143,143	0
58	MG	BA	3413	1/1	0.89	0.18	105,105,105,105	1
58	MG	DA	3292	1/1	0.89	0.48	49,49,49,49	0
58	MG	BA	3132	1/1	0.89	0.27	36,36,36,36	0
58	MG	BA	3443	1/1	0.89	0.34	100,100,100,100	0
58	MG	BA	3280	1/1	0.89	0.08	87,87,87,87	0
58	MG	DA	3270	1/1	0.89	0.12	44,44,44,44	0
58	MG	CA	1631	1/1	0.89	0.32	88,88,88,88	0
58	MG	DA	3305	1/1	0.89	0.33	60,60,60,60	0
58	MG	CA	1748	1/1	0.89	0.24	88,88,88,88	1
58	MG	BA	3072	1/1	0.89	0.49	67,67,67,67	0
58	MG	AA	1614	1/1	0.89	0.18	76,76,76,76	0
58	MG	DA	3157	1/1	0.89	0.25	47,47,47,47	1
58	MG	BA	3416	1/1	0.89	1.92	95,95,95,95	0
58	MG	DA	3424	1/1	0.89	0.21	53,53,53,53	0
58	MG	BA	3343	1/1	0.89	0.38	55,55,55,55	1
58	MG	AA	1622	1/1	0.89	0.23	45,45,45,45	0
58	MG	BA	3282	1/1	0.89	0.19	121,121,121,121	0
58	MG	AA	1751	1/1	0.89	0.27	75,75,75,75	0
58	MG	CA	1648	1/1	0.89	0.23	108,108,108,108	0
58	MG	CW	102	1/1	0.89	1.00	98,98,98,98	1
58	MG	CA	1715	1/1	0.89	0.14	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3369	1/1	0.89	0.32	96,96,96,96	0
58	MG	BA	3301	1/1	0.89	0.72	67,67,67,67	1
58	MG	BA	3172	1/1	0.89	0.25	78,78,78,78	0
58	MG	AA	1782	1/1	0.89	0.59	71,71,71,71	0
58	MG	BA	3103	1/1	0.89	0.28	68,68,68,68	0
58	MG	CA	1814	1/1	0.89	0.70	115,115,115,115	1
58	MG	DA	3164	1/1	0.89	0.35	63,63,63,63	0
58	MG	AW	105	1/1	0.89	0.13	116,116,116,116	0
58	MG	DA	3239	1/1	0.89	0.23	63,63,63,63	0
58	MG	DA	3142	1/1	0.89	0.93	125,125,125,125	0
58	MG	BA	3274	1/1	0.89	0.12	54,54,54,54	0
58	MG	AA	1641	1/1	0.89	0.08	65,65,65,65	0
58	MG	BA	3286	1/1	0.89	0.43	66,66,66,66	0
58	MG	DA	3028	1/1	0.89	0.32	63,63,63,63	0
58	MG	B2	602	1/1	0.89	0.31	112,112,112,112	0
58	MG	AV	106	1/1	0.89	0.15	119,119,119,119	0
58	MG	BA	3245	1/1	0.89	0.55	81,81,81,81	0
58	MG	CA	1795	1/1	0.89	0.21	55,55,55,55	0
58	MG	DA	3326	1/1	0.89	0.32	134,134,134,134	0
58	MG	CA	1711	1/1	0.89	0.08	95,95,95,95	0
58	MG	BA	3159	1/1	0.89	0.30	52,52,52,52	1
58	MG	DA	3295	1/1	0.89	0.16	85,85,85,85	0
58	MG	AA	1639	1/1	0.89	0.20	57,57,57,57	0
58	MG	AA	1794	1/1	0.89	0.20	70,70,70,70	0
58	MG	DA	3308	1/1	0.89	0.26	48,48,48,48	0
58	MG	DA	3356	1/1	0.89	0.69	78,78,78,78	1
58	MG	DA	3226	1/1	0.89	0.33	121,121,121,121	0
58	MG	CA	1761	1/1	0.89	0.63	94,94,94,94	0
58	MG	BA	3433	1/1	0.89	0.14	121,121,121,121	0
58	MG	CA	1670	1/1	0.89	0.85	84,84,84,84	0
58	MG	BA	3207	1/1	0.90	0.09	59,59,59,59	0
60	ZN	B9	101	1/1	0.90	0.50	199,199,199,199	0
58	MG	BA	3326	1/1	0.90	0.61	111,111,111,111	1
58	MG	DA	3112	1/1	0.90	0.32	70,70,70,70	0
58	MG	DA	3248	1/1	0.90	0.30	62,62,62,62	0
58	MG	DA	3118	1/1	0.90	0.10	29,29,29,29	0
58	MG	BA	3254	1/1	0.90	0.18	74,74,74,74	0
58	MG	BA	3044	1/1	0.90	0.50	115,115,115,115	0
58	MG	CW	120	1/1	0.90	0.29	117,117,117,117	1
58	MG	CA	1757	1/1	0.90	0.40	76,76,76,76	0
58	MG	DA	3004	1/1	0.90	0.34	54,54,54,54	0
58	MG	DA	3016	1/1	0.90	0.18	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3226	1/1	0.90	0.34	33,33,33,33	0
58	MG	BA	3332	1/1	0.90	0.15	138,138,138,138	0
58	MG	DA	3210	1/1	0.90	0.15	145,145,145,145	0
58	MG	BA	3218	1/1	0.90	0.21	87,87,87,87	0
58	MG	DA	3104	1/1	0.90	0.26	60,60,60,60	0
58	MG	DA	3182	1/1	0.90	0.40	65,65,65,65	0
58	MG	AA	1659	1/1	0.90	0.83	88,88,88,88	0
58	MG	BA	3134	1/1	0.90	0.28	70,70,70,70	0
58	MG	DA	3217	1/1	0.90	0.47	109,109,109,109	0
58	MG	CA	1655	1/1	0.90	0.11	99,99,99,99	0
58	MG	DB	207	1/1	0.90	0.07	79,79,79,79	0
58	MG	DA	3155	1/1	0.90	0.20	53,53,53,53	1
58	MG	DA	3158	1/1	0.90	0.39	51,51,51,51	0
58	MG	BA	3421	1/1	0.90	0.24	110,110,110,110	0
58	MG	BA	3156	1/1	0.90	0.69	89,89,89,89	0
58	MG	BA	3189	1/1	0.90	0.33	54,54,54,54	0
58	MG	BA	3036	1/1	0.90	0.72	90,90,90,90	0
58	MG	DA	3417	1/1	0.90	0.32	71,71,71,71	0
58	MG	DA	3257	1/1	0.90	0.17	99,99,99,99	0
58	MG	BA	3131	1/1	0.90	0.09	60,60,60,60	0
58	MG	CA	1759	1/1	0.90	0.88	88,88,88,88	1
58	MG	DA	3122	1/1	0.90	0.20	49,49,49,49	0
58	MG	CA	1681	1/1	0.90	0.13	69,69,69,69	0
58	MG	CA	1736	1/1	0.90	0.28	73,73,73,73	0
58	MG	AA	1708	1/1	0.90	0.46	93,93,93,93	0
58	MG	AA	1786	1/1	0.90	0.24	55,55,55,55	0
58	MG	AU	101	1/1	0.90	0.53	117,117,117,117	0
58	MG	DA	3266	1/1	0.90	0.09	87,87,87,87	0
58	MG	BA	3224	1/1	0.90	0.36	96,96,96,96	0
58	MG	CA	1717	1/1	0.90	0.11	67,67,67,67	0
58	MG	BA	3029	1/1	0.90	0.40	63,63,63,63	0
58	MG	BA	3042	1/1	0.90	0.14	35,35,35,35	0
58	MG	BB	216	1/1	0.91	0.30	94,94,94,94	1
58	MG	CA	1741	1/1	0.91	0.32	130,130,130,130	1
58	MG	CA	1803	1/1	0.91	0.06	70,70,70,70	0
58	MG	D7	101	1/1	0.91	0.18	51,51,51,51	0
58	MG	DA	3109	1/1	0.91	0.22	43,43,43,43	0
58	MG	AA	1727	1/1	0.91	0.16	62,62,62,62	0
