



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:22 PM UTC

PDB ID : 4V87 / pdb_00004v87
Title : Crystal structure analysis of ribosomal decoding.
Authors : Demeshkina, N.; Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-09-20
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

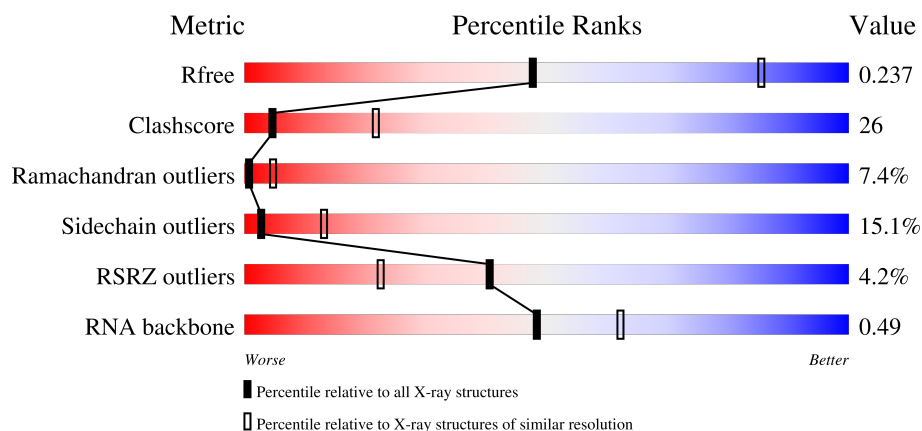
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	2912	2% 41% 45% 14%
1	DA	2912	2% 40% 44% 16%
2	AB	122	% 38% 44% 18%
2	DB	122	2% 33% 48% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AD	272	% 46% 42% 11%
3	DD	272	% 47% 42% 10%
4	AE	205	3% 33% 48% 17%
4	DE	205	8% 29% 44% 21% 5%
5	AF	208	% 46% 40% 11%
5	DF	208	4% 40% 42% 17%
6	AG	181	2% 42% 44% 13%
6	DG	181	6% 41% 49% 10%
7	AH	170	6% 37% 42% 18%
7	DH	170	14% 40% 42% 18%
8	AK	146	5% 33% 50% 14%
8	DK	146	9% 38% 43% 17%
9	AM	138	4% 33% 51% 15%
9	DM	138	4% 38% 50% 12%
10	AN	122	61% 30% 9%
10	DN	122	% 55% 41%
11	AO	150	7% 32% 43% 24%
11	DO	150	5% 32% 38% 21% 9%
12	AP	141	7% 30% 46% 19% 5%
12	DP	141	13% 28% 39% 27% 6%
13	A0	118	% 41% 44% 13%
13	D0	118	% 42% 48% 9%
14	AQ	111	5% 33% 48% 19%
14	DQ	111	7% 32% 55% 10%
15	AR	137	4% 31% 50% 18%

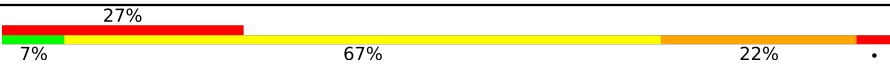
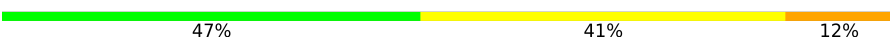
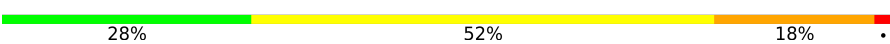
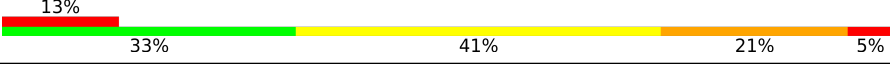
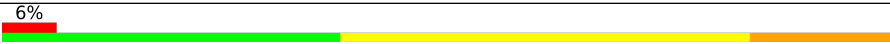
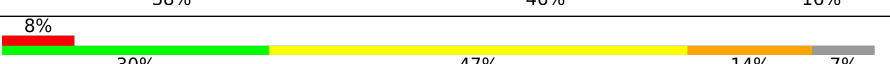
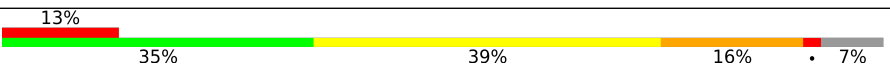
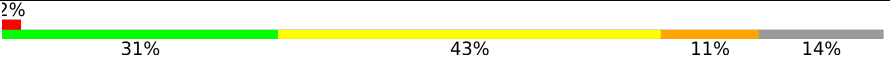
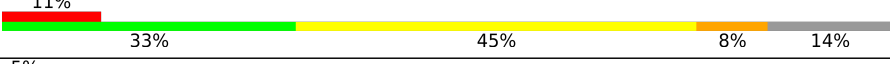
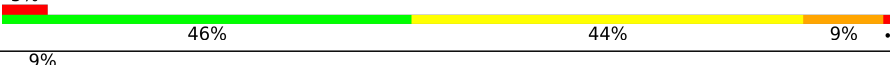
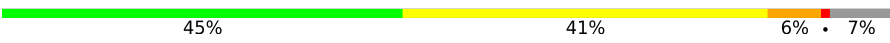
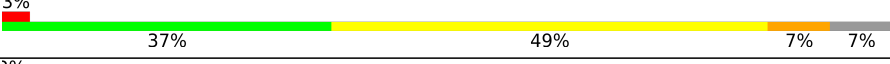
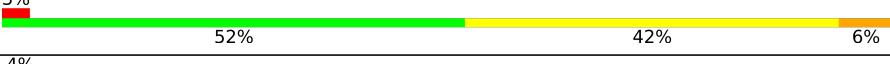
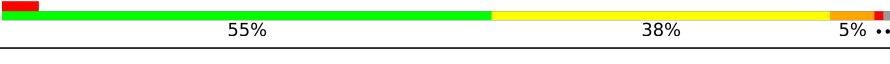
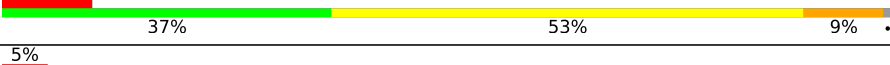
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	DR	137	
16	A1	117	
16	D1	117	
17	A2	101	
17	D2	101	
18	AS	113	
18	DS	113	
19	AT	92	
19	DT	92	
20	AU	102	
20	DU	102	
21	AV	179	
21	DV	179	
22	A3	77	
22	D3	77	
23	AZ	97	
23	DZ	97	
24	AW	69	
24	DW	69	
25	AX	59	
25	DX	59	
26	A4	66	
26	D4	66	
27	A5	59	
27	D5	59	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	A6	45	
28	D6	45	
29	A7	49	
29	D7	49	
30	A8	61	
30	D8	61	
31	BA	1506	
31	CA	1506	
32	BE	256	
32	CE	256	
33	BF	239	
33	CF	239	
34	BG	208	
34	CG	208	
35	BH	162	
35	CH	162	
36	BI	101	
36	CI	101	
37	BJ	156	
37	CJ	156	
38	BK	138	
38	CK	138	
39	BL	128	
39	CL	128	
40	BM	105	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	CM	105	
41	BN	129	
41	CN	129	
42	BO	132	
42	CO	132	
43	BP	126	
43	CP	126	
44	BQ	61	
44	CQ	61	
45	BR	89	
45	CR	89	
46	BS	88	
46	CS	88	
47	BT	105	
47	CT	105	
48	BU	88	
48	CU	88	
49	BV	93	
49	CV	93	
50	BW	106	
50	CW	106	
51	BX	27	
51	CX	27	
52	BB	87	
52	CB	87	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	BC	77	
53	BD	77	
53	CC	77	
53	CD	77	
54	B1	10	
54	C1	10	

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
55	MG	AA	3058	-	-	-	X
55	MG	AA	3077	-	-	-	X
55	MG	AA	3108	-	-	-	X
55	MG	AA	3132	-	-	-	X
55	MG	AA	3236	-	-	-	X
55	MG	AA	3317	-	-	-	X
55	MG	AA	3326	-	-	-	X
55	MG	AA	3353	-	-	-	X
55	MG	AA	3431	-	-	-	X
55	MG	AA	3509	-	-	-	X
55	MG	AA	3518	-	-	-	X
55	MG	AA	3521	-	-	-	X
55	MG	AA	3558	-	-	-	X
55	MG	AE	304	-	-	-	X
55	MG	BA	1628	-	-	-	X
55	MG	BA	1636	-	-	-	X
55	MG	BA	1678	-	-	-	X
55	MG	BA	1709	-	-	-	X
55	MG	BA	1712	-	-	-	X
55	MG	BA	1751	-	-	-	X
55	MG	BA	1778	-	-	-	X
55	MG	BA	1784	-	-	-	X
55	MG	BA	1831	-	-	-	X
55	MG	BA	1838	-	-	-	X
55	MG	CA	1634	-	-	-	X
55	MG	CA	1747	-	-	-	X
55	MG	CA	1777	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3004	-	-	-	X
55	MG	DA	3060	-	-	-	X
55	MG	DA	3272	-	-	-	X
55	MG	DA	3324	-	-	-	X
55	MG	DA	3332	-	-	-	X
55	MG	DA	3357	-	-	-	X
55	MG	DA	3372	-	-	-	X
55	MG	DA	3397	-	-	-	X
55	MG	DA	3404	-	-	-	X
55	MG	DA	3438	-	-	-	X
55	MG	DA	3447	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299628 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 RNA (2909-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	DA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	161	U	-	insertion	GB AP008226.1
AA	654A	A	G	conflict	GB AP008226.1
AA	654E	C	G	conflict	GB AP008226.1
AA	654P	G	C	conflict	GB AP008226.1
AA	654T	A	C	conflict	GB AP008226.1
AA	1058	U	G	conflict	GB AP008226.1
AA	1080	A	C	conflict	GB AP008226.1
DA	166	U	-	expression tag	GB AP008226.1
DA	654A	A	G	conflict	GB AP008226.1
DA	654E	C	G	conflict	GB AP008226.1
DA	654P	G	C	conflict	GB AP008226.1
DA	654T	A	C	conflict	GB AP008226.1
DA	1058	U	G	conflict	GB AP008226.1
DA	1080	A	C	conflict	GB AP008226.1

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
2	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	272	Total	C	N	O	S	0	0	0
			2116	1335	420	358	3			
3	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			
4	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	203	Total	C	N	O	S	0	0	1
			1586	1011	298	275	2			
5	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	170	Total	C	N	O	S	0	0	0
			1308	829	245	233	1			
7	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1137	726	201	209	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AM	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			
9	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
10	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
11	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	D0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			
15	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
18	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AT	92	Total	C	N	O	0	0	0
			726	471	131	124			
19	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	102	Total	C	N	O	S	0	0	0
			786	505	150	126	5			
20	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
21	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
23	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	59	Total	C	N	O		0	0	0
			469	298	90	81				
25	DX	59	Total	C	N	O		0	0	0
			469	298	90	81				

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			390	241	79	66	4			
28	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
29	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
30	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
31	CA	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
32	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
33	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
34	CG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
35	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
36	CI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
37	CJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
38	CK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
39	CL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
41	CN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
42	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
43	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
44	CQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
45	CR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
46	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
47	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BU	72	Total	C	N	O	0	0	0
			591	376	117	98			
48	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
49	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
50	CW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BX	25	Total	C	N	O	0	0	0
			217	134	52	31			
51	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 52 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			
52	CB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	BD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	18	C	U	conflict	GB AP012306.1
BD	18	C	U	conflict	GB AP012306.1
CC	18	C	U	conflict	GB AP012306.1
CD	18	C	U	conflict	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B1	10	Total	C	N	O	P	0	0	0
			205	92	28	75	10			
54	C1	10	Total	C	N	O	P	0	0	0
			205	92	28	75	10			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	630	Total Mg 630 630	0	0
55	AB	17	Total Mg 17 17	0	0
55	AD	2	Total Mg 2 2	0	0
55	AE	4	Total Mg 4 4	0	0
55	AF	3	Total Mg 3 3	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	A1	1	Total Mg 1 1	0	0
55	A2	1	Total Mg 1 1	0	0
55	AU	1	Total Mg 1 1	0	0
55	A3	1	Total Mg 1 1	0	0
55	A5	2	Total Mg 2 2	0	0
55	A6	1	Total Mg 1 1	0	0
55	A7	1	Total Mg 1 1	0	0
55	BA	244	Total Mg 244 244	0	0
55	BG	1	Total Mg 1 1	0	0
55	BN	2	Total Mg 2 2	0	0
55	BQ	2	Total Mg 2 2	0	0
55	BB	8	Total Mg 8 8	0	0
55	BC	9	Total Mg 9 9	0	0
55	BD	1	Total Mg 1 1	0	0
55	B1	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CA	209	Total 209	Mg 209	0	0
55	CG	3	Total 3	Mg 3	0	0
55	CH	1	Total 1	Mg 1	0	0
55	CS	1	Total 1	Mg 1	0	0
55	CB	5	Total 5	Mg 5	0	0
55	CC	8	Total 8	Mg 8	0	0
55	DA	528	Total 528	Mg 528	0	0
55	DB	14	Total 14	Mg 14	0	0
55	DE	3	Total 3	Mg 3	0	0
55	DP	1	Total 1	Mg 1	0	0
55	D0	1	Total 1	Mg 1	0	0
55	D1	2	Total 2	Mg 2	0	0
55	DU	1	Total 1	Mg 1	0	0
55	D3	1	Total 1	Mg 1	0	0
55	D5	1	Total 1	Mg 1	0	0

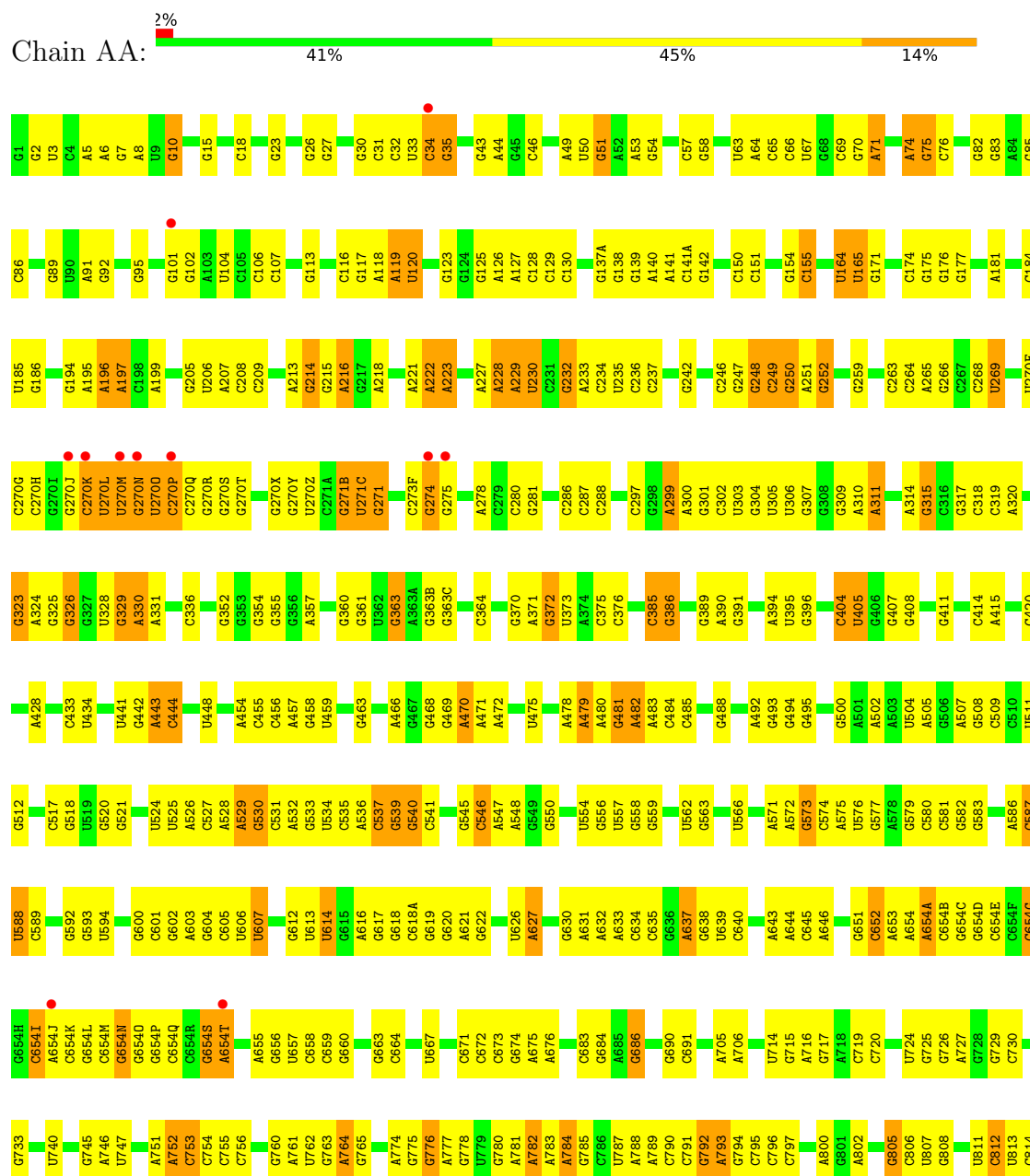
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BG	1	Total 1	Zn 1	0	0
56	BQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

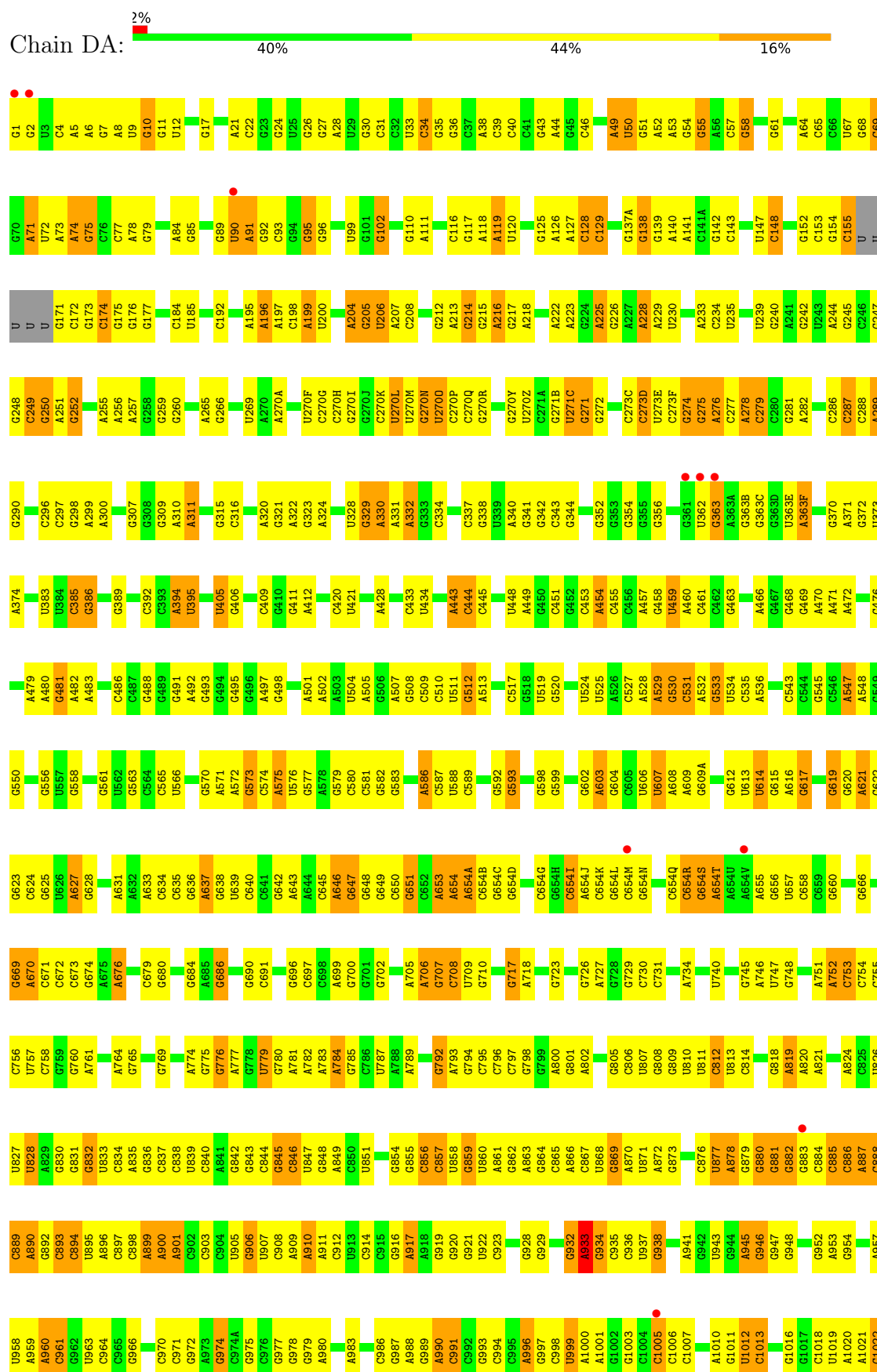
• Molecule 1: RNA (2909-MER)



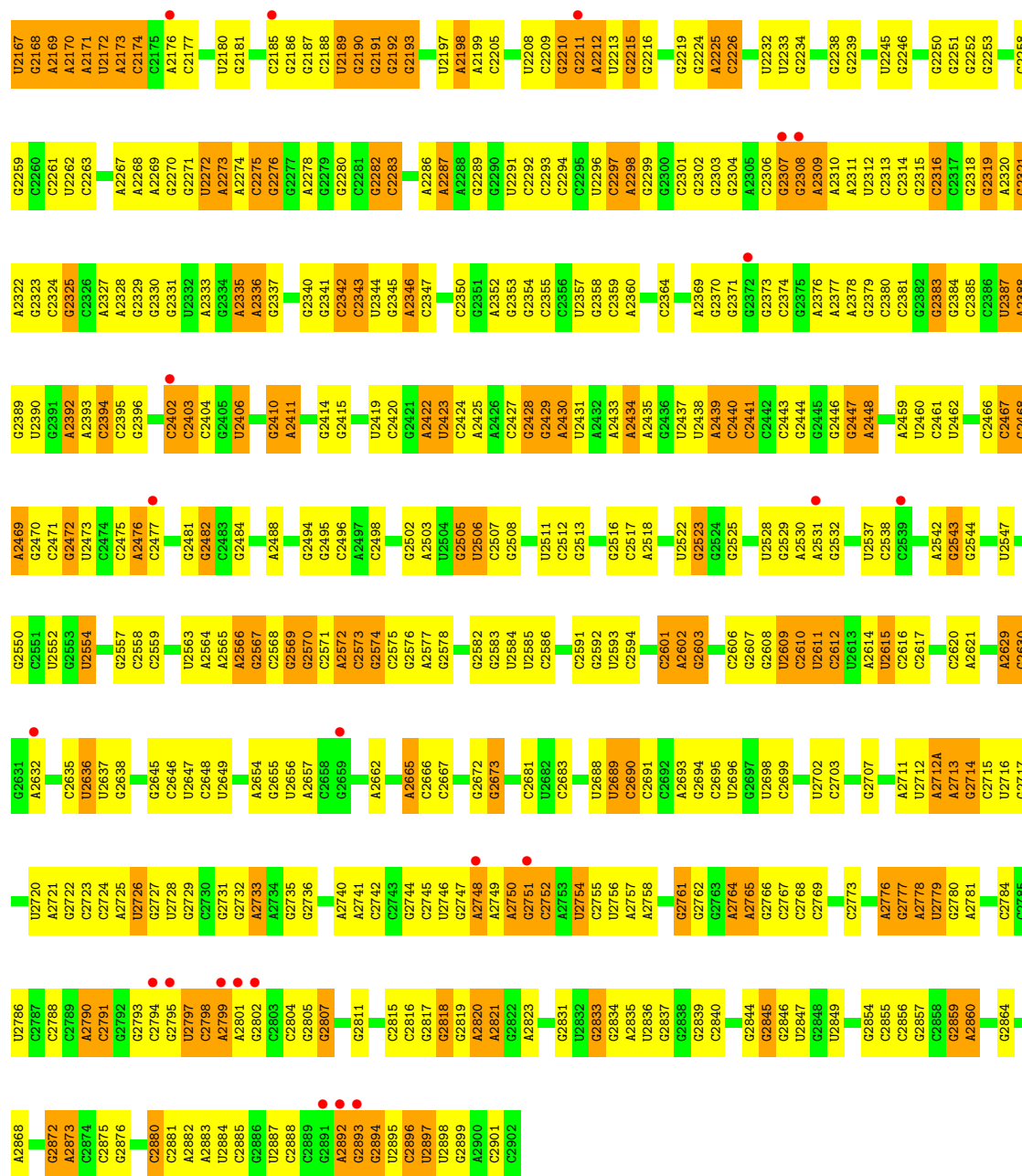
C1827	A1749	G1651	C1548	G1478	G1410	G1328	G1244	G1168	C1100	G1039	C971	A890	C815
G1828	G1750	A1652	C1549	G1479	G1411	U1329	A1247	G1169	U1101	G1042	G972	C892	C816
A1829	C1754	A1653	C1550	G1480	A1412	C1330	G1250	G1170	A1102	G1043	A973	C893	C817
U1834	G1755	A1654	C1551	U1482	A1413	A1331	G1251	G1171	A1103	C974A	C894	C894	G818
G1835	U1756	A1655	G1552	G1483	G1414	G1332	G1252	G1172	U1104	G975	C895	U895	A819
	G1757	C1656	C1553	A1486	U1415	C1333	G1253	A1174	U1105	A1045	C896	A896	A820
	G1758	C1657	C1554	G1487	G1416	G1337	A1254	U1175	G1106	G1046	C976	C897	A821
C1843		C1658	C1555	G1488	G1417	G1338	G1255	G1176		A1047	G977	C898	A822
A1847	A1762	A1665	A1558	C1493	G1418	G1339	G1256	G1177	G1110	A1048	G978	A899	A824
	G1764	G1666	G1559	A1494	A1419	G1344	G1263	C1178	A1111	A1049	G979	A900	C825
U1851		A1667	G1560	A1495	U1420	C1345	U1264	C1179	G1112	A1050		A901	U826
G1858	G1769	A1668	G1561	A1496	G1421		A1265	C1180	U1113	G1051	C982	C902	U827
A1859	G1770	A1669	A1570	U1497	G1422	G1348	A1266	C1181		G1052	A983	C903	U828
G1860	A1771	C1670	A1571	C1498	G1423	A1349	A1267	A1182	C1116	C1053	C904	C904	A829
G1861	A1772	G1674	C1575	C1502	A1427	U1352	A1268	C1185	G1117	A1054	U905	U905	
G1862	A1773	G1678	U1576	U1503	C1428	U1353	A1269	G1186	C1118	G1055	U906	U906	U833
G1863	U1778	C1577	C1577	G1504	G1429	A1354	C1270	U1188	C1119	A1056	U907	U907	C834
U1864	A1780	G1681	U1578	C1505	C1430	G1355	G1271	U1189	G1122	A1057	C908	C908	
G1869		C1686	A1579	C1506	U1431	G1356	A1272	A1190	G1123	U1058	A909	A909	C838
	A1783	G1687	A1580	A1507	U1432	U1357	U1273	G1191	G1124	U1060	C991	A910	C840
G1872	A1784	U1687	G1581	U1508	U1433	G1358	A1274	G1195	G1125	U1061	C992		
G1878	A1785	C1582	C1582	A1510	A1434	A1359	A1275	G1196	A1127	G1063	C993	C915	C844
	A1786	A1583	G1583	A1511	G1436	A1360	G1277	C1201		U1064	C995	A917	C846
C1882	A1787	C1585	U1585	G1512	C1437	G1364	A1278	G1202	U1130	U1065	A996	A918	U847
G1883	G1787	A1586	A1586	C1513	G1441	A1365	U1288	G1203	G1131	U1066	A1000	A919	G848
A1884	C1788	U1691	C1587	U1514	G1442	A1366	U1289	A1204	C1135	A1067	A1001	G919	G849
A1885	A1789	U1692	C1588	U1515	G1443	G1367	C1290	U1205	G1136	G1068	G1002	G929	C850
C1886	C1790	C1694	C1589	G1517	G1444	G1369	C1291	G1206	G1137	A1069	G1003		U851
G1887	A1791	U1695	U1590	U1518	G1444		C1292	G1207	U1138	A1070	C1004	G932	C856
G1888	G1792	G1698	G1591	G1519	A1444A	U1372	C1293	C1208	G1139	C1072	C1005	A933	C857
A1889	C1793	C1592	C1592	G1521	G1448	A1373	C1294	U1209	U1140	A1073	C1006	G938	U858
C1894	C1795	G1594	G1594	G1522	A1449	G1374	C1297	U1210	U1141	G1074	C1007		U859
C1895	U1796	G1595		G1525	G1449A	C1376	G1298	U1211	U1142	C1075		U860	
	C1797		C1600	G1526	A1453	G1377	G1299	G1212	A1142A	C1076	U1011	A941	
G1899	U1798	G1705	G1601	G1527	U1454	A1378	U1300	G1215	A1143	A1077	U1012	G942	A863
A1900	C1800	U1706	C1601	A1528	G1455	A1379	A1301	G1216	G1144	U1078	C1013	U943	G864
C1902	A1801	U1709	C1607	A1529	G1456	G1380		C1217	C1145	G1079	U1014	G944	C865
G1903	A1802	C1710	A1608	G1530	G1458	G1381	G1309	G1218	C1146	A1080	G1015	A945	A866
	A1803		A1609	C1531	G1459	C1382	G1310	G1219	C1147	U1081	G1016	G946	
G1906	C1804	G1718	A1610	C1532	A1460	A1383	G1311	C1220	A1148	U1082	C1017	G950	C867
G1907	U1805	G1725	C1617	G1533	G1461	C1384	U1312	C1221	U1083	U1083	U1018	G951	U868
C1908		G1726	A1618	G1534	C1464	C1385	G1313	G1222	A1084	A1084	U1019	G952	G869
	A1810	G1727	A1618	U1535	C1465	C1386	C1314	A1227	A1085	A1085	A1020	G953	A870
A1913	G1811	U1728	A1637	A1536	G1466	G1387	U1315	G1228	C1152	A1086	G1022	G954	U871
C1914	A1812	A1729	C1638	G1537	C1467	G1388	G1316	G1229	G1153	A1087	U1023	C955	A872
U1915	G1813	U1730	U1639	G1538	C1468	G1389	A1317	G1230	A1155	U1089	G1024	G956	G873
A1916	A1732	U1731	A1640	G1539	A1469	U1396	C1318	G1231	C1158	U1090	U1025	A957	G879
A1918	G1733	C1733	A1641	U1540	G1470	C1403	C1320	G1235	U1159	G1091	U1026	U958	G880
A1919	A1819	G1734	G1642	G1541	A1471	C1405	A1322	G1236	G1160	A1092	A1027	A959	G881
C1920	U1820	C1735	G1643	U1542	A1471	U1405	U1323	A1237	C1161	C1093	A1029	A960	G882
	A1821	C1741	A1543	A1544		U1406	G1324	U1240	G1162	U1094		C961	G883
C1924	A1825	G1742	C1544	C1545	C1474	U1407	G1325	A1241	U1165	A1095	U1033	G966	C884
C1925	G1743	G1648	A1545	G1475	G1476	C1407	U1326		U1166	A1096		C967	C885
U1926		G1650	C1547	C1477	A1477	C1408	G1327		U1167	U1097	G1036	C968	C886
						C1409				A1098	G1037	U969	A887
											C1038		C888
													C889

A2851	G2100	C2163	G2246	C2316	C2381	A2450	U2537	A2614	C2699	C2773	A2851
G2852	G2101	C2164	A2247	C2317	G2382	G2458	C2536	U2615	C2700	C2774	G2852
C2853	U2102	G2165	G2250	G2318	G2383	G2461	G2543	C2617	C2701	A2775	C2853
C2855	C2103	G2166	G2251	G2319	G2384	U2462	G2544	C2618	U2702	U2778	C2855
C2856	U2022	U2167	G2255	G2320	C2385	U2462	G2545	C2619	C2703	A2779	C2856
G2857	G2023	G2168	G2256	G2321	G2386	C2465	U2546	C2620	A2705	G2780	G2857
A2860	G2024	A2169	G2257	G2322	G2389	C2466	G2550	G2627	G2706	A2781	A2860
C2863	C2025	A2170	G2258	G2323	U2390	C2467	G2551	A2628	G2707	G2782	C2863
U2864	G2026	A2171	U2257	G2324	G2391	C2468	U2552	A2629	C2710	G2783	U2864
U2865	A2030	U2172	G2259	G2325	A2392	C2469	U2553	G2630	A2711	C2784	U2865
U2866	A1937	U2173	G2262	G2326	A2393	A2469	G2554	C2635	U2712	U2785	U2866
U2867	A1938	A2174	U2263	A2327	C2394	C2470	U2555	U2636	A2713	G2787	U2867
C2871	U1939	G2175	C2263	G2328	G2397	G2471	G2556	U2637	A2714	C2788	A2868
G2872	A1952	A2176	A2266	G2330	U2401	U2472	G2557	U2638	U2715	A2789	C2869
C2875	C2036	C2177	A2267	G2331	C2402	C2473	G2558	U2639	G2716	A2790	C2870
G2876	G2037	C2178	A2268	U2332	C2403	C2474	U2562	C2645	U2717	C2794	C2871
G2877	U2038	C2179	A2269	A2333	C2404	C2475	U2563	C2646	G2718	G2795	C2872
C2881	C2039	G2181	A2270	G2334	G2405	G2476	A2564	U2647	U2719	U2797	C2881
C2882	A2042	G2182	G2271	A2335	U2406	C2477	A2565	U2648	G2720	C2798	C2882
A2883	C2043	C2183	A2272	A2336	U2407	C2480	U2566	U2649	A2721	U2799	A2883
G2886	G1964	G2184	A2273	G2337	U2408	G2481	G2567	C2652	G2722	A2801	G2886
U2887	C2050	G2186	A2274	G2340	U2409	G2482	C2568	U2653	C2723	G2802	U2887
C2888	G2051	G2187	G2275	G2341	G2410	A2488	A2572	U2654	U2726	G2805	C2888
C2889	G1967	G2188	G2276	C2342	G2411	G2489	C2573	A2654	G2727	U2807	C2889
A2892	G1968	C2127	G2277	C2343	G2412	G2490	G2574	U2655	U2728	U2797	A2892
G2893	G1969	C2128	C2281	U2344	G2413	G2491	G2575	U2656	G2729	C2798	G2893
G2894	A1970	G2129	G2282	A2345	C2414	U2492	G2576	U2657	C2730	U2809	G2894
U2895	C2055	U2130	C2283	G2346	G2415	U2493	A2577	A2660	G2731	A2810	U2895
C2896	A1971	G2131	C2284	A2347	U2416	U2494	G2578	U2661	G2732	G2811	C2896
U2897	A1972	G2132	C2285	U2348	U2417	G2495	G2579	U2662	A2733	G2812	U2897
U2898	G2056	U2133	C2286	G2349	C2420	G2496	U2580	G2663	C2745	C2815	U2898
C2899	G1989	C2134	G2287	G2350	G2421	C2497	G2581	U2664	U2746	C2816	C2899
A2900	C1990	A2060	U2291	C2351	A2422	U2503	U2585	C2665	G2747	G2817	A2900
C2901	U1991	G2066	C2292	G2352	G2423	U2504	G2586	C2666	A2748	G2818	C2901
C2902	U1993	C2067	C2293	C2353	G2424	G2505	C2591	C2667	U2749	C2819	C2902
C2907	U1994	G2068	C2294	G2354	A2430	U2506	U2592	U2673	G2751	A2820	C2907
C2908	C1995	A2069	C2297	A2360	U2439	U2511	U2593	C2678	C2752	A2821	C2908
G2012	C1996	C2077	A2298	C2364	A2433	C2512	C2594	A2679	C2755	G2830	G2012
A2013	C2078	G2087	G2299	G2365	A2434	G2513	G2599	C2680	U2756	G2833	A2013
A2014	C2079	G2088	G2303	A2366	A2435	U2514	A2600	C2681	A2757	U2758	A2014
A2015	G2081	A2082	G2304	G2369	G2436	C2515	C2601	U2682	G2759	A2835	A2015
U2016	G2083	G2082	A2305	G2370	U2437	A2518	G2603	C2683	C2760	U2836	U2016
U2017	U2086	G2087	G2306	G2371	A2438	G2525	U2604	U2688	G2761	G2837	U2017
G2094	G2086	G2087	G2307	G2372	C2440	G2526	U2605	U2689	G2762	C2841	G2094
C2095	G2087	G2087	G2308	G2373	C2441	U2528	G2606	C2690	G2763	G2845	C2095
U2096	G2094	G2094	G2309	G2374	C2442	G2529	G2607	A2693	A2764	G2846	U2096
A2158	G2157	G2157	A2310	A2375	C2443	A2530	G2608	C2694	U2765	G2847	A2158
A2169	G2158	G2158	A2311	A2376	G2444	A2531	U2609	C2695	G2766	U2847	A2169
U2243	G2159	G2159	U2312	A2377	G2445	A2532	C2610	U2696	C2767	U2848	U2243
U2244	G2162	G2162	C2313	A2378	G2446	A2533	U2611	G2697	C2771	A2850	U2244
U2245	G2162	G2162	C2314	A2379	G2447	A2534	U2612	U2698	C2772		U2245