58	MG	AA	1738	1/1	0.91	0.58	89,89,89,89	0
58	MG	DA	3284	1/1	0.91	0.24	70,70,70,70	0
58	MG	BA	3442	1/1	0.91	0.09	67,67,67,67	0
58	MG	DA	3222	1/1	0.91	0.38	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CW	118	1/1	0.91	0.14	95,95,95,95	1
58	MG	BA	3372	1/1	0.91	0.82	105,105,105,105	0
58	MG	BA	3426	1/1	0.91	0.37	76,76,76,76	0
58	MG	DA	3272	1/1	0.91	0.22	51,51,51,51	0
58	MG	BA	3064	1/1	0.91	0.36	39,39,39,39	0
58	MG	BA	3025	1/1	0.91	0.33	42,42,42,42	0
58	MG	CW	101	1/1	0.91	0.41	94,94,94,94	1
58	MG	AW	102	1/1	0.91	0.16	78,78,78,78	1
58	MG	BB	207	1/1	0.91	0.09	81,81,81,81	0
58	MG	CA	1668	1/1	0.91	0.09	80,80,80,80	0
58	MG	AA	1636	1/1	0.91	0.16	44,44,44,44	1
58	MG	BA	3417	1/1	0.91	0.28	49,49,49,49	0
58	MG	DA	3074	1/1	0.91	0.12	40,40,40,40	0
58	MG	BA	3407	1/1	0.91	0.39	82,82,82,82	0
58	MG	DV	201	1/1	0.91	0.33	95,95,95,95	0
58	MG	AA	1721	1/1	0.91	0.22	55,55,55,55	0
58	MG	AA	1715	1/1	0.91	0.26	63,63,63,63	0
58	MG	BA	3079	1/1	0.91	0.17	28,28,28,28	0
58	MG	CA	1720	1/1	0.91	0.14	79,79,79,79	0
58	MG	DA	3133	1/1	0.91	0.18	52,52,52,52	0
58	MG	DA	3403	1/1	0.91	0.50	72,72,72,72	0
58	MG	DA	3436	1/1	0.91	0.23	60,60,60,60	0
58	MG	DA	3012	1/1	0.91	0.61	70,70,70,70	0
58	MG	DA	3022	1/1	0.91	0.16	69,69,69,69	0
58	MG	AA	1726	1/1	0.91	0.32	65,65,65,65	0
58	MG	DA	3437	1/1	0.91	0.36	52,52,52,52	0
58	MG	DA	3017	1/1	0.91	0.20	58,58,58,58	0
58	MG	AA	1735	1/1	0.91	0.25	58,58,58,58	0
58	MG	DA	3278	1/1	0.91	0.05	116,116,116,116	0
58	MG	CA	1652	1/1	0.91	0.18	113,113,113,113	0
58	MG	AA	1621	1/1	0.91	0.13	55,55,55,55	0
58	MG	AA	1673	1/1	0.91	0.27	53,53,53,53	0
58	MG	AA	1705	1/1	0.91	0.12	35,35,35,35	0
58	MG	AA	1653	1/1	0.91	0.54	82,82,82,82	1
58	MG	AW	106	1/1	0.91	0.27	103,103,103,103	0
58	MG	DA	3008	1/1	0.91	0.83	70,70,70,70	0
58	MG	DA	3034	1/1	0.91	0.24	54,54,54,54	0
58	MG	AA	1787	1/1	0.91	0.23	58,58,58,58	0
58	MG	AA	1746	1/1	0.91	0.11	57,57,57,57	0
58	MG	CA	1662	1/1	0.91	0.12	114,114,114,114	0
58	MG	BA	3418	1/1	0.91	0.30	61,61,61,61	0
58	MG	BA	3430	1/1	0.92	0.16	92,92,92,92	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3352	1/1	0.92	0.58	70,70,70,70	0
58	MG	BA	3165	1/1	0.92	0.15	63,63,63,63	0
58	MG	CA	1781	1/1	0.92	0.36	82,82,82,82	0
58	MG	DA	3441	1/1	0.92	0.44	74,74,74,74	0
58	MG	DA	3280	1/1	0.92	0.53	107,107,107,107	0
58	MG	BA	3110	1/1	0.92	0.31	47,47,47,47	0
58	MG	CV	103	1/1	0.92	0.09	89,89,89,89	0
58	MG	BA	3111	1/1	0.92	0.17	38,38,38,38	0
58	MG	DA	3204	1/1	0.92	0.09	33,33,33,33	0
58	MG	DA	3147	1/1	0.92	0.25	105,105,105,105	0
58	MG	DA	3274	1/1	0.92	0.23	141,141,141,141	0
58	MG	CA	1605	1/1	0.92	0.12	72,72,72,72	0
58	MG	BA	3222	1/1	0.92	0.07	57,57,57,57	0
58	MG	CA	1620	1/1	0.92	0.61	65,65,65,65	0
58	MG	DA	3064	1/1	0.92	0.48	61,61,61,61	0
58	MG	AA	1617	1/1	0.92	0.50	66,66,66,66	0
58	MG	BA	3310	1/1	0.92	0.41	36,36,36,36	0
58	MG	AA	1806	1/1	0.92	0.07	68,68,68,68	0
58	MG	BA	3182	1/1	0.92	0.30	107,107,107,107	0
58	MG	BA	3208	1/1	0.92	0.21	59,59,59,59	0
58	MG	CA	1703	1/1	0.92	0.36	71,71,71,71	0
58	MG	AA	1720	1/1	0.92	0.14	56,56,56,56	0
58	MG	DA	3027	1/1	0.92	0.35	50,50,50,50	0
58	MG	AA	1644	1/1	0.92	0.13	57,57,57,57	0
58	MG	AA	1690	1/1	0.92	0.20	69,69,69,69	0
58	MG	BA	3139	1/1	0.92	0.29	59,59,59,59	0
58	MG	DA	3091	1/1	0.92	0.53	84,84,84,84	0
58	MG	AA	1775	1/1	0.92	0.04	68,68,68,68	0
58	MG	AA	1680	1/1	0.92	0.13	79,79,79,79	0
58	MG	BA	3101	1/1	0.92	0.37	58,58,58,58	0
58	MG	AA	1714	1/1	0.92	0.25	86,86,86,86	0
58	MG	AA	1640	1/1	0.92	0.54	56,56,56,56	0
58	MG	BA	3333	1/1	0.92	0.37	79,79,79,79	1
58	MG	BA	3085	1/1	0.92	0.20	49,49,49,49	0
58	MG	BA	3088	1/1	0.92	0.29	69,69,69,69	0
58	MG	AA	1664	1/1	0.92	0.24	55,55,55,55	0
58	MG	DA	3238	1/1	0.92	0.53	135,135,135,135	0
58	MG	AW	111	1/1	0.92	0.10	24,24,24,24	1
58	MG	BA	3033	1/1	0.92	0.32	63,63,63,63	0
58	MG	BB	215	1/1	0.92	0.20	88,88,88,88	1
58	MG	DA	3050	1/1	0.92	0.57	45,45,45,45	0
58	MG	AA	1634	1/1	0.92	0.14	106,106,106,106	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3168	1/1	0.92	0.17	62,62,62,62	0
58	MG	DA	3233	1/1	0.92	0.22	50,50,50,50	0
58	MG	BA	3035	1/1	0.92	0.18	70,70,70,70	0
58	MG	DA	3425	1/1	0.92	0.12	76,76,76,76	0
58	MG	DA	3349	1/1	0.92	0.16	103,103,103,103	0
58	MG	AA	1674	1/1	0.92	0.44	63,63,63,63	0
58	MG	BA	3014	1/1	0.92	0.11	40,40,40,40	0
58	MG	DA	3119	1/1	0.92	0.18	50,50,50,50	0
58	MG	DA	3342	1/1	0.92	0.17	62,62,62,62	1
58	MG	D2	102	1/1	0.92	0.41	50,50,50,50	1
58	MG	BA	3277	1/1	0.92	0.12	58,58,58,58	0
58	MG	CA	1633	1/1	0.92	0.10	73,73,73,73	0