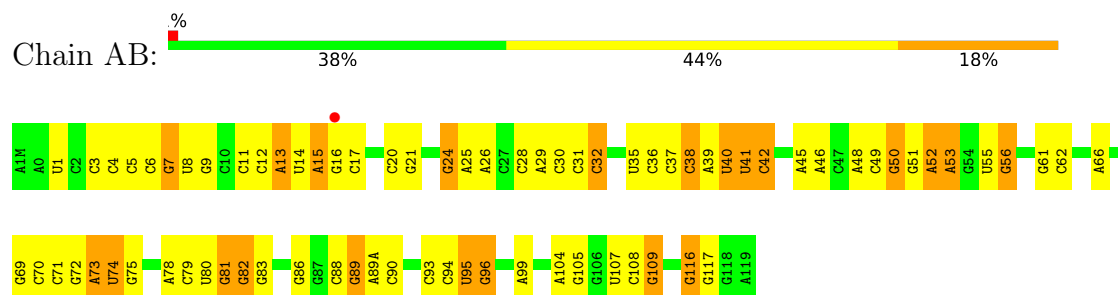
• Molecule 1: RNA (2909-MER)



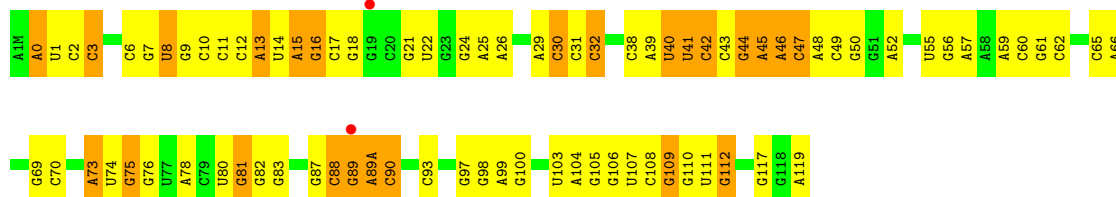
G2104	G2029	A1936	G1828	A1755	A1641	G1542	A1472	A1392	A1317	G1244	G1154	G1089	U1023
C2107	A2030	A1937	A1829	G1756	G1642	A1543	G1473	A1393	G1318	G1244	A1154	U1090	G1024
C2108	A2031	A1938		U1757	G1645	C1544	G1475		G1319	A1246	A1156	G1091	U1025
	G2032		U1833	G1758	G1646	A1545	G1476	U1396	C1320	A1247		C1092	U1026
	A2033	C1942	U1834	A1759	G1647	C1547	A1477	U1397	A1321	G1248	G1160	U1094	A1027
	U2034		G1835	A1760	G1648	C1548	G1478		U1323	U1249		A1095	U1033
	G2035	U1946	C1836	G1761	G1649	C1549	G1479	G1401	U1324	G1250	G1164	A1096	U1034
	C2036	C1947	C1837	A1762	G1650	C1557	G1480	G1402	G1325	C1251	U1165	A1097	U1035
	C2039		G1839	G1763	A1651	A1558	U1482		U1405	A1252	C1166	G1098	U1036
	G2040			G1764	A1652	G1559	G1483	U1406	C1327	A1253		G1099	
	U2041				G1653	G1560	G1484	U1407	G1328	A1254	G1169		G1039
	A2042	G1954	A1847	G1770	A1654		G1485	C1408	U1329	U1255	G1170	C1102	G1040
	C2043		A1854	C1771		G1568	A1486		C1330	G1256	G1171		C1041
		U1955		C1657	C1657	A1569	G1487		A1331	C1257			C1042
	C2050	C1957	G1858	A1773	C1658	A1570	G1488	G1416	G1332		G1173	U1105	G1043
	A2051	C1957		A1774		A1571	U1489	G1417		C1258	A1174	G1106	A1044
	G2052	C1958	U1864	U1775	A1665	C1575	A1490	G1418	A1336	G1259	U1175	U1107	A1045
	C2053		G1869	G1776	G1666	C1576	U1491	U1420	G1337	G1260	A1177	C1109	A1046
	A2054	U1963		U1777	G1667	C1577	G1492	G1421	G1338	A1262	C1178	G1110	A1047
	C2055	G1964	A1872	U1778	A1668	C1578	A1493		G1339		C1179	G1111	G1048
	G2056	A1966	G1878	U1779	A1669	U1578	A1494	G1426	U1340	G1265	C1180	G1112	C1049
	A2057	C1967	C1879	A1780	C1670	A1579	A1495	G1427	U1341	A1266	C1181	U1113	A1050
	C2058	G1968	C1890	C1781	U1671	U1580	A1496	A1427	A1342	U1267	A1182	G1114	G1051
	A2059	A1969		C1782	C1672	G1581	U1497	C1428	A1349	A1268	G1183	G1115	C1052
	U2060	A1970	A1884	A1783	U1673	C1582	C1498	G1429	C1345	A1269		C1116	C1053
	G2061	A1971		A1784	G1674	A1583	C1499	G1430	G1346	C1270	G1187		A1054
	A2062	A1972	C1887	A1785	C1675	C1585	G1500	U1431	G1347	A1271	U1188	C1119	G1055
	C2063	G1973	A1786	A1676	A1677	A1586	C1501	A1439	G1348	A1272	A1189		G1056
	A2064	C1974	A1889	A1787	A1677	A1587	C1502		A1349	U1273	A1190	G1122	A1057
	C2065				U1678	C1588	U1503	G1436		A1274	G1191		U1058
	G2066	A1981	G1899	C1790	U1679	C1592	C1504	G1437	U1352			G1125	G1059
	C2067	A1990	A1900	A1791	U1680	C1593	C1505	U1437	A1353	A1278	U1198	A1126	U1060
	U2068	G1989	C1901			G1594	C1506	A1438	A1354	G1279	U1199	A1127	U1061
	G2070	U1991	A1902	U1794	C1686	G1595	C1507		G1355		C1200	G1062	G1062
		G1992		C1795	G1687	A1596	A1508	G1442	U1356	G1283	C1201	A1129	G1063
	U2074	U1993	G1906	U1796	U1688	A1597	C1509	G1443	G1357	A1284	U1130	G1064	G1064
	C2075	C1994	C1907	C1797	A1689	C1598	A1510	G1444	G1358	G1285	G1203	G1131	U1065
			C1908	U1798		C1599		A1444	A1359	A1286	U1204	A1132	U1066
	U2079	C1999	G1910	G1799	G1696	C1599	C1515	G1445	A1360	A1287	U1205	C1135	G1068
	G2080	G2000	G1910	C1800	G1697	G1600	U1516	A1445	A1361	U1288		C1136	U1069
	C2081	A2001	G1914	G1801	A1698	G1601	G1517	C1446	G1361	C1289	A1210	G1137	A1070
	A2082	G2002	U1915	A1802	G1699	U1602	C1518		A1365		U1211	G1138	G1071
			A1916	A1700	A1700		G1519	A1449		U1292	G1212	G1139	C1072
	U2086	C2006		A1701		G1606		G1449A	G1368	C1293		G1140	A1073
	C2087	C2007	A1917		C1607	C1607	G1522	G1450	G1369		C1217	U1141	G1074
			A1918	U1716	A1608	A1608	G1525			C1297	A1220	U1142	C1075
	U2092	G2010	G1919	G1717	A1609	A1609	G1526	G1455	U1372	G1299	A1142A	A1143	G1076
	G2094	G2011	A1812	G1718	A1610	A1610	G1527			U1300	G1225	G1144	A1077
	C2095	G2012	G1813	G1725		A1614	A1528	G1458	G1379	A1301	G1226	G1148	
	U2096	A2013	G1814	G1728	G1728	G1615		G1459	G1380	A1227	G1228	A1149	U1082
	C2097	A2014	A1815	U1729	A1729	A1616	G1534	A1460	A1384	G1309	C1145	C1146	U1081
	U2098	A2015	G1816	U1730	A1616	A1616	U1535	G1461	G1385	G1310	C1147	C1147	U1082
				G1731	C1625	C1625	A1536	G1464	C1386	G1311	G1231	A1148	U1083
	G2100	A2020	A1819	G1731	C1625	C1625	C1537	G1465	C1387	G1312	G1232	G1149	A1084
	C2101	C2021	U1820	G1742	G1635	G1635	G1538	G1466	G1388	U1313		C1150	A1085
	U2102	G2022	G1743	G1743	C1638	C1638	G1539	G1467	G1389	C1314	G1239	G1151	A1086
	G2103		C1754				U1541	A1471	U1391	U1316	U1240	C1152	G1087
											A1241	G1153	A1088



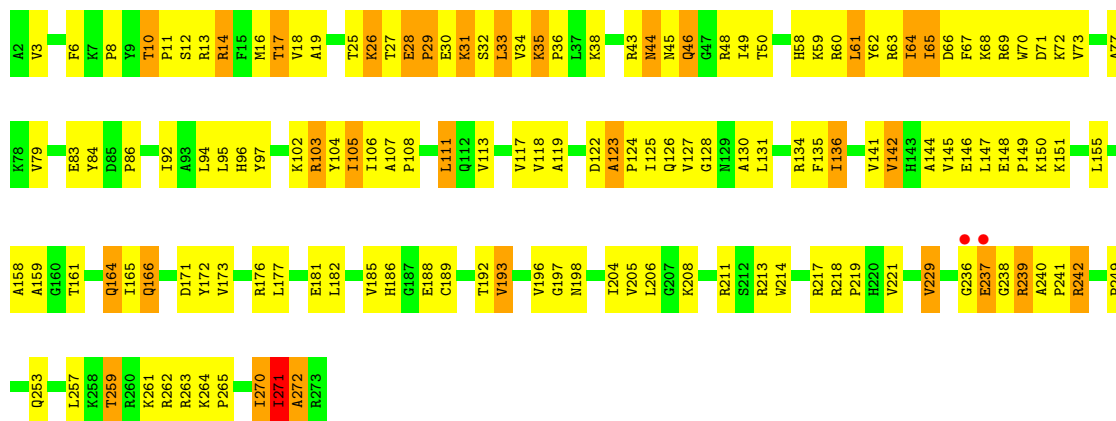
• Molecule 2: 5S RIBOSOMAL RNA



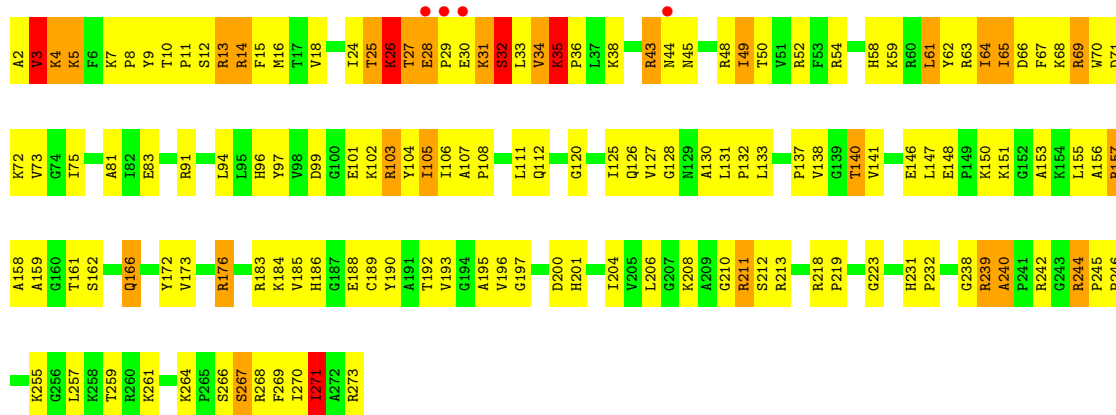
• Molecule 2: 5S RIBOSOMAL RNA



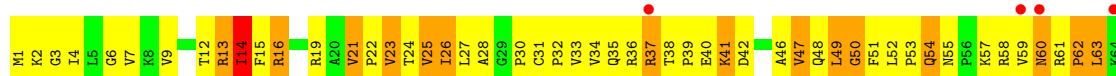
• Molecule 3: 50S ribosomal protein L2

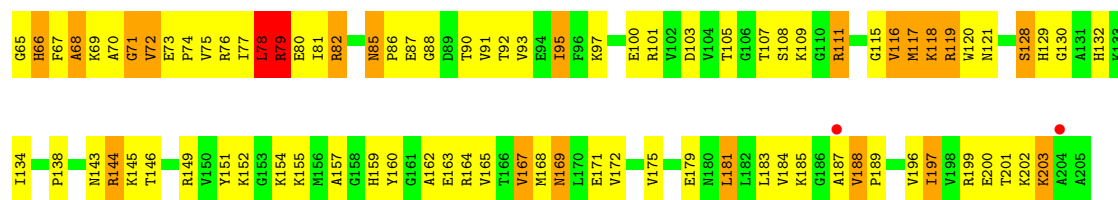


• Molecule 3: 50S ribosomal protein L2

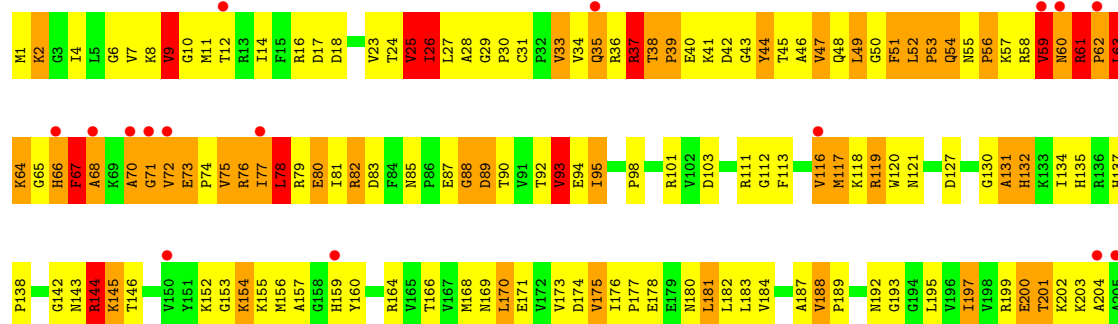


• Molecule 4: 50S ribosomal protein L3

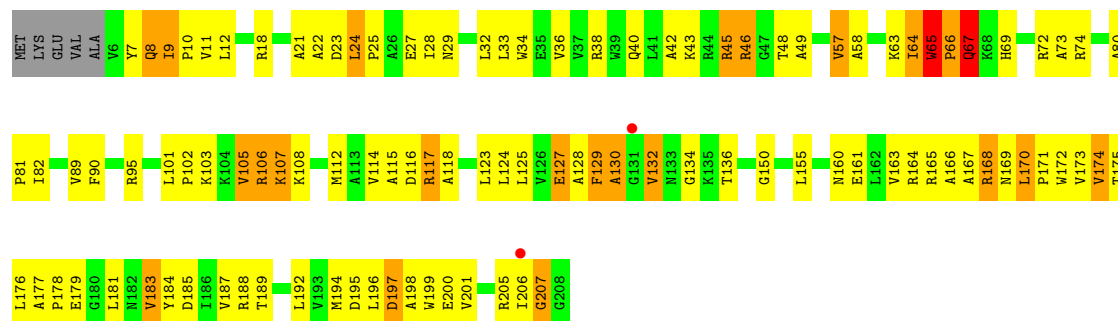




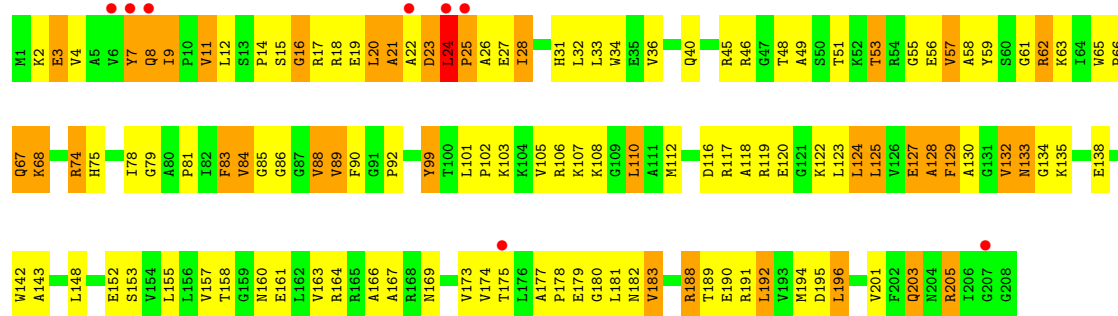
• Molecule 4: 50S ribosomal protein L3



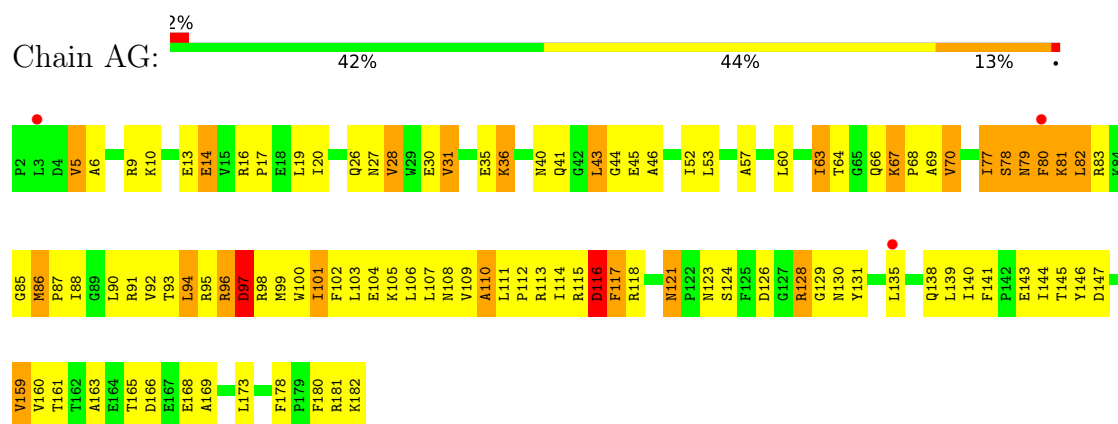
• Molecule 5: 50S ribosomal protein L4



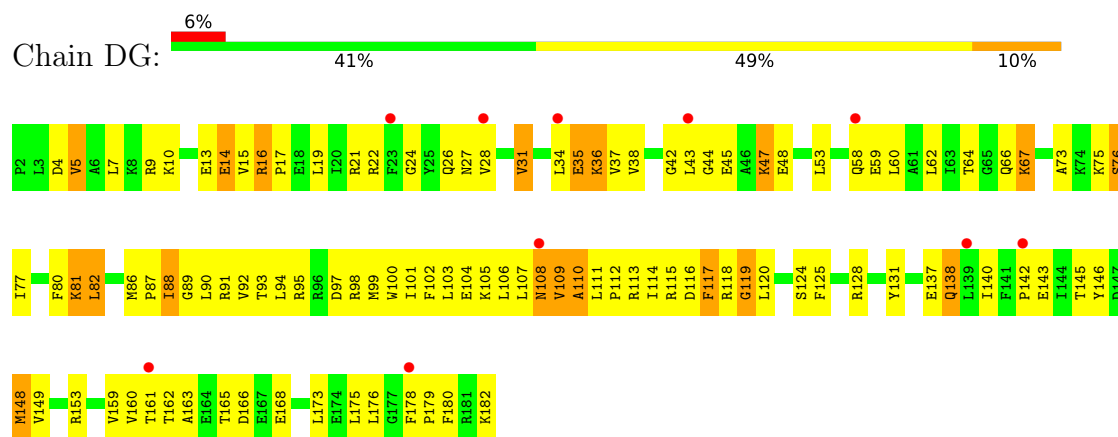
• Molecule 5: 50S ribosomal protein L4



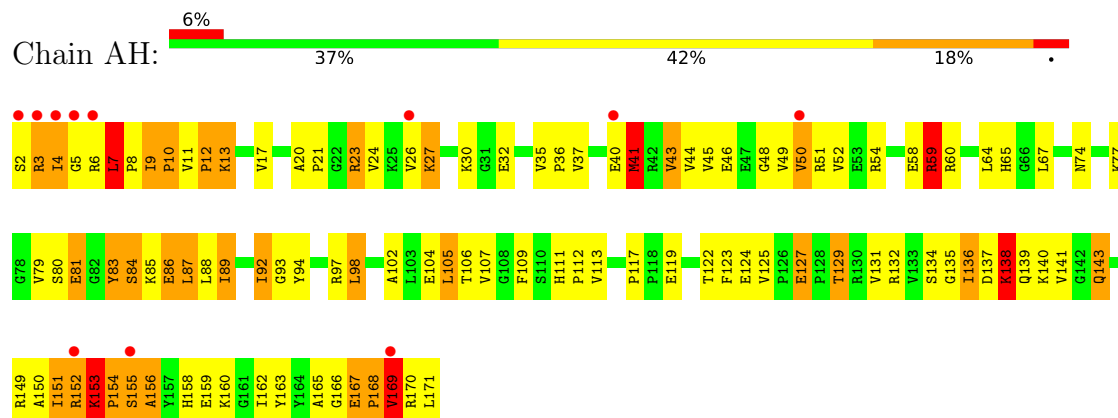
• Molecule 6: 50S ribosomal protein L5



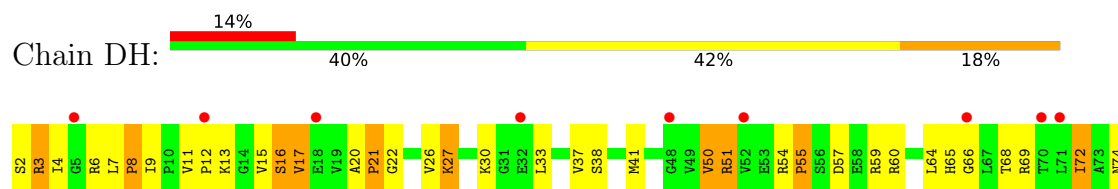
- Molecule 6: 50S ribosomal protein L5

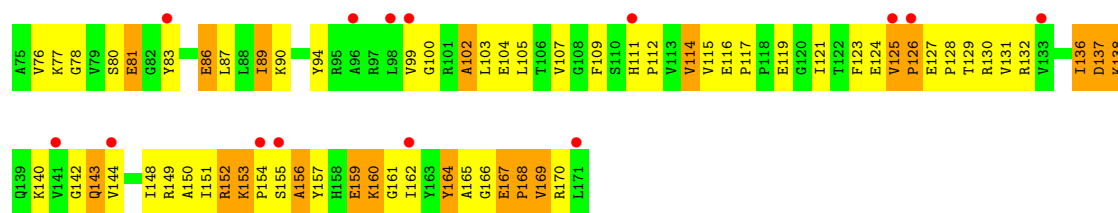


- Molecule 7: 50S ribosomal protein L6

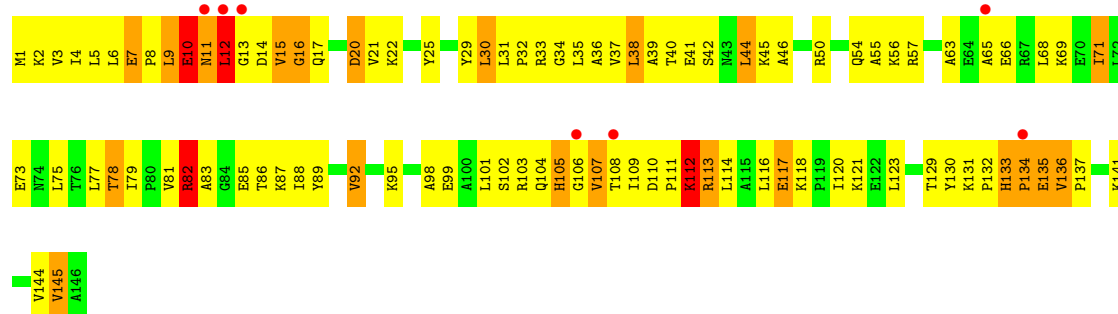


- Molecule 7: 50S ribosomal protein L6

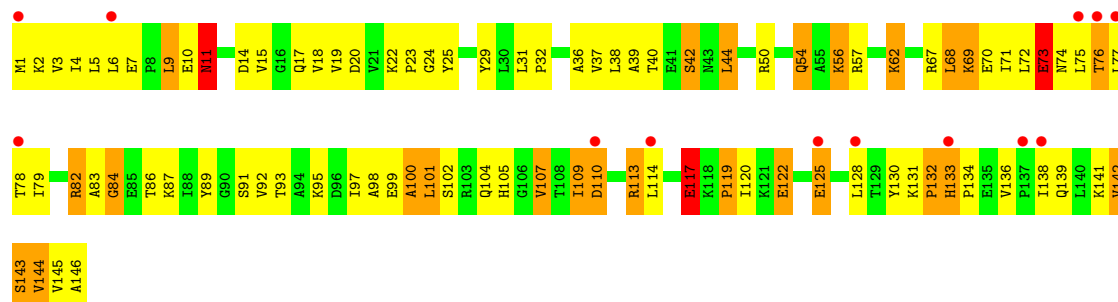




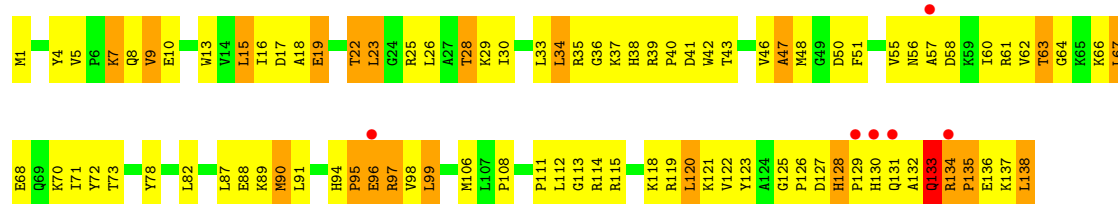
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9

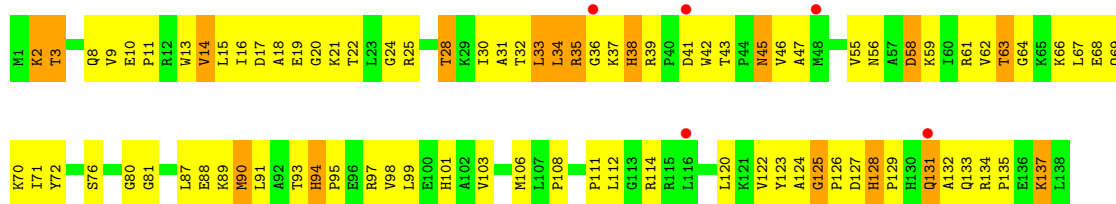


• Molecule 9: 50S ribosomal protein L13



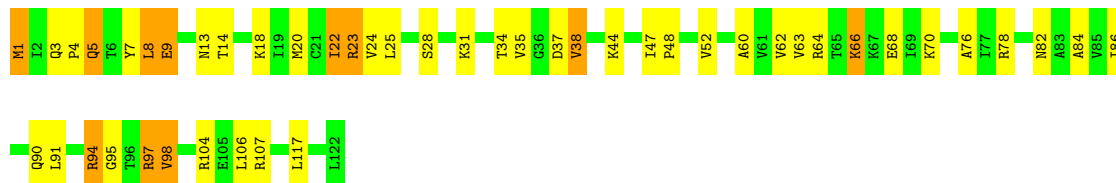
• Molecule 9: 50S ribosomal protein L13





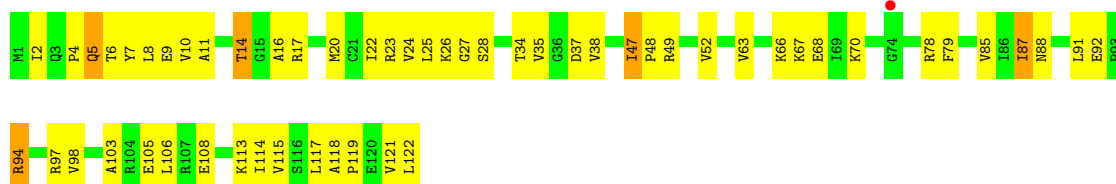
• Molecule 10: 50S ribosomal protein L14

Chain AN: 61% 30% 9%



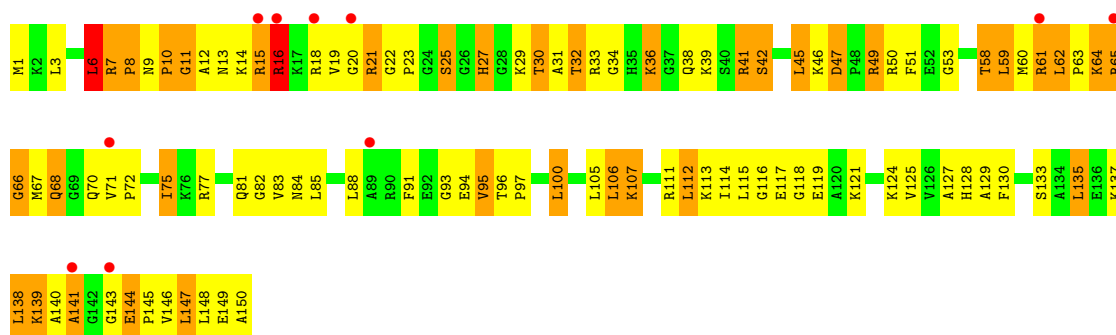
• Molecule 10: 50S ribosomal protein L14

Chain DN: 55% 41% .



• Molecule 11: 50S ribosomal protein L15

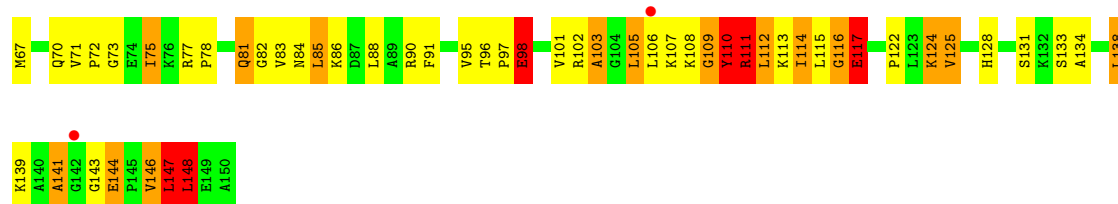
Chain AO: 7% 32% 43% 24% .



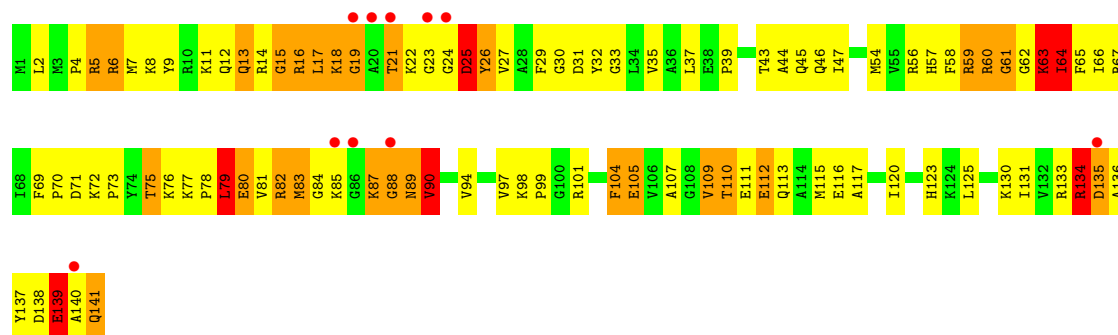
• Molecule 11: 50S ribosomal protein L15

Chain DO: 5% 32% 38% 21% 9%

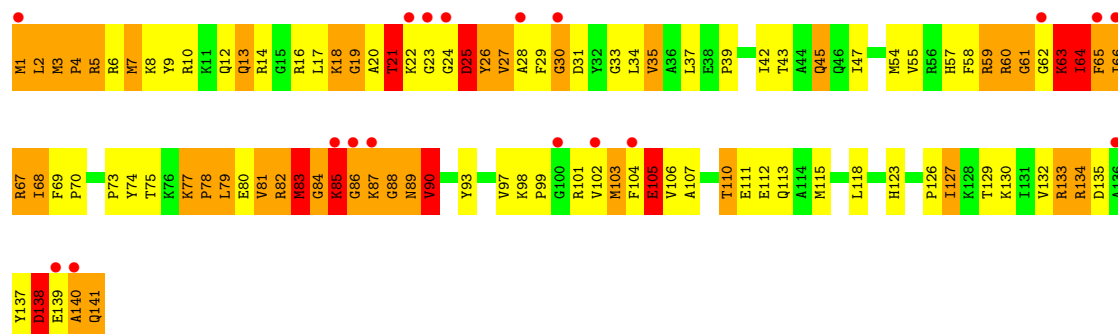




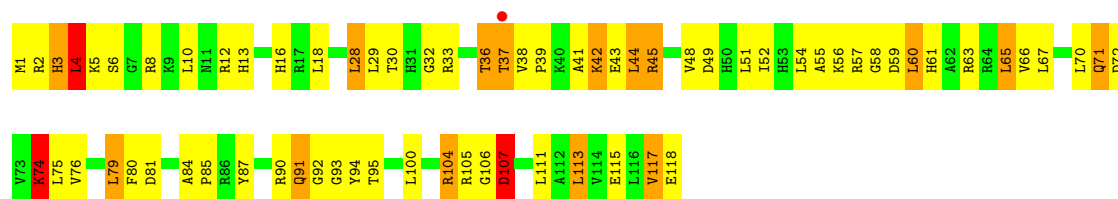
• Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16

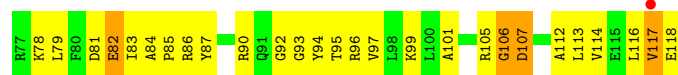


• Molecule 13: 50S ribosomal protein L17

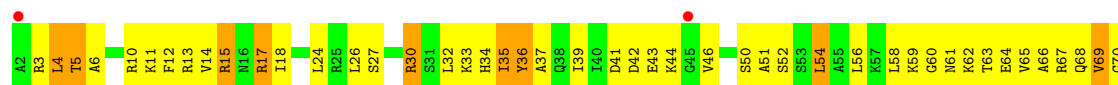


• Molecule 13: 50S ribosomal protein L17

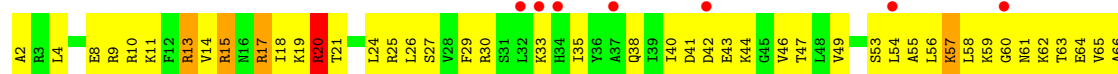




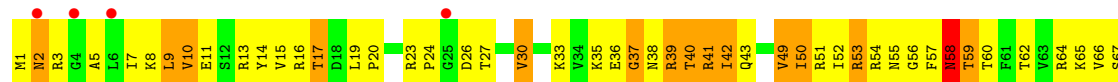
• Molecule 14: 50S ribosomal protein L18



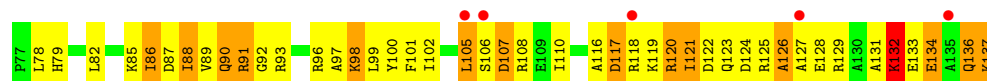
• Molecule 14: 50S ribosomal protein L18



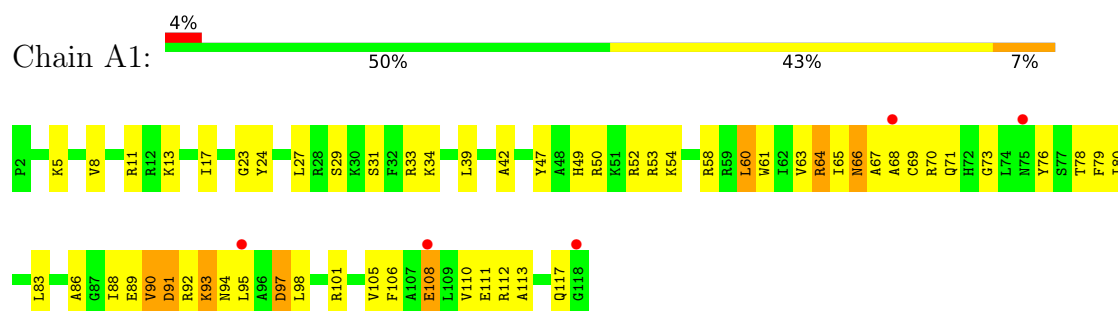
• Molecule 15: 50S ribosomal protein L19



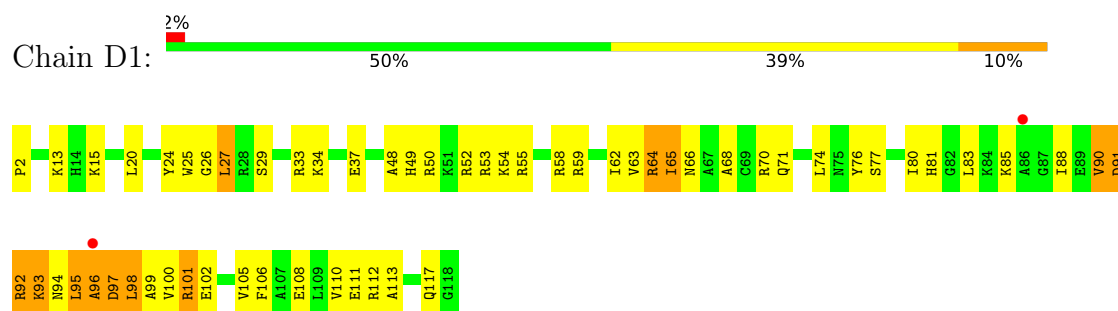
• Molecule 15: 50S ribosomal protein L19



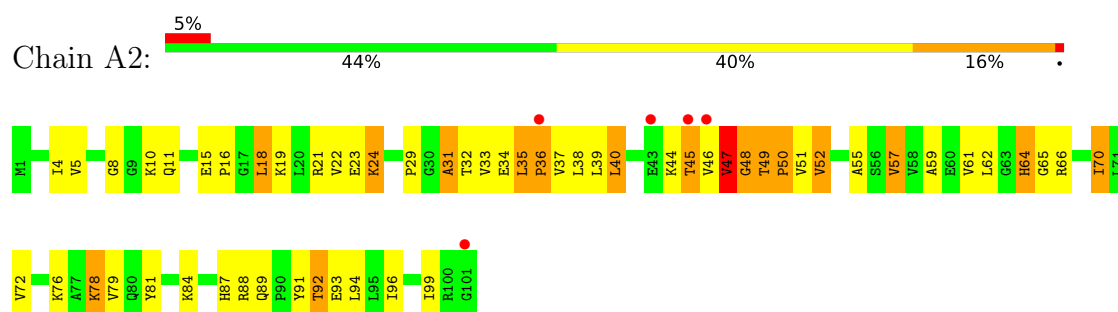
- Molecule 16: 50S ribosomal protein L20



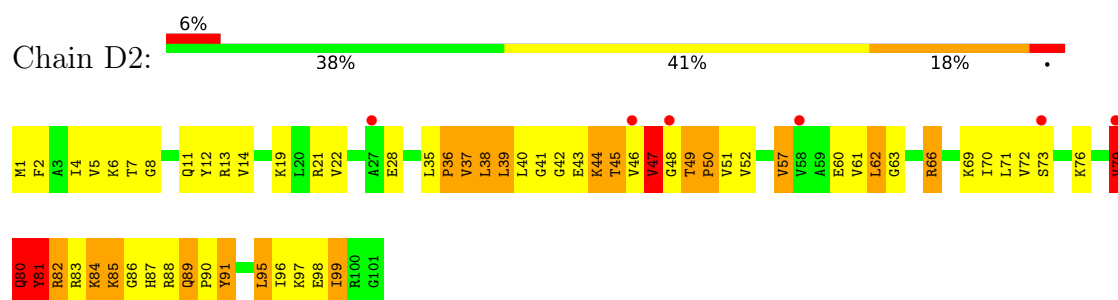
- Molecule 16: 50S ribosomal protein L20



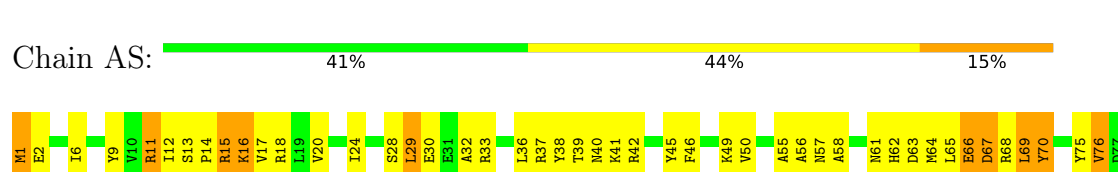
- Molecule 17: 50S ribosomal protein L21

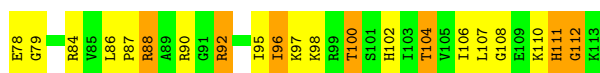


- Molecule 17: 50S ribosomal protein L21

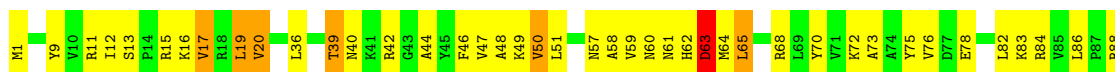


- Molecule 18: 50S ribosomal protein L22

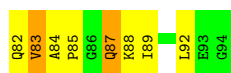
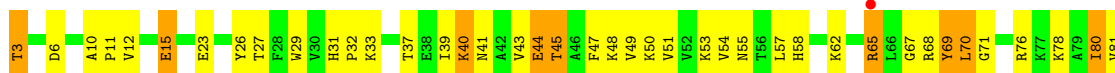




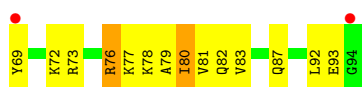
- Molecule 18: 50S ribosomal protein L22



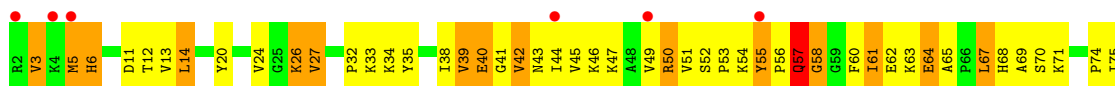
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23

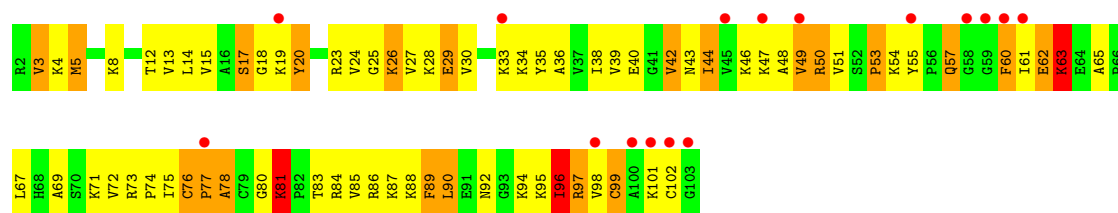


- Molecule 20: 50S ribosomal protein L24

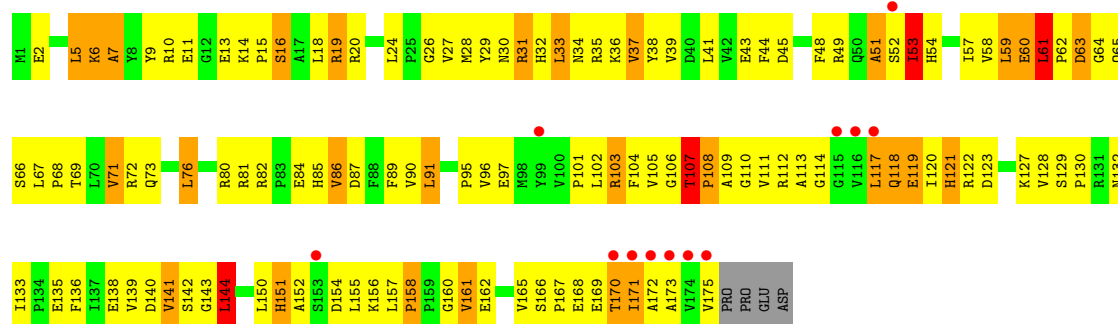


- Molecule 20: 50S ribosomal protein L24

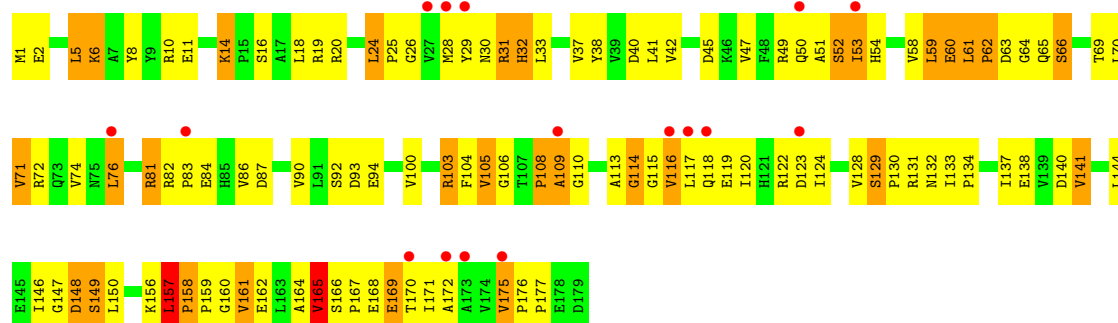




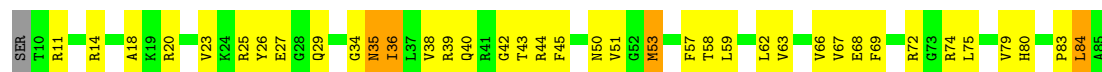
• Molecule 21: 50S ribosomal protein L25



• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27

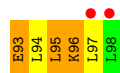
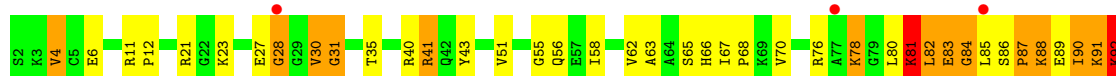




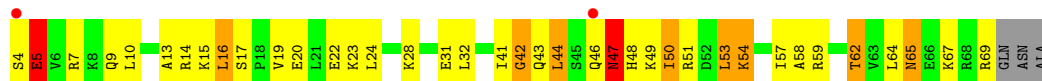
- Molecule 23: 50S ribosomal protein L28



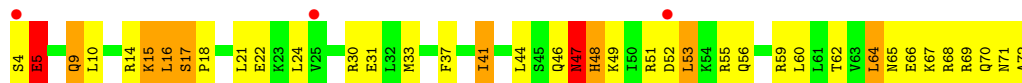
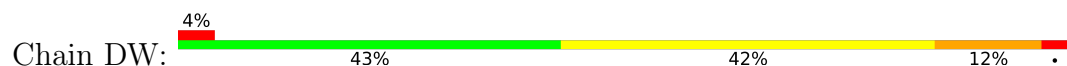
- Molecule 23: 50S ribosomal protein L28



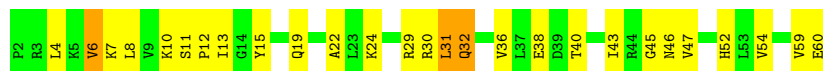
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

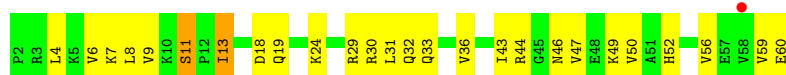


- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30

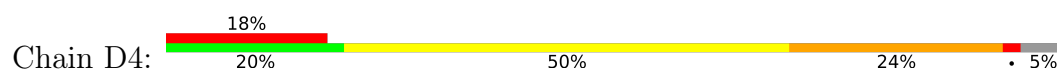




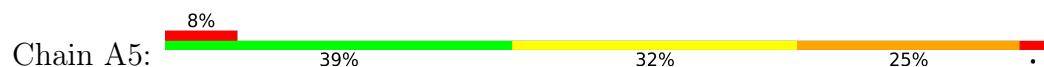
- Molecule 26: 50S ribosomal protein L31



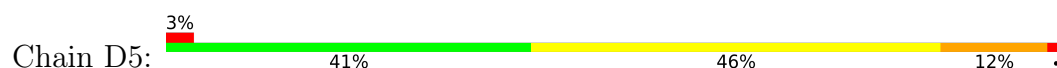
- Molecule 26: 50S ribosomal protein L31



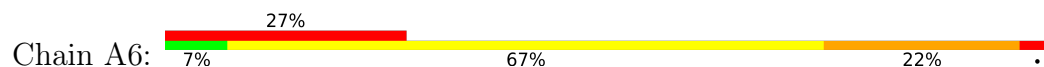
- Molecule 27: 50S ribosomal protein L32



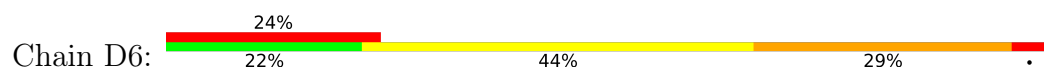
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

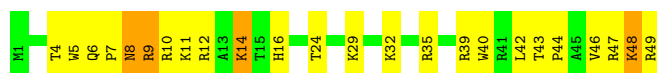


- Molecule 28: 50S ribosomal protein L33





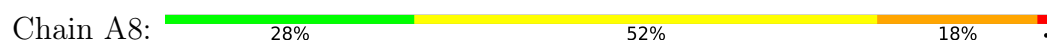
- Molecule 29: 50S ribosomal protein L34



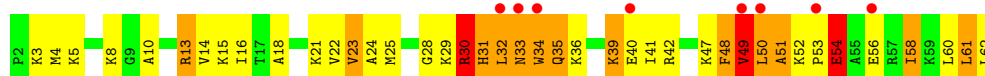
- Molecule 29: 50S ribosomal protein L34



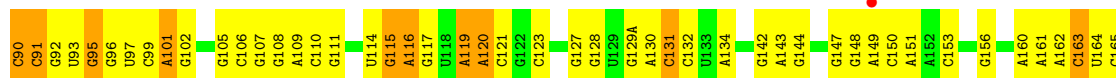
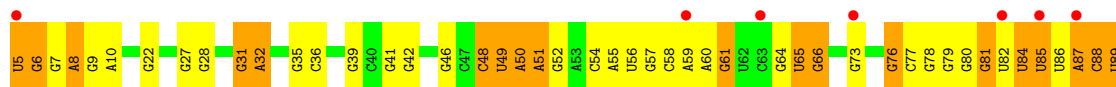
- Molecule 30: 50S ribosomal protein L35

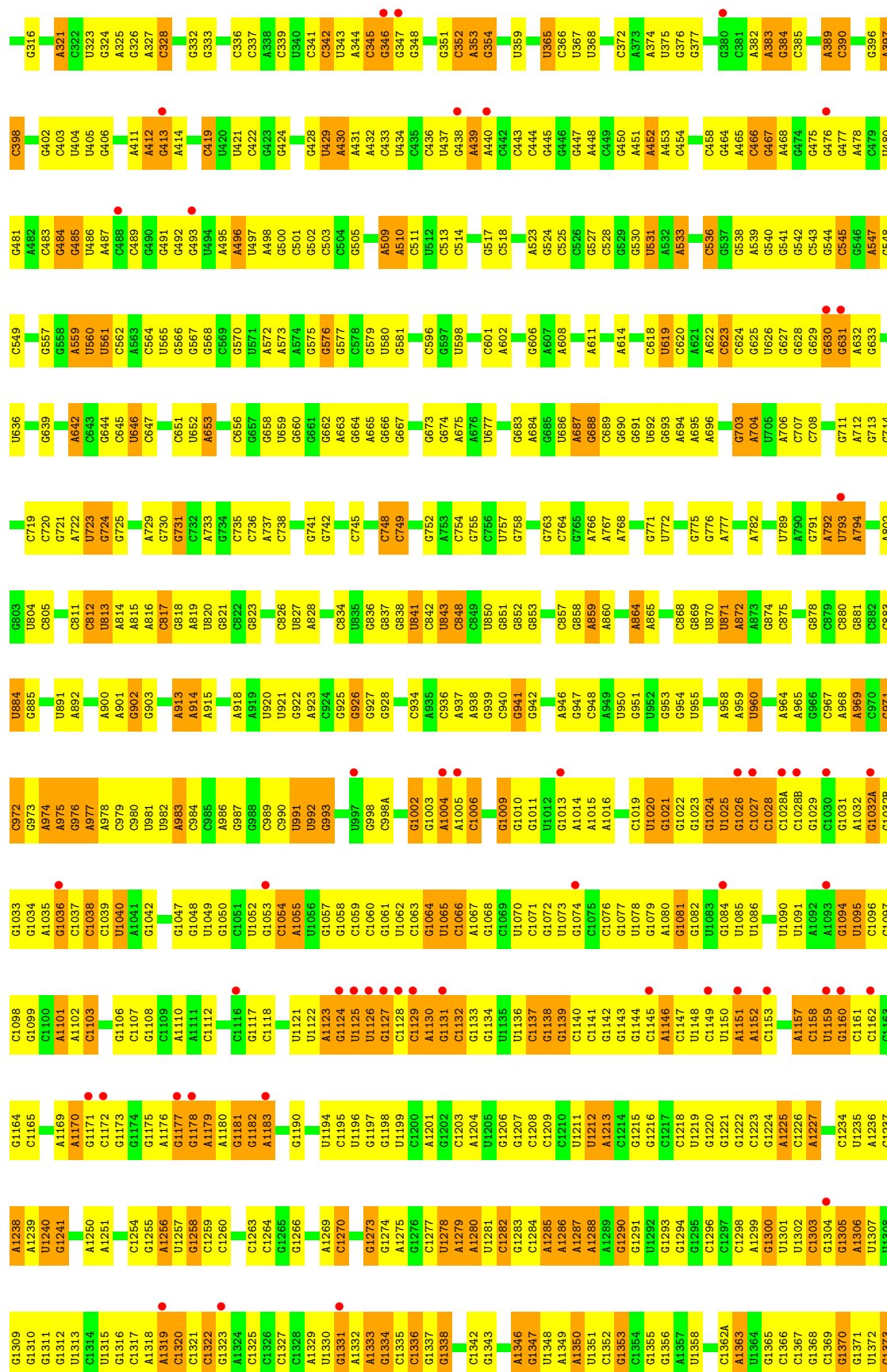


- Molecule 30: 50S ribosomal protein L35



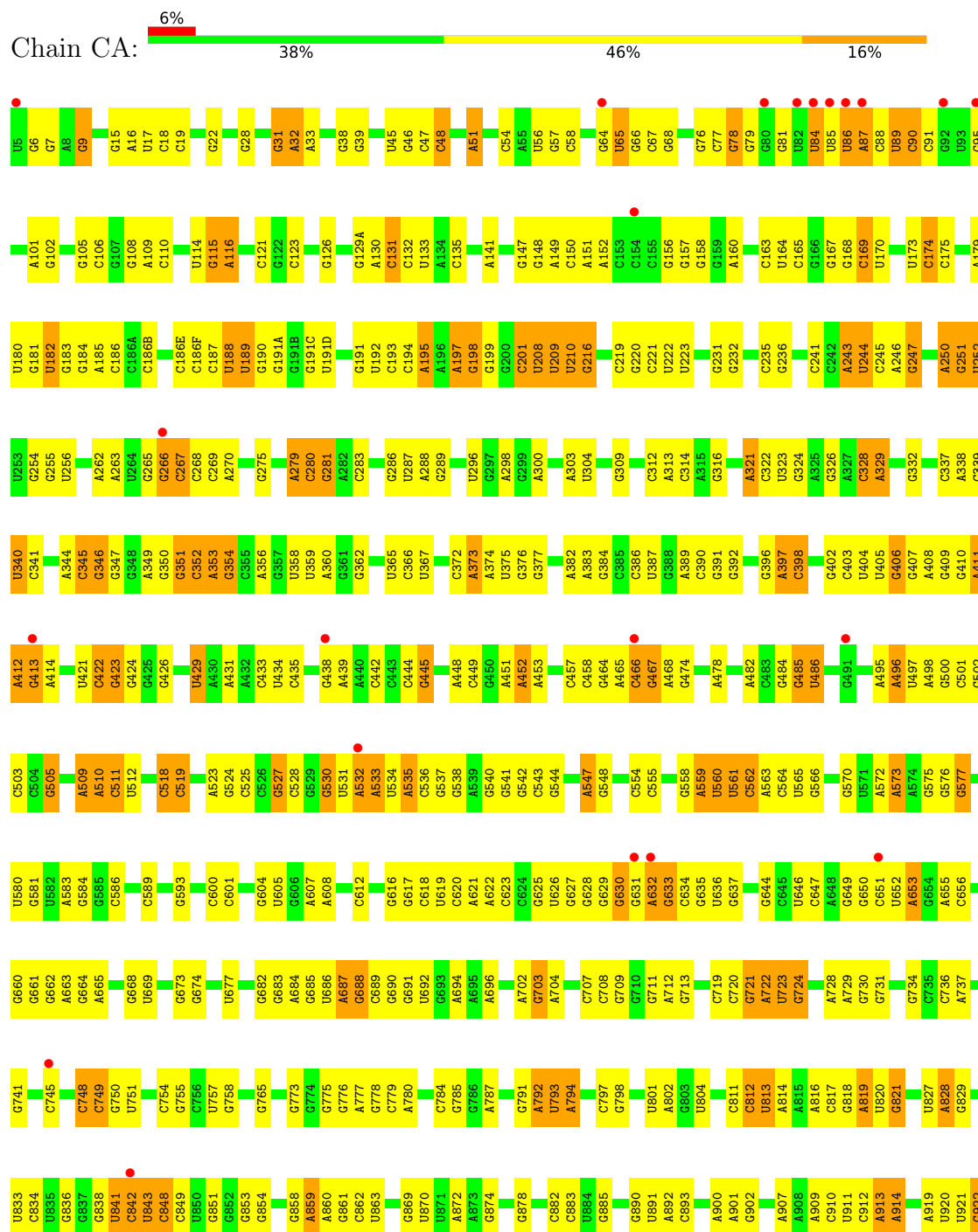
- Molecule 31: 16S ribosomal RNA

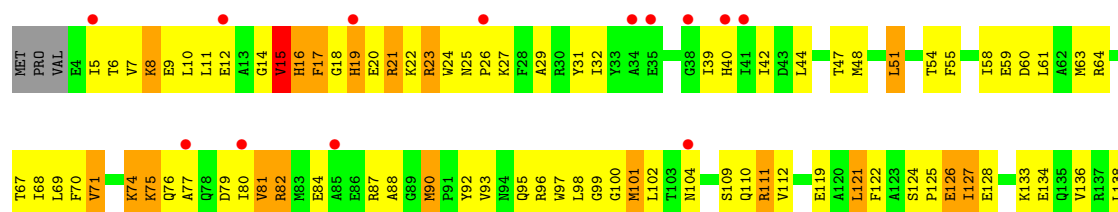


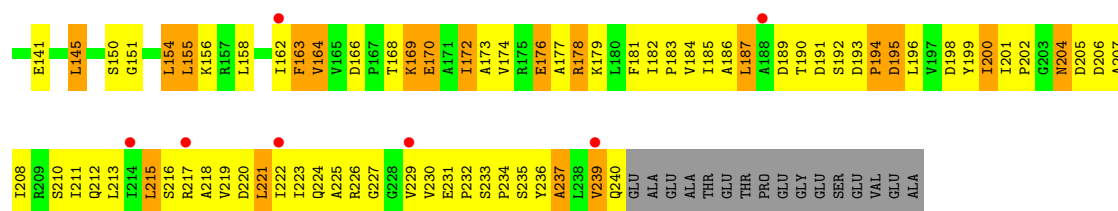




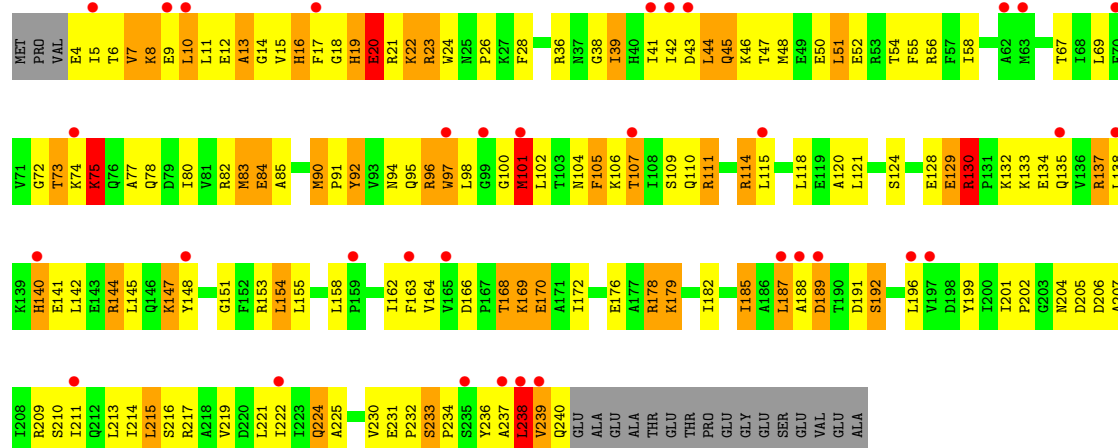
- Molecule 31: 16S ribosomal RNA



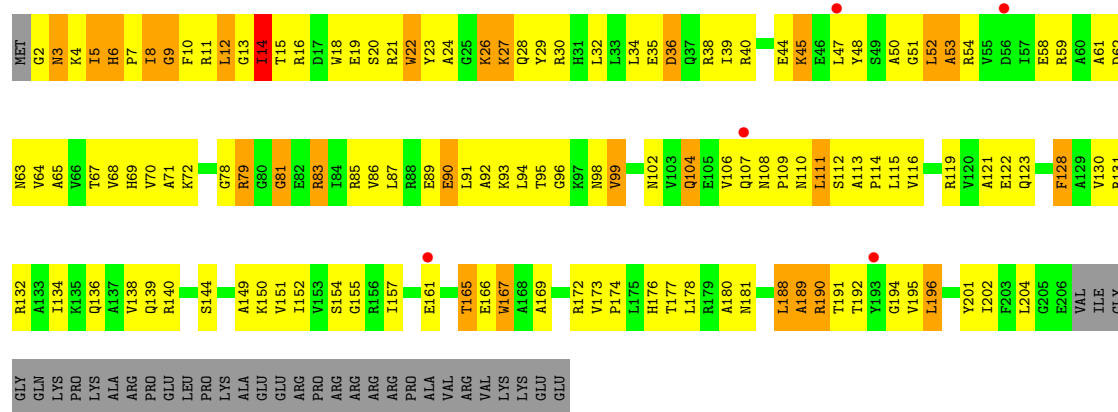




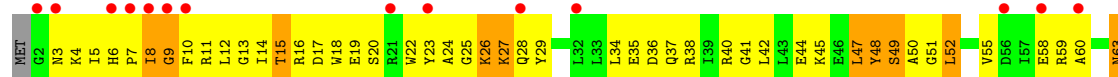
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

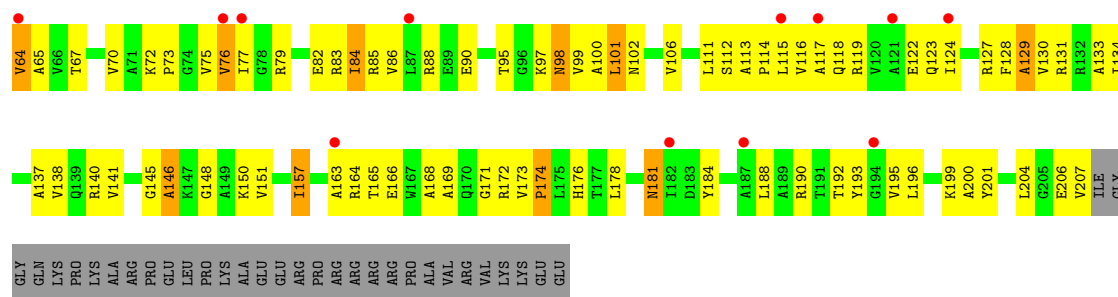


• Molecule 33: 30S RIBOSOMAL PROTEIN S3

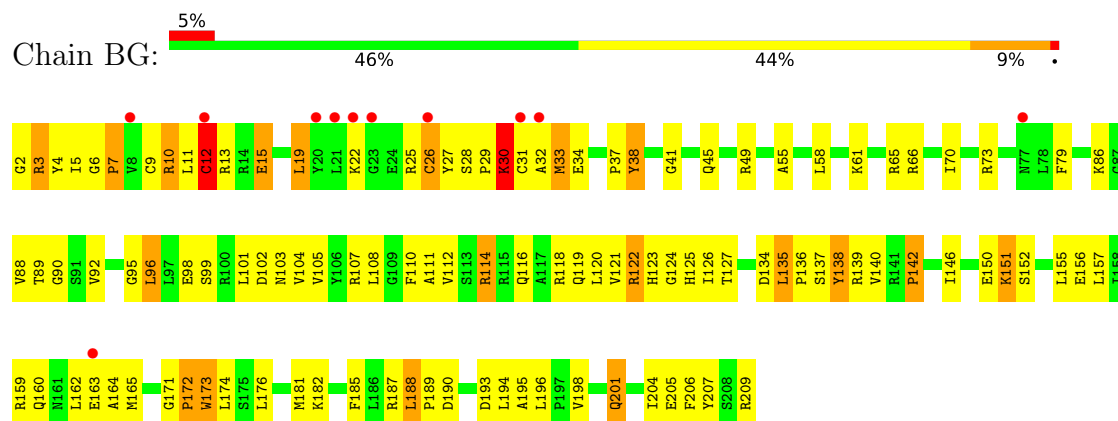


• Molecule 33: 30S RIBOSOMAL PROTEIN S3

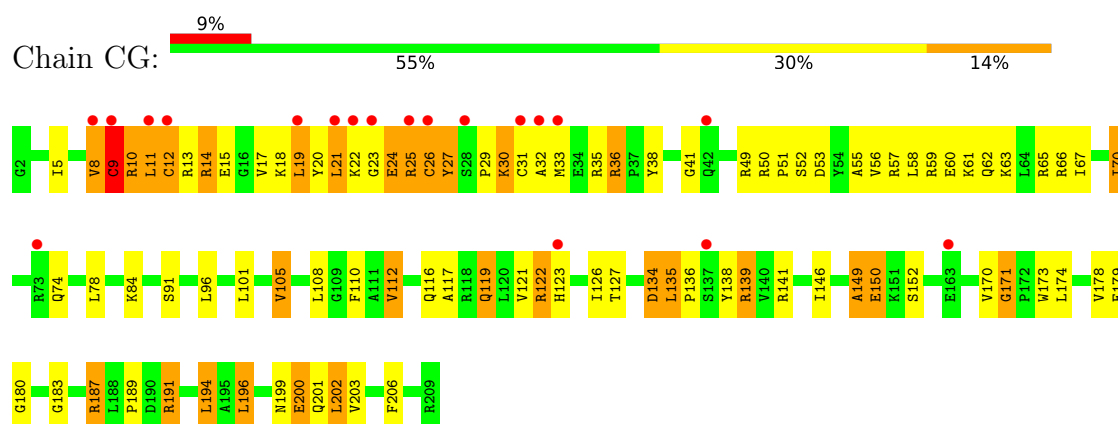




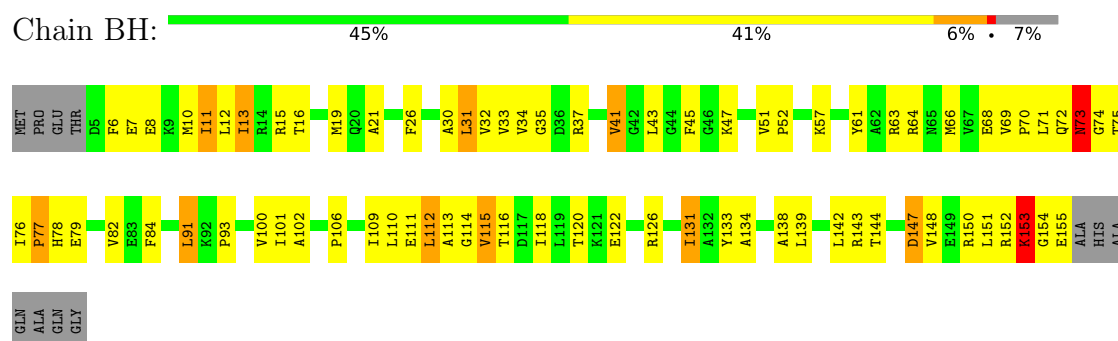
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



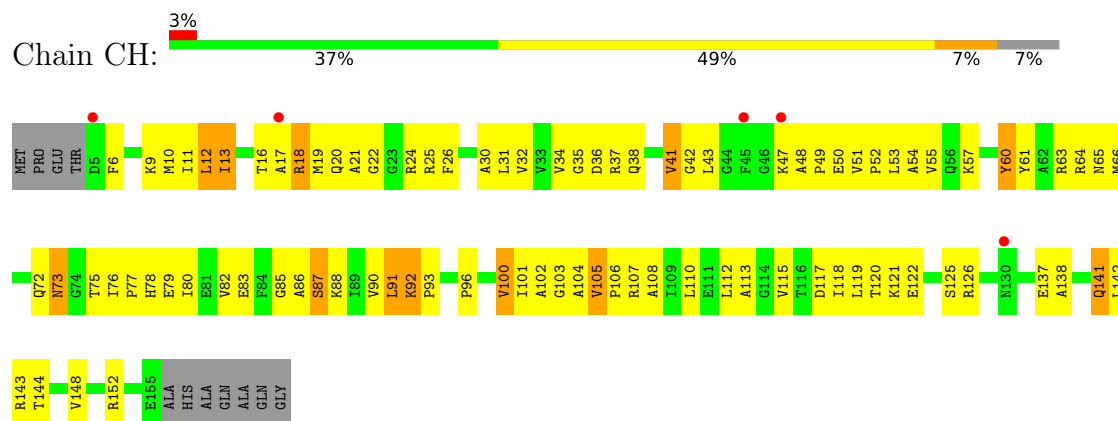
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