59	PAR	AA	1814	42/42	0.93	0.22	80,85,103,108	0
58	MG	BA	3037	1/1	0.93	0.14	61,61,61,61	0
58	MG	CA	1706	1/1	0.93	0.18	56,56,56,56	0
58	MG	AA	1710	1/1	0.93	0.12	82,82,82,82	0
58	MG	DA	3340	1/1	0.93	0.68	63,63,63,63	1
58	MG	CW	111	1/1	0.93	0.73	89,89,89,89	1
58	MG	CL	201	1/1	0.93	0.54	51,51,51,51	0
58	MG	AW	109	1/1	0.93	0.15	50,50,50,50	1
58	MG	AA	1642	1/1	0.93	0.20	34,34,34,34	0
58	MG	BA	3017	1/1	0.93	0.22	69,69,69,69	0
58	MG	BA	3204	1/1	0.93	0.15	51,51,51,51	0
58	MG	DA	3405	1/1	0.93	0.66	129,129,129,129	0
58	MG	BA	3120	1/1	0.93	0.29	87,87,87,87	0
58	MG	DA	3177	1/1	0.93	0.14	103,103,103,103	0
58	MG	BA	3185	1/1	0.93	0.18	69,69,69,69	0
58	MG	CA	1693	1/1	0.93	0.29	74,74,74,74	0
58	MG	DA	3260	1/1	0.93	0.09	29,29,29,29	0
58	MG	AA	1625	1/1	0.93	0.20	39,39,39,39	0
58	MG	BA	3137	1/1	0.93	0.33	61,61,61,61	0
58	MG	DB	204	1/1	0.93	0.77	148,148,148,148	0
58	MG	BA	3399	1/1	0.93	0.21	70,70,70,70	1
58	MG	BA	3094	1/1	0.93	0.40	63,63,63,63	0
58	MG	AA	1627	1/1	0.93	0.57	74,74,74,74	0
58	MG	DA	3143	1/1	0.93	0.72	63,63,63,63	0
58	MG	DA	3200	1/1	0.93	0.45	57,57,57,57	0
58	MG	DA	3024	1/1	0.93	0.30	37,37,37,37	0
58	MG	BA	3297	1/1	0.93	0.57	51,51,51,51	0
58	MG	DB	206	1/1	0.93	0.19	78,78,78,78	0
58	MG	CA	1752	1/1	0.93	0.16	94,94,94,94	0
58	MG	DE	302	1/1	0.93	0.53	83,83,83,83	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3422	1/1	0.93	0.29	69,69,69,69	0
58	MG	AA	1698	1/1	0.93	0.28	61,61,61,61	0
58	MG	AA	1754	1/1	0.93	0.17	114,114,114,114	0
58	MG	DA	3338	1/1	0.93	0.19	123,123,123,123	0
58	MG	BX	101	1/1	0.93	0.30	69,69,69,69	0
58	MG	BA	3250	1/1	0.93	0.48	65,65,65,65	0
58	MG	BA	3180	1/1	0.93	0.26	93,93,93,93	0
58	MG	DA	3240	1/1	0.93	0.32	51,51,51,51	0
58	MG	AA	1809	1/1	0.93	0.20	88,88,88,88	0
58	MG	BW	201	1/1	0.93	0.37	120,120,120,120	0
58	MG	AV	104	1/1	0.93	0.37	98,98,98,98	1
58	MG	AA	1770	1/1	0.93	0.21	55,55,55,55	0
58	MG	CW	113	1/1	0.93	0.24	41,41,41,41	1
58	MG	BA	3449	1/1	0.93	0.46	107,107,107,107	1
58	MG	BA	3412	1/1	0.93	0.28	67,67,67,67	0
58	MG	BA	3320	1/1	0.93	0.07	40,40,40,40	0
58	MG	DA	3137	1/1	0.93	0.44	39,39,39,39	0
58	MG	BA	3167	1/1	0.93	0.44	55,55,55,55	0
58	MG	CA	1734	1/1	0.93	0.21	144,144,144,144	1
58	MG	AA	1713	1/1	0.93	0.21	82,82,82,82	0
58	MG	DB	210	1/1	0.93	0.20	51,51,51,51	1
58	MG	AA	1628	1/1	0.93	0.31	71,71,71,71	0
58	MG	AA	1657	1/1	0.93	0.37	73,73,73,73	0
58	MG	AA	1701	1/1	0.93	0.34	61,61,61,61	0
58	MG	AA	1722	1/1	0.93	0.18	67,67,67,67	0
58	MG	BA	3018	1/1	0.93	0.14	80,80,80,80	0
58	MG	DN	203	1/1	0.93	0.12	109,109,109,109	1
58	MG	DA	3354	1/1	0.93	0.24	110,110,110,110	0
58	MG	DA	3202	1/1	0.93	0.06	38,38,38,38	0
58	MG	CA	1674	1/1	0.93	0.55	89,89,89,89	0
58	MG	AA	1768	1/1	0.93	0.33	100,100,100,100	0
58	MG	CA	1746	1/1	0.93	0.21	87,87,87,87	0
58	MG	DA	3407	1/1	0.93	0.29	140,140,140,140	0
58	MG	CA	1796	1/1	0.93	0.09	51,51,51,51	1
58	MG	BA	3334	1/1	0.93	0.11	137,137,137,137	0
58	MG	AA	1732	1/1	0.94	0.20	64,64,64,64	1
58	MG	BA	3107	1/1	0.94	0.30	46,46,46,46	0
58	MG	B5	101	1/1	0.94	0.36	50,50,50,50	0
58	MG	CA	1640	1/1	0.94	0.60	61,61,61,61	0
58	MG	AA	1781	1/1	0.94	0.20	89,89,89,89	0
58	MG	DA	3229	1/1	0.94	0.12	101,101,101,101	0
58	MG	DA	3221	1/1	0.94	0.31	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	1707	1/1	0.94	0.09	82,82,82,82	0
58	MG	AA	1699	1/1	0.94	0.20	106,106,106,106	0
58	MG	DA	3169	1/1	0.94	0.05	52,52,52,52	0
58	MG	CA	1666	1/1	0.94	0.47	75,75,75,75	0
58	MG	BA	3145	1/1	0.94	0.46	61,61,61,61	0
58	MG	DA	3110	1/1	0.94	0.17	38,38,38,38	0
58	MG	AW	115	1/1	0.94	0.15	130,130,130,130	0
58	MG	CA	1713	1/1	0.94	0.23	54,54,54,54	0
58	MG	BA	3059	1/1	0.94	0.22	45,45,45,45	0
58	MG	DA	3236	1/1	0.94	0.42	37,37,37,37	0
58	MG	BA	3356	1/1	0.94	0.30	67,67,67,67	0
58	MG	BA	3031	1/1	0.94	0.31	35,35,35,35	0
58	MG	DA	3324	1/1	0.94	0.29	104,104,104,104	1
58	MG	DA	3184	1/1	0.94	0.26	56,56,56,56	0
58	MG	CA	1723	1/1	0.94	0.08	47,47,47,47	0
58	MG	BA	3252	1/1	0.94	0.12	46,46,46,46	0
58	MG	BA	3387	1/1	0.94	0.18	107,107,107,107	0
58	MG	AA	1665	1/1	0.94	0.48	55,55,55,55	0
58	MG	BA	3448	1/1	0.94	0.05	67,67,67,67	0
58	MG	CA	1792	1/1	0.94	0.22	70,70,70,70	1
58	MG	DA	3130	1/1	0.94	0.13	80,80,80,80	0
58	MG	CA	1622	1/1	0.94	0.14	36,36,36,36	0
58	MG	BA	3063	1/1	0.94	0.25	20,20,20,20	0
58	MG	DA	3058	1/1	0.94	0.23	49,49,49,49	0
58	MG	DA	3235	1/1	0.94	0.22	44,44,44,44	0
58	MG	DA	3026	1/1	0.94	0.47	49,49,49,49	0
58	MG	BA	3247	1/1	0.94	0.16	33,33,33,33	0
58	MG	AA	1759	1/1	0.94	0.22	70,70,70,70	1
58	MG	DA	3073	1/1	0.94	0.33	55,55,55,55	0