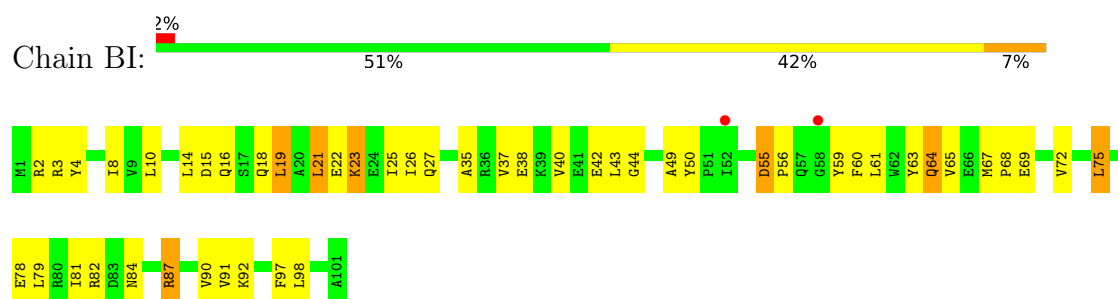
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



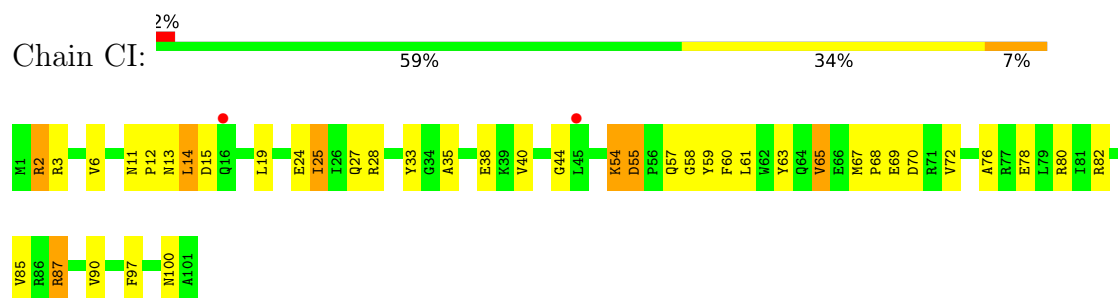
- Molecule 35: 30S RIBOSOMAL PROTEIN S5



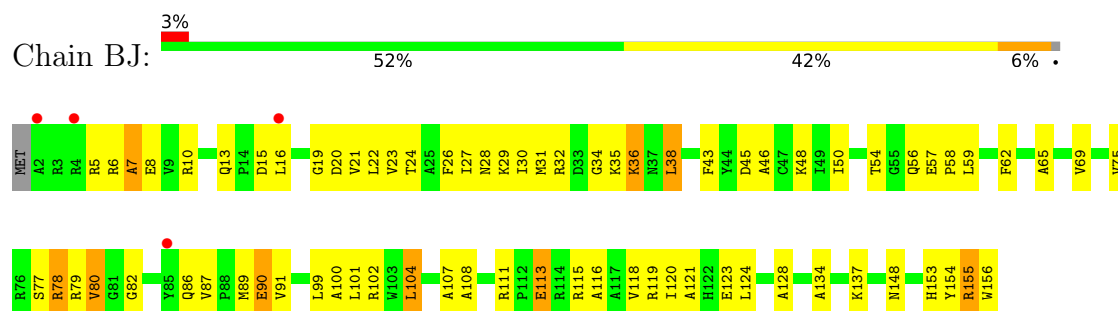
- Molecule 36: 30S RIBOSOMAL PROTEIN S6



- Molecule 36: 30S RIBOSOMAL PROTEIN S6

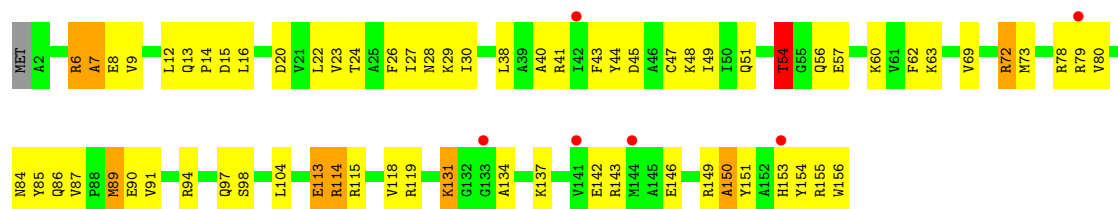


- Molecule 37: 30S RIBOSOMAL PROTEIN S7



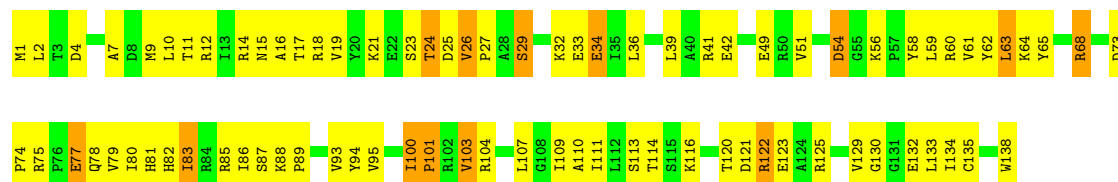
- Molecule 37: 30S RIBOSOMAL PROTEIN S7





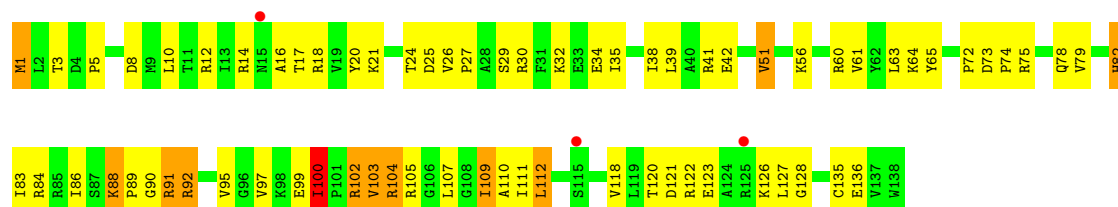
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain BK: 41% 50% 9%



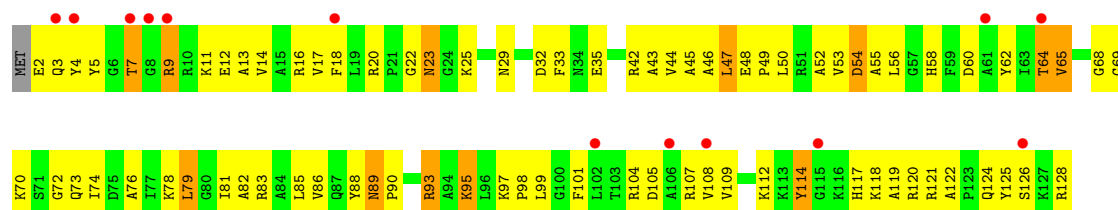
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain CK: 2% 49% 42% 8%



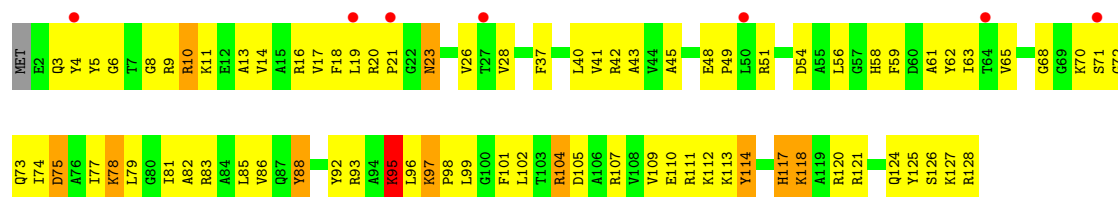
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain BL: 10% 37% 53% 9%

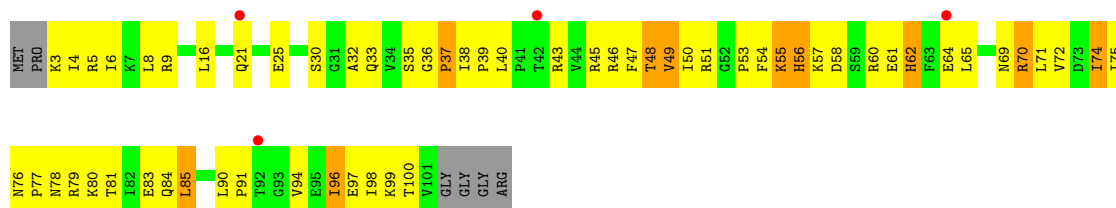


• Molecule 39: 30S RIBOSOMAL PROTEIN S9

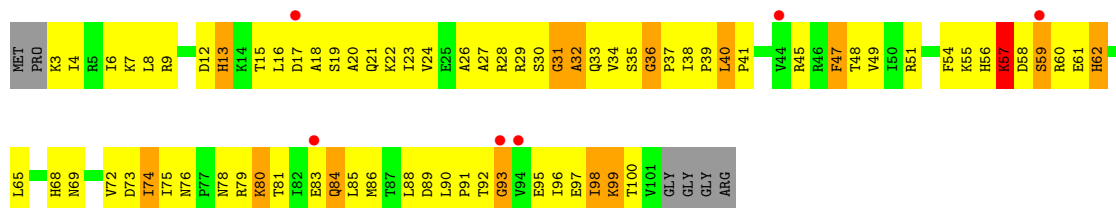
Chain CL: 5% 38% 53% 8%



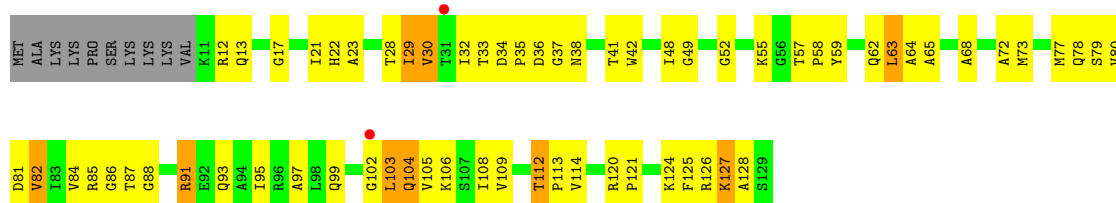
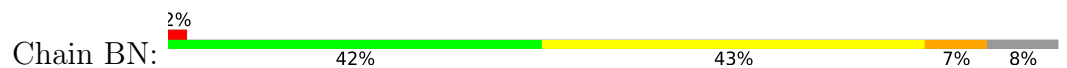
• Molecule 40: 30S RIBOSOMAL PROTEIN S10



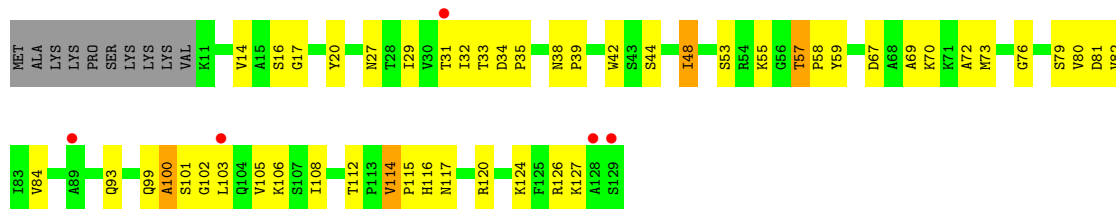
• Molecule 40: 30S RIBOSOMAL PROTEIN S10



• Molecule 41: 30S RIBOSOMAL PROTEIN S11

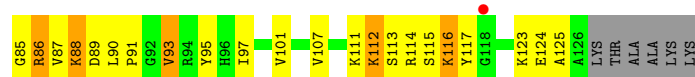


• Molecule 41: 30S RIBOSOMAL PROTEIN S11

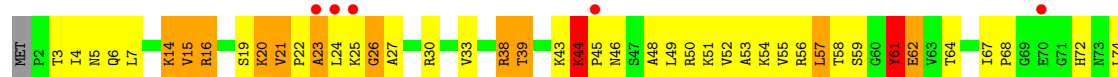


• Molecule 42: 30S RIBOSOMAL PROTEIN S12

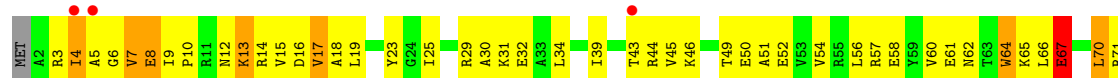
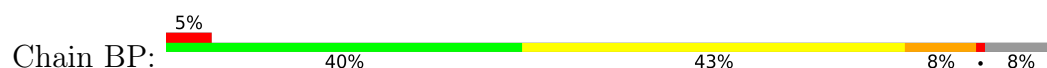




• Molecule 42: 30S RIBOSOMAL PROTEIN S12



• Molecule 43: 30S RIBOSOMAL PROTEIN S13



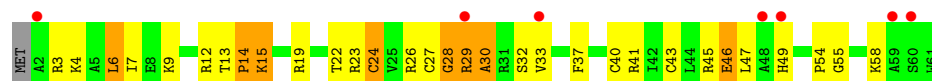
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



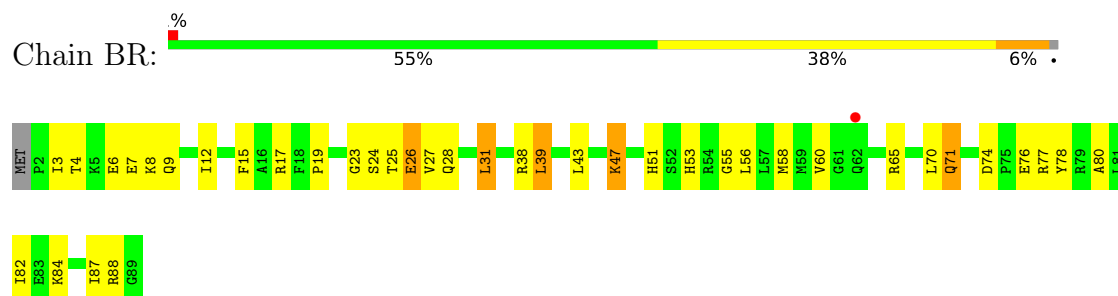
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



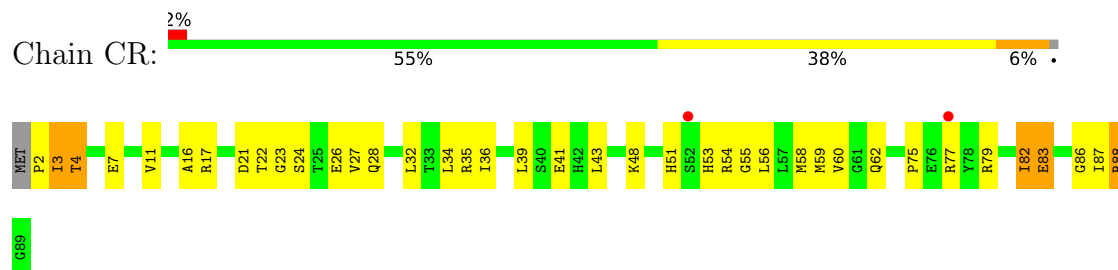
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



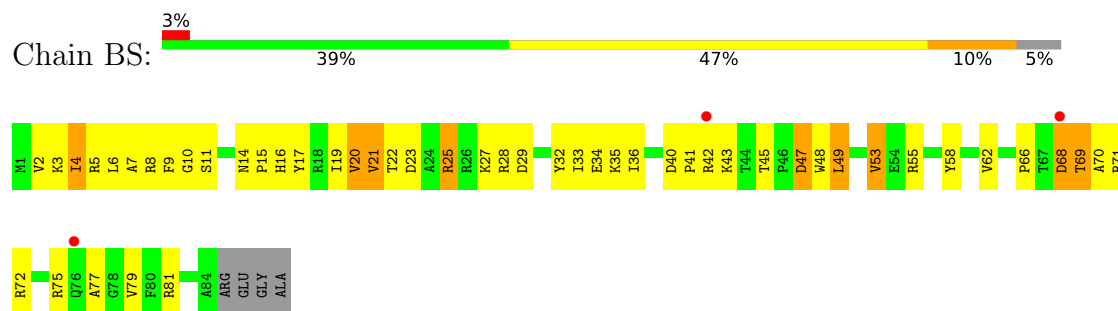
- Molecule 45: 30S RIBOSOMAL PROTEIN S15



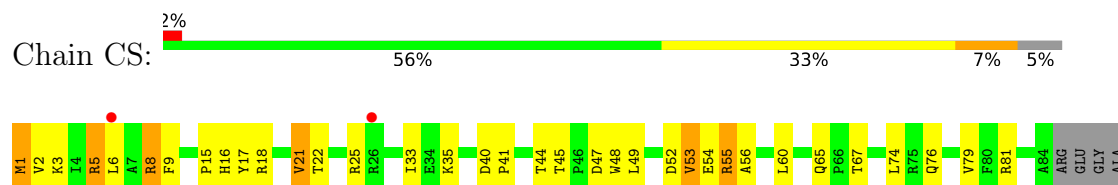
- Molecule 45: 30S RIBOSOMAL PROTEIN S15



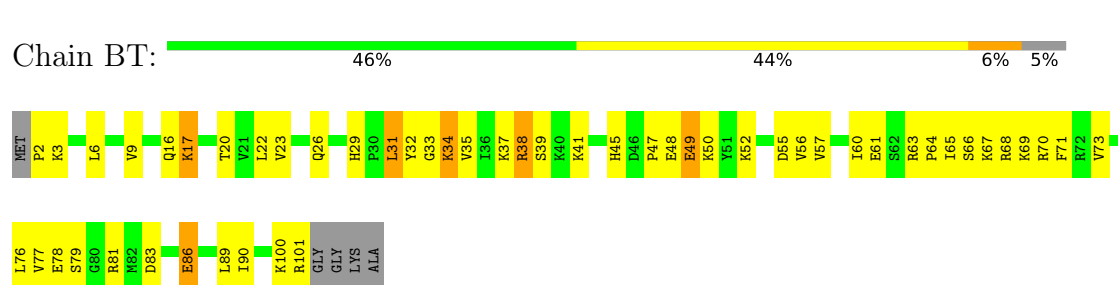
- Molecule 46: 30S RIBOSOMAL PROTEIN S16



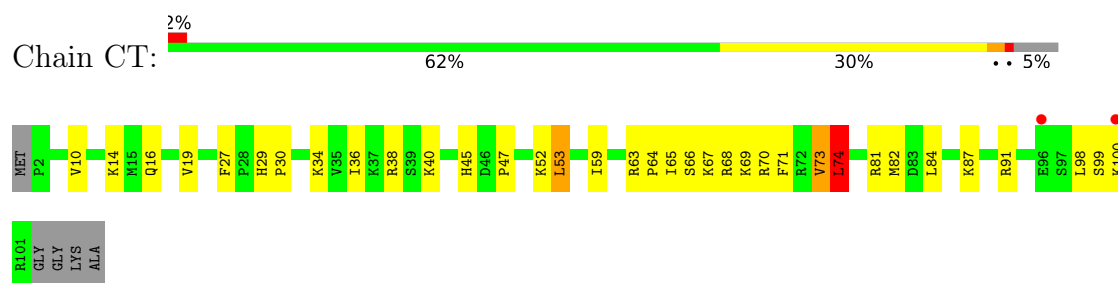
- Molecule 46: 30S RIBOSOMAL PROTEIN S16



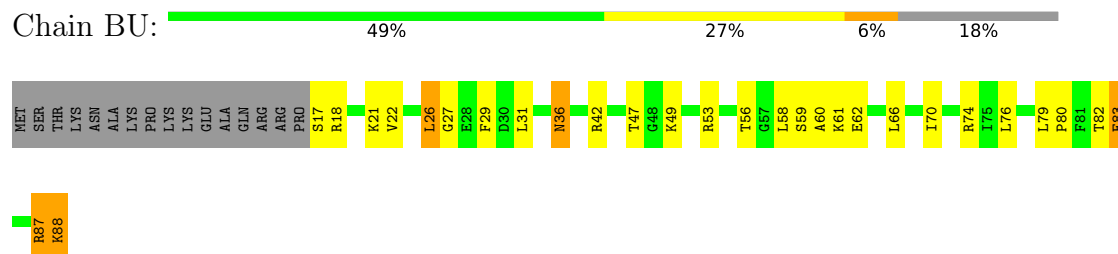
- Molecule 47: 30S RIBOSOMAL PROTEIN S17



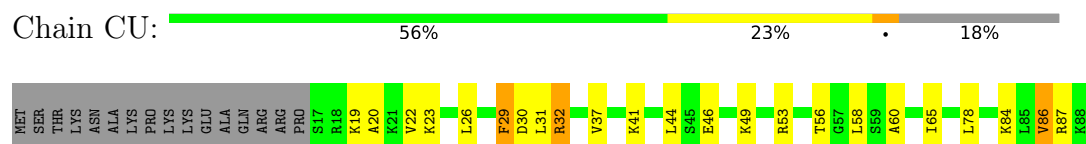
- Molecule 47: 30S RIBOSOMAL PROTEIN S17



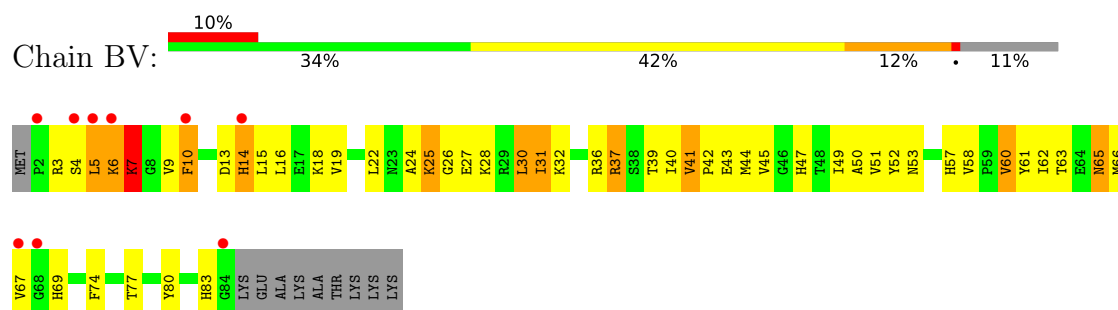
● Molecule 48: 30S RIBOSOMAL PROTEIN S18



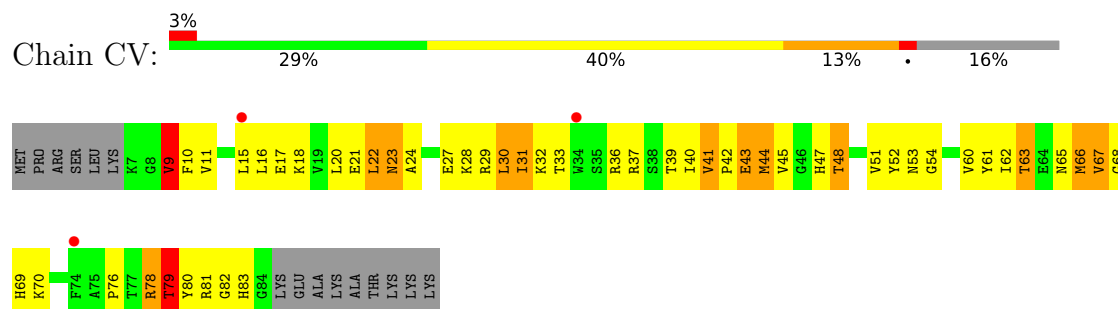
● Molecule 48: 30S RIBOSOMAL PROTEIN S18



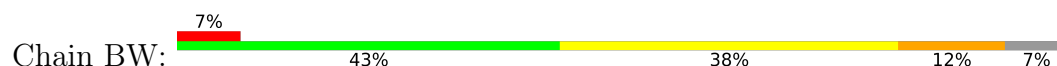
• Molecule 49: 30S RIBOSOMAL PROTEIN S19

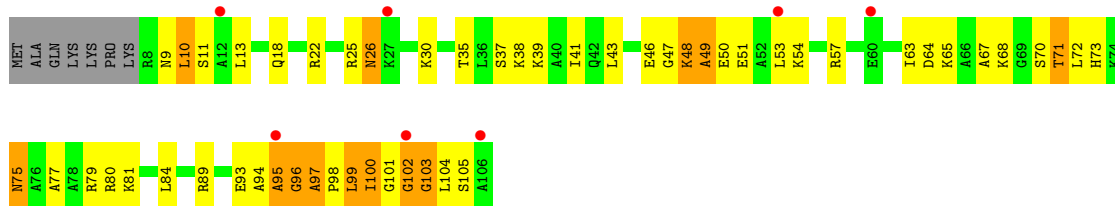


● Molecule 49: 30S RIBOSOMAL PROTEIN S19

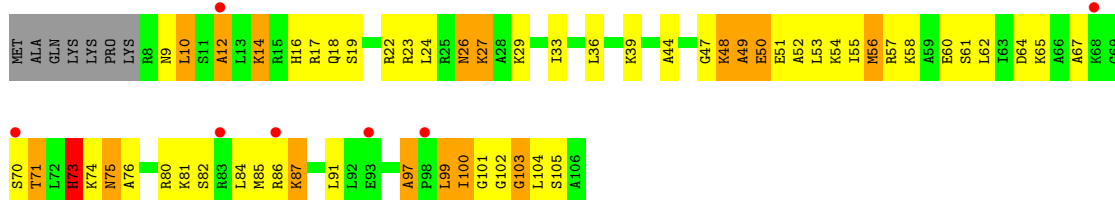


● Molecule 50: 30S RIBOSOMAL PROTEIN S20





• Molecule 50: 30S RIBOSOMAL PROTEIN S20



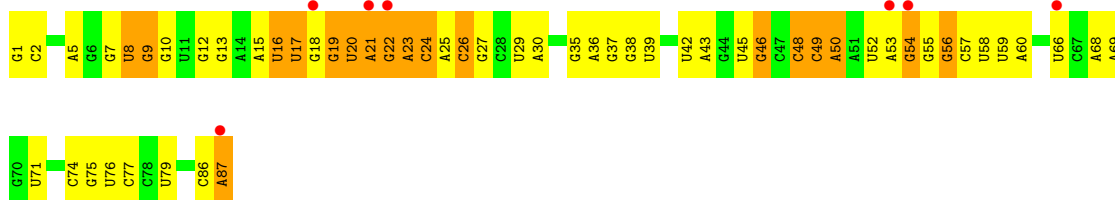
• Molecule 51: 30S RIBOSOMAL PROTEIN THX



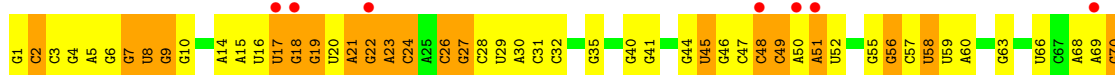
• Molecule 51: 30S RIBOSOMAL PROTEIN THX



• Molecule 52: TRNA-LEU

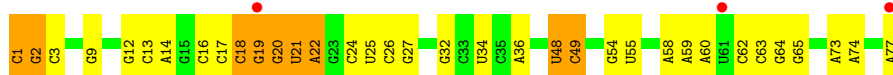


• Molecule 52: TRNA-LEU

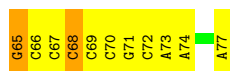
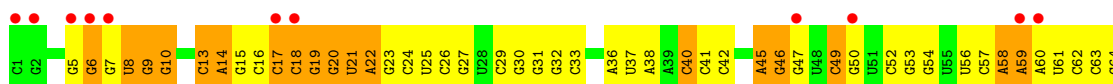




● Molecule 53: TRNA-FMET



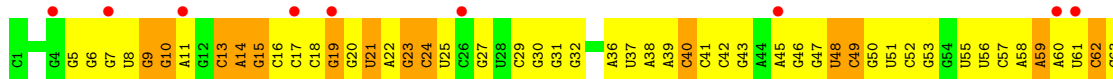
● Molecule 53: TRNA-FMET



● Molecule 53: TRNA-FMET



● Molecule 53: TRNA-FMET

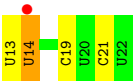


● Molecule 54: MRNA



● Molecule 54: MRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.19Å 451.05Å 621.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.76 – 3.10 153.76 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.76-3.10) 93.2 (153.76-3.10)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_810)	Depositor
R, R_{free}	0.201 , 0.240 0.202 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 99.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299628	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.21	0/70233	0.36	0/109643
1	DA	0.19	0/70122	0.35	2/109469 (0.0%)
2	AB	0.17	0/2928	0.33	0/4568
2	DB	0.15	0/2928	0.32	0/4568
3	AD	0.40	0/2166	0.88	3/2919 (0.1%)
3	DD	0.37	0/2165	0.85	3/2919 (0.1%)
4	AE	0.34	0/1602	0.89	5/2160 (0.2%)
4	DE	0.37	0/1601	0.90	9/2160 (0.4%)
5	AF	0.42	1/1621 (0.1%)	0.87	2/2196 (0.1%)
5	DF	0.32	0/1662	0.86	4/2249 (0.2%)
6	AG	0.30	0/1499	0.74	1/2016 (0.0%)
6	DG	0.28	0/1499	0.74	2/2016 (0.1%)
7	AH	0.34	0/1333	0.84	0/1802
7	DH	0.33	0/1332	0.96	3/1802 (0.2%)
8	AK	0.34	0/1152	0.76	1/1558 (0.1%)
8	DK	0.32	0/1151	0.77	1/1558 (0.1%)
9	AM	0.33	0/1132	0.78	0/1525
9	DM	0.29	0/1131	0.79	0/1525
10	AN	0.33	0/943	0.79	0/1269
10	DN	0.32	0/943	0.77	0/1269
11	AO	0.37	0/1162	0.90	3/1544 (0.2%)
11	DO	0.35	0/1162	0.87	3/1544 (0.2%)
12	AP	0.32	0/1143	0.70	2/1527 (0.1%)
12	DP	0.57	1/1143 (0.1%)	0.67	0/1527
13	A0	0.33	0/982	0.75	0/1312
13	D0	0.33	0/974	0.75	0/1302
14	AQ	0.32	0/892	0.76	0/1187
14	DQ	0.29	0/892	0.72	0/1187
15	AR	0.34	0/1156	0.85	2/1542 (0.1%)
15	DR	0.31	0/1155	0.76	1/1542 (0.1%)
16	A1	0.35	0/982	0.83	2/1306 (0.2%)
16	D1	0.32	0/982	0.76	1/1306 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.32	0/790	0.81	0/1057
17	D2	0.39	0/790	0.81	2/1057 (0.2%)
18	AS	0.34	0/911	0.75	1/1220 (0.1%)
18	DS	0.35	0/911	0.76	0/1220
19	AT	0.38	0/740	0.76	0/993
19	DT	0.34	0/739	0.82	3/993 (0.3%)
20	AU	0.38	0/799	0.84	0/1064
20	DU	0.37	0/798	0.81	2/1064 (0.2%)
21	AV	0.28	0/1427	0.77	0/1935
21	DV	0.28	0/1460	0.79	4/1982 (0.2%)
22	A3	0.31	0/615	0.73	1/819 (0.1%)
22	D3	0.30	0/621	0.78	0/827
23	AZ	0.34	0/770	0.73	0/1022
23	DZ	0.31	0/770	0.81	0/1022
24	AW	0.35	0/560	0.89	1/741 (0.1%)
24	DW	0.29	0/583	0.78	1/771 (0.1%)
25	AX	0.32	0/474	0.78	0/635
25	DX	0.29	0/474	0.81	2/635 (0.3%)
26	A4	0.30	0/545	0.76	1/733 (0.1%)
26	D4	0.32	0/527	0.81	0/709
27	A5	0.39	0/473	1.00	4/639 (0.6%)
27	D5	0.34	0/473	0.84	2/639 (0.3%)
28	A6	0.36	0/397	0.90	2/529 (0.4%)
28	D6	0.35	0/396	0.84	0/529
29	A7	0.39	0/438	0.75	2/575 (0.3%)
29	D7	0.34	0/438	0.82	2/575 (0.3%)
30	A8	0.41	0/494	0.98	2/649 (0.3%)
30	D8	0.42	0/494	1.01	4/649 (0.6%)
31	BA	0.16	0/36234	0.32	0/56554
31	CA	0.16	0/36237	0.32	0/56558
32	BE	0.28	0/1959	0.74	2/2642 (0.1%)
32	CE	0.28	0/1959	0.79	2/2642 (0.1%)
33	BF	0.28	0/1629	0.69	1/2195 (0.0%)
33	CF	0.28	0/1636	0.71	0/2205
34	BG	0.33	0/1733	0.77	4/2318 (0.2%)
34	CG	0.31	0/1733	0.77	2/2318 (0.1%)
35	BH	0.30	0/1171	0.76	0/1576
35	CH	0.30	0/1171	0.82	2/1576 (0.1%)
36	BI	0.29	0/856	0.72	0/1154
36	CI	0.29	0/856	0.73	2/1154 (0.2%)
37	BJ	0.29	0/1276	0.73	0/1709
37	CJ	0.28	0/1276	0.74	0/1709
38	BK	0.30	0/1136	0.79	2/1527 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CK	0.28	0/1136	0.78	2/1527 (0.1%)
39	BL	0.27	0/1029	0.72	0/1379
39	CL	0.26	0/1029	0.73	0/1379
40	BM	0.30	0/814	0.79	0/1095
40	CM	0.28	0/814	0.78	0/1095
41	BN	0.31	0/900	0.78	2/1213 (0.2%)
41	CN	0.30	0/900	0.77	2/1213 (0.2%)
42	BO	0.33	0/991	0.78	0/1327
42	CO	0.32	0/991	0.75	1/1327 (0.1%)
43	BP	0.29	0/938	0.79	0/1258
43	CP	0.29	0/943	0.73	0/1265
44	BQ	0.31	0/501	0.83	2/664 (0.3%)
44	CQ	0.27	0/501	0.75	1/664 (0.2%)
45	BR	0.31	0/745	0.69	0/992
45	CR	0.29	0/745	0.68	0/992
46	BS	0.27	0/721	0.73	0/970
46	CS	0.29	0/721	0.67	0/970
47	BT	0.27	0/847	0.74	0/1131
47	CT	0.27	0/847	0.75	0/1131
48	BU	0.30	0/596	0.74	0/790
48	CU	0.29	0/596	0.71	0/790
49	BV	0.29	0/680	0.81	0/915
49	CV	0.27	0/638	0.75	1/860 (0.1%)
50	BW	0.28	0/765	0.71	0/1007
50	CW	0.31	0/765	0.78	1/1007 (0.1%)
51	BX	0.27	0/221	0.74	0/288
51	CX	0.26	0/221	0.71	0/288
52	BB	0.12	0/2080	0.26	0/3242
52	CB	0.12	0/2080	0.26	0/3242
53	BC	0.15	0/1835	0.30	0/2859
53	BD	0.09	0/1835	0.25	0/2859
53	CC	0.14	0/1835	0.29	0/2859
53	CD	0.09	0/1835	0.25	0/2859
54	B1	0.17	0/226	0.28	0/348
54	C1	0.24	0/226	0.32	0/348
All	All	0.23	2/324084 (0.0%)	0.50	115/485290 (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
7	AH	0	1
42	BO	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	DP	141	GLN	C-OXT	16.97	1.57	1.23
5	AF	207	GLY	C-N	-6.80	1.23	1.33