58	MG	DA	3288	1/1	0.94	0.27	32,32,32,32	0
58	MG	BA	3010	1/1	0.94	0.24	40,40,40,40	0
58	MG	BA	3105	1/1	0.94	0.44	55,55,55,55	0
58	MG	CA	1768	1/1	0.94	0.29	65,65,65,65	1
58	MG	DA	3438	1/1	0.94	0.67	97,97,97,97	0
58	MG	AA	1800	1/1	0.94	0.22	59,59,59,59	1
58	MG	BA	3402	1/1	0.94	0.42	59,59,59,59	0
58	MG	BA	3195	1/1	0.94	0.27	48,48,48,48	0
58	MG	CA	1760	1/1	0.94	0.19	85,85,85,85	1
58	MG	DA	3271	1/1	0.94	0.09	62,62,62,62	0
58	MG	DA	3060	1/1	0.94	0.49	35,35,35,35	0
58	MG	DA	3413	1/1	0.94	0.27	96,96,96,96	0
58	MG	BA	3243	1/1	0.94	0.30	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	1741	1/1	0.94	0.45	72,72,72,72	0
58	MG	BA	3003	1/1	0.94	0.39	68,68,68,68	0
58	MG	DA	3129	1/1	0.94	0.12	58,58,58,58	1
58	MG	AA	1801	1/1	0.94	0.09	71,71,71,71	0
58	MG	BA	3171	1/1	0.94	0.14	59,59,59,59	0
58	MG	BA	3169	1/1	0.94	0.17	83,83,83,83	0
58	MG	CA	1777	1/1	0.94	0.30	99,99,99,99	0
58	MG	CA	1800	1/1	0.94	0.23	108,108,108,108	0
58	MG	AW	113	1/1	0.94	0.23	45,45,45,45	1
58	MG	DA	3131	1/1	0.94	0.27	40,40,40,40	0
58	MG	DA	3174	1/1	0.94	0.15	77,77,77,77	0
58	MG	CA	1802	1/1	0.94	0.11	70,70,70,70	1
58	MG	CA	1702	1/1	0.94	0.32	88,88,88,88	0
58	MG	BA	3439	1/1	0.94	0.34	52,52,52,52	0
58	MG	AA	1804	1/1	0.94	0.16	49,49,49,49	0
58	MG	DF	301	1/1	0.94	0.22	90,90,90,90	0
58	MG	DA	3267	1/1	0.94	0.37	79,79,79,79	0
58	MG	CA	1630	1/1	0.94	0.23	81,81,81,81	0
58	MG	AA	1605	1/1	0.94	0.13	53,53,53,53	0
58	MG	BA	3203	1/1	0.94	0.49	86,86,86,86	0
58	MG	BA	3184	1/1	0.94	0.08	52,52,52,52	0
58	MG	BA	3086	1/1	0.94	0.32	36,36,36,36	0
58	MG	CA	1788	1/1	0.94	0.07	75,75,75,75	0
58	MG	BA	3129	1/1	0.94	0.46	63,63,63,63	0
58	MG	DA	3176	1/1	0.94	0.16	49,49,49,49	0
58	MG	DA	3002	1/1	0.94	0.10	63,63,63,63	0
59	PAR	CA	1817	42/42	0.94	0.23	72,78,95,100	0
58	MG	CA	1794	1/1	0.94	0.77	77,77,77,77	0
58	MG	AA	1671	1/1	0.94	0.41	61,61,61,61	0
58	MG	BA	3196	1/1	0.94	0.39	60,60,60,60	0
58	MG	DA	3126	1/1	0.94	0.22	24,24,24,24	0
58	MG	BA	3124	1/1	0.94	0.40	40,40,40,40	0
58	MG	DA	3010	1/1	0.94	0.09	51,51,51,51	0
58	MG	CA	1790	1/1	0.94	0.10	84,84,84,84	0
58	MG	BA	3052	1/1	0.94	0.59	134,134,134,134	1
58	MG	BA	3098	1/1	0.94	0.33	45,45,45,45	0
58	MG	AA	1737	1/1	0.94	0.30	78,78,78,78	0
58	MG	DA	3149	1/1	0.94	0.48	73,73,73,73	0
58	MG	DB	209	1/1	0.94	0.09	117,117,117,117	0
58	MG	BB	212	1/1	0.94	0.12	59,59,59,59	1
58	MG	BA	3318	1/1	0.94	0.37	110,110,110,110	0
58	MG	DA	3429	1/1	0.94	0.14	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3283	1/1	0.94	0.06	100,100,100,100	0
58	MG	BA	3382	1/1	0.94	0.32	86,86,86,86	0
58	MG	DA	3105	1/1	0.95	0.39	52,52,52,52	0
58	MG	DA	3030	1/1	0.95	0.21	24,24,24,24	0
58	MG	BA	3075	1/1	0.95	0.17	36,36,36,36	0
58	MG	BA	3383	1/1	0.95	0.19	89,89,89,89	0
58	MG	AA	1810	1/1	0.95	0.30	36,36,36,36	0
58	MG	DA	3123	1/1	0.95	0.42	40,40,40,40	0
58	MG	BA	3264	1/1	0.95	0.09	27,27,27,27	0
58	MG	DA	3132	1/1	0.95	0.17	34,34,34,34	0
58	MG	DA	3020	1/1	0.95	0.33	15,15,15,15	0
58	MG	BA	3162	1/1	0.95	0.17	51,51,51,51	0
58	MG	DA	3415	1/1	0.95	0.37	70,70,70,70	0
58	MG	DA	3412	1/1	0.95	0.20	109,109,109,109	0
58	MG	BD	301	1/1	0.95	0.16	44,44,44,44	0
58	MG	CA	1695	1/1	0.95	0.37	49,49,49,49	1
58	MG	AA	1717	1/1	0.95	0.32	48,48,48,48	0
58	MG	AA	1750	1/1	0.95	0.74	97,97,97,97	0
58	MG	CA	1657	1/1	0.95	0.15	78,78,78,78	0
58	MG	DA	3256	1/1	0.95	0.27	82,82,82,82	1
58	MG	DA	3261	1/1	0.95	0.37	32,32,32,32	0
58	MG	CA	1728	1/1	0.95	0.10	86,86,86,86	0
58	MG	DA	3063	1/1	0.95	0.38	35,35,35,35	0
58	MG	BA	3092	1/1	0.95	0.56	100,100,100,100	0
58	MG	BA	3338	1/1	0.95	0.09	121,121,121,121	0
58	MG	DA	3082	1/1	0.95	0.26	37,37,37,37	0
58	MG	DA	3294	1/1	0.95	0.57	63,63,63,63	0
58	MG	BA	3405	1/1	0.95	0.36	53,53,53,53	0
58	MG	DA	3121	1/1	0.95	0.29	44,44,44,44	0
58	MG	BA	3376	1/1	0.95	0.21	68,68,68,68	1
58	MG	CA	1607	1/1	0.95	0.11	52,52,52,52	0
58	MG	BO	201	1/1	0.95	0.22	44,44,44,44	0
58	MG	BA	3379	1/1	0.95	0.20	110,110,110,110	0
58	MG	BA	3126	1/1	0.95	0.53	47,47,47,47	0
58	MG	BA	3360	1/1	0.95	0.14	60,60,60,60	0
58	MG	DA	3193	1/1	0.95	0.16	62,62,62,62	0
58	MG	BA	3212	1/1	0.95	0.19	75,75,75,75	0
58	MG	DA	3373	1/1	0.95	0.28	78,78,78,78	1
58	MG	CA	1689	1/1	0.95	0.14	138,138,138,138	0
58	MG	DA	3087	1/1	0.95	0.25	45,45,45,45	0
58	MG	AX	103	1/1	0.95	0.21	98,98,98,98	0
58	MG	AV	102	1/1	0.95	0.13	85,85,85,85	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3168	1/1	0.95	0.12	72,72,72,72	0
58	MG	DA	3085	1/1	0.95	0.56	60,60,60,60	0
58	MG	AA	1733	1/1	0.95	0.19	91,91,91,91	1
58	MG	BA	3306	1/1	0.95	0.48	67,67,67,67	0
58	MG	DB	203	1/1	0.95	0.06	89,89,89,89	0
58	MG	D1	102	1/1	0.95	0.09	54,54,54,54	1
58	MG	CA	1754	1/1	0.95	0.10	93,93,93,93	0
58	MG	AA	1811	1/1	0.95	0.15	93,93,93,93	0
58	MG	CA	1721	1/1	0.95	0.34	94,94,94,94	0
58	MG	DA	3419	1/1	0.95	0.13	83,83,83,83	0
58	MG	DA	3214	1/1	0.95	0.10	131,131,131,131	0
58	MG	DA	3051	1/1	0.95	0.11	110,110,110,110	1
58	MG	CA	1611	1/1	0.95	0.23	61,61,61,61	0
58	MG	BA	3358	1/1	0.95	0.17	60,60,60,60	0
58	MG	B7	101	1/1	0.95	1.07	73,73,73,73	1
58	MG	DA	3365	1/1	0.95	0.19	135,135,135,135	1
58	MG	BA	3125	1/1	0.95	0.20	64,64,64,64	0
58	MG	BA	3194	1/1	0.95	0.12	43,43,43,43	0
58	MG	BA	3390	1/1	0.95	0.19	57,57,57,57	0
58	MG	AA	1667	1/1	0.95	0.09	56,56,56,56	0
58	MG	CA	1637	1/1	0.95	0.21	40,40,40,40	0
58	MG	DA	3228	1/1	0.95	0.49	75,75,75,75	0
58	MG	DA	3392	1/1	0.95	0.32	74,74,74,74	0
58	MG	BA	3342	1/1	0.95	0.34	92,92,92,92	0
58	MG	AA	1757	1/1	0.95	0.13	71,71,71,71	0
58	MG	DA	3111	1/1	0.95	0.21	44,44,44,44	0
58	MG	CV	106	1/1	0.95	0.11	93,93,93,93	0
58	MG	CA	1699	1/1	0.95	0.14	44,44,44,44	0
58	MG	DA	3041	1/1	0.95	0.30	56,56,56,56	0
58	MG	DA	3173	1/1	0.95	0.15	46,46,46,46	0
58	MG	BA	3444	1/1	0.95	0.09	90,90,90,90	0
58	MG	BA	3452	1/1	0.95	0.37	114,114,114,114	1
58	MG	BA	3330	1/1	0.95	0.30	114,114,114,114	1
58	MG	BE	301	1/1	0.95	0.21	30,30,30,30	0
58	MG	BA	3116	1/1	0.95	0.16	38,38,38,38	0
58	MG	DA	3186	1/1	0.95	0.16	49,49,49,49	0
58	MG	DX	101	1/1	0.95	0.23	51,51,51,51	0
58	MG	DA	3072	1/1	0.95	0.40	31,31,31,31	0
58	MG	DA	3185	1/1	0.95	0.20	40,40,40,40	0
58	MG	AA	1646	1/1	0.95	0.21	47,47,47,47	0
58	MG	CA	1646	1/1	0.95	0.24	64,64,64,64	0
58	MG	BA	3392	1/1	0.95	0.26	79,79,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3366	1/1	0.95	0.15	77,77,77,77	0
58	MG	AW	107	1/1	0.95	0.09	74,74,74,74	1
58	MG	DA	3416	1/1	0.95	0.28	114,114,114,114	0
58	MG	CA	1654	1/1	0.96	0.27	76,76,76,76	1
58	MG	AA	1623	1/1	0.96	0.17	106,106,106,106	0
58	MG	BA	3078	1/1	0.96	0.15	23,23,23,23	0
58	MG	AA	1793	1/1	0.96	0.39	106,106,106,106	0
58	MG	DA	3047	1/1	0.96	0.34	27,27,27,27	0
58	MG	D5	101	1/1	0.96	0.16	51,51,51,51	0
58	MG	BA	3082	1/1	0.96	0.24	63,63,63,63	0
58	MG	AA	1706	1/1	0.96	0.06	63,63,63,63	0
58	MG	BA	3095	1/1	0.96	0.26	40,40,40,40	0
58	MG	AA	1648	1/1	0.96	0.15	95,95,95,95	0
58	MG	DA	3208	1/1	0.96	0.10	76,76,76,76	0
58	MG	DA	3211	1/1	0.96	0.31	61,61,61,61	0
58	MG	BA	3440	1/1	0.96	0.41	93,93,93,93	0
58	MG	DA	3378	1/1	0.96	0.28	72,72,72,72	0
58	MG	AA	1716	1/1	0.96	0.07	46,46,46,46	0
58	MG	CA	1625	1/1	0.96	0.20	40,40,40,40	0
58	MG	BN	202	1/1	0.96	0.12	97,97,97,97	1
58	MG	DA	3207	1/1	0.96	0.09	60,60,60,60	0
58	MG	BA	3056	1/1	0.96	0.13	53,53,53,53	0
58	MG	CA	1811	1/1	0.96	0.15	165,165,165,165	0
58	MG	DA	3099	1/1	0.96	0.52	45,45,45,45	0
58	MG	DA	3081	1/1	0.96	0.29	96,96,96,96	0
58	MG	DA	3014	1/1	0.96	0.27	28,28,28,28	0
58	MG	DA	3382	1/1	0.96	0.14	59,59,59,59	0
58	MG	BA	3049	1/1	0.96	0.31	35,35,35,35	0
58	MG	DB	218	1/1	0.96	0.15	82,82,82,82	1
58	MG	CA	1692	1/1	0.96	0.12	92,92,92,92	0
58	MG	AA	1630	1/1	0.96	0.18	84,84,84,84	0
58	MG	BA	3368	1/1	0.96	0.18	74,74,74,74	0
58	MG	DA	3212	1/1	0.96	0.13	60,60,60,60	0
58	MG	BV	201	1/1	0.96	0.54	101,101,101,101	0
58	MG	DA	3402	1/1	0.96	0.13	178,178,178,178	0
58	MG	AX	101	1/1	0.96	0.18	85,85,85,85	0
58	MG	BA	3414	1/1	0.96	0.12	78,78,78,78	0
58	MG	AA	1613	1/1	0.96	0.37	53,53,53,53	0
58	MG	DA	3113	1/1	0.96	0.42	42,42,42,42	0
58	MG	DA	3433	1/1	0.96	0.09	94,94,94,94	1
58	MG	BA	3077	1/1	0.96	0.28	55,55,55,55	0
58	MG	BA	3106	1/1	0.96	0.42	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3229	1/1	0.96	0.12	117,117,117,117	0
58	MG	BA	3076	1/1	0.96	0.29	40,40,40,40	0
58	MG	CA	1685	1/1	0.96	0.10	101,101,101,101	0
58	MG	DA	3097	1/1	0.96	0.30	53,53,53,53	0
58	MG	CA	1624	1/1	0.96	0.33	99,99,99,99	0
58	MG	DA	3054	1/1	0.96	0.33	45,45,45,45	0
58	MG	BP	201	1/1	0.96	0.14	66,66,66,66	0
58	MG	BA	3143	1/1	0.96	0.17	90,90,90,90	0
58	MG	AA	1663	1/1	0.96	0.20	31,31,31,31	0
58	MG	BA	3266	1/1	0.96	0.16	64,64,64,64	0
58	MG	CA	1771	1/1	0.96	0.12	47,47,47,47	0
58	MG	BA	3210	1/1	0.96	0.22	43,43,43,43	0
58	MG	CA	1733	1/1	0.96	0.07	49,49,49,49	1
58	MG	BA	3020	1/1	0.96	0.34	41,41,41,41	0
58	MG	DA	3444	1/1	0.96	0.07	70,70,70,70	0
58	MG	BA	3053	1/1	0.96	0.25	18,18,18,18	0
58	MG	DA	3078	1/1	0.96	0.19	24,24,24,24	0
58	MG	BA	3303	1/1	0.96	0.32	89,89,89,89	0
58	MG	DA	3083	1/1	0.96	0.16	32,32,32,32	0
58	MG	CA	1632	1/1	0.96	0.09	73,73,73,73	0
58	MG	DA	3136	1/1	0.96	0.29	44,44,44,44	0