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	DH	125	VAL	CA-C-N	12.88	135.94	119.84
7	DH	125	VAL	C-N-CA	12.88	135.94	119.84
4	DE	67	PHE	N-CA-C	-9.29	101.86	113.01
16	A1	97	ASP	N-CA-C	-8.71	101.92	112.54
24	AW	5	GLU	N-CA-C	-8.26	103.20	113.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AH	153	LYS	Peptide
42	BO	44	LYS	Peptide

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	62707	0	31614	1926	1
1	DA	62607	0	31565	1983	1
2	AB	2617	0	1328	92	0
2	DB	2617	0	1328	98	0
3	AD	2116	0	2195	200	0
3	DD	2115	0	2195	189	0
4	AE	1569	0	1634	167	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DE	1568	0	1634	185	0
5	AF	1586	0	1632	117	0
5	DF	1627	0	1680	131	0
6	AG	1474	0	1535	129	0
6	DG	1474	0	1535	106	0
7	AH	1308	0	1382	146	0
7	DH	1307	0	1382	109	1
8	AK	1137	0	1223	96	0
8	DK	1136	0	1223	97	0
9	AM	1105	0	1180	104	0
9	DM	1104	0	1180	88	0
10	AN	933	0	996	39	0
10	DN	933	0	996	39	0
11	AO	1145	0	1228	160	0
11	DO	1145	0	1228	184	0
12	AP	1122	0	1179	188	0
12	DP	1122	0	1179	209	0
13	A0	968	0	1033	71	0
13	D0	960	0	1021	72	0
14	AQ	882	0	943	94	0
14	DQ	882	0	943	75	0
15	AR	1142	0	1202	96	0
15	DR	1141	0	1202	103	0
16	A1	964	0	1022	84	0
16	D1	964	0	1022	91	0
17	A2	779	0	852	76	0
17	D2	779	0	852	119	0
18	AS	900	0	964	63	0
18	DS	900	0	964	43	0
19	AT	726	0	778	54	0
19	DT	725	0	778	58	0
20	AU	786	0	878	79	0
20	DU	785	0	878	103	0
21	AV	1397	0	1430	124	0
21	DV	1428	0	1454	102	0
22	A3	607	0	628	42	0
22	D3	613	0	633	45	0
23	AZ	763	0	848	44	0
23	DZ	763	0	848	53	0
24	AW	558	0	610	31	0
24	DW	581	0	629	49	0
25	AX	469	0	518	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DX	469	0	518	24	0
26	A4	533	0	522	79	0
26	D4	515	0	510	82	0
27	A5	459	0	480	54	0
27	D5	459	0	480	43	0
28	A6	390	0	404	66	0
28	D6	389	0	404	51	0
29	A7	430	0	480	19	0
29	D7	430	0	480	29	0
30	A8	488	0	560	83	0
30	D8	488	0	560	89	0
31	BA	32369	0	16339	1085	1
31	CA	32372	0	16338	1080	2
32	BE	1924	0	1975	167	0
32	CE	1924	0	1975	177	0
33	BF	1605	0	1668	121	0
33	CF	1612	0	1677	122	0
34	BG	1703	0	1764	127	0
34	CG	1703	0	1763	98	1
35	BH	1155	0	1213	66	0
35	CH	1155	0	1213	81	0
36	BI	843	0	857	43	1
36	CI	843	0	857	38	0
37	BJ	1257	0	1296	68	0
37	CJ	1257	0	1296	65	0
38	BK	1116	0	1177	72	0
38	CK	1116	0	1177	54	0
39	BL	1010	0	1037	91	0
39	CL	1010	0	1037	97	0
40	BM	801	0	849	75	0
40	CM	801	0	849	74	0
41	BN	885	0	904	61	0
41	CN	885	0	904	35	0
42	BO	975	0	1062	53	0
42	CO	975	0	1062	69	0
43	BP	928	0	987	67	0
43	CP	933	0	992	74	0
44	BQ	492	0	529	48	0
44	CQ	492	0	530	40	0
45	BR	734	0	771	35	0
45	CR	734	0	771	36	0
46	BS	705	0	725	44	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	CS	705	0	725	35	0
47	BT	834	0	904	49	0
47	CT	834	0	904	32	0
48	BU	591	0	662	25	0
48	CU	591	0	662	20	0
49	BV	665	0	686	69	0
49	CV	624	0	636	66	0
50	BW	763	0	861	62	0
50	CW	763	0	861	51	0
51	BX	217	0	234	17	0
51	CX	217	0	234	21	0
52	BB	1861	0	938	50	0
52	CB	1861	0	938	63	0
53	BC	1643	0	837	47	0
53	BD	1643	0	837	65	0
53	CC	1643	0	837	51	0
53	CD	1643	0	837	77	0
54	B1	205	0	105	7	0
54	C1	205	0	105	5	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A2	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	2	0	0	0	0
55	A6	1	0	0	0	0
55	A7	1	0	0	0	0
55	AA	630	0	0	0	0
55	AB	17	0	0	0	0
55	AD	2	0	0	0	0
55	AE	4	0	0	0	0
55	AF	3	0	0	0	0
55	AO	3	0	0	0	0
55	AU	1	0	0	0	0
55	B1	2	0	0	0	0
55	BA	244	0	0	0	0
55	BB	8	0	0	0	0
55	BC	9	0	0	0	0
55	BD	1	0	0	0	0
55	BG	1	0	0	0	0
55	BN	2	0	0	0	0
55	BQ	2	0	0	0	0
55	CA	209	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CB	5	0	0	0	0
55	CC	8	0	0	0	0
55	CG	3	0	0	0	0
55	CH	1	0	0	0	0
55	CS	1	0	0	0	0
55	D0	1	0	0	0	0
55	D1	2	0	0	0	0
55	D3	1	0	0	0	0
55	D5	1	0	0	0	0
55	DA	528	0	0	0	0
55	DB	14	0	0	0	0
55	DE	3	0	0	0	0
55	DP	1	0	0	0	0
55	DU	1	0	0	0	0
56	BG	1	0	0	0	0
56	BQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299628	0	200976	12914	4

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 26.

The worst 5 of 12914 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)
6:AG:108:ASN:HA	26:A4:38:LYS:CG	1.41	1.51
6:AG:108:ASN:CA	26:A4:38:LYS:HG2	1.46	1.45
1:AA:1056:G:H21	1:AA:1103:A:N6	1.13	1.45
1:DA:226:G:H21	1:DA:228:A:N6	0.93	1.41
1:DA:226:G:N2	1:DA:228:A:H61	1.15	1.40

All (4) 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:BA:85:U:O2'	7:DH:100:GLY:O[3_555]	1.87	0.33
1:AA:2137:C:OP1	31:CA:999:U:O2'[4_555]	1.89	0.31
36:BI:15:ASP:OD2	34:CG:27:TYR:OH[4_555]	2.05	0.15
31:CA:86:U:O2'	1:DA:276:A:OP2[3_545]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
3	AD	270/272 (99%)	226 (84%)	31 (12%)	13 (5%)	2	11
3	DD	270/272 (99%)	231 (86%)	25 (9%)	14 (5%)	1	10
4	AE	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	0	3
4	DE	203/205 (99%)	128 (63%)	41 (20%)	34 (17%)	0	0
5	AF	201/208 (97%)	177 (88%)	13 (6%)	11 (6%)	1	9
5	DF	206/208 (99%)	162 (79%)	25 (12%)	19 (9%)	0	3
6	AG	179/181 (99%)	147 (82%)	21 (12%)	11 (6%)	1	7
6	DG	179/181 (99%)	141 (79%)	27 (15%)	11 (6%)	1	7
7	AH	168/170 (99%)	116 (69%)	22 (13%)	30 (18%)	0	0
7	DH	168/170 (99%)	108 (64%)	37 (22%)	23 (14%)	0	1
8	AK	144/146 (99%)	97 (67%)	27 (19%)	20 (14%)	0	1
8	DK	144/146 (99%)	106 (74%)	26 (18%)	12 (8%)	0	4
9	AM	136/138 (99%)	105 (77%)	18 (13%)	13 (10%)	0	3
9	DM	136/138 (99%)	108 (79%)	20 (15%)	8 (6%)	1	8
10	AN	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	7	30
10	DN	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	16	47
11	AO	148/150 (99%)	106 (72%)	25 (17%)	17 (12%)	0	1
11	DO	148/150 (99%)	92 (62%)	28 (19%)	28 (19%)	0	0
12	AP	139/141 (99%)	95 (68%)	25 (18%)	19 (14%)	0	1
12	DP	139/141 (99%)	91 (66%)	20 (14%)	28 (20%)	0	0
13	A0	116/118 (98%)	93 (80%)	15 (13%)	8 (7%)	1	5
13	D0	115/118 (98%)	93 (81%)	17 (15%)	5 (4%)	2	12
14	AQ	109/111 (98%)	77 (71%)	24 (22%)	8 (7%)	1	5
14	DQ	109/111 (98%)	78 (72%)	21 (19%)	10 (9%)	0	3
15	AR	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	DR	135/137 (98%)	103 (76%)	23 (17%)	9 (7%)	1	6
16	A1	115/117 (98%)	101 (88%)	7 (6%)	7 (6%)	1	7
16	D1	115/117 (98%)	93 (81%)	15 (13%)	7 (6%)	1	7
17	A2	99/101 (98%)	83 (84%)	9 (9%)	7 (7%)	1	5
17	D2	99/101 (98%)	73 (74%)	14 (14%)	12 (12%)	0	1
18	AS	111/113 (98%)	92 (83%)	14 (13%)	5 (4%)	2	12
18	DS	111/113 (98%)	99 (89%)	10 (9%)	2 (2%)	6	28
19	AT	90/92 (98%)	83 (92%)	6 (7%)	1 (1%)	11	39
19	DT	90/92 (98%)	75 (83%)	12 (13%)	3 (3%)	3	17
20	AU	100/102 (98%)	68 (68%)	19 (19%)	13 (13%)	0	1
20	DU	100/102 (98%)	61 (61%)	22 (22%)	17 (17%)	0	0
21	AV	173/179 (97%)	112 (65%)	36 (21%)	25 (14%)	0	0
21	DV	177/179 (99%)	120 (68%)	27 (15%)	30 (17%)	0	0
22	A3	74/77 (96%)	57 (77%)	15 (20%)	2 (3%)	4	20
22	D3	75/77 (97%)	62 (83%)	13 (17%)	0	100	100
23	AZ	95/97 (98%)	78 (82%)	10 (10%)	7 (7%)	1	5
23	DZ	95/97 (98%)	77 (81%)	7 (7%)	11 (12%)	0	1
24	AW	64/69 (93%)	56 (88%)	3 (5%)	5 (8%)	1	4
24	DW	67/69 (97%)	56 (84%)	5 (8%)	6 (9%)	0	3
25	AX	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
25	DX	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	6	28
26	A4	64/66 (97%)	38 (59%)	16 (25%)	10 (16%)	0	0
26	D4	61/66 (92%)	24 (39%)	25 (41%)	12 (20%)	0	0
27	A5	57/59 (97%)	40 (70%)	10 (18%)	7 (12%)	0	1
27	D5	57/59 (97%)	46 (81%)	7 (12%)	4 (7%)	1	5
28	A6	43/45 (96%)	25 (58%)	12 (28%)	6 (14%)	0	1
28	D6	43/45 (96%)	25 (58%)	12 (28%)	6 (14%)	0	1
29	A7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	5	25
29	D7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
30	A8	59/61 (97%)	50 (85%)	5 (8%)	4 (7%)	1	5
30	D8	59/61 (97%)	39 (66%)	11 (19%)	9 (15%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BE	235/256 (92%)	170 (72%)	47 (20%)	18 (8%)	1	4
32	CE	235/256 (92%)	188 (80%)	23 (10%)	24 (10%)	0	3
33	BF	203/239 (85%)	141 (70%)	46 (23%)	16 (8%)	1	4
33	CF	204/239 (85%)	152 (74%)	37 (18%)	15 (7%)	1	5
34	BG	206/208 (99%)	168 (82%)	27 (13%)	11 (5%)	1	10
34	CG	206/208 (99%)	171 (83%)	30 (15%)	5 (2%)	4	22
35	BH	149/162 (92%)	129 (87%)	14 (9%)	6 (4%)	2	13
35	CH	149/162 (92%)	134 (90%)	11 (7%)	4 (3%)	4	20
36	BI	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	25
36	CI	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	41
37	BJ	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	18	49
37	CJ	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	6	25
38	BK	136/138 (99%)	115 (85%)	14 (10%)	7 (5%)	1	10
38	CK	136/138 (99%)	122 (90%)	11 (8%)	3 (2%)	5	24
39	BL	125/128 (98%)	100 (80%)	22 (18%)	3 (2%)	4	22
39	CL	125/128 (98%)	102 (82%)	19 (15%)	4 (3%)	3	18
40	BM	97/105 (92%)	76 (78%)	19 (20%)	2 (2%)	5	25
40	CM	97/105 (92%)	75 (77%)	13 (13%)	9 (9%)	0	3
41	BN	117/129 (91%)	97 (83%)	15 (13%)	5 (4%)	2	12
41	CN	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	4	21
42	BO	123/132 (93%)	101 (82%)	13 (11%)	9 (7%)	1	5
42	CO	123/132 (93%)	96 (78%)	19 (15%)	8 (6%)	1	6
43	BP	114/126 (90%)	86 (75%)	20 (18%)	8 (7%)	1	5
43	CP	115/126 (91%)	83 (72%)	22 (19%)	10 (9%)	0	4
44	BQ	58/61 (95%)	42 (72%)	11 (19%)	5 (9%)	0	4
44	CQ	58/61 (95%)	41 (71%)	11 (19%)	6 (10%)	0	2
45	BR	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	5	23
45	CR	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	10	37
46	BS	82/88 (93%)	65 (79%)	14 (17%)	3 (4%)	2	15
46	CS	82/88 (93%)	69 (84%)	13 (16%)	0	100	100
47	BT	98/105 (93%)	85 (87%)	11 (11%)	2 (2%)	6	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	CT	98/105 (93%)	92 (94%)	4 (4%)	2 (2%)	6	25
48	BU	70/88 (80%)	60 (86%)	8 (11%)	2 (3%)	3	19
48	CU	70/88 (80%)	63 (90%)	7 (10%)	0	100	100
49	BV	81/93 (87%)	63 (78%)	11 (14%)	7 (9%)	0	4
49	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	0	3
50	BW	97/106 (92%)	75 (77%)	12 (12%)	10 (10%)	0	2
50	CW	97/106 (92%)	73 (75%)	13 (13%)	11 (11%)	0	2
51	BX	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	12
51	CX	23/27 (85%)	19 (83%)	0	4 (17%)	0	0
All	All	11342/11844 (96%)	8910 (79%)	1590 (14%)	842 (7%)	1	5

5 of 842 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	26	LYS
3	AD	28	GLU
3	AD	33	LEU
3	AD	122	ASP
3	AD	237	GLU

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	
3	AD	214/214 (100%)	181 (85%)	33 (15%)	2	12
3	DD	214/214 (100%)	175 (82%)	39 (18%)	2	8
4	AE	165/165 (100%)	129 (78%)	36 (22%)	1	5
4	DE	165/165 (100%)	133 (81%)	32 (19%)	1	7
5	AF	161/165 (98%)	136 (84%)	25 (16%)	2	12
5	DF	165/165 (100%)	139 (84%)	26 (16%)	2	12
6	AG	155/155 (100%)	134 (86%)	21 (14%)	4	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	DG	155/155 (100%)	138 (89%)	17 (11%)	6	24
7	AH	142/142 (100%)	118 (83%)	24 (17%)	2	10
7	DH	142/142 (100%)	129 (91%)	13 (9%)	8	31
8	AK	122/122 (100%)	105 (86%)	17 (14%)	3	15
8	DK	122/122 (100%)	102 (84%)	20 (16%)	2	11
9	AM	117/117 (100%)	94 (80%)	23 (20%)	1	6
9	DM	117/117 (100%)	98 (84%)	19 (16%)	2	11
10	AN	100/100 (100%)	87 (87%)	13 (13%)	4	18
10	DN	100/100 (100%)	88 (88%)	12 (12%)	5	21
11	AO	116/116 (100%)	85 (73%)	31 (27%)	0	2
11	DO	116/116 (100%)	84 (72%)	32 (28%)	0	1
12	AP	111/111 (100%)	85 (77%)	26 (23%)	1	4
12	DP	111/111 (100%)	80 (72%)	31 (28%)	0	1
13	A0	101/101 (100%)	81 (80%)	20 (20%)	1	6
13	D0	100/101 (99%)	86 (86%)	14 (14%)	3	15
14	AQ	87/87 (100%)	66 (76%)	21 (24%)	1	3
14	DQ	87/87 (100%)	73 (84%)	14 (16%)	2	11
15	AR	120/120 (100%)	95 (79%)	25 (21%)	1	5
15	DR	120/120 (100%)	91 (76%)	29 (24%)	1	3
16	A1	93/93 (100%)	85 (91%)	8 (9%)	10	34
16	D1	93/93 (100%)	87 (94%)	6 (6%)	15	44
17	A2	82/82 (100%)	66 (80%)	16 (20%)	1	6
17	D2	82/82 (100%)	70 (85%)	12 (15%)	3	14
18	AS	92/92 (100%)	73 (79%)	19 (21%)	1	5
18	DS	92/92 (100%)	76 (83%)	16 (17%)	2	9
19	AT	74/74 (100%)	58 (78%)	16 (22%)	1	5
19	DT	74/74 (100%)	61 (82%)	13 (18%)	2	9
20	AU	85/85 (100%)	67 (79%)	18 (21%)	1	5
20	DU	85/85 (100%)	68 (80%)	17 (20%)	1	6
21	AV	154/158 (98%)	132 (86%)	22 (14%)	3	14
21	DV	158/158 (100%)	144 (91%)	14 (9%)	9	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	A3	61/62 (98%)	56 (92%)	5 (8%)	10	36
22	D3	62/62 (100%)	59 (95%)	3 (5%)	23	54
23	AZ	82/82 (100%)	70 (85%)	12 (15%)	3	14
23	DZ	82/82 (100%)	70 (85%)	12 (15%)	3	14
24	AW	62/64 (97%)	48 (77%)	14 (23%)	1	4
24	DW	64/64 (100%)	54 (84%)	10 (16%)	2	12
25	AX	51/51 (100%)	46 (90%)	5 (10%)	7	29
25	DX	51/51 (100%)	48 (94%)	3 (6%)	18	48
26	A4	59/59 (100%)	48 (81%)	11 (19%)	1	8
26	D4	57/59 (97%)	50 (88%)	7 (12%)	4	20
27	A5	51/51 (100%)	39 (76%)	12 (24%)	1	3
27	D5	51/51 (100%)	41 (80%)	10 (20%)	1	6
28	A6	44/44 (100%)	36 (82%)	8 (18%)	2	8
28	D6	44/44 (100%)	33 (75%)	11 (25%)	0	2
29	A7	42/42 (100%)	35 (83%)	7 (17%)	2	10
29	D7	42/42 (100%)	35 (83%)	7 (17%)	2	10
30	A8	51/51 (100%)	39 (76%)	12 (24%)	1	3
30	D8	51/51 (100%)	42 (82%)	9 (18%)	2	9
32	BE	205/220 (93%)	173 (84%)	32 (16%)	2	12
32	CE	205/220 (93%)	172 (84%)	33 (16%)	2	11
33	BF	159/188 (85%)	134 (84%)	25 (16%)	2	12
33	CF	160/188 (85%)	145 (91%)	15 (9%)	8	31
34	BG	180/180 (100%)	161 (89%)	19 (11%)	6	26
34	CG	180/180 (100%)	147 (82%)	33 (18%)	2	8
35	BH	116/123 (94%)	102 (88%)	14 (12%)	5	20
35	CH	116/123 (94%)	101 (87%)	15 (13%)	4	18
36	BI	90/90 (100%)	79 (88%)	11 (12%)	5	20
36	CI	90/90 (100%)	82 (91%)	8 (9%)	9	33
37	BJ	126/127 (99%)	112 (89%)	14 (11%)	6	24
37	CJ	126/127 (99%)	107 (85%)	19 (15%)	3	13
38	BK	119/119 (100%)	110 (92%)	9 (8%)	12	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	CK	119/119 (100%)	108 (91%)	11 (9%)	8	31
39	BL	98/99 (99%)	81 (83%)	17 (17%)	2	9
39	CL	98/99 (99%)	86 (88%)	12 (12%)	5	20
40	BM	89/92 (97%)	79 (89%)	10 (11%)	6	24
40	CM	89/92 (97%)	77 (86%)	12 (14%)	4	16
41	BN	90/99 (91%)	81 (90%)	9 (10%)	7	29
41	CN	90/99 (91%)	79 (88%)	11 (12%)	5	20
42	BO	104/109 (95%)	90 (86%)	14 (14%)	4	16
42	CO	104/109 (95%)	91 (88%)	13 (12%)	4	19
43	BP	94/101 (93%)	85 (90%)	9 (10%)	8	30
43	CP	94/101 (93%)	82 (87%)	12 (13%)	4	18
44	BQ	49/50 (98%)	41 (84%)	8 (16%)	2	11
44	CQ	49/50 (98%)	46 (94%)	3 (6%)	17	46
45	BR	79/80 (99%)	74 (94%)	5 (6%)	16	45
45	CR	79/80 (99%)	72 (91%)	7 (9%)	9	33
46	BS	72/74 (97%)	63 (88%)	9 (12%)	4	19
46	CS	72/74 (97%)	61 (85%)	11 (15%)	3	12
47	BT	95/97 (98%)	86 (90%)	9 (10%)	8	30
47	CT	95/97 (98%)	87 (92%)	8 (8%)	10	35
48	BU	63/77 (82%)	57 (90%)	6 (10%)	8	30
48	CU	63/77 (82%)	56 (89%)	7 (11%)	6	24
49	BV	72/80 (90%)	60 (83%)	12 (17%)	2	10
49	CV	67/80 (84%)	53 (79%)	14 (21%)	1	5
50	BW	76/82 (93%)	68 (90%)	8 (10%)	6	26
50	CW	76/82 (93%)	65 (86%)	11 (14%)	3	14
51	BX	20/22 (91%)	19 (95%)	1 (5%)	22	53
51	CX	20/22 (91%)	19 (95%)	1 (5%)	22	53
All	All	9584/9828 (98%)	8139 (85%)	1445 (15%)	3	13

5 of 1445 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	CP	58	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	DM	28	THR
46	CS	53	VAL
43	CP	32	GLU
4	DE	35	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 291 such sidechains are listed below:

Mol	Chain	Res	Type
9	DM	101	HIS
27	D5	4	HIS
12	DP	45	GLN
18	DS	102	HIS
32	BE	212	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	556 (19%)	51 (1%)
1	DA	2905/2912 (99%)	601 (20%)	50 (1%)
2	AB	121/122 (99%)	24 (19%)	0
2	DB	121/122 (99%)	28 (23%)	0
31	BA	1506/1506 (100%)	291 (19%)	32 (2%)
31	CA	1505/1506 (99%)	315 (20%)	42 (2%)
52	BB	86/87 (98%)	26 (30%)	4 (4%)
52	CB	86/87 (98%)	30 (34%)	3 (3%)
53	BC	77/77 (100%)	12 (15%)	3 (3%)
53	BD	76/77 (98%)	25 (32%)	2 (2%)
53	CC	76/77 (98%)	14 (18%)	3 (3%)
53	CD	76/77 (98%)	16 (21%)	2 (2%)
54	B1	9/10 (90%)	2 (22%)	0
54	C1	9/10 (90%)	2 (22%)	0
All	All	9564/9582 (99%)	1942 (20%)	192 (2%)

5 of 1942 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	15	G
1	AA	23	G
1	AA	34	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	35	G

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	993	G
1	DA	71	A
31	CA	1128	C
31	CA	1442	G
1	DA	654(S)	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1720 ligands modelled in this entry, 1720 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2912/2912 (100%)	-0.04	53 (1%) 67 47	38, 71, 209, 243	0
1	DA	2907/2912 (99%)	0.14	58 (1%) 65 44	49, 82, 229, 246	0
2	AB	122/122 (100%)	0.41	1 (0%) 82 65	73, 98, 119, 180	0
2	DB	122/122 (100%)	0.80	2 (1%) 70 49	87, 121, 145, 200	0
3	AD	272/272 (100%)	-0.21	2 (0%) 84 68	38, 61, 83, 107	0
3	DD	272/272 (100%)	-0.01	4 (1%) 72 52	45, 69, 94, 125	0
4	AE	205/205 (100%)	0.25	6 (2%) 53 32	44, 82, 133, 147	0
4	DE	205/205 (100%)	0.36	16 (7%) 19 10	51, 90, 144, 167	0
5	AF	203/208 (97%)	-0.05	2 (0%) 79 61	40, 74, 116, 133	0
5	DF	208/208 (100%)	0.32	8 (3%) 44 25	54, 96, 161, 183	0
6	AG	181/181 (100%)	0.32	3 (1%) 69 48	91, 110, 140, 149	0
6	DG	181/181 (100%)	0.60	10 (5%) 30 16	112, 138, 161, 171	0
7	AH	170/170 (100%)	0.55	11 (6%) 25 13	80, 110, 129, 154	0
7	DH	170/170 (100%)	1.00	23 (13%) 7 4	150, 196, 217, 230	0
8	AK	146/146 (100%)	0.57	7 (4%) 35 19	75, 124, 142, 149	0
8	DK	146/146 (100%)	0.59	13 (8%) 15 8	76, 127, 150, 154	0
9	AM	138/138 (100%)	0.29	6 (4%) 40 22	63, 86, 124, 137	0
9	DM	138/138 (100%)	0.36	5 (3%) 46 26	74, 105, 136, 148	0
10	AN	122/122 (100%)	-0.19	0 100 100	54, 74, 92, 103	0
10	DN	122/122 (100%)	0.01	1 (0%) 82 65	62, 84, 106, 123	0
11	AO	150/150 (100%)	0.45	10 (6%) 24 13	45, 82, 112, 166	0
11	DO	150/150 (100%)	0.50	8 (5%) 32 17	50, 100, 140, 180	0
12	AP	141/141 (100%)	0.48	10 (7%) 22 12	58, 85, 110, 134	0
12	DP	141/141 (100%)	0.73	18 (12%) 7 4	58, 101, 131, 154	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	0.02	1 (0%) 82 65	55, 80, 102, 114	0
13	D0	117/118 (99%)	0.16	1 (0%) 81 63	58, 78, 100, 119	0
14	AQ	111/111 (100%)	0.37	5 (4%) 38 20	75, 96, 120, 136	0
14	DQ	111/111 (100%)	0.62	8 (7%) 21 11	80, 118, 143, 165	0
15	AR	137/137 (100%)	0.26	5 (3%) 46 26	69, 89, 140, 171	0
15	DR	137/137 (100%)	0.36	6 (4%) 39 21	70, 94, 158, 186	0
16	A1	117/117 (100%)	0.14	5 (4%) 40 22	46, 74, 108, 149	0
16	D1	117/117 (100%)	0.25	2 (1%) 69 48	59, 95, 138, 157	0
17	A2	101/101 (100%)	0.28	5 (4%) 34 18	47, 96, 125, 142	0
17	D2	101/101 (100%)	0.67	6 (5%) 28 15	57, 121, 140, 151	0
18	AS	113/113 (100%)	-0.24	0 100 100	46, 70, 106, 155	0
18	DS	113/113 (100%)	-0.04	1 (0%) 81 63	61, 74, 107, 155	0
19	AT	92/92 (100%)	-0.07	1 (1%) 78 59	54, 68, 98, 112	0
19	DT	92/92 (100%)	0.26	4 (4%) 40 22	64, 86, 112, 128	0
20	AU	102/102 (100%)	0.63	10 (9%) 13 7	70, 97, 148, 168	0
20	DU	102/102 (100%)	0.86	16 (15%) 5 2	85, 113, 163, 184	0
21	AV	175/179 (97%)	0.61	12 (6%) 23 12	87, 125, 190, 195	0
21	DV	179/179 (100%)	0.79	16 (8%) 15 8	112, 156, 209, 216	0
22	A3	76/77 (98%)	-0.03	0 100 100	56, 75, 95, 135	0
22	D3	77/77 (100%)	0.21	2 (2%) 57 36	66, 88, 113, 152	0
23	AZ	97/97 (100%)	0.09	4 (4%) 41 23	50, 69, 126, 161	0
23	DZ	97/97 (100%)	0.29	5 (5%) 33 17	52, 78, 131, 156	0
24	AW	66/69 (95%)	0.12	2 (3%) 52 31	60, 77, 97, 134	0
24	DW	69/69 (100%)	0.40	3 (4%) 40 22	79, 105, 134, 172	0
25	AX	59/59 (100%)	0.01	0 100 100	63, 80, 112, 127	0
25	DX	59/59 (100%)	0.17	1 (1%) 69 48	74, 100, 138, 162	0
26	A4	66/66 (100%)	1.08	5 (7%) 20 11	117, 153, 177, 184	0
26	D4	63/66 (95%)	1.03	12 (19%) 3 1	143, 184, 193, 201	0
27	A5	59/59 (100%)	0.62	5 (8%) 16 9	43, 85, 167, 172	0
27	D5	59/59 (100%)	0.31	2 (3%) 48 28	55, 83, 177, 186	0
28	A6	45/45 (100%)	1.49	12 (26%) 1 1	107, 136, 159, 163	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/45 (100%)	1.55	11 (24%) 2 1	121, 158, 176, 182	0
29	A7	49/49 (100%)	-0.38	0 100 100	38, 47, 95, 123	0
29	D7	49/49 (100%)	-0.36	0 100 100	49, 58, 115, 133	0
30	A8	61/61 (100%)	0.21	0 100 100	55, 68, 85, 108	0
30	D8	61/61 (100%)	0.67	8 (13%) 7 4	65, 81, 103, 120	0
31	BA	1506/1506 (100%)	0.47	64 (4%) 40 22	54, 103, 187, 244	0
31	CA	1506/1506 (100%)	0.58	85 (5%) 30 16	59, 109, 187, 245	0
32	BE	237/256 (92%)	0.77	20 (8%) 17 9	107, 142, 181, 191	0
32	CE	237/256 (92%)	0.96	34 (14%) 6 3	117, 158, 190, 208	0
33	BF	205/239 (85%)	0.35	5 (2%) 59 38	88, 118, 150, 162	0
33	CF	206/239 (86%)	0.97	26 (12%) 8 4	119, 143, 172, 183	0
34	BG	208/208 (100%)	0.62	11 (5%) 32 17	84, 110, 135, 149	0
34	CG	208/208 (100%)	0.52	19 (9%) 15 8	74, 101, 128, 142	0
35	BH	151/162 (93%)	0.16	0 100 100	79, 101, 129, 159	0
35	CH	151/162 (93%)	0.58	5 (3%) 49 29	90, 114, 139, 162	0
36	BI	101/101 (100%)	0.27	2 (1%) 65 44	77, 102, 122, 143	0
36	CI	101/101 (100%)	0.20	2 (1%) 65 44	73, 98, 121, 149	0
37	BJ	155/156 (99%)	0.44	4 (2%) 57 36	101, 122, 156, 167	0
37	CJ	155/156 (99%)	0.63	6 (3%) 43 24	105, 127, 158, 166	0
38	BK	138/138 (100%)	0.39	0 100 100	84, 108, 123, 132	0
38	CK	138/138 (100%)	0.44	3 (2%) 62 41	93, 118, 131, 141	0
39	BL	127/128 (99%)	0.77	13 (10%) 12 6	91, 141, 160, 169	0
39	CL	127/128 (99%)	0.78	7 (5%) 30 16	107, 151, 168, 172	0
40	BM	99/105 (94%)	0.68	4 (4%) 42 23	87, 140, 171, 176	0
40	CM	99/105 (94%)	0.88	6 (6%) 27 15	113, 154, 173, 176	0
41	BN	119/129 (92%)	0.25	2 (1%) 69 48	63, 101, 133, 162	0
41	CN	119/129 (92%)	0.42	5 (4%) 40 22	77, 103, 141, 166	0
42	BO	125/132 (94%)	-0.07	1 (0%) 82 65	61, 78, 116, 162	0
42	CO	125/132 (94%)	0.38	6 (4%) 35 19	70, 97, 130, 168	0
43	BP	116/126 (92%)	0.51	6 (5%) 33 17	87, 124, 144, 158	0
43	CP	117/126 (92%)	0.81	7 (5%) 27 15	105, 152, 166, 174	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	60/61 (98%)	0.57	3 (5%) 34 18	84, 107, 124, 134	0
44	CQ	60/61 (98%)	0.96	7 (11%) 9 5	120, 136, 153, 161	0
45	BR	88/89 (98%)	0.22	1 (1%) 78 59	73, 97, 120, 126	0
45	CR	88/89 (98%)	0.35	2 (2%) 61 39	75, 105, 129, 135	0
46	BS	84/88 (95%)	0.42	3 (3%) 46 26	98, 113, 141, 173	0
46	CS	84/88 (95%)	0.25	2 (2%) 59 38	79, 96, 122, 161	0
47	BT	100/105 (95%)	0.19	0 100 100	85, 105, 123, 137	0
47	CT	100/105 (95%)	0.32	2 (2%) 65 44	81, 104, 126, 143	0
48	BU	72/88 (81%)	0.22	0 100 100	75, 102, 140, 169	0
48	CU	72/88 (81%)	0.19	0 100 100	86, 109, 150, 165	0
49	BV	83/93 (89%)	0.76	9 (10%) 11 6	103, 129, 145, 156	0
49	CV	78/93 (83%)	0.81	3 (3%) 44 25	137, 160, 180, 183	0
50	BW	99/106 (93%)	0.64	7 (7%) 22 12	101, 123, 152, 162	0
50	CW	99/106 (93%)	0.47	7 (7%) 22 12	79, 110, 149, 164	0
51	BX	25/27 (92%)	0.42	0 100 100	93, 114, 133, 155	0
51	CX	25/27 (92%)	0.96	1 (4%) 42 23	110, 134, 152, 170	0
52	BB	87/87 (100%)	0.96	7 (8%) 18 10	83, 164, 192, 209	0
52	CB	87/87 (100%)	1.08	8 (9%) 14 8	99, 167, 196, 209	0
53	BC	77/77 (100%)	0.36	3 (3%) 43 24	66, 101, 139, 152	0
53	BD	77/77 (100%)	1.17	11 (14%) 6 3	75, 226, 239, 242	0
53	CC	77/77 (100%)	0.64	3 (3%) 43 24	77, 110, 148, 162	0
53	CD	77/77 (100%)	1.38	11 (14%) 6 3	78, 227, 239, 242	0
54	B1	10/10 (100%)	0.10	1 (10%) 12 6	73, 80, 132, 141	0
54	C1	10/10 (100%)	0.42	1 (10%) 12 6	81, 98, 145, 150	0
All	All	21111/21426 (98%)	0.35	888 (4%) 40 22	38, 99, 184, 246	0

The worst 5 of 888 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	BG	12	CYS	8.0
31	BA	1129	C	7.7
27	A5	2	ALA	7.4
12	AP	23	GLY	7.1
34	BG	26	CYS	7.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1667	1/1	-0.08	0.22	144,144,144,144	0
55	MG	BA	1692	1/1	0.19	0.21	132,132,132,132	0
55	MG	BA	1742	1/1	0.25	0.22	133,133,133,133	0
55	MG	DA	3124	1/1	0.26	0.23	111,111,111,111	0
55	MG	CA	1704	1/1	0.30	0.29	129,129,129,129	0
55	MG	BA	1638	1/1	0.32	0.36	123,123,123,123	0
55	MG	BA	1784	1/1	0.35	0.50	106,106,106,106	0
55	MG	CA	1753	1/1	0.38	0.26	129,129,129,129	0
55	MG	BA	1758	1/1	0.42	0.15	110,110,110,110	0
55	MG	CA	1730	1/1	0.42	0.35	118,118,118,118	0
55	MG	DA	3010	1/1	0.43	0.25	121,121,121,121	0
55	MG	CA	1719	1/1	0.47	0.32	157,157,157,157	0
55	MG	DA	3272	1/1	0.48	0.50	117,117,117,117	0
55	MG	BA	1714	1/1	0.49	0.17	127,127,127,127	0
55	MG	DA	3526	1/1	0.49	0.21	92,92,92,92	0
55	MG	CA	1748	1/1	0.51	0.38	91,91,91,91	0
55	MG	BA	1713	1/1	0.51	0.28	107,107,107,107	0
55	MG	CA	1626	1/1	0.52	0.28	103,103,103,103	0
55	MG	CA	1802	1/1	0.52	0.27	107,107,107,107	0
55	MG	BA	1712	1/1	0.54	0.44	125,125,125,125	0
55	MG	AA	3406	1/1	0.57	0.33	99,99,99,99	0
55	MG	DB	206	1/1	0.58	0.37	122,122,122,122	0
55	MG	AA	3318	1/1	0.59	0.32	120,120,120,120	0
55	MG	BA	1787	1/1	0.59	0.38	107,107,107,107	0
55	MG	AA	3370	1/1	0.59	0.28	103,103,103,103	0
55	MG	CA	1800	1/1	0.60	0.14	102,102,102,102	0
55	MG	DA	3497	1/1	0.60	0.17	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BB	105	1/1	0.61	0.27	115,115,115,115	0
55	MG	CA	1759	1/1	0.61	0.40	100,100,100,100	0
55	MG	BD	101	1/1	0.61	0.15	108,108,108,108	0
55	MG	AA	3076	1/1	0.61	0.25	109,109,109,109	0
55	MG	BA	1831	1/1	0.61	0.42	116,116,116,116	0
55	MG	CA	1659	1/1	0.62	0.34	111,111,111,111	0
55	MG	CA	1789	1/1	0.62	0.26	117,117,117,117	0
55	MG	CB	101	1/1	0.62	0.23	102,102,102,102	0
55	MG	BA	1829	1/1	0.63	0.28	102,102,102,102	0
55	MG	DA	3433	1/1	0.64	0.21	110,110,110,110	0
55	MG	BA	1751	1/1	0.64	0.40	122,122,122,122	0
55	MG	CA	1699	1/1	0.64	0.10	106,106,106,106	0
55	MG	CB	104	1/1	0.64	0.21	114,114,114,114	0
55	MG	DB	214	1/1	0.64	0.11	99,99,99,99	0
55	MG	AA	3518	1/1	0.65	0.59	71,71,71,71	0
55	MG	DA	3444	1/1	0.65	0.22	82,82,82,82	0
55	MG	BA	1609	1/1	0.65	0.31	84,84,84,84	0
55	MG	AA	3431	1/1	0.65	0.46	197,197,197,197	0
55	MG	BA	1686	1/1	0.65	0.36	94,94,94,94	0
55	MG	AA	3443	1/1	0.65	0.29	95,95,95,95	0
55	MG	DA	3352	1/1	0.66	0.27	77,77,77,77	0
55	MG	DA	3412	1/1	0.66	0.26	97,97,97,97	0
55	MG	CA	1747	1/1	0.66	0.49	114,114,114,114	0
55	MG	AA	3419	1/1	0.66	0.28	102,102,102,102	0
55	MG	DA	3473	1/1	0.67	0.25	103,103,103,103	0
55	MG	CA	1795	1/1	0.67	0.34	110,110,110,110	0
55	MG	DA	3163	1/1	0.67	0.12	97,97,97,97	0
55	MG	BA	1834	1/1	0.67	0.24	86,86,86,86	0
55	MG	DA	3343	1/1	0.67	0.25	145,145,145,145	0
55	MG	DA	3060	1/1	0.68	0.44	85,85,85,85	0
55	MG	AA	3230	1/1	0.68	0.30	112,112,112,112	0
55	MG	AA	3521	1/1	0.68	0.47	87,87,87,87	0
55	MG	DA	3248	1/1	0.68	0.23	98,98,98,98	0
55	MG	BA	1828	1/1	0.68	0.37	85,85,85,85	0
55	MG	CA	1734	1/1	0.68	0.29	92,92,92,92	0
55	MG	BA	1778	1/1	0.68	0.74	93,93,93,93	0
55	MG	DA	3382	1/1	0.68	0.14	84,84,84,84	0
55	MG	BA	1678	1/1	0.69	0.61	75,75,75,75	0
55	MG	DA	3038	1/1	0.69	0.15	102,102,102,102	0
55	MG	DA	3498	1/1	0.69	0.26	90,90,90,90	0
55	MG	BG	301	1/1	0.69	0.27	110,110,110,110	0
55	MG	DA	3377	1/1	0.69	0.32	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
55	MG	DA	3447	1/1	0.69	0.58	86,86,86,86	0
55	MG	DA	3045	1/1	0.70	0.38	79,79,79,79	0
55	MG	DA	3065	1/1	0.70	0.29	95,95,95,95	0
55	MG	CA	1806	1/1	0.71	0.31	115,115,115,115	0
55	MG	BA	1647	1/1	0.71	0.21	93,93,93,93	0
55	MG	AA	3378	1/1	0.71	0.25	86,86,86,86	0
55	MG	CC	108	1/1	0.71	0.26	110,110,110,110	0
55	MG	DA	3004	1/1	0.71	0.47	91,91,91,91	0
55	MG	AA	3450	1/1	0.71	0.35	84,84,84,84	0
55	MG	AA	3236	1/1	0.71	0.60	93,93,93,93	0
55	MG	CA	1657	1/1	0.71	0.32	94,94,94,94	0
55	MG	AA	3055	1/1	0.71	0.30	100,100,100,100	0
55	MG	CA	1762	1/1	0.71	0.22	105,105,105,105	0
55	MG	AE	304	1/1	0.71	0.53	85,85,85,85	0
55	MG	AA	3426	1/1	0.71	0.29	123,123,123,123	0
55	MG	BA	1718	1/1	0.71	0.24	104,104,104,104	0
55	MG	AA	3058	1/1	0.71	0.52	85,85,85,85	0
55	MG	BA	1621	1/1	0.72	0.25	116,116,116,116	0
55	MG	BA	1636	1/1	0.72	0.42	92,92,92,92	0
55	MG	DA	3438	1/1	0.72	0.80	102,102,102,102	0
55	MG	BB	106	1/1	0.72	0.21	120,120,120,120	0
55	MG	AA	3241	1/1	0.72	0.15	101,101,101,101	0
55	MG	DA	3285	1/1	0.72	0.21	109,109,109,109	0
55	MG	AA	3451	1/1	0.72	0.27	85,85,85,85	0
55	MG	AA	3573	1/1	0.72	0.21	47,47,47,47	0
55	MG	DA	3357	1/1	0.72	0.76	89,89,89,89	0
55	MG	AA	3505	1/1	0.72	0.26	103,103,103,103	0
55	MG	AA	3508	1/1	0.72	0.29	96,96,96,96	0
55	MG	DA	3429	1/1	0.73	0.13	94,94,94,94	0
55	MG	DA	3299	1/1	0.73	0.20	92,92,92,92	0
55	MG	DA	3312	1/1	0.73	0.20	101,101,101,101	0
55	MG	DA	3332	1/1	0.73	0.68	90,90,90,90	0
55	MG	AA	3251	1/1	0.73	0.23	97,97,97,97	0
55	MG	DA	3472	1/1	0.73	0.19	85,85,85,85	0
55	MG	BC	102	1/1	0.73	0.20	100,100,100,100	0
55	MG	AA	3411	1/1	0.73	0.34	84,84,84,84	0
55	MG	AA	3460	1/1	0.73	0.38	89,89,89,89	0
55	MG	BA	1804	1/1	0.73	0.26	80,80,80,80	0
55	MG	AA	3353	1/1	0.73	0.41	105,105,105,105	0
55	MG	DA	3422	1/1	0.73	0.16	96,96,96,96	0
55	MG	CA	1720	1/1	0.74	0.22	108,108,108,108	0
55	MG	BA	1810	1/1	0.74	0.28	110,110,110,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1823	1/1	0.74	0.15	93,93,93,93	0
55	MG	BA	1611	1/1	0.74	0.33	97,97,97,97	0
55	MG	CC	101	1/1	0.74	0.25	110,110,110,110	0
55	MG	BA	1765	1/1	0.74	0.31	99,99,99,99	0
55	MG	AA	3465	1/1	0.74	0.28	88,88,88,88	0
55	MG	DA	3455	1/1	0.74	0.29	95,95,95,95	0
55	MG	BA	1674	1/1	0.74	0.39	113,113,113,113	0
55	MG	BA	1749	1/1	0.74	0.25	95,95,95,95	0
55	MG	BA	1798	1/1	0.74	0.37	89,89,89,89	0
55	MG	CA	1713	1/1	0.74	0.17	109,109,109,109	0
55	MG	AA	3188	1/1	0.74	0.25	72,72,72,72	0
55	MG	DA	3066	1/1	0.74	0.16	83,83,83,83	0
55	MG	DA	3410	1/1	0.74	0.32	99,99,99,99	0
55	MG	BA	1838	1/1	0.75	0.45	101,101,101,101	0
55	MG	CA	1634	1/1	0.75	0.43	90,90,90,90	0
55	MG	CA	1723	1/1	0.75	0.22	93,93,93,93	0
55	MG	CA	1727	1/1	0.75	0.27	84,84,84,84	0
55	MG	DA	3059	1/1	0.75	0.30	104,104,104,104	0
55	MG	BA	1841	1/1	0.75	0.22	105,105,105,105	0
55	MG	DA	3063	1/1	0.75	0.18	86,86,86,86	0
55	MG	AF	303	1/1	0.75	0.21	77,77,77,77	0
55	MG	AA	3346	1/1	0.75	0.10	98,98,98,98	0
55	MG	AA	3262	1/1	0.75	0.20	71,71,71,71	0
55	MG	DA	3502	1/1	0.75	0.15	96,96,96,96	0
55	MG	BA	1732	1/1	0.75	0.14	94,94,94,94	0
55	MG	DA	3244	1/1	0.75	0.26	106,106,106,106	0
55	MG	AA	3430	1/1	0.75	0.14	88,88,88,88	0
55	MG	BA	1735	1/1	0.76	0.33	80,80,80,80	0
55	MG	BA	1649	1/1	0.76	0.23	85,85,85,85	0
55	MG	DA	3340	1/1	0.76	0.26	107,107,107,107	0
55	MG	AA	3317	1/1	0.76	0.43	95,95,95,95	0
55	MG	AA	3249	1/1	0.76	0.18	92,92,92,92	0
55	MG	BA	1753	1/1	0.76	0.13	91,91,91,91	0
55	MG	DA	3054	1/1	0.76	0.19	105,105,105,105	0
55	MG	DA	3477	1/1	0.76	0.28	125,125,125,125	0
55	MG	DA	3253	1/1	0.76	0.20	83,83,83,83	0
55	MG	DA	3398	1/1	0.76	0.31	107,107,107,107	0
55	MG	DA	3263	1/1	0.76	0.26	88,88,88,88	0
55	MG	CA	1631	1/1	0.76	0.38	95,95,95,95	0
55	MG	AA	3495	1/1	0.76	0.26	98,98,98,98	0
55	MG	AA	3388	1/1	0.76	0.32	119,119,119,119	0
55	MG	AA	3102	1/1	0.77	0.21	108,108,108,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3404	1/1	0.77	0.44	91,91,91,91	0
55	MG	CA	1661	1/1	0.77	0.28	105,105,105,105	0
55	MG	CA	1662	1/1	0.77	0.37	102,102,102,102	0
55	MG	DA	3261	1/1	0.77	0.23	89,89,89,89	0
55	MG	AA	3380	1/1	0.77	0.30	84,84,84,84	0
55	MG	BA	1723	1/1	0.77	0.28	95,95,95,95	0
55	MG	DA	3278	1/1	0.77	0.20	116,116,116,116	0
55	MG	AA	3288	1/1	0.77	0.21	73,73,73,73	0
55	MG	CA	1773	1/1	0.77	0.15	115,115,115,115	0
55	MG	CA	1710	1/1	0.77	0.24	105,105,105,105	0
55	MG	BA	1698	1/1	0.77	0.20	73,73,73,73	0
55	MG	AA	3326	1/1	0.77	0.57	81,81,81,81	0
55	MG	DA	3342	1/1	0.77	0.26	96,96,96,96	0
55	MG	BA	1785	1/1	0.77	0.32	91,91,91,91	0
55	MG	BA	1745	1/1	0.77	0.23	90,90,90,90	0
55	MG	DA	3109	1/1	0.77	0.35	97,97,97,97	0
55	MG	DA	3372	1/1	0.77	0.50	108,108,108,108	0
55	MG	CA	1635	1/1	0.77	0.24	87,87,87,87	0
55	MG	DB	208	1/1	0.77	0.17	114,114,114,114	0
55	MG	DB	212	1/1	0.77	0.12	94,94,94,94	0
55	MG	AD	301	1/1	0.77	0.12	100,100,100,100	0
55	MG	DA	3225	1/1	0.78	0.26	64,64,64,64	0
55	MG	AA	3108	1/1	0.78	0.49	79,79,79,79	0
55	MG	AA	3223	1/1	0.78	0.19	72,72,72,72	0
55	MG	DA	3249	1/1	0.78	0.21	87,87,87,87	0
55	MG	AA	3560	1/1	0.78	0.21	84,84,84,84	0
55	MG	AA	3120	1/1	0.78	0.11	92,92,92,92	0
55	MG	CA	1665	1/1	0.78	0.29	101,101,101,101	0
55	MG	BA	1746	1/1	0.78	0.38	95,95,95,95	0
55	MG	CA	1687	1/1	0.78	0.12	99,99,99,99	0
55	MG	BA	1709	1/1	0.78	0.45	101,101,101,101	0
55	MG	CA	1763	1/1	0.78	0.30	96,96,96,96	0
55	MG	BA	1637	1/1	0.78	0.19	93,93,93,93	0
55	MG	DA	3324	1/1	0.78	0.60	89,89,89,89	0
55	MG	CA	1777	1/1	0.78	0.43	95,95,95,95	0
55	MG	DA	3478	1/1	0.78	0.20	99,99,99,99	0
55	MG	AB	216	1/1	0.78	0.35	112,112,112,112	0
55	MG	CA	1630	1/1	0.78	0.12	76,76,76,76	0
55	MG	AA	3145	1/1	0.78	0.27	98,98,98,98	0
55	MG	DA	3520	1/1	0.78	0.19	99,99,99,99	0
55	MG	DA	3068	1/1	0.78	0.34	100,100,100,100	0
55	MG	DB	204	1/1	0.78	0.28	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3076	1/1	0.78	0.14	96,96,96,96	0
55	MG	AA	3333	1/1	0.78	0.28	80,80,80,80	0
55	MG	AA	3509	1/1	0.78	0.43	80,80,80,80	0
55	MG	CH	201	1/1	0.78	0.31	96,96,96,96	0
55	MG	AA	3393	1/1	0.79	0.23	91,91,91,91	0
55	MG	BQ	101	1/1	0.79	0.32	99,99,99,99	0
55	MG	DA	3301	1/1	0.79	0.38	91,91,91,91	0
55	MG	DA	3309	1/1	0.79	0.29	69,69,69,69	0
55	MG	AA	3131	1/1	0.79	0.12	88,88,88,88	0
55	MG	BA	1741	1/1	0.79	0.24	124,124,124,124	0
55	MG	CB	102	1/1	0.79	0.15	94,94,94,94	0
55	MG	AB	203	1/1	0.79	0.32	70,70,70,70	0
55	MG	DA	3132	1/1	0.79	0.28	56,56,56,56	0
55	MG	CA	1749	1/1	0.79	0.17	106,106,106,106	0
55	MG	BC	104	1/1	0.79	0.24	106,106,106,106	0
55	MG	AA	3164	1/1	0.79	0.18	102,102,102,102	0
55	MG	BA	1628	1/1	0.79	0.47	86,86,86,86	0
55	MG	DA	3500	1/1	0.79	0.17	100,100,100,100	0
55	MG	BA	1833	1/1	0.79	0.18	88,88,88,88	0
55	MG	DA	3504	1/1	0.79	0.33	119,119,119,119	0
55	MG	AA	3132	1/1	0.79	0.46	89,89,89,89	0
55	MG	DA	3393	1/1	0.79	0.18	93,93,93,93	0
55	MG	DA	3397	1/1	0.79	0.61	150,150,150,150	0
55	MG	BA	1788	1/1	0.79	0.29	108,108,108,108	0
55	MG	AA	3446	1/1	0.79	0.26	93,93,93,93	0
55	MG	CA	1637	1/1	0.79	0.20	97,97,97,97	0
55	MG	CA	1643	1/1	0.79	0.24	97,97,97,97	0
55	MG	AA	3077	1/1	0.80	0.43	94,94,94,94	0
55	MG	AA	3349	1/1	0.80	0.17	79,79,79,79	0
55	MG	BA	1747	1/1	0.80	0.14	97,97,97,97	0
55	MG	AA	3623	1/1	0.80	0.28	107,107,107,107	0
55	MG	AA	3629	1/1	0.80	0.18	107,107,107,107	0
55	MG	DA	3440	1/1	0.80	0.15	92,92,92,92	0
55	MG	BA	1752	1/1	0.80	0.23	116,116,116,116	0
55	MG	BB	107	1/1	0.80	0.18	97,97,97,97	0
55	MG	DA	3453	1/1	0.80	0.46	94,94,94,94	0
55	MG	DA	3315	1/1	0.80	0.18	82,82,82,82	0
55	MG	DA	3077	1/1	0.80	0.37	82,82,82,82	0
55	MG	CA	1742	1/1	0.80	0.27	93,93,93,93	0
55	MG	DA	3116	1/1	0.80	0.37	96,96,96,96	0
55	MG	BA	1726	1/1	0.80	0.41	98,98,98,98	0
55	MG	DA	3128	1/1	0.80	0.29	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1695	1/1	0.80	0.19	101,101,101,101	0
55	MG	AA	3435	1/1	0.80	0.18	137,137,137,137	0
55	MG	CA	1685	1/1	0.80	0.32	85,85,85,85	0
55	MG	CA	1612	1/1	0.80	0.20	91,91,91,91	0
55	MG	DA	3505	1/1	0.80	0.11	87,87,87,87	0
55	MG	DA	3247	1/1	0.80	0.35	71,71,71,71	0
55	MG	BA	1775	1/1	0.80	0.20	100,100,100,100	0
55	MG	DA	3023	1/1	0.80	0.57	107,107,107,107	0
55	MG	BA	1648	1/1	0.80	0.23	77,77,77,77	0
55	MG	CA	1769	1/1	0.80	0.28	109,109,109,109	0
55	MG	DA	3405	1/1	0.80	0.39	97,97,97,97	0
55	MG	AA	3558	1/1	0.80	0.40	110,110,110,110	0
55	MG	BA	1690	1/1	0.81	0.18	109,109,109,109	0
55	MG	AA	3005	1/1	0.81	0.31	38,38,38,38	0
55	MG	AA	3434	1/1	0.81	0.17	65,65,65,65	0
55	MG	CA	1761	1/1	0.81	0.29	96,96,96,96	0
55	MG	DA	3046	1/1	0.81	0.24	60,60,60,60	0
55	MG	AA	3355	1/1	0.81	0.39	87,87,87,87	0
55	MG	DA	3431	1/1	0.81	0.26	93,93,93,93	0
55	MG	DA	3432	1/1	0.81	0.24	89,89,89,89	0
55	MG	DA	3056	1/1	0.81	0.22	100,100,100,100	0
55	MG	DA	3283	1/1	0.81	0.49	78,78,78,78	0
55	MG	BA	1707	1/1	0.81	0.33	94,94,94,94	0
55	MG	BA	1639	1/1	0.81	0.43	94,94,94,94	0
55	MG	CA	1616	1/1	0.81	0.22	90,90,90,90	0
55	MG	DA	3449	1/1	0.81	0.27	96,96,96,96	0
55	MG	CA	1621	1/1	0.81	0.30	84,84,84,84	0
55	MG	AA	3366	1/1	0.81	0.34	78,78,78,78	0
55	MG	CA	1715	1/1	0.81	0.34	99,99,99,99	0
55	MG	DA	3318	1/1	0.81	0.50	93,93,93,93	0
55	MG	AA	3600	1/1	0.81	0.44	79,79,79,79	0
55	MG	AA	3420	1/1	0.81	0.28	107,107,107,107	0
55	MG	DA	3084	1/1	0.81	0.20	87,87,87,87	0
55	MG	BA	1669	1/1	0.81	0.35	76,76,76,76	0
55	MG	AA	3215	1/1	0.81	0.29	55,55,55,55	0
55	MG	BA	1624	1/1	0.81	0.23	92,92,92,92	0
55	MG	DA	3125	1/1	0.81	0.22	86,86,86,86	0
55	MG	DA	3360	1/1	0.81	0.35	96,96,96,96	0
55	MG	BA	1681	1/1	0.81	0.23	79,79,79,79	0
55	MG	BA	1683	1/1	0.81	0.11	112,112,112,112	0
55	MG	CA	1745	1/1	0.81	0.20	87,87,87,87	0
55	MG	DA	3390	1/1	0.81	0.12	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
55	MG	BB	104	1/1	0.81	0.11	103,103,103,103	0
55	MG	DB	210	1/1	0.81	0.35	76,76,76,76	0
55	MG	AA	3394	1/1	0.81	0.16	85,85,85,85	0
55	MG	DA	3007	1/1	0.81	0.14	75,75,75,75	0
55	MG	DA	3185	1/1	0.82	0.24	64,64,64,64	0
55	MG	CA	1606	1/1	0.82	0.24	96,96,96,96	0
55	MG	AA	3458	1/1	0.82	0.58	105,105,105,105	0
55	MG	CA	1614	1/1	0.82	0.40	95,95,95,95	0
55	MG	AA	3391	1/1	0.82	0.16	90,90,90,90	0
55	MG	BA	1819	1/1	0.82	0.30	107,107,107,107	0
55	MG	AA	3591	1/1	0.82	0.48	80,80,80,80	0
55	MG	DA	3425	1/1	0.82	0.16	88,88,88,88	0
55	MG	CA	1627	1/1	0.82	0.28	102,102,102,102	0
55	MG	CA	1744	1/1	0.82	0.18	70,70,70,70	0
55	MG	DA	3271	1/1	0.82	0.23	76,76,76,76	0
55	MG	DA	3025	1/1	0.82	0.17	111,111,111,111	0
55	MG	BA	1625	1/1	0.82	0.20	61,61,61,61	0
55	MG	DA	3439	1/1	0.82	0.07	92,92,92,92	0
55	MG	AA	3277	1/1	0.82	0.34	98,98,98,98	0
55	MG	AA	3620	1/1	0.82	0.40	99,99,99,99	0
55	MG	DA	3446	1/1	0.82	0.38	98,98,98,98	0
55	MG	DA	3294	1/1	0.82	0.33	93,93,93,93	0
55	MG	AA	3478	1/1	0.82	0.15	93,93,93,93	0
55	MG	AA	3032	1/1	0.82	0.20	60,60,60,60	0
55	MG	BA	1710	1/1	0.82	0.40	99,99,99,99	0
55	MG	AA	3301	1/1	0.82	0.25	113,113,113,113	0
55	MG	BA	1844	1/1	0.82	0.16	95,95,95,95	0
55	MG	AB	207	1/1	0.82	0.13	97,97,97,97	0
55	MG	BN	202	1/1	0.82	0.16	104,104,104,104	0
55	MG	AB	215	1/1	0.82	0.17	92,92,92,92	0
55	MG	AA	3095	1/1	0.82	0.20	75,75,75,75	0
55	MG	AA	3444	1/1	0.82	0.21	87,87,87,87	0
55	MG	AA	3352	1/1	0.82	0.15	91,91,91,91	0
55	MG	CA	1797	1/1	0.82	0.21	94,94,94,94	0
55	MG	AA	3387	1/1	0.82	0.26	102,102,102,102	0
55	MG	DA	3123	1/1	0.82	0.36	73,73,73,73	0
55	MG	DA	3525	1/1	0.82	0.32	88,88,88,88	0
55	MG	DA	3366	1/1	0.82	0.17	97,97,97,97	0
55	MG	AA	3224	1/1	0.82	0.29	77,77,77,77	0
55	MG	DA	3376	1/1	0.82	0.12	88,88,88,88	0
55	MG	BA	1791	1/1	0.82	0.22	89,89,89,89	0
55	MG	CA	1809	1/1	0.82	0.22	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BC	105	1/1	0.82	0.27	95,95,95,95	0
55	MG	BA	1739	1/1	0.82	0.20	79,79,79,79	0
55	MG	CA	1754	1/1	0.83	0.17	84,84,84,84	0
55	MG	DA	3267	1/1	0.83	0.36	74,74,74,74	0
55	MG	AA	3367	1/1	0.83	0.24	101,101,101,101	0
55	MG	AA	3192	1/1	0.83	0.26	90,90,90,90	0
55	MG	AA	3343	1/1	0.83	0.38	94,94,94,94	0
55	MG	AA	3422	1/1	0.83	0.48	73,73,73,73	0
55	MG	AA	3466	1/1	0.83	0.42	106,106,106,106	0
55	MG	AA	3193	1/1	0.83	0.21	94,94,94,94	0
55	MG	AA	3486	1/1	0.83	0.35	96,96,96,96	0
55	MG	CA	1786	1/1	0.83	0.28	97,97,97,97	0
55	MG	DA	3302	1/1	0.83	0.40	91,91,91,91	0
55	MG	AA	3148	1/1	0.83	0.25	70,70,70,70	0
55	MG	AA	3496	1/1	0.83	0.36	91,91,91,91	0
55	MG	AA	3103	1/1	0.83	0.20	75,75,75,75	0
55	MG	AA	3066	1/1	0.83	0.29	103,103,103,103	0
55	MG	BA	1800	1/1	0.83	0.17	101,101,101,101	0
55	MG	DA	3466	1/1	0.83	0.28	78,78,78,78	0
55	MG	BA	1736	1/1	0.83	0.23	89,89,89,89	0
55	MG	AA	3254	1/1	0.83	0.30	97,97,97,97	0
55	MG	BA	1814	1/1	0.83	0.25	86,86,86,86	0
55	MG	AA	3364	1/1	0.83	0.34	89,89,89,89	0
55	MG	DA	3480	1/1	0.83	0.29	56,56,56,56	0
55	MG	AO	202	1/1	0.83	0.25	74,74,74,74	0
55	MG	CA	1622	1/1	0.83	0.33	74,74,74,74	0
55	MG	DA	3135	1/1	0.83	0.20	64,64,64,64	0
55	MG	BA	1824	1/1	0.83	0.53	97,97,97,97	0
55	MG	DA	3176	1/1	0.83	0.15	78,78,78,78	0
55	MG	BA	1744	1/1	0.83	0.26	93,93,93,93	0
55	MG	DA	3518	1/1	0.83	0.18	63,63,63,63	0
55	MG	BA	1684	1/1	0.83	0.18	100,100,100,100	0
55	MG	DA	3521	1/1	0.83	0.22	89,89,89,89	0
55	MG	DA	3236	1/1	0.83	0.25	57,57,57,57	0
55	MG	DA	3241	1/1	0.83	0.30	85,85,85,85	0
55	MG	AA	3398	1/1	0.83	0.22	91,91,91,91	0
55	MG	AA	3556	1/1	0.83	0.37	85,85,85,85	0
55	MG	DA	3021	1/1	0.83	0.23	61,61,61,61	0
55	MG	BA	1616	1/1	0.83	0.15	92,92,92,92	0
55	MG	AA	3399	1/1	0.83	0.13	71,71,71,71	0
55	MG	AA	3258	1/1	0.83	0.21	80,80,80,80	0
55	MG	AA	3500	1/1	0.84	0.22	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3388	1/1	0.84	0.13	85,85,85,85	0
55	MG	BA	1750	1/1	0.84	0.29	79,79,79,79	0
55	MG	DA	3183	1/1	0.84	0.21	59,59,59,59	0
55	MG	AB	201	1/1	0.84	0.16	91,91,91,91	0
55	MG	DA	3215	1/1	0.84	0.28	50,50,50,50	0
55	MG	CA	1623	1/1	0.84	0.13	98,98,98,98	0
55	MG	CC	107	1/1	0.84	0.48	102,102,102,102	0
55	MG	DA	3239	1/1	0.84	0.44	75,75,75,75	0
55	MG	CA	1625	1/1	0.84	0.23	85,85,85,85	0
55	MG	AA	3297	1/1	0.84	0.24	63,63,63,63	0
55	MG	AA	3071	1/1	0.84	0.24	99,99,99,99	0
55	MG	BA	1754	1/1	0.84	0.15	80,80,80,80	0
55	MG	AA	3179	1/1	0.84	0.46	70,70,70,70	0
55	MG	BA	1763	1/1	0.84	0.15	93,93,93,93	0
55	MG	AA	3257	1/1	0.84	0.15	84,84,84,84	0
55	MG	DA	3437	1/1	0.84	0.27	140,140,140,140	0
55	MG	DA	3033	1/1	0.84	0.24	94,94,94,94	0
55	MG	AA	3231	1/1	0.84	0.37	120,120,120,120	0
55	MG	CA	1638	1/1	0.84	0.34	93,93,93,93	0
55	MG	AA	3523	1/1	0.84	0.19	87,87,87,87	0
55	MG	DA	3276	1/1	0.84	0.16	86,86,86,86	0
55	MG	CA	1655	1/1	0.84	0.47	87,87,87,87	0
55	MG	BA	1729	1/1	0.84	0.15	85,85,85,85	0
55	MG	AA	3534	1/1	0.84	0.15	100,100,100,100	0
55	MG	AA	3202	1/1	0.84	0.32	55,55,55,55	0
55	MG	AA	3468	1/1	0.84	0.16	92,92,92,92	0
55	MG	CA	1770	1/1	0.84	0.14	75,75,75,75	0
55	MG	AA	3184	1/1	0.84	0.45	90,90,90,90	0
55	MG	DA	3308	1/1	0.84	0.28	95,95,95,95	0
55	MG	AA	3374	1/1	0.84	0.32	96,96,96,96	0
55	MG	CA	1782	1/1	0.84	0.26	104,104,104,104	0
55	MG	AA	3490	1/1	0.84	0.16	88,88,88,88	0
55	MG	DA	3078	1/1	0.84	0.15	87,87,87,87	0
55	MG	BA	1802	1/1	0.84	0.24	69,69,69,69	0
55	MG	DA	3325	1/1	0.84	0.24	70,70,70,70	0
55	MG	DA	3326	1/1	0.84	0.31	63,63,63,63	0
55	MG	DA	3103	1/1	0.84	0.13	82,82,82,82	0
55	MG	DA	3334	1/1	0.84	0.32	95,95,95,95	0
55	MG	CA	1689	1/1	0.84	0.17	87,87,87,87	0
55	MG	CA	1694	1/1	0.84	0.40	94,94,94,94	0
55	MG	AA	3047	1/1	0.84	0.22	87,87,87,87	0
55	MG	AA	3295	1/1	0.84	0.29	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1803	1/1	0.84	0.24	87,87,87,87	0
55	MG	AA	3497	1/1	0.84	0.24	105,105,105,105	0
55	MG	AA	3624	1/1	0.84	0.20	80,80,80,80	0
55	MG	DA	3133	1/1	0.84	0.40	77,77,77,77	0
55	MG	BA	1822	1/1	0.84	0.21	107,107,107,107	0
55	MG	DA	3136	1/1	0.84	0.18	97,97,97,97	0
55	MG	AA	3506	1/1	0.85	0.18	73,73,73,73	0
55	MG	AB	202	1/1	0.85	0.26	86,86,86,86	0
55	MG	DA	3365	1/1	0.85	0.34	89,89,89,89	0
55	MG	CA	1664	1/1	0.85	0.28	97,97,97,97	0
55	MG	AA	3182	1/1	0.85	0.30	77,77,77,77	0
55	MG	AA	3461	1/1	0.85	0.27	78,78,78,78	0
55	MG	AA	3463	1/1	0.85	0.46	108,108,108,108	0
55	MG	AA	3165	1/1	0.85	0.34	71,71,71,71	0
55	MG	AA	3310	1/1	0.85	0.18	74,74,74,74	0
55	MG	AA	3532	1/1	0.85	0.12	89,89,89,89	0
55	MG	DA	3392	1/1	0.85	0.18	106,106,106,106	0
55	MG	DA	3213	1/1	0.85	0.21	94,94,94,94	0
55	MG	DA	3396	1/1	0.85	0.19	89,89,89,89	0
55	MG	AA	3259	1/1	0.85	0.10	91,91,91,91	0
55	MG	AA	3477	1/1	0.85	0.11	65,65,65,65	0
55	MG	DA	3403	1/1	0.85	0.13	78,78,78,78	0
55	MG	DA	3227	1/1	0.85	0.27	81,81,81,81	0
55	MG	BA	1605	1/1	0.85	0.33	69,69,69,69	0
55	MG	BA	1702	1/1	0.85	0.31	98,98,98,98	0
55	MG	DA	3240	1/1	0.85	0.42	80,80,80,80	0
55	MG	BA	1770	1/1	0.85	0.29	106,106,106,106	0
55	MG	CA	1717	1/1	0.85	0.22	106,106,106,106	0
55	MG	DA	3426	1/1	0.85	0.20	94,94,94,94	0
55	MG	AA	3186	1/1	0.85	0.17	77,77,77,77	0
55	MG	AA	3559	1/1	0.85	0.11	93,93,93,93	0
55	MG	DA	3018	1/1	0.85	0.18	85,85,85,85	0
55	MG	AA	3324	1/1	0.85	0.16	60,60,60,60	0
55	MG	AA	3488	1/1	0.85	0.18	94,94,94,94	0
55	MG	BA	1622	1/1	0.85	0.23	84,84,84,84	0
55	MG	CA	1731	1/1	0.85	0.41	85,85,85,85	0
55	MG	AA	3264	1/1	0.85	0.29	74,74,74,74	0
55	MG	DA	3442	1/1	0.85	0.36	96,96,96,96	0
55	MG	BA	1790	1/1	0.85	0.15	83,83,83,83	0
55	MG	CA	1617	1/1	0.85	0.33	91,91,91,91	0