58	MG	BA	3225	1/1	0.96	0.35	38,38,38,38	0
58	MG	AA	1749	1/1	0.96	0.42	117,117,117,117	0
58	MG	BA	3030	1/1	0.96	0.32	70,70,70,70	0
58	MG	DA	3385	1/1	0.96	0.23	138,138,138,138	0
58	MG	CA	1641	1/1	0.96	0.12	39,39,39,39	0
58	MG	DA	3446	1/1	0.96	0.08	51,51,51,51	0
58	MG	CA	1667	1/1	0.96	0.11	147,147,147,147	0
58	MG	DA	3095	1/1	0.96	0.13	33,33,33,33	0
58	MG	CA	1628	1/1	0.96	0.34	80,80,80,80	0
58	MG	BA	3119	1/1	0.96	0.06	24,24,24,24	0
58	MG	DA	3080	1/1	0.96	0.17	35,35,35,35	0
58	MG	CA	1786	1/1	0.96	0.07	53,53,53,53	0
58	MG	CA	1608	1/1	0.96	0.21	80,80,80,80	0
58	MG	B1	101	1/1	0.96	0.08	29,29,29,29	1
58	MG	DA	3243	1/1	0.96	0.16	45,45,45,45	0
58	MG	DA	3172	1/1	0.96	0.27	42,42,42,42	0
58	MG	DA	3076	1/1	0.96	0.26	48,48,48,48	0
58	MG	BA	3434	1/1	0.96	0.15	90,90,90,90	0
58	MG	DA	3188	1/1	0.97	0.18	123,123,123,123	0
58	MG	BA	3366	1/1	0.97	0.29	60,60,60,60	0
58	MG	CA	1738	1/1	0.97	0.37	95,95,95,95	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3109	1/1	0.97	0.04	28,28,28,28	0
58	MG	BA	3032	1/1	0.97	0.17	68,68,68,68	0
58	MG	BA	3315	1/1	0.97	0.40	100,100,100,100	1
58	MG	CA	1676	1/1	0.97	0.27	88,88,88,88	0
58	MG	BA	3415	1/1	0.97	0.15	80,80,80,80	0
58	MG	CA	1809	1/1	0.97	0.17	56,56,56,56	1
58	MG	CA	1698	1/1	0.97	0.10	106,106,106,106	0
58	MG	DA	3386	1/1	0.97	0.20	49,49,49,49	0
58	MG	AA	1784	1/1	0.97	0.14	66,66,66,66	0
58	MG	BA	3133	1/1	0.97	0.27	56,56,56,56	0
58	MG	BF	302	1/1	0.97	0.18	93,93,93,93	0
58	MG	DA	3079	1/1	0.97	0.24	22,22,22,22	0
58	MG	BA	3067	1/1	0.97	0.28	34,34,34,34	0
58	MG	DA	3432	1/1	0.97	0.10	91,91,91,91	0
58	MG	DA	3116	1/1	0.97	0.28	30,30,30,30	0
58	MG	CA	1718	1/1	0.97	0.24	71,71,71,71	0
58	MG	DA	3353	1/1	0.97	0.20	58,58,58,58	0
58	MG	DA	3153	1/1	0.97	0.16	45,45,45,45	1
58	MG	DA	3276	1/1	0.97	0.21	75,75,75,75	0
58	MG	DA	3310	1/1	0.97	0.27	110,110,110,110	1
58	MG	BA	3039	1/1	0.97	0.22	45,45,45,45	0
58	MG	BA	3395	1/1	0.97	0.34	70,70,70,70	0
58	MG	CA	1758	1/1	0.97	0.08	110,110,110,110	0
58	MG	DA	3160	1/1	0.97	0.19	96,96,96,96	0
58	MG	CA	1664	1/1	0.97	0.25	40,40,40,40	0
58	MG	DA	3307	1/1	0.97	0.29	30,30,30,30	0
58	MG	BB	206	1/1	0.97	0.30	130,130,130,130	0
58	MG	CA	1683	1/1	0.97	0.19	84,84,84,84	0
58	MG	BA	3087	1/1	0.97	0.17	47,47,47,47	0
58	MG	BA	3047	1/1	0.97	0.29	34,34,34,34	0
58	MG	AA	1739	1/1	0.97	0.24	102,102,102,102	0
58	MG	BV	202	1/1	0.97	0.18	136,136,136,136	1
58	MG	DA	3108	1/1	0.97	0.12	32,32,32,32	0
58	MG	DA	3427	1/1	0.97	0.19	133,133,133,133	0
58	MG	BA	3205	1/1	0.97	0.27	59,59,59,59	0
58	MG	BA	3406	1/1	0.97	0.13	38,38,38,38	0
58	MG	BA	3240	1/1	0.97	0.32	32,32,32,32	0
58	MG	BA	3026	1/1	0.97	0.20	52,52,52,52	0
58	MG	BA	3093	1/1	0.97	0.29	37,37,37,37	0
58	MG	AA	1649	1/1	0.97	0.32	53,53,53,53	0
58	MG	DD	301	1/1	0.97	0.26	27,27,27,27	0
58	MG	BA	3073	1/1	0.97	0.42	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3215	1/1	0.97	0.10	82,82,82,82	0
58	MG	DA	3371	1/1	0.97	0.10	98,98,98,98	1
58	MG	DA	3232	1/1	0.97	0.38	55,55,55,55	0
58	MG	BA	3138	1/1	0.97	0.37	37,37,37,37	0
58	MG	BA	3265	1/1	0.97	0.36	32,32,32,32	0
58	MG	AA	1611	1/1	0.97	0.21	48,48,48,48	0
58	MG	BA	3438	1/1	0.97	0.33	71,71,71,71	0
58	MG	DA	3150	1/1	0.97	0.10	46,46,46,46	0
58	MG	BA	3040	1/1	0.97	0.15	33,33,33,33	0
58	MG	AA	1798	1/1	0.97	0.17	135,135,135,135	0
58	MG	BA	3046	1/1	0.97	0.25	64,64,64,64	0
58	MG	CA	1623	1/1	0.97	0.10	74,74,74,74	0
58	MG	DA	3418	1/1	0.97	0.14	60,60,60,60	0
58	MG	BA	3258	1/1	0.97	0.22	100,100,100,100	0
58	MG	CA	1812	1/1	0.97	0.22	39,39,39,39	0
58	MG	BA	3127	1/1	0.97	0.15	35,35,35,35	0
58	MG	BA	3215	1/1	0.97	0.37	51,51,51,51	0
58	MG	CA	1798	1/1	0.97	0.06	89,89,89,89	1
58	MG	BA	3370	1/1	0.97	0.34	110,110,110,110	1
58	MG	CA	1766	1/1	0.97	0.21	44,44,44,44	0
58	MG	DA	3152	1/1	0.97	0.15	65,65,65,65	1
58	MG	D2	103	1/1	0.97	0.17	78,78,78,78	0
58	MG	DA	3044	1/1	0.97	0.37	66,66,66,66	0
58	MG	DA	3312	1/1	0.97	0.18	101,101,101,101	0
58	MG	BA	3048	1/1	0.97	0.42	32,32,32,32	0
58	MG	CA	1700	1/1	0.97	0.14	102,102,102,102	0
58	MG	DA	3285	1/1	0.97	0.07	36,36,36,36	0
58	MG	DA	3145	1/1	0.97	0.44	36,36,36,36	0
58	MG	DA	3125	1/1	0.97	0.44	53,53,53,53	0
58	MG	DA	3007	1/1	0.97	0.45	40,40,40,40	0
58	MG	DA	3065	1/1	0.97	0.17	41,41,41,41	0
58	MG	DA	3092	1/1	0.97	0.29	29,29,29,29	0
58	MG	DA	3367	1/1	0.97	0.50	127,127,127,127	0
58	MG	DA	3031	1/1	0.97	0.18	31,31,31,31	0
58	MG	DA	3442	1/1	0.97	0.13	71,71,71,71	0
58	MG	CX	103	1/1	0.97	0.08	97,97,97,97	0
58	MG	CA	1735	1/1	0.97	0.12	74,74,74,74	0
58	MG	DA	3001	1/1	0.97	0.09	92,92,92,92	0