55	MG	AA	3599	1/1	0.85	0.28	84,84,84,84	0
55	MG	BA	1626	1/1	0.85	0.29	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1724	1/1	0.85	0.21	100,100,100,100	0
55	MG	AA	3274	1/1	0.85	0.27	77,77,77,77	0
55	MG	BA	1727	1/1	0.85	0.32	125,125,125,125	0
55	MG	DA	3469	1/1	0.85	0.19	64,64,64,64	0
55	MG	BA	1806	1/1	0.85	0.20	75,75,75,75	0
55	MG	BA	1728	1/1	0.85	0.08	90,90,90,90	0
55	MG	AA	3604	1/1	0.85	0.15	84,84,84,84	0
55	MG	BA	1818	1/1	0.85	0.15	82,82,82,82	0
55	MG	DA	3311	1/1	0.85	0.12	80,80,80,80	0
55	MG	DA	3485	1/1	0.85	0.23	40,40,40,40	0
55	MG	DA	3496	1/1	0.85	0.31	85,85,85,85	0
55	MG	AA	3618	1/1	0.85	0.25	76,76,76,76	0
55	MG	AA	3619	1/1	0.85	0.26	94,94,94,94	0
55	MG	AA	3447	1/1	0.85	0.10	51,51,51,51	0
55	MG	DA	3085	1/1	0.85	0.12	89,89,89,89	0
55	MG	DA	3086	1/1	0.85	0.18	98,98,98,98	0
55	MG	CA	1640	1/1	0.85	0.25	78,78,78,78	0
55	MG	DA	3331	1/1	0.85	0.12	76,76,76,76	0
55	MG	AA	3176	1/1	0.85	0.32	38,38,38,38	0
55	MG	DA	3115	1/1	0.85	0.30	76,76,76,76	0
55	MG	CA	1780	1/1	0.85	0.18	124,124,124,124	0
55	MG	AA	3190	1/1	0.85	0.51	83,83,83,83	0
55	MG	AA	3091	1/1	0.85	0.30	69,69,69,69	0
55	MG	DA	3346	1/1	0.85	0.42	83,83,83,83	0
55	MG	DB	207	1/1	0.85	0.23	98,98,98,98	0
55	MG	DA	3349	1/1	0.85	0.25	83,83,83,83	0
55	MG	BA	1654	1/1	0.85	0.34	74,74,74,74	0
55	MG	DA	3353	1/1	0.85	0.34	70,70,70,70	0
55	MG	DA	3355	1/1	0.85	0.29	93,93,93,93	0
55	MG	DU	201	1/1	0.85	0.24	72,72,72,72	0
55	MG	D3	101	1/1	0.85	0.25	68,68,68,68	0
55	MG	AA	3302	1/1	0.86	0.23	84,84,84,84	0
55	MG	BA	1759	1/1	0.86	0.23	97,97,97,97	0
55	MG	DA	3137	1/1	0.86	0.17	78,78,78,78	0
55	MG	DA	3156	1/1	0.86	0.71	62,62,62,62	0
55	MG	AA	3529	1/1	0.86	0.28	78,78,78,78	0
55	MG	DA	3167	1/1	0.86	0.12	72,72,72,72	0
55	MG	BA	1764	1/1	0.86	0.29	93,93,93,93	0
55	MG	CA	1680	1/1	0.86	0.30	68,68,68,68	0
55	MG	AA	3630	1/1	0.86	0.21	92,92,92,92	0
55	MG	DA	3192	1/1	0.86	0.22	51,51,51,51	0
55	MG	DA	3204	1/1	0.86	0.21	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1766	1/1	0.86	0.20	116,116,116,116	0
55	MG	BB	101	1/1	0.86	0.12	88,88,88,88	0
55	MG	BA	1767	1/1	0.86	0.23	101,101,101,101	0
55	MG	AA	3307	1/1	0.86	0.47	75,75,75,75	0
55	MG	CA	1702	1/1	0.86	0.28	74,74,74,74	0
55	MG	CA	1703	1/1	0.86	0.10	88,88,88,88	0
55	MG	CC	106	1/1	0.86	0.27	115,115,115,115	0
55	MG	DA	3423	1/1	0.86	0.37	102,102,102,102	0
55	MG	AA	3272	1/1	0.86	0.23	86,86,86,86	0
55	MG	CA	1707	1/1	0.86	0.55	88,88,88,88	0
55	MG	DA	3427	1/1	0.86	0.20	78,78,78,78	0
55	MG	AA	3555	1/1	0.86	0.17	68,68,68,68	0
55	MG	DA	3430	1/1	0.86	0.26	102,102,102,102	0
55	MG	AA	3314	1/1	0.86	0.16	82,82,82,82	0
55	MG	AB	211	1/1	0.86	0.23	105,105,105,105	0
55	MG	AA	3363	1/1	0.86	0.17	80,80,80,80	0
55	MG	AA	3078	1/1	0.86	0.14	84,84,84,84	0
55	MG	BA	1665	1/1	0.86	0.28	66,66,66,66	0
55	MG	AA	3237	1/1	0.86	0.15	81,81,81,81	0
55	MG	CA	1724	1/1	0.86	0.31	88,88,88,88	0
55	MG	CA	1613	1/1	0.86	0.40	84,84,84,84	0
55	MG	DA	3274	1/1	0.86	0.57	80,80,80,80	0
55	MG	BA	1794	1/1	0.86	0.49	94,94,94,94	0
55	MG	BA	1672	1/1	0.86	0.25	104,104,104,104	0
55	MG	AA	3561	1/1	0.86	0.18	88,88,88,88	0
55	MG	DA	3055	1/1	0.86	0.39	80,80,80,80	0
55	MG	BA	1737	1/1	0.86	0.13	102,102,102,102	0
55	MG	DA	3057	1/1	0.86	0.31	81,81,81,81	0
55	MG	BA	1677	1/1	0.86	0.34	92,92,92,92	0
55	MG	AA	3323	1/1	0.86	0.55	93,93,93,93	0
55	MG	DA	3062	1/1	0.86	0.11	85,85,85,85	0
55	MG	BA	1808	1/1	0.86	0.29	69,69,69,69	0
55	MG	AA	3414	1/1	0.86	0.14	68,68,68,68	0
55	MG	BA	1604	1/1	0.86	0.32	77,77,77,77	0
55	MG	DA	3481	1/1	0.86	0.32	45,45,45,45	0
55	MG	AA	3452	1/1	0.86	0.33	95,95,95,95	0
55	MG	DA	3489	1/1	0.86	0.41	57,57,57,57	0
55	MG	AA	3415	1/1	0.86	0.23	86,86,86,86	0
55	MG	CA	1755	1/1	0.86	0.53	94,94,94,94	0
55	MG	CA	1756	1/1	0.86	0.21	93,93,93,93	0
55	MG	AA	3017	1/1	0.86	0.24	59,59,59,59	0
55	MG	DA	3328	1/1	0.86	0.23	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
55	MG	BA	1615	1/1	0.86	0.27	104,104,104,104	0
55	MG	AA	3242	1/1	0.86	0.29	58,58,58,58	0
55	MG	DA	3516	1/1	0.86	0.18	60,60,60,60	0
55	MG	DA	3091	1/1	0.86	0.38	52,52,52,52	0
55	MG	BA	1825	1/1	0.86	0.22	104,104,104,104	0
55	MG	AA	3122	1/1	0.86	0.24	87,87,87,87	0
55	MG	DA	3522	1/1	0.86	0.36	85,85,85,85	0
55	MG	AA	3298	1/1	0.86	0.28	80,80,80,80	0
55	MG	DA	3344	1/1	0.86	0.46	93,93,93,93	0
55	MG	CA	1654	1/1	0.86	0.20	88,88,88,88	0
55	MG	AA	3621	1/1	0.86	0.16	100,100,100,100	0
55	MG	AA	3094	1/1	0.86	0.16	81,81,81,81	0
55	MG	BA	1755	1/1	0.86	0.14	106,106,106,106	0
55	MG	CA	1785	1/1	0.86	0.25	81,81,81,81	0
55	MG	DA	3131	1/1	0.86	0.17	93,93,93,93	0
55	MG	CA	1660	1/1	0.86	0.17	76,76,76,76	0
55	MG	DA	3362	1/1	0.86	0.18	86,86,86,86	0
55	MG	BA	1835	1/1	0.86	0.40	82,82,82,82	0
55	MG	CA	1609	1/1	0.87	0.25	108,108,108,108	0
55	MG	DA	3003	1/1	0.87	0.22	70,70,70,70	0
55	MG	BA	1731	1/1	0.87	0.29	67,67,67,67	0
55	MG	DA	3198	1/1	0.87	0.27	68,68,68,68	0
55	MG	AA	3181	1/1	0.87	0.21	92,92,92,92	0
55	MG	BA	1799	1/1	0.87	0.27	85,85,85,85	0
55	MG	DA	3391	1/1	0.87	0.24	86,86,86,86	0
55	MG	BA	1734	1/1	0.87	0.29	96,96,96,96	0
55	MG	DA	3218	1/1	0.87	0.46	75,75,75,75	0
55	MG	AA	3535	1/1	0.87	0.16	82,82,82,82	0
55	MG	AA	3541	1/1	0.87	0.12	94,94,94,94	0
55	MG	AA	3101	1/1	0.87	0.08	69,69,69,69	0
55	MG	AB	210	1/1	0.87	0.46	71,71,71,71	0
55	MG	DA	3036	1/1	0.87	0.49	87,87,87,87	0
55	MG	AA	3235	1/1	0.87	0.21	86,86,86,86	0
55	MG	DA	3408	1/1	0.87	0.16	61,61,61,61	0
55	MG	DA	3243	1/1	0.87	0.17	83,83,83,83	0
55	MG	DA	3043	1/1	0.87	0.21	81,81,81,81	0
55	MG	DA	3414	1/1	0.87	0.30	74,74,74,74	0
55	MG	DA	3246	1/1	0.87	0.34	66,66,66,66	0
55	MG	AA	3046	1/1	0.87	0.21	54,54,54,54	0
55	MG	AA	3493	1/1	0.87	0.26	89,89,89,89	0
55	MG	AA	3208	1/1	0.87	0.18	66,66,66,66	0
55	MG	AA	3345	1/1	0.87	0.16	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3256	1/1	0.87	0.30	82,82,82,82	0
55	MG	DA	3257	1/1	0.87	0.15	75,75,75,75	0
55	MG	AA	3568	1/1	0.87	0.24	29,29,29,29	0
55	MG	AA	3570	1/1	0.87	0.16	49,49,49,49	0
55	MG	BA	1601	1/1	0.87	0.48	65,65,65,65	0
55	MG	DA	3435	1/1	0.87	0.23	104,104,104,104	0
55	MG	AA	3418	1/1	0.87	0.50	85,85,85,85	0
55	MG	AA	3498	1/1	0.87	0.28	86,86,86,86	0
55	MG	DA	3273	1/1	0.87	0.11	108,108,108,108	0
55	MG	BA	1607	1/1	0.87	0.12	87,87,87,87	0
55	MG	DA	3275	1/1	0.87	0.35	81,81,81,81	0
55	MG	CA	1650	1/1	0.87	0.22	90,90,90,90	0
55	MG	CA	1653	1/1	0.87	0.33	73,73,73,73	0
55	MG	DA	3281	1/1	0.87	0.18	75,75,75,75	0
55	MG	AA	3593	1/1	0.87	0.29	90,90,90,90	0
55	MG	DA	3070	1/1	0.87	0.31	73,73,73,73	0
55	MG	DA	3288	1/1	0.87	0.21	82,82,82,82	0
55	MG	AA	3596	1/1	0.87	0.28	87,87,87,87	0
55	MG	BA	1700	1/1	0.87	0.26	97,97,97,97	0
55	MG	AA	3303	1/1	0.87	0.20	91,91,91,91	0
55	MG	DA	3082	1/1	0.87	0.24	83,83,83,83	0
55	MG	DA	3474	1/1	0.87	0.29	103,103,103,103	0
55	MG	BA	1762	1/1	0.87	0.23	85,85,85,85	0
55	MG	BA	1705	1/1	0.87	0.39	70,70,70,70	0
55	MG	AA	3171	1/1	0.87	0.14	81,81,81,81	0
55	MG	AA	3043	1/1	0.87	0.21	83,83,83,83	0
55	MG	AA	3424	1/1	0.87	0.26	77,77,77,77	0
55	MG	DA	3107	1/1	0.87	0.32	89,89,89,89	0
55	MG	DA	3321	1/1	0.87	0.24	81,81,81,81	0
55	MG	AA	3390	1/1	0.87	0.20	73,73,73,73	0
55	MG	DA	3111	1/1	0.87	0.38	67,67,67,67	0
55	MG	BB	102	1/1	0.87	0.18	86,86,86,86	0
55	MG	CA	1682	1/1	0.87	0.28	97,97,97,97	0
55	MG	DA	3120	1/1	0.87	0.30	78,78,78,78	0
55	MG	AA	3512	1/1	0.87	0.46	71,71,71,71	0
55	MG	DA	3507	1/1	0.87	0.25	88,88,88,88	0
55	MG	AA	3428	1/1	0.87	0.24	106,106,106,106	0
55	MG	AA	3246	1/1	0.87	0.37	73,73,73,73	0
55	MG	DA	3519	1/1	0.87	0.29	114,114,114,114	0
55	MG	CA	1690	1/1	0.87	0.33	74,74,74,74	0
55	MG	CA	1691	1/1	0.87	0.23	69,69,69,69	0
55	MG	BA	1631	1/1	0.87	0.11	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CG	303	1/1	0.87	0.17	100,100,100,100	0
55	MG	DA	3348	1/1	0.87	0.23	77,77,77,77	0
55	MG	DA	3527	1/1	0.87	0.28	96,96,96,96	0
55	MG	BB	108	1/1	0.87	0.24	106,106,106,106	0
55	MG	AA	3126	1/1	0.87	0.17	63,63,63,63	0
55	MG	AA	3627	1/1	0.87	0.28	108,108,108,108	0
55	MG	DA	3142	1/1	0.87	0.27	51,51,51,51	0
55	MG	DA	3151	1/1	0.87	0.27	75,75,75,75	0
55	MG	AA	3471	1/1	0.87	0.16	69,69,69,69	0
55	MG	DB	213	1/1	0.87	0.13	90,90,90,90	0
55	MG	AA	3226	1/1	0.87	0.29	85,85,85,85	0
55	MG	CA	1601	1/1	0.87	0.27	95,95,95,95	0
55	MG	BA	1640	1/1	0.87	0.28	80,80,80,80	0
55	MG	DA	3268	1/1	0.88	0.20	82,82,82,82	0
55	MG	DA	3101	1/1	0.88	0.40	57,57,57,57	0
55	MG	DA	3407	1/1	0.88	0.12	80,80,80,80	0
55	MG	AA	3287	1/1	0.88	0.23	88,88,88,88	0
55	MG	CA	1714	1/1	0.88	0.16	115,115,115,115	0
55	MG	AA	3312	1/1	0.88	0.13	88,88,88,88	0
55	MG	AA	3233	1/1	0.88	0.10	74,74,74,74	0
55	MG	DA	3417	1/1	0.88	0.26	83,83,83,83	0
55	MG	DA	3114	1/1	0.88	0.53	70,70,70,70	0
55	MG	AA	3554	1/1	0.88	0.18	86,86,86,86	0
55	MG	AA	3360	1/1	0.88	0.27	89,89,89,89	0
55	MG	DA	3117	1/1	0.88	0.22	68,68,68,68	0
55	MG	DA	3284	1/1	0.88	0.18	81,81,81,81	0
55	MG	AA	3294	1/1	0.88	0.46	99,99,99,99	0
55	MG	DA	3121	1/1	0.88	0.20	99,99,99,99	0
55	MG	AA	3261	1/1	0.88	0.16	30,30,30,30	0
55	MG	AA	3013	1/1	0.88	0.21	49,49,49,49	0
55	MG	AA	3449	1/1	0.88	0.14	76,76,76,76	0
55	MG	AB	208	1/1	0.88	0.22	87,87,87,87	0
55	MG	DA	3304	1/1	0.88	0.24	106,106,106,106	0
55	MG	DA	3307	1/1	0.88	0.34	77,77,77,77	0
55	MG	AA	3049	1/1	0.88	0.20	106,106,106,106	0
55	MG	CA	1736	1/1	0.88	0.23	90,90,90,90	0
55	MG	AA	3369	1/1	0.88	0.25	85,85,85,85	0
55	MG	CA	1647	1/1	0.88	0.32	65,65,65,65	0
55	MG	BA	1768	1/1	0.88	0.17	86,86,86,86	0
55	MG	BA	1769	1/1	0.88	0.34	86,86,86,86	0
55	MG	BA	1643	1/1	0.88	0.19	80,80,80,80	0
55	MG	DA	3451	1/1	0.88	0.23	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AB	214	1/1	0.88	0.05	88,88,88,88	0
55	MG	AA	3299	1/1	0.88	0.23	94,94,94,94	0
55	MG	AA	3453	1/1	0.88	0.20	47,47,47,47	0
55	MG	DA	3164	1/1	0.88	0.21	65,65,65,65	0
55	MG	DA	3329	1/1	0.88	0.27	80,80,80,80	0
55	MG	DA	3041	1/1	0.88	0.20	91,91,91,91	0
55	MG	DA	3042	1/1	0.88	0.09	84,84,84,84	0
55	MG	DA	3180	1/1	0.88	0.31	50,50,50,50	0
55	MG	DA	3339	1/1	0.88	0.36	77,77,77,77	0
55	MG	BA	1652	1/1	0.88	0.19	86,86,86,86	0
55	MG	AA	3372	1/1	0.88	0.22	77,77,77,77	0
55	MG	BA	1664	1/1	0.88	0.20	52,52,52,52	0
55	MG	AD	302	1/1	0.88	0.15	44,44,44,44	0
55	MG	DA	3494	1/1	0.88	0.42	81,81,81,81	0
55	MG	AA	3123	1/1	0.88	0.29	47,47,47,47	0
55	MG	DA	3207	1/1	0.88	0.19	61,61,61,61	0
55	MG	AA	3213	1/1	0.88	0.56	50,50,50,50	0
55	MG	CA	1766	1/1	0.88	0.23	75,75,75,75	0
55	MG	AA	3379	1/1	0.88	0.14	88,88,88,88	0
55	MG	DA	3221	1/1	0.88	0.41	66,66,66,66	0
55	MG	BA	1675	1/1	0.88	0.18	89,89,89,89	0
55	MG	BC	108	1/1	0.88	0.24	101,101,101,101	0
55	MG	AA	3061	1/1	0.88	0.17	75,75,75,75	0
55	MG	AA	3602	1/1	0.88	0.12	70,70,70,70	0
55	MG	AA	3384	1/1	0.88	0.38	79,79,79,79	0
55	MG	DA	3368	1/1	0.88	0.20	87,87,87,87	0
55	MG	AA	3613	1/1	0.88	0.10	104,104,104,104	0
55	MG	DA	3374	1/1	0.88	0.33	72,72,72,72	0
55	MG	AA	3306	1/1	0.88	0.32	63,63,63,63	0
55	MG	DA	3075	1/1	0.88	0.34	80,80,80,80	0
55	MG	CA	1788	1/1	0.88	0.30	68,68,68,68	0
55	MG	DB	201	1/1	0.88	0.20	77,77,77,77	0
55	MG	CA	1695	1/1	0.88	0.31	77,77,77,77	0
55	MG	AA	3285	1/1	0.88	0.26	77,77,77,77	0
55	MG	DA	3081	1/1	0.88	0.18	73,73,73,73	0
55	MG	BA	1811	1/1	0.88	0.26	86,86,86,86	0
55	MG	DB	209	1/1	0.88	0.24	103,103,103,103	0
55	MG	BA	1614	1/1	0.88	0.28	93,93,93,93	0
55	MG	BA	1815	1/1	0.88	0.48	81,81,81,81	0
55	MG	AA	3530	1/1	0.88	0.10	65,65,65,65	0
55	MG	AA	3475	1/1	0.88	0.23	67,67,67,67	0
55	MG	D1	202	1/1	0.88	0.18	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3399	1/1	0.88	0.24	97,97,97,97	0
55	MG	DA	3096	1/1	0.88	0.22	47,47,47,47	0
55	MG	CA	1644	1/1	0.89	0.14	59,59,59,59	0
55	MG	DA	3354	1/1	0.89	0.38	92,92,92,92	0
55	MG	AB	209	1/1	0.89	0.22	103,103,103,103	0
55	MG	AA	3330	1/1	0.89	0.12	61,61,61,61	0
55	MG	DA	3358	1/1	0.89	0.23	90,90,90,90	0
55	MG	BA	1653	1/1	0.89	0.28	91,91,91,91	0
55	MG	AA	3037	1/1	0.89	0.17	50,50,50,50	0
55	MG	AA	3334	1/1	0.89	0.18	73,73,73,73	0
55	MG	AA	3479	1/1	0.89	0.20	97,97,97,97	0
55	MG	BA	1666	1/1	0.89	0.30	74,74,74,74	0
55	MG	DA	3370	1/1	0.89	0.28	85,85,85,85	0
55	MG	CA	1798	1/1	0.89	0.25	96,96,96,96	0
55	MG	BA	1830	1/1	0.89	0.24	96,96,96,96	0
55	MG	DA	3375	1/1	0.89	0.12	82,82,82,82	0
55	MG	AA	3480	1/1	0.89	0.13	77,77,77,77	0
55	MG	BA	1670	1/1	0.89	0.22	62,62,62,62	0
55	MG	DA	3379	1/1	0.89	0.52	99,99,99,99	0
55	MG	AA	3483	1/1	0.89	0.21	70,70,70,70	0
55	MG	DA	3170	1/1	0.89	0.30	66,66,66,66	0
55	MG	AA	3121	1/1	0.89	0.37	93,93,93,93	0
55	MG	BA	1837	1/1	0.89	0.27	88,88,88,88	0
55	MG	CA	1668	1/1	0.89	0.30	75,75,75,75	0
55	MG	DA	3184	1/1	0.89	0.22	71,71,71,71	0
55	MG	CA	1672	1/1	0.89	0.34	76,76,76,76	0
55	MG	DA	3190	1/1	0.89	0.16	46,46,46,46	0
55	MG	DA	3191	1/1	0.89	0.26	47,47,47,47	0
55	MG	CA	1675	1/1	0.89	0.30	65,65,65,65	0
55	MG	CB	103	1/1	0.89	0.20	110,110,110,110	0
55	MG	DA	3200	1/1	0.89	0.38	66,66,66,66	0
55	MG	AA	3147	1/1	0.89	0.36	77,77,77,77	0
55	MG	AA	3260	1/1	0.89	0.16	70,70,70,70	0
55	MG	BA	1843	1/1	0.89	0.14	87,87,87,87	0
55	MG	AA	3491	1/1	0.89	0.35	93,93,93,93	0
55	MG	A3	101	1/1	0.89	0.44	80,80,80,80	0
55	MG	A5	102	1/1	0.89	0.16	75,75,75,75	0
55	MG	AA	3578	1/1	0.89	0.15	52,52,52,52	0
55	MG	AA	3437	1/1	0.89	0.19	105,105,105,105	0
55	MG	DA	3232	1/1	0.89	0.12	75,75,75,75	0
55	MG	BA	1689	1/1	0.89	0.17	110,110,110,110	0
55	MG	DA	3237	1/1	0.89	0.42	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3012	1/1	0.89	0.14	64,64,64,64	0
55	MG	DA	3015	1/1	0.89	0.12	83,83,83,83	0
55	MG	DA	3017	1/1	0.89	0.25	88,88,88,88	0
55	MG	CA	1696	1/1	0.89	0.20	79,79,79,79	0
55	MG	DA	3019	1/1	0.89	0.31	66,66,66,66	0
55	MG	AA	3438	1/1	0.89	0.14	77,77,77,77	0
55	MG	AA	3441	1/1	0.89	0.07	76,76,76,76	0
55	MG	DA	3024	1/1	0.89	0.16	100,100,100,100	0
55	MG	BA	1608	1/1	0.89	0.31	63,63,63,63	0
55	MG	AA	3203	1/1	0.89	0.32	53,53,53,53	0
55	MG	DA	3035	1/1	0.89	0.24	102,102,102,102	0
55	MG	AA	3207	1/1	0.89	0.32	44,44,44,44	0
55	MG	CA	1708	1/1	0.89	0.22	91,91,91,91	0
55	MG	BA	1612	1/1	0.89	0.23	90,90,90,90	0
55	MG	CA	1711	1/1	0.89	0.26	88,88,88,88	0
55	MG	DA	3448	1/1	0.89	0.20	75,75,75,75	0
55	MG	BA	1771	1/1	0.89	0.16	100,100,100,100	0
55	MG	DA	3450	1/1	0.89	0.31	86,86,86,86	0
55	MG	AA	3069	1/1	0.89	0.36	64,64,64,64	0
55	MG	BC	106	1/1	0.89	0.18	80,80,80,80	0
55	MG	DA	3454	1/1	0.89	0.23	108,108,108,108	0
55	MG	DA	3051	1/1	0.89	0.24	81,81,81,81	0
55	MG	BA	1776	1/1	0.89	0.14	84,84,84,84	0
55	MG	AA	3354	1/1	0.89	0.35	79,79,79,79	0
55	MG	BA	1783	1/1	0.89	0.17	91,91,91,91	0
55	MG	CA	1721	1/1	0.89	0.16	94,94,94,94	0
55	MG	DA	3279	1/1	0.89	0.25	66,66,66,66	0
55	MG	CA	1604	1/1	0.89	0.19	78,78,78,78	0
55	MG	AA	3269	1/1	0.89	0.33	72,72,72,72	0
55	MG	CA	1725	1/1	0.89	0.23	75,75,75,75	0
55	MG	CA	1607	1/1	0.89	0.27	77,77,77,77	0
55	MG	BA	1618	1/1	0.89	0.29	94,94,94,94	0
55	MG	AA	3210	1/1	0.89	0.24	58,58,58,58	0
55	MG	CA	1732	1/1	0.89	0.18	93,93,93,93	0
55	MG	AA	3405	1/1	0.89	0.25	86,86,86,86	0
55	MG	AA	3048	1/1	0.89	0.18	63,63,63,63	0
55	MG	AA	3098	1/1	0.89	0.18	71,71,71,71	0
55	MG	DA	3305	1/1	0.89	0.13	83,83,83,83	0
55	MG	CA	1743	1/1	0.89	0.40	71,71,71,71	0
55	MG	AA	3279	1/1	0.89	0.10	81,81,81,81	0
55	MG	AA	3219	1/1	0.89	0.30	60,60,60,60	0
55	MG	DA	3506	1/1	0.89	0.41	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
55	MG	DA	3310	1/1	0.89	0.22	80,80,80,80	0
55	MG	DA	3513	1/1	0.89	0.23	103,103,103,103	0
55	MG	BA	1630	1/1	0.89	0.15	105,105,105,105	0
55	MG	DA	3517	1/1	0.89	0.28	62,62,62,62	0
55	MG	AA	3526	1/1	0.89	0.20	57,57,57,57	0
55	MG	BA	1801	1/1	0.89	0.11	93,93,93,93	0
55	MG	CA	1752	1/1	0.89	0.09	70,70,70,70	0
55	MG	AA	3417	1/1	0.89	0.12	78,78,78,78	0
55	MG	AA	3221	1/1	0.89	0.24	51,51,51,51	0
55	MG	BA	1730	1/1	0.89	0.25	97,97,97,97	0
55	MG	AA	3113	1/1	0.89	0.33	55,55,55,55	0
55	MG	CA	1633	1/1	0.89	0.39	79,79,79,79	0
55	MG	DA	3108	1/1	0.89	0.23	69,69,69,69	0
55	MG	DB	202	1/1	0.89	0.25	101,101,101,101	0
55	MG	CA	1760	1/1	0.89	0.30	103,103,103,103	0
55	MG	AA	3533	1/1	0.89	0.14	89,89,89,89	0
55	MG	AA	3371	1/1	0.89	0.18	69,69,69,69	0
55	MG	CA	1636	1/1	0.89	0.26	80,80,80,80	0
55	MG	CA	1765	1/1	0.89	0.34	97,97,97,97	0
55	MG	AB	204	1/1	0.89	0.27	94,94,94,94	0
55	MG	DB	211	1/1	0.89	0.28	104,104,104,104	0
55	MG	DA	3118	1/1	0.89	0.55	72,72,72,72	0
55	MG	CA	1767	1/1	0.89	0.20	94,94,94,94	0
55	MG	AA	3292	1/1	0.89	0.22	80,80,80,80	0
55	MG	BA	1817	1/1	0.89	0.32	92,92,92,92	0
55	MG	CA	1642	1/1	0.89	0.22	78,78,78,78	0
55	MG	AA	3173	1/1	0.89	0.33	70,70,70,70	0
55	MG	AA	3511	1/1	0.90	0.22	51,51,51,51	0
55	MG	DA	3186	1/1	0.90	0.36	56,56,56,56	0
55	MG	DA	3188	1/1	0.90	0.32	48,48,48,48	0
55	MG	AA	3448	1/1	0.90	0.18	85,85,85,85	0
55	MG	DA	3373	1/1	0.90	0.17	90,90,90,90	0
55	MG	AA	3109	1/1	0.90	0.12	33,33,33,33	0
55	MG	AA	3520	1/1	0.90	0.39	97,97,97,97	0
55	MG	AA	3141	1/1	0.90	0.34	37,37,37,37	0
55	MG	AB	206	1/1	0.90	0.22	97,97,97,97	0
55	MG	AA	3044	1/1	0.90	0.43	54,54,54,54	0
55	MG	DA	3206	1/1	0.90	0.23	65,65,65,65	0
55	MG	AA	3183	1/1	0.90	0.09	79,79,79,79	0
55	MG	BA	1668	1/1	0.90	0.37	73,73,73,73	0
55	MG	BA	1761	1/1	0.90	0.33	85,85,85,85	0
55	MG	AA	3222	1/1	0.90	0.16	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3026	1/1	0.90	0.16	35,35,35,35	0
55	MG	AA	3410	1/1	0.90	0.12	99,99,99,99	0
55	MG	AB	212	1/1	0.90	0.23	76,76,76,76	0
55	MG	DA	3029	1/1	0.90	0.12	92,92,92,92	0
55	MG	BC	109	1/1	0.90	0.24	92,92,92,92	0
55	MG	AA	3100	1/1	0.90	0.14	79,79,79,79	0
55	MG	AA	3412	1/1	0.90	0.47	88,88,88,88	0
55	MG	AA	3162	1/1	0.90	0.27	45,45,45,45	0
55	MG	BA	1679	1/1	0.90	0.25	86,86,86,86	0
55	MG	AA	3362	1/1	0.90	0.26	86,86,86,86	0
55	MG	BA	1682	1/1	0.90	0.28	98,98,98,98	0
55	MG	AA	3543	1/1	0.90	0.28	61,61,61,61	0
55	MG	AA	3416	1/1	0.90	0.23	70,70,70,70	0
55	MG	DA	3415	1/1	0.90	0.14	84,84,84,84	0
55	MG	AA	3304	1/1	0.90	0.22	59,59,59,59	0
55	MG	CA	1615	1/1	0.90	0.18	92,92,92,92	0
55	MG	DA	3251	1/1	0.90	0.15	50,50,50,50	0
55	MG	BA	1687	1/1	0.90	0.32	74,74,74,74	0
55	MG	DA	3255	1/1	0.90	0.25	83,83,83,83	0
55	MG	AA	3263	1/1	0.90	0.18	56,56,56,56	0
55	MG	CA	1620	1/1	0.90	0.32	70,70,70,70	0
55	MG	CA	1741	1/1	0.90	0.16	83,83,83,83	0
55	MG	AA	3476	1/1	0.90	0.17	94,94,94,94	0
55	MG	AA	3079	1/1	0.90	0.20	100,100,100,100	0
55	MG	A6	101	1/1	0.90	0.27	121,121,121,121	0
55	MG	AA	3191	1/1	0.90	0.31	61,61,61,61	0
55	MG	BA	1699	1/1	0.90	0.20	58,58,58,58	0
55	MG	DA	3067	1/1	0.90	0.27	75,75,75,75	0
55	MG	AA	3270	1/1	0.90	0.19	96,96,96,96	0
55	MG	AA	3041	1/1	0.90	0.29	62,62,62,62	0
55	MG	BA	1703	1/1	0.90	0.24	118,118,118,118	0
55	MG	DA	3443	1/1	0.90	0.26	94,94,94,94	0
55	MG	BA	1704	1/1	0.90	0.21	87,87,87,87	0
55	MG	AA	3481	1/1	0.90	0.28	66,66,66,66	0
55	MG	AA	3167	1/1	0.90	0.26	51,51,51,51	0
55	MG	DA	3080	1/1	0.90	0.15	114,114,114,114	0
55	MG	AA	3195	1/1	0.90	0.22	62,62,62,62	0
55	MG	BA	1610	1/1	0.90	0.29	53,53,53,53	0
55	MG	DA	3286	1/1	0.90	0.11	86,86,86,86	0
55	MG	AA	3429	1/1	0.90	0.37	85,85,85,85	0
55	MG	AA	3489	1/1	0.90	0.16	93,93,93,93	0
55	MG	DA	3297	1/1	0.90	0.28	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3458	1/1	0.90	0.22	88,88,88,88	0
55	MG	BA	1613	1/1	0.90	0.11	96,96,96,96	0
55	MG	AA	3594	1/1	0.90	0.22	97,97,97,97	0
55	MG	BA	1722	1/1	0.90	0.20	90,90,90,90	0
55	MG	DA	3097	1/1	0.90	0.25	42,42,42,42	0
55	MG	CA	1645	1/1	0.90	0.54	71,71,71,71	0
55	MG	AA	3373	1/1	0.90	0.25	71,71,71,71	0
55	MG	CA	1768	1/1	0.90	0.39	115,115,115,115	0
55	MG	CA	1648	1/1	0.90	0.20	65,65,65,65	0
55	MG	AA	3598	1/1	0.90	0.18	84,84,84,84	0
55	MG	CA	1772	1/1	0.90	0.17	76,76,76,76	0
55	MG	CA	1651	1/1	0.90	0.20	79,79,79,79	0
55	MG	DA	3314	1/1	0.90	0.15	78,78,78,78	0
55	MG	AA	3322	1/1	0.90	0.14	83,83,83,83	0
55	MG	DA	3317	1/1	0.90	0.17	87,87,87,87	0
55	MG	CA	1779	1/1	0.90	0.24	82,82,82,82	0
55	MG	DA	3319	1/1	0.90	0.31	68,68,68,68	0
55	MG	AA	3168	1/1	0.90	0.24	64,64,64,64	0
55	MG	DA	3323	1/1	0.90	0.37	85,85,85,85	0
55	MG	AA	3494	1/1	0.90	0.30	88,88,88,88	0
55	MG	CA	1656	1/1	0.90	0.17	87,87,87,87	0
55	MG	AA	3282	1/1	0.90	0.40	87,87,87,87	0
55	MG	CA	1787	1/1	0.90	0.27	84,84,84,84	0
55	MG	AA	3610	1/1	0.90	0.23	34,34,34,34	0
55	MG	AA	3611	1/1	0.90	0.29	54,54,54,54	0
55	MG	CA	1790	1/1	0.90	0.23	75,75,75,75	0
55	MG	AA	3284	1/1	0.90	0.47	80,80,80,80	0
55	MG	AA	3383	1/1	0.90	0.12	70,70,70,70	0
55	MG	AA	3439	1/1	0.90	0.08	93,93,93,93	0
55	MG	DA	3341	1/1	0.90	0.32	62,62,62,62	0
55	MG	BA	1633	1/1	0.90	0.30	75,75,75,75	0
55	MG	CA	1666	1/1	0.90	0.30	76,76,76,76	0
55	MG	BA	1635	1/1	0.90	0.18	87,87,87,87	0
55	MG	DA	3345	1/1	0.90	0.16	75,75,75,75	0
55	MG	DA	3140	1/1	0.90	0.31	49,49,49,49	0