58	MG	BA	3099	1/1	0.97	0.11	59,59,59,59	0
58	MG	CA	1696	1/1	0.97	0.24	59,59,59,59	0
58	MG	BA	3179	1/1	0.97	0.10	48,48,48,48	0
58	MG	CA	1740	1/1	0.97	0.25	132,132,132,132	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	1782	1/1	0.97	0.31	160,160,160,160	0
58	MG	BA	3080	1/1	0.97	0.22	32,32,32,32	0
58	MG	BA	3388	1/1	0.97	0.16	66,66,66,66	0
58	MG	DA	3350	1/1	0.97	0.16	65,65,65,65	1
58	MG	BA	3028	1/1	0.97	0.25	45,45,45,45	0
58	MG	BA	3015	1/1	0.97	0.30	47,47,47,47	0
58	MG	BA	3188	1/1	0.97	0.13	47,47,47,47	0
58	MG	BA	3420	1/1	0.97	0.26	93,93,93,93	0
58	MG	BA	3022	1/1	0.97	0.40	64,64,64,64	0
58	MG	DA	3315	1/1	0.97	0.06	29,29,29,29	0
58	MG	AA	1724	1/1	0.97	0.17	109,109,109,109	0
58	MG	AA	1684	1/1	0.97	0.16	97,97,97,97	0
58	MG	DA	3192	1/1	0.97	0.21	65,65,65,65	0
58	MG	DA	3062	1/1	0.97	0.33	13,13,13,13	0
58	MG	DA	3019	1/1	0.97	0.27	21,21,21,21	0
58	MG	BA	3248	1/1	0.97	0.08	22,22,22,22	0
58	MG	BA	3427	1/1	0.97	0.28	106,106,106,106	0
58	MG	DA	3066	1/1	0.98	0.20	22,22,22,22	0
58	MG	DA	3451	1/1	0.98	0.15	105,105,105,105	0
58	MG	DA	3011	1/1	0.98	0.32	27,27,27,27	0
58	MG	BA	3051	1/1	0.98	0.54	45,45,45,45	0
58	MG	BA	3397	1/1	0.98	0.19	112,112,112,112	1
58	MG	AV	107	1/1	0.98	0.55	76,76,76,76	0
58	MG	DA	3381	1/1	0.98	0.16	149,149,149,149	0
58	MG	DA	3406	1/1	0.98	0.08	87,87,87,87	1
58	MG	BA	3241	1/1	0.98	0.25	31,31,31,31	0
58	MG	BA	3027	1/1	0.98	0.33	25,25,25,25	0
58	MG	AA	1736	1/1	0.98	0.36	60,60,60,60	1
58	MG	DA	3046	1/1	0.98	0.25	30,30,30,30	0
58	MG	AA	1795	1/1	0.98	0.08	91,91,91,91	1
58	MG	AX	102	1/1	0.98	0.13	85,85,85,85	0
58	MG	CA	1610	1/1	0.98	0.20	46,46,46,46	0
58	MG	DA	3075	1/1	0.98	0.20	33,33,33,33	0
58	MG	BA	3140	1/1	0.98	0.15	75,75,75,75	0
58	MG	AA	1654	1/1	0.98	0.22	129,129,129,129	0
58	MG	BA	3324	1/1	0.98	0.28	121,121,121,121	0
58	MG	BA	3281	1/1	0.98	0.27	54,54,54,54	0
58	MG	BA	3054	1/1	0.98	0.23	38,38,38,38	0
58	MG	BA	3069	1/1	0.98	0.42	31,31,31,31	0
58	MG	DA	3355	1/1	0.98	0.10	37,37,37,37	0
58	MG	DA	3023	1/1	0.98	0.52	61,61,61,61	0
58	MG	CA	1669	1/1	0.98	0.30	118,118,118,118	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3439	1/1	0.98	0.15	65,65,65,65	1
58	MG	DA	3068	1/1	0.98	0.27	22,22,22,22	0
58	MG	BA	3357	1/1	0.98	0.08	56,56,56,56	0
58	MG	BA	3311	1/1	0.98	0.33	71,71,71,71	1
58	MG	DA	3098	1/1	0.98	0.23	60,60,60,60	0
58	MG	DA	3061	1/1	0.98	0.28	43,43,43,43	0
58	MG	DA	3084	1/1	0.98	0.22	35,35,35,35	0
58	MG	DA	3396	1/1	0.98	0.07	83,83,83,83	0
58	MG	BA	3045	1/1	0.98	0.16	69,69,69,69	0
58	MG	BA	3090	1/1	0.98	0.26	40,40,40,40	0
58	MG	DA	3225	1/1	0.98	0.13	115,115,115,115	0
58	MG	BA	3312	1/1	0.98	0.34	32,32,32,32	0
58	MG	DA	3052	1/1	0.98	0.21	9,9,9,9	0
58	MG	BA	3041	1/1	0.98	0.09	78,78,78,78	0
58	MG	DA	3139	1/1	0.98	0.16	106,106,106,106	0
58	MG	DA	3383	1/1	0.98	0.11	76,76,76,76	0
58	MG	AV	101	1/1	0.98	0.24	34,34,34,34	0
58	MG	BA	3193	1/1	0.98	0.47	56,56,56,56	0
58	MG	BA	3122	1/1	0.98	0.17	30,30,30,30	0
58	MG	BA	3038	1/1	0.98	0.23	35,35,35,35	0
58	MG	BA	3084	1/1	0.98	0.16	39,39,39,39	0
60	ZN	CN	101	1/1	0.98	0.16	109,109,109,109	0
58	MG	AA	1777	1/1	0.98	0.33	57,57,57,57	0
58	MG	BA	3083	1/1	0.98	0.34	47,47,47,47	0
58	MG	DA	3339	1/1	0.98	0.41	85,85,85,85	1
58	MG	DA	3397	1/1	0.98	0.09	48,48,48,48	1
58	MG	BA	3155	1/1	0.98	0.10	31,31,31,31	1
58	MG	DA	3352	1/1	0.98	0.10	52,52,52,52	0
58	MG	BA	3058	1/1	0.98	0.32	49,49,49,49	0
58	MG	DA	3037	1/1	0.98	0.17	32,32,32,32	0
58	MG	DA	3237	1/1	0.98	0.35	40,40,40,40	0
58	MG	DA	3244	1/1	0.98	0.12	22,22,22,22	0
58	MG	DA	3190	1/1	0.98	0.44	49,49,49,49	0
58	MG	BA	3268	1/1	0.98	0.28	73,73,73,73	0
58	MG	DA	3242	1/1	0.98	0.30	22,22,22,22	0
58	MG	BA	3112	1/1	0.98	0.11	35,35,35,35	0
58	MG	BA	3197	1/1	0.98	0.38	71,71,71,71	0
58	MG	BA	3152	1/1	0.98	0.14	30,30,30,30	0
58	MG	DA	3306	1/1	0.98	0.18	45,45,45,45	1
58	MG	AA	1607	1/1	0.98	0.12	50,50,50,50	0
58	MG	BA	3374	1/1	0.98	0.20	95,95,95,95	0
58	MG	DA	3086	1/1	0.98	0.19	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	1642	1/1	0.98	0.37	52,52,52,52	0
58	MG	BA	3175	1/1	0.98	0.29	70,70,70,70	0
58	MG	CA	1704	1/1	0.98	0.07	41,41,41,41	0
58	MG	DA	3094	1/1	0.98	0.27	43,43,43,43	0
58	MG	CA	1604	1/1	0.98	0.13	107,107,107,107	0
58	MG	DA	3025	1/1	0.98	0.18	42,42,42,42	0
58	MG	CA	1776	1/1	0.98	0.04	72,72,72,72	0
58	MG	DA	3337	1/1	0.98	0.11	82,82,82,82	0
58	MG	BA	3246	1/1	0.98	0.29	24,24,24,24	0
58	MG	BA	3408	1/1	0.98	0.20	64,64,64,64	1
58	MG	DA	3015	1/1	0.98	0.17	45,45,45,45	0
58	MG	BA	3384	1/1	0.98	0.49	83,83,83,83	0
58	MG	BA	3096	1/1	0.98	0.11	33,33,33,33	0
58	MG	AA	1756	1/1	0.98	0.49	64,64,64,64	0
58	MG	CA	1765	1/1	0.98	0.17	114,114,114,114	0
58	MG	DA	3101	1/1	0.98	0.12	71,71,71,71	0
58	MG	DA	3029	1/1	0.98	0.23	25,25,25,25	0
58	MG	DA	3021	1/1	0.98	0.40	59,59,59,59	0
58	MG	BA	3016	1/1	0.98	0.17	50,50,50,50	0
58	MG	CA	1714	1/1	0.98	0.48	102,102,102,102	0
58	MG	BA	3114	1/1	0.98	0.49	44,44,44,44	0
58	MG	BA	3219	1/1	0.98	0.10	106,106,106,106	0
58	MG	DA	3400	1/1	0.98	0.51	33,33,33,33	0
58	MG	BA	3021	1/1	0.98	0.37	24,24,24,24	0
58	MG	BA	3391	1/1	0.98	0.15	33,33,33,33	0
58	MG	AA	1637	1/1	0.98	0.20	44,44,44,44	0
58	MG	DA	3281	1/1	0.98	0.28	65,65,65,65	0
58	MG	DA	3038	1/1	0.98	0.24	53,53,53,53	0
58	MG	DA	3450	1/1	0.98	0.20	120,120,120,120	1
58	MG	DA	3055	1/1	0.98	0.13	44,44,44,44	0
58	MG	BA	3081	1/1	0.98	0.13	46,46,46,46	0
58	MG	DA	3384	1/1	0.98	0.25	67,67,67,67	0
58	MG	DA	3067	1/1	0.98	0.22	31,31,31,31	0
60	ZN	CD	301	1/1	0.98	0.28	87,87,87,87	0
58	MG	DA	3134	1/1	0.98	0.14	32,32,32,32	0
58	MG	BA	3066	1/1	0.99	0.14	39,39,39,39	0
58	MG	DA	3077	1/1	0.99	0.21	16,16,16,16	0
58	MG	DA	3263	1/1	0.99	0.34	57,57,57,57	0
58	MG	DA	3053	1/1	0.99	0.18	31,31,31,31	0
58	MG	DA	3096	1/1	0.99	0.19	43,43,43,43	0
58	MG	DA	3368	1/1	0.99	0.11	57,57,57,57	1
58	MG	BA	3147	1/1	0.99	0.23	20,20,20,20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3019	1/1	0.99	0.43	41,41,41,41	0
58	MG	BA	3043	1/1	0.99	0.27	63,63,63,63	0
58	MG	DA	3045	1/1	0.99	0.27	50,50,50,50	0
58	MG	DA	3114	1/1	0.99	0.46	33,33,33,33	0
58	MG	DA	3138	1/1	0.99	0.14	25,25,25,25	0
58	MG	AA	1792	1/1	0.99	0.10	78,78,78,78	0
58	MG	BA	3011	1/1	0.99	0.10	42,42,42,42	0
60	ZN	AN	101	1/1	0.99	0.17	106,106,106,106	0
58	MG	DB	212	1/1	0.99	0.05	30,30,30,30	1
58	MG	AA	1610	1/1	0.99	0.17	43,43,43,43	0
58	MG	BA	3057	1/1	0.99	0.22	35,35,35,35	0
58	MG	DA	3057	1/1	0.99	0.28	18,18,18,18	0
58	MG	CV	101	1/1	0.99	0.20	25,25,25,25	0
58	MG	DA	3106	1/1	0.99	0.36	36,36,36,36	0
58	MG	BA	3364	1/1	0.99	0.12	96,96,96,96	1
58	MG	DA	3369	1/1	0.99	0.10	117,117,117,117	0
58	MG	BA	3062	1/1	0.99	0.33	32,32,32,32	0
58	MG	BA	3091	1/1	0.99	0.39	34,34,34,34	0
58	MG	BA	3354	1/1	0.99	0.17	50,50,50,50	1
58	MG	BA	3425	1/1	0.99	0.17	108,108,108,108	0
60	ZN	AD	302	1/1	0.99	0.27	56,56,56,56	0
58	MG	BA	3359	1/1	0.99	0.13	92,92,92,92	0
58	MG	BA	3146	1/1	0.99	0.39	31,31,31,31	0
58	MG	BA	3117	1/1	0.99	0.34	38,38,38,38	0
58	MG	AA	1651	1/1	0.99	0.27	95,95,95,95	0
58	MG	DA	3329	1/1	0.99	0.27	83,83,83,83	1
58	MG	DA	3328	1/1	0.99	0.15	103,103,103,103	0
58	MG	BA	3239	1/1	0.99	0.14	48,48,48,48	0
58	MG	BA	3102	1/1	0.99	0.23	49,49,49,49	0
58	MG	DA	3247	1/1	0.99	0.14	96,96,96,96	1
58	MG	BA	3348	1/1	0.99	0.09	78,78,78,78	1
58	MG	BA	3190	1/1	0.99	0.19	41,41,41,41	0
58	MG	BA	3441	1/1	0.99	0.10	61,61,61,61	1
58	MG	CA	1694	1/1	0.99	0.14	124,124,124,124	1
58	MG	CA	1806	1/1	0.99	0.18	29,29,29,29	0
58	MG	BA	3012	1/1	0.99	0.24	27,27,27,27	0
58	MG	BA	3024	1/1	0.99	0.40	36,36,36,36	0
58	MG	DA	3316	1/1	0.99	0.28	41,41,41,41	0
58	MG	BA	3068	1/1	0.99	0.33	40,40,40,40	0
58	MG	DE	301	1/1	0.99	0.39	38,38,38,38	0
58	MG	BA	3251	1/1	0.99	0.10	58,58,58,58	1
58	MG	BA	3335	1/1	0.99	0.10	89,89,89,89	1

*Continued on next page...*

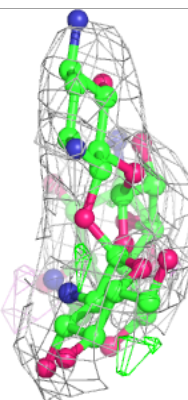
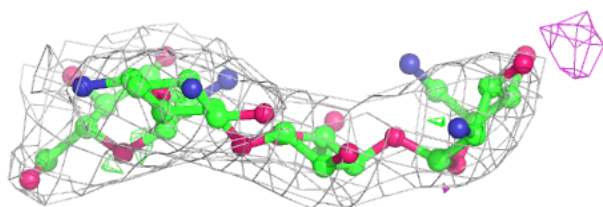
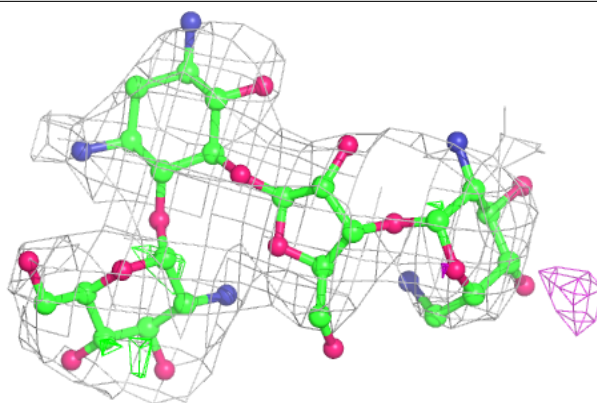
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	1603	1/1	0.99	0.15	101,101,101,101	0
58	MG	BA	3115	1/1	0.99	0.54	42,42,42,42	0
58	MG	BA	3135	1/1	0.99	0.15	34,34,34,34	0
58	MG	BA	3385	1/1	0.99	0.12	88,88,88,88	1
58	MG	DA	3090	1/1	0.99	0.42	25,25,25,25	0
58	MG	CA	1778	1/1	0.99	0.48	68,68,68,68	0
58	MG	DA	3394	1/1	0.99	0.20	48,48,48,48	1
58	MG	BA	3361	1/1	0.99	0.08	107,107,107,107	1
58	MG	DA	3039	1/1	0.99	0.28	45,45,45,45	0
58	MG	BA	3211	1/1	0.99	0.20	55,55,55,55	0
58	MG	BA	3008	1/1	0.99	0.37	31,31,31,31	0
58	MG	DA	3089	1/1	0.99	0.26	45,45,45,45	0
58	MG	BA	3097	1/1	0.99	0.16	46,46,46,46	0
58	MG	BA	3322	1/1	0.99	0.25	42,42,42,42	0
58	MG	BA	3435	1/1	0.99	0.08	80,80,80,80	1
58	MG	BA	3216	1/1	0.99	0.20	90,90,90,90	0
58	MG	DA	3359	1/1	0.99	0.17	84,84,84,84	1
58	MG	CA	1793	1/1	1.00	0.11	103,103,103,103	0

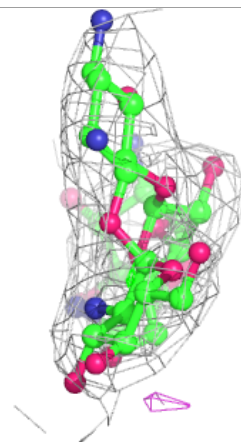
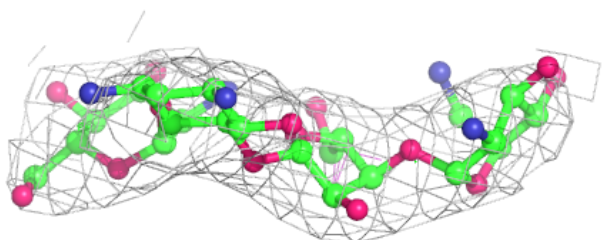
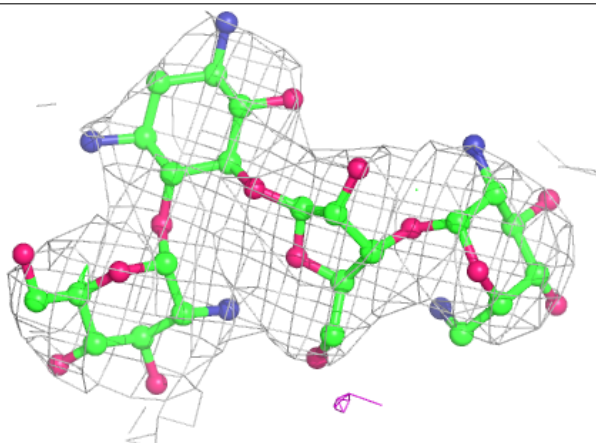
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around PAR AA 1814:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PAR CA 1817:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.