55	MG	AA	3093	1/1	0.90	0.14	55,55,55,55	0
55	MG	DB	205	1/1	0.90	0.32	90,90,90,90	0
55	MG	AA	3172	1/1	0.90	0.22	102,102,102,102	0
55	MG	DA	3350	1/1	0.90	0.21	79,79,79,79	0
55	MG	CA	1673	1/1	0.90	0.22	65,65,65,65	0
55	MG	AA	3129	1/1	0.90	0.31	75,75,75,75	0
55	MG	CA	1679	1/1	0.90	0.16	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1839	1/1	0.90	0.23	61,61,61,61	0
55	MG	AA	3338	1/1	0.90	0.18	72,72,72,72	0
55	MG	AA	3004	1/1	0.90	0.16	37,37,37,37	0
55	MG	DA	3359	1/1	0.90	0.16	75,75,75,75	0
55	MG	AA	3628	1/1	0.90	0.14	89,89,89,89	0
55	MG	AA	3510	1/1	0.90	0.26	73,73,73,73	0
55	MG	BN	201	1/1	0.90	0.21	67,67,67,67	0
55	MG	BA	1826	1/1	0.91	0.25	73,73,73,73	0
55	MG	AA	3617	1/1	0.91	0.12	92,92,92,92	0
55	MG	DA	3195	1/1	0.91	0.14	73,73,73,73	0
55	MG	AA	3516	1/1	0.91	0.21	57,57,57,57	0
55	MG	DA	3199	1/1	0.91	0.17	49,49,49,49	0
55	MG	DA	3027	1/1	0.91	0.23	93,93,93,93	0
55	MG	AA	3245	1/1	0.91	0.24	81,81,81,81	0
55	MG	CA	1641	1/1	0.91	0.11	101,101,101,101	0
55	MG	AA	3467	1/1	0.91	0.17	83,83,83,83	0
55	MG	BA	1832	1/1	0.91	0.19	100,100,100,100	0
55	MG	DA	3037	1/1	0.91	0.10	84,84,84,84	0
55	MG	DA	3381	1/1	0.91	0.26	89,89,89,89	0
55	MG	AA	3283	1/1	0.91	0.29	74,74,74,74	0
55	MG	DA	3039	1/1	0.91	0.28	82,82,82,82	0
55	MG	DA	3389	1/1	0.91	0.30	85,85,85,85	0
55	MG	AA	3050	1/1	0.91	0.20	69,69,69,69	0
55	MG	AA	3472	1/1	0.91	0.13	81,81,81,81	0
55	MG	BA	1688	1/1	0.91	0.20	76,76,76,76	0
55	MG	DA	3234	1/1	0.91	0.36	55,55,55,55	0
55	MG	AA	3626	1/1	0.91	0.34	63,63,63,63	0
55	MG	AA	3051	1/1	0.91	0.20	51,51,51,51	0
55	MG	DA	3238	1/1	0.91	0.32	80,80,80,80	0
55	MG	DA	3047	1/1	0.91	0.22	84,84,84,84	0
55	MG	DA	3402	1/1	0.91	0.18	73,73,73,73	0
55	MG	DA	3050	1/1	0.91	0.50	78,78,78,78	0
55	MG	AA	3024	1/1	0.91	0.26	35,35,35,35	0
55	MG	DA	3053	1/1	0.91	0.14	86,86,86,86	0
55	MG	BA	1694	1/1	0.91	0.11	99,99,99,99	0
55	MG	AA	3220	1/1	0.91	0.16	44,44,44,44	0
55	MG	CA	1757	1/1	0.91	0.18	83,83,83,83	0
55	MG	BA	1696	1/1	0.91	0.38	90,90,90,90	0
55	MG	DA	3058	1/1	0.91	0.47	75,75,75,75	0
55	MG	AA	3289	1/1	0.91	0.29	62,62,62,62	0
55	MG	AA	3337	1/1	0.91	0.41	88,88,88,88	0
55	MG	DA	3254	1/1	0.91	0.32	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3061	1/1	0.91	0.27	67,67,67,67	0
55	MG	AA	3256	1/1	0.91	0.15	65,65,65,65	0
55	MG	BA	1629	1/1	0.91	0.10	100,100,100,100	0
55	MG	DA	3260	1/1	0.91	0.16	82,82,82,82	0
55	MG	AA	3339	1/1	0.91	0.17	95,95,95,95	0
55	MG	AA	3482	1/1	0.91	0.17	82,82,82,82	0
55	MG	BA	1632	1/1	0.91	0.20	72,72,72,72	0
55	MG	AA	3111	1/1	0.91	0.32	43,43,43,43	0
55	MG	DA	3069	1/1	0.91	0.30	82,82,82,82	0
55	MG	DA	3434	1/1	0.91	0.09	75,75,75,75	0
55	MG	AA	3484	1/1	0.91	0.11	86,86,86,86	0
55	MG	BA	1781	1/1	0.91	0.41	57,57,57,57	0
55	MG	CA	1771	1/1	0.91	0.24	64,64,64,64	0
55	MG	CA	1669	1/1	0.91	0.17	67,67,67,67	0
55	MG	BA	1782	1/1	0.91	0.34	88,88,88,88	0
55	MG	DA	3441	1/1	0.91	0.18	67,67,67,67	0
55	MG	CA	1775	1/1	0.91	0.31	66,66,66,66	0
55	MG	CA	1776	1/1	0.91	0.13	91,91,91,91	0
55	MG	AA	3149	1/1	0.91	0.27	49,49,49,49	0
55	MG	DA	3445	1/1	0.91	0.18	72,72,72,72	0
55	MG	DA	3282	1/1	0.91	0.29	55,55,55,55	0
55	MG	AA	3151	1/1	0.91	0.33	61,61,61,61	0
55	MG	CA	1677	1/1	0.91	0.23	68,68,68,68	0
55	MG	AA	3086	1/1	0.91	0.31	70,70,70,70	0
55	MG	CA	1784	1/1	0.91	0.45	102,102,102,102	0
55	MG	BC	107	1/1	0.91	0.12	88,88,88,88	0
55	MG	BA	1786	1/1	0.91	0.24	72,72,72,72	0
55	MG	DA	3099	1/1	0.91	0.22	51,51,51,51	0
55	MG	DA	3298	1/1	0.91	0.13	95,95,95,95	0
55	MG	DA	3100	1/1	0.91	0.33	62,62,62,62	0
55	MG	DA	3462	1/1	0.91	0.24	67,67,67,67	0
55	MG	CA	1684	1/1	0.91	0.36	77,77,77,77	0
55	MG	AA	3012	1/1	0.91	0.28	45,45,45,45	0
55	MG	DA	3471	1/1	0.91	0.42	89,89,89,89	0
55	MG	AA	3029	1/1	0.91	0.24	50,50,50,50	0
55	MG	B1	102	1/1	0.91	0.09	69,69,69,69	0
55	MG	CA	1793	1/1	0.91	0.26	78,78,78,78	0
55	MG	DA	3475	1/1	0.91	0.21	81,81,81,81	0
55	MG	AA	3062	1/1	0.91	0.11	73,73,73,73	0
55	MG	AA	3400	1/1	0.91	0.23	86,86,86,86	0
55	MG	CA	1605	1/1	0.91	0.35	72,72,72,72	0
55	MG	CA	1799	1/1	0.91	0.25	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
55	MG	AA	3404	1/1	0.91	0.12	89,89,89,89	0
55	MG	AA	3064	1/1	0.91	0.21	77,77,77,77	0
55	MG	DA	3490	1/1	0.91	0.12	49,49,49,49	0
55	MG	DA	3491	1/1	0.91	0.15	43,43,43,43	0
55	MG	AA	3030	1/1	0.91	0.21	51,51,51,51	0
55	MG	CA	1611	1/1	0.91	0.16	76,76,76,76	0
55	MG	CA	1807	1/1	0.91	0.32	121,121,121,121	0
55	MG	AA	3407	1/1	0.91	0.20	84,84,84,84	0
55	MG	DA	3499	1/1	0.91	0.29	78,78,78,78	0
55	MG	AA	3361	1/1	0.91	0.21	88,88,88,88	0
55	MG	CA	1705	1/1	0.91	0.21	86,86,86,86	0
55	MG	CS	101	1/1	0.91	0.17	84,84,84,84	0
55	MG	BA	1658	1/1	0.91	0.30	54,54,54,54	0
55	MG	AA	3504	1/1	0.91	0.37	103,103,103,103	0
55	MG	AA	3006	1/1	0.91	0.50	60,60,60,60	0
55	MG	DA	3512	1/1	0.91	0.35	70,70,70,70	0
55	MG	AA	3036	1/1	0.91	0.20	34,34,34,34	0
55	MG	BA	1667	1/1	0.91	0.33	78,78,78,78	0
55	MG	DA	3138	1/1	0.91	0.40	71,71,71,71	0
55	MG	CC	104	1/1	0.91	0.18	90,90,90,90	0
55	MG	DA	3335	1/1	0.91	0.27	72,72,72,72	0
55	MG	DA	3141	1/1	0.91	0.24	44,44,44,44	0
55	MG	CC	105	1/1	0.91	0.23	74,74,74,74	0
55	MG	AA	3507	1/1	0.91	0.15	62,62,62,62	0
55	MG	DA	3524	1/1	0.91	0.24	99,99,99,99	0
55	MG	AA	3273	1/1	0.91	0.22	63,63,63,63	0
55	MG	DA	3157	1/1	0.91	0.17	51,51,51,51	0
55	MG	DA	3158	1/1	0.91	0.18	77,77,77,77	0
55	MG	DA	3528	1/1	0.91	0.14	87,87,87,87	0
55	MG	DA	3159	1/1	0.91	0.23	52,52,52,52	0
55	MG	BA	1602	1/1	0.91	0.18	65,65,65,65	0
55	MG	CA	1624	1/1	0.91	0.26	83,83,83,83	0
55	MG	DA	3166	1/1	0.91	0.25	86,86,86,86	0
55	MG	AA	3603	1/1	0.91	0.18	65,65,65,65	0
55	MG	DA	3351	1/1	0.91	0.28	70,70,70,70	0
55	MG	AA	3010	1/1	0.91	0.37	52,52,52,52	0
55	MG	BA	1743	1/1	0.91	0.31	58,58,58,58	0
55	MG	BA	1820	1/1	0.91	0.31	97,97,97,97	0
55	MG	AA	3275	1/1	0.91	0.24	65,65,65,65	0
55	MG	DA	3356	1/1	0.91	0.10	80,80,80,80	0
55	MG	BA	1676	1/1	0.91	0.21	81,81,81,81	0
55	MG	CA	1729	1/1	0.91	0.33	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
55	MG	AA	3135	1/1	0.91	0.23	66,66,66,66	0
55	MG	AA	3244	1/1	0.91	0.20	69,69,69,69	0
55	MG	DA	3022	1/1	0.91	0.11	66,66,66,66	0
55	MG	BA	1673	1/1	0.92	0.33	80,80,80,80	0
55	MG	DA	3209	1/1	0.92	0.35	54,54,54,54	0
55	MG	DA	3210	1/1	0.92	0.25	51,51,51,51	0
55	MG	A0	201	1/1	0.92	0.22	46,46,46,46	0
55	MG	AA	3576	1/1	0.92	0.14	36,36,36,36	0
55	MG	CA	1658	1/1	0.92	0.28	78,78,78,78	0
55	MG	DA	3219	1/1	0.92	0.14	79,79,79,79	0
55	MG	CA	1764	1/1	0.92	0.31	67,67,67,67	0
55	MG	BA	1842	1/1	0.92	0.20	88,88,88,88	0
55	MG	DA	3226	1/1	0.92	0.24	57,57,57,57	0
55	MG	DA	3383	1/1	0.92	0.25	79,79,79,79	0
55	MG	DA	3385	1/1	0.92	0.16	90,90,90,90	0
55	MG	DA	3387	1/1	0.92	0.30	45,45,45,45	0
55	MG	AA	3577	1/1	0.92	0.23	42,42,42,42	0
55	MG	AA	3072	1/1	0.92	0.21	75,75,75,75	0
55	MG	AA	3588	1/1	0.92	0.28	63,63,63,63	0
55	MG	CA	1663	1/1	0.92	0.27	72,72,72,72	0
55	MG	BA	1757	1/1	0.92	0.23	88,88,88,88	0
55	MG	AA	3074	1/1	0.92	0.42	81,81,81,81	0
55	MG	DA	3394	1/1	0.92	0.19	70,70,70,70	0
55	MG	AA	3592	1/1	0.92	0.16	69,69,69,69	0
55	MG	AA	3319	1/1	0.92	0.16	61,61,61,61	0
55	MG	AA	3455	1/1	0.92	0.31	61,61,61,61	0
55	MG	DA	3242	1/1	0.92	0.42	61,61,61,61	0
55	MG	BB	103	1/1	0.92	0.33	87,87,87,87	0
55	MG	AA	3502	1/1	0.92	0.17	81,81,81,81	0
55	MG	AA	3075	1/1	0.92	0.07	71,71,71,71	0
55	MG	DA	3073	1/1	0.92	0.17	69,69,69,69	0
55	MG	DA	3406	1/1	0.92	0.14	72,72,72,72	0
55	MG	DA	3074	1/1	0.92	0.34	89,89,89,89	0
55	MG	AA	3459	1/1	0.92	0.22	110,110,110,110	0
55	MG	DA	3409	1/1	0.92	0.10	70,70,70,70	0
55	MG	CA	1781	1/1	0.92	0.30	92,92,92,92	0
55	MG	AA	3166	1/1	0.92	0.34	63,63,63,63	0
55	MG	CA	1783	1/1	0.92	0.19	72,72,72,72	0
55	MG	CA	1678	1/1	0.92	0.18	67,67,67,67	0
55	MG	DA	3416	1/1	0.92	0.18	75,75,75,75	0
55	MG	AA	3025	1/1	0.92	0.28	46,46,46,46	0
55	MG	DA	3421	1/1	0.92	0.09	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BC	101	1/1	0.92	0.23	58,58,58,58	0
55	MG	DA	3083	1/1	0.92	0.36	108,108,108,108	0
55	MG	AA	3204	1/1	0.92	0.37	56,56,56,56	0
55	MG	DA	3262	1/1	0.92	0.14	39,39,39,39	0
55	MG	BC	103	1/1	0.92	0.22	65,65,65,65	0
55	MG	DA	3266	1/1	0.92	0.28	97,97,97,97	0
55	MG	AA	3464	1/1	0.92	0.18	83,83,83,83	0
55	MG	DA	3087	1/1	0.92	0.33	48,48,48,48	0
55	MG	DA	3269	1/1	0.92	0.26	86,86,86,86	0
55	MG	AA	3606	1/1	0.92	0.13	77,77,77,77	0
55	MG	DA	3093	1/1	0.92	0.15	51,51,51,51	0
55	MG	CA	1792	1/1	0.92	0.32	91,91,91,91	0
55	MG	AA	3127	1/1	0.92	0.20	47,47,47,47	0
55	MG	CA	1794	1/1	0.92	0.24	72,72,72,72	0
55	MG	AA	3376	1/1	0.92	0.32	67,67,67,67	0
55	MG	DA	3277	1/1	0.92	0.19	77,77,77,77	0
55	MG	BA	1619	1/1	0.92	0.26	67,67,67,67	0
55	MG	DA	3102	1/1	0.92	0.33	72,72,72,72	0
55	MG	DA	3280	1/1	0.92	0.15	80,80,80,80	0
55	MG	CA	1693	1/1	0.92	0.28	73,73,73,73	0
55	MG	BA	1777	1/1	0.92	0.12	88,88,88,88	0
55	MG	AA	3421	1/1	0.92	0.37	64,64,64,64	0
55	MG	AA	3248	1/1	0.92	0.26	53,53,53,53	0
55	MG	DA	3110	1/1	0.92	0.21	84,84,84,84	0
55	MG	AA	3470	1/1	0.92	0.11	59,59,59,59	0
55	MG	CA	1700	1/1	0.92	0.27	60,60,60,60	0
55	MG	DA	3291	1/1	0.92	0.42	70,70,70,70	0
55	MG	DA	3452	1/1	0.92	0.21	91,91,91,91	0
55	MG	DA	3293	1/1	0.92	0.17	67,67,67,67	0
55	MG	AA	3423	1/1	0.92	0.24	69,69,69,69	0
55	MG	AA	3023	1/1	0.92	0.32	52,52,52,52	0
55	MG	CG	302	1/1	0.92	0.19	83,83,83,83	0
55	MG	BA	1627	1/1	0.92	0.19	62,62,62,62	0
55	MG	AA	3034	1/1	0.92	0.42	61,61,61,61	0
55	MG	DA	3468	1/1	0.92	0.15	53,53,53,53	0
55	MG	AA	3525	1/1	0.92	0.19	67,67,67,67	0
55	MG	DA	3303	1/1	0.92	0.37	61,61,61,61	0
55	MG	AA	3382	1/1	0.92	0.22	83,83,83,83	0
55	MG	BA	1711	1/1	0.92	0.37	86,86,86,86	0
55	MG	AA	3625	1/1	0.92	0.29	70,70,70,70	0
55	MG	CA	1712	1/1	0.92	0.19	86,86,86,86	0
55	MG	DA	3476	1/1	0.92	0.15	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3130	1/1	0.92	0.34	64,64,64,64	0
55	MG	AA	3027	1/1	0.92	0.28	49,49,49,49	0
55	MG	CC	102	1/1	0.92	0.22	69,69,69,69	0
55	MG	AA	3175	1/1	0.92	0.25	70,70,70,70	0
55	MG	BA	1716	1/1	0.92	0.16	90,90,90,90	0
55	MG	DA	3487	1/1	0.92	0.17	59,59,59,59	0
55	MG	BA	1717	1/1	0.92	0.19	79,79,79,79	0
55	MG	AA	3531	1/1	0.92	0.23	53,53,53,53	0
55	MG	BA	1720	1/1	0.92	0.37	71,71,71,71	0
55	MG	DA	3139	1/1	0.92	0.26	51,51,51,51	0
55	MG	DA	3320	1/1	0.92	0.21	73,73,73,73	0
55	MG	BA	1721	1/1	0.92	0.25	109,109,109,109	0
55	MG	DA	3322	1/1	0.92	0.31	83,83,83,83	0
55	MG	AA	3217	1/1	0.92	0.25	58,58,58,58	0
55	MG	AA	3133	1/1	0.92	0.19	38,38,38,38	0
55	MG	DA	3144	1/1	0.92	0.35	68,68,68,68	0
55	MG	AA	3178	1/1	0.92	0.25	49,49,49,49	0
55	MG	DA	3153	1/1	0.92	0.21	54,54,54,54	0
55	MG	AA	3347	1/1	0.92	0.12	92,92,92,92	0
55	MG	BA	1813	1/1	0.92	0.21	80,80,80,80	0
55	MG	DA	3508	1/1	0.92	0.29	77,77,77,77	0
55	MG	AA	3134	1/1	0.92	0.22	59,59,59,59	0
55	MG	AA	3085	1/1	0.92	0.27	62,62,62,62	0
55	MG	DA	3161	1/1	0.92	0.41	73,73,73,73	0
55	MG	DA	3162	1/1	0.92	0.39	70,70,70,70	0
55	MG	AA	3545	1/1	0.92	0.27	72,72,72,72	0
55	MG	AA	3546	1/1	0.92	0.13	33,33,33,33	0
55	MG	CA	1735	1/1	0.92	0.19	86,86,86,86	0
55	MG	AA	3547	1/1	0.92	0.20	45,45,45,45	0
55	MG	DA	3169	1/1	0.92	0.28	68,68,68,68	0
55	MG	CA	1737	1/1	0.92	0.19	109,109,109,109	0
55	MG	DA	3171	1/1	0.92	0.25	81,81,81,81	0
55	MG	DA	3347	1/1	0.92	0.37	66,66,66,66	0
55	MG	CA	1740	1/1	0.92	0.14	75,75,75,75	0
55	MG	BA	1650	1/1	0.92	0.28	78,78,78,78	0
55	MG	AA	3485	1/1	0.92	0.19	96,96,96,96	0
55	MG	AA	3053	1/1	0.92	0.27	59,59,59,59	0
55	MG	AA	3487	1/1	0.92	0.07	78,78,78,78	0
55	MG	AA	3557	1/1	0.92	0.26	68,68,68,68	0
55	MG	BA	1661	1/1	0.92	0.21	49,49,49,49	0
55	MG	BA	1740	1/1	0.92	0.21	72,72,72,72	0
55	MG	AA	3087	1/1	0.92	0.17	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
55	MG	AA	3008	1/1	0.92	0.24	42,42,42,42	0
55	MG	AA	3114	1/1	0.92	0.24	41,41,41,41	0
55	MG	DA	3196	1/1	0.92	0.32	82,82,82,82	0
55	MG	AA	3117	1/1	0.92	0.27	62,62,62,62	0
55	MG	DA	3361	1/1	0.92	0.48	102,102,102,102	0
55	MG	AA	3562	1/1	0.92	0.11	96,96,96,96	0
55	MG	DE	303	1/1	0.92	0.24	52,52,52,52	0
55	MG	AA	3150	1/1	0.92	0.38	58,58,58,58	0
55	MG	AA	3234	1/1	0.92	0.16	83,83,83,83	0
55	MG	AA	3057	1/1	0.92	0.15	52,52,52,52	0
55	MG	CA	1739	1/1	0.93	0.34	69,69,69,69	0
55	MG	DA	3222	1/1	0.93	0.26	57,57,57,57	0
55	MG	AA	3115	1/1	0.93	0.29	56,56,56,56	0
55	MG	AA	3271	1/1	0.93	0.27	68,68,68,68	0
55	MG	AA	3325	1/1	0.93	0.22	78,78,78,78	0
55	MG	DA	3228	1/1	0.93	0.25	71,71,71,71	0
55	MG	AA	3389	1/1	0.93	0.22	89,89,89,89	0
55	MG	BA	1773	1/1	0.93	0.13	79,79,79,79	0
55	MG	AA	3001	1/1	0.93	0.30	49,49,49,49	0
55	MG	AA	3118	1/1	0.93	0.21	74,74,74,74	0
55	MG	AA	3392	1/1	0.93	0.25	94,94,94,94	0
55	MG	AA	3462	1/1	0.93	0.10	69,69,69,69	0
55	MG	CA	1750	1/1	0.93	0.27	91,91,91,91	0
55	MG	DA	3395	1/1	0.93	0.15	80,80,80,80	0
55	MG	BA	1779	1/1	0.93	0.09	105,105,105,105	0
55	MG	AA	3331	1/1	0.93	0.30	79,79,79,79	0
55	MG	AA	3539	1/1	0.93	0.50	54,54,54,54	0
55	MG	AA	3185	1/1	0.93	0.11	43,43,43,43	0
55	MG	DA	3401	1/1	0.93	0.25	75,75,75,75	0
55	MG	CA	1629	1/1	0.93	0.12	82,82,82,82	0
55	MG	AA	3542	1/1	0.93	0.26	40,40,40,40	0
55	MG	AA	3070	1/1	0.93	0.29	66,66,66,66	0
55	MG	AA	3276	1/1	0.93	0.23	59,59,59,59	0
55	MG	AE	303	1/1	0.93	0.13	91,91,91,91	0
55	MG	AA	3022	1/1	0.93	0.20	43,43,43,43	0
55	MG	BA	1789	1/1	0.93	0.19	69,69,69,69	0
55	MG	AF	301	1/1	0.93	0.19	75,75,75,75	0
55	MG	AA	3402	1/1	0.93	0.53	94,94,94,94	0
55	MG	BA	1792	1/1	0.93	0.24	94,94,94,94	0
55	MG	DA	3413	1/1	0.93	0.13	96,96,96,96	0
55	MG	AA	3553	1/1	0.93	0.22	100,100,100,100	0
55	MG	BA	1796	1/1	0.93	0.23	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1691	1/1	0.93	0.41	60,60,60,60	0
55	MG	AO	203	1/1	0.93	0.33	63,63,63,63	0
55	MG	DA	3419	1/1	0.93	0.28	90,90,90,90	0
55	MG	DA	3420	1/1	0.93	0.33	73,73,73,73	0
55	MG	DA	3264	1/1	0.93	0.17	76,76,76,76	0
55	MG	AA	3403	1/1	0.93	0.07	74,74,74,74	0
55	MG	AA	3155	1/1	0.93	0.26	61,61,61,61	0
55	MG	AA	3340	1/1	0.93	0.24	61,61,61,61	0
55	MG	AA	3342	1/1	0.93	0.38	65,65,65,65	0
55	MG	A7	101	1/1	0.93	0.17	69,69,69,69	0
55	MG	DA	3428	1/1	0.93	0.20	79,79,79,79	0
55	MG	AA	3054	1/1	0.93	0.18	52,52,52,52	0
55	MG	DA	3094	1/1	0.93	0.30	45,45,45,45	0
55	MG	AA	3011	1/1	0.93	0.28	38,38,38,38	0
55	MG	AA	3125	1/1	0.93	0.34	49,49,49,49	0
55	MG	BA	1812	1/1	0.93	0.46	76,76,76,76	0
55	MG	AA	3240	1/1	0.93	0.43	76,76,76,76	0
55	MG	AA	3413	1/1	0.93	0.21	82,82,82,82	0
55	MG	AA	3563	1/1	0.93	0.15	75,75,75,75	0
55	MG	BA	1708	1/1	0.93	0.20	78,78,78,78	0
55	MG	DA	3105	1/1	0.93	0.28	72,72,72,72	0
55	MG	DA	3106	1/1	0.93	0.24	46,46,46,46	0
55	MG	AA	3348	1/1	0.93	0.10	92,92,92,92	0
55	MG	AA	3045	1/1	0.93	0.17	50,50,50,50	0
55	MG	AA	3572	1/1	0.93	0.21	40,40,40,40	0
55	MG	AA	3351	1/1	0.93	0.30	84,84,84,84	0
55	MG	AA	3575	1/1	0.93	0.20	40,40,40,40	0
55	MG	DA	3113	1/1	0.93	0.19	44,44,44,44	0
55	MG	AA	3196	1/1	0.93	0.19	60,60,60,60	0
55	MG	AA	3035	1/1	0.93	0.15	46,46,46,46	0
55	MG	AA	3059	1/1	0.93	0.15	84,84,84,84	0
55	MG	BA	1617	1/1	0.93	0.29	64,64,64,64	0
55	MG	BA	1719	1/1	0.93	0.28	91,91,91,91	0
55	MG	AA	3583	1/1	0.93	0.22	44,44,44,44	0
55	MG	AA	3584	1/1	0.93	0.28	94,94,94,94	0
55	MG	BA	1620	1/1	0.93	0.22	58,58,58,58	0
55	MG	CA	1801	1/1	0.93	0.32	71,71,71,71	0
55	MG	DA	3457	1/1	0.93	0.24	62,62,62,62	0
55	MG	AA	3587	1/1	0.93	0.09	28,28,28,28	0
55	MG	AA	3169	1/1	0.93	0.09	74,74,74,74	0
55	MG	CA	1805	1/1	0.93	0.22	81,81,81,81	0
55	MG	DA	3467	1/1	0.93	0.23	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3357	1/1	0.93	0.27	61,61,61,61	0
55	MG	AA	3247	1/1	0.93	0.27	76,76,76,76	0
55	MG	CA	1808	1/1	0.93	0.25	73,73,73,73	0
55	MG	DA	3134	1/1	0.93	0.34	56,56,56,56	0
55	MG	DA	3313	1/1	0.93	0.39	75,75,75,75	0
55	MG	AA	3205	1/1	0.93	0.28	43,43,43,43	0
55	MG	CG	301	1/1	0.93	0.26	86,86,86,86	0
55	MG	DA	3316	1/1	0.93	0.14	87,87,87,87	0
55	MG	AA	3130	1/1	0.93	0.12	59,59,59,59	0
55	MG	CA	1686	1/1	0.93	0.41	68,68,68,68	0
55	MG	DA	3479	1/1	0.93	0.35	87,87,87,87	0
55	MG	AA	3250	1/1	0.93	0.19	73,73,73,73	0
55	MG	AA	3028	1/1	0.93	0.22	51,51,51,51	0
55	MG	AA	3252	1/1	0.93	0.23	68,68,68,68	0
55	MG	BA	1733	1/1	0.93	0.30	88,88,88,88	0
55	MG	DA	3143	1/1	0.93	0.32	69,69,69,69	0
55	MG	AA	3209	1/1	0.93	0.22	71,71,71,71	0
55	MG	AA	3368	1/1	0.93	0.25	83,83,83,83	0
55	MG	DA	3492	1/1	0.93	0.30	48,48,48,48	0
55	MG	CB	105	1/1	0.93	0.16	80,80,80,80	0
55	MG	DA	3327	1/1	0.93	0.36	85,85,85,85	0
55	MG	AA	3433	1/1	0.93	0.30	77,77,77,77	0
55	MG	BA	1634	1/1	0.93	0.23	68,68,68,68	0
55	MG	CA	1698	1/1	0.93	0.15	104,104,104,104	0
55	MG	AA	3015	1/1	0.93	0.21	30,30,30,30	0
55	MG	DA	3160	1/1	0.93	0.30	65,65,65,65	0
55	MG	DA	3503	1/1	0.93	0.09	52,52,52,52	0
55	MG	AA	3212	1/1	0.93	0.31	56,56,56,56	0
55	MG	AA	3608	1/1	0.93	0.34	69,69,69,69	0
55	MG	AA	3503	1/1	0.93	0.07	72,72,72,72	0
55	MG	AA	3080	1/1	0.93	0.35	52,52,52,52	0
55	MG	AA	3214	1/1	0.93	0.37	66,66,66,66	0
55	MG	DA	3509	1/1	0.93	0.34	65,65,65,65	0
55	MG	DA	3511	1/1	0.93	0.25	65,65,65,65	0
55	MG	BA	1641	1/1	0.93	0.21	62,62,62,62	0
55	MG	DA	3168	1/1	0.93	0.27	49,49,49,49	0
55	MG	DA	3514	1/1	0.93	0.34	49,49,49,49	0
55	MG	BA	1642	1/1	0.93	0.25	69,69,69,69	0
55	MG	AA	3311	1/1	0.93	0.29	58,58,58,58	0
55	MG	BA	1644	1/1	0.93	0.20	78,78,78,78	0
55	MG	AA	3081	1/1	0.93	0.24	41,41,41,41	0
55	MG	AA	3442	1/1	0.93	0.22	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3177	1/1	0.93	0.15	45,45,45,45	0
55	MG	AA	3377	1/1	0.93	0.17	85,85,85,85	0
55	MG	BA	1651	1/1	0.93	0.48	73,73,73,73	0
55	MG	AA	3445	1/1	0.93	0.21	69,69,69,69	0
55	MG	BA	1756	1/1	0.93	0.21	96,96,96,96	0
55	MG	AA	3315	1/1	0.93	0.18	68,68,68,68	0
55	MG	DA	3026	1/1	0.93	0.22	82,82,82,82	0
55	MG	B1	101	1/1	0.93	0.29	64,64,64,64	0
55	MG	DA	3194	1/1	0.93	0.23	59,59,59,59	0
55	MG	DA	3028	1/1	0.93	0.14	71,71,71,71	0
55	MG	AA	3084	1/1	0.93	0.16	40,40,40,40	0
55	MG	AA	3038	1/1	0.93	0.29	70,70,70,70	0
55	MG	CA	1602	1/1	0.93	0.28	81,81,81,81	0
55	MG	CA	1728	1/1	0.93	0.23	58,58,58,58	0
55	MG	CA	1603	1/1	0.93	0.26	75,75,75,75	0
55	MG	AA	3519	1/1	0.93	0.14	91,91,91,91	0
55	MG	BA	1662	1/1	0.93	0.26	80,80,80,80	0
55	MG	DA	3371	1/1	0.93	0.66	82,82,82,82	0
55	MG	AA	3381	1/1	0.93	0.36	88,88,88,88	0
55	MG	CA	1733	1/1	0.93	0.44	66,66,66,66	0
55	MG	AA	3180	1/1	0.93	0.20	56,56,56,56	0
55	MG	D0	201	1/1	0.93	0.15	78,78,78,78	0
55	MG	D1	201	1/1	0.93	0.32	73,73,73,73	0
55	MG	AA	3522	1/1	0.93	0.15	67,67,67,67	0
55	MG	AA	3039	1/1	0.93	0.32	80,80,80,80	0
55	MG	AA	3524	1/1	0.93	0.08	72,72,72,72	0
55	MG	AA	3211	1/1	0.94	0.21	43,43,43,43	0
55	MG	DA	3287	1/1	0.94	0.18	62,62,62,62	0
55	MG	CA	1697	1/1	0.94	0.27	56,56,56,56	0
55	MG	AA	3007	1/1	0.94	0.12	33,33,33,33	0
55	MG	AA	3501	1/1	0.94	0.24	73,73,73,73	0
55	MG	AA	3128	1/1	0.94	0.31	54,54,54,54	0
55	MG	DA	3295	1/1	0.94	0.14	66,66,66,66	0
55	MG	AA	3056	1/1	0.94	0.25	64,64,64,64	0
55	MG	AA	3267	1/1	0.94	0.26	80,80,80,80	0
55	MG	AA	3300	1/1	0.94	0.13	77,77,77,77	0
55	MG	DA	3424	1/1	0.94	0.08	79,79,79,79	0
55	MG	BA	1693	1/1	0.94	0.10	80,80,80,80	0
55	MG	CA	1706	1/1	0.94	0.28	77,77,77,77	0
55	MG	AA	3009	1/1	0.94	0.31	48,48,48,48	0
55	MG	CA	1628	1/1	0.94	0.13	86,86,86,86	0
55	MG	DA	3064	1/1	0.94	0.26	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3306	1/1	0.94	0.23	73,73,73,73	0
55	MG	AA	3216	1/1	0.94	0.34	56,56,56,56	0
55	MG	DA	3175	1/1	0.94	0.13	70,70,70,70	0
55	MG	AA	3105	1/1	0.94	0.31	64,64,64,64	0
55	MG	DA	3177	1/1	0.94	0.23	51,51,51,51	0
55	MG	DA	3178	1/1	0.94	0.22	45,45,45,45	0
55	MG	AA	3565	1/1	0.94	0.27	81,81,81,81	0
55	MG	AA	3344	1/1	0.94	0.10	71,71,71,71	0
55	MG	AA	3154	1/1	0.94	0.34	55,55,55,55	0
55	MG	AA	3083	1/1	0.94	0.17	47,47,47,47	0
55	MG	DA	3072	1/1	0.94	0.26	98,98,98,98	0
55	MG	CA	1716	1/1	0.94	0.24	78,78,78,78	0
55	MG	AA	3199	1/1	0.94	0.26	66,66,66,66	0
55	MG	CA	1718	1/1	0.94	0.14	78,78,78,78	0
55	MG	AA	3514	1/1	0.94	0.09	59,59,59,59	0
55	MG	DA	3193	1/1	0.94	0.16	49,49,49,49	0
55	MG	AA	3386	1/1	0.94	0.28	74,74,74,74	0
55	MG	AA	3161	1/1	0.94	0.24	41,41,41,41	0
55	MG	DA	3079	1/1	0.94	0.18	83,83,83,83	0
55	MG	AB	213	1/1	0.94	0.23	54,54,54,54	0
55	MG	AA	3473	1/1	0.94	0.22	70,70,70,70	0
55	MG	AA	3581	1/1	0.94	0.13	67,67,67,67	0
55	MG	BA	1772	1/1	0.94	0.10	89,89,89,89	0
55	MG	DA	3205	1/1	0.94	0.34	60,60,60,60	0
55	MG	AA	3582	1/1	0.94	0.20	33,33,33,33	0
55	MG	DA	3456	1/1	0.94	0.14	83,83,83,83	0
55	MG	CA	1646	1/1	0.94	0.28	56,56,56,56	0
55	MG	AB	217	1/1	0.94	0.26	109,109,109,109	0
55	MG	AA	3052	1/1	0.94	0.58	74,74,74,74	0
55	MG	DA	3465	1/1	0.94	0.35	51,51,51,51	0
55	MG	DA	3211	1/1	0.94	0.25	49,49,49,49	0
55	MG	DA	3088	1/1	0.94	0.35	49,49,49,49	0
55	MG	DA	3214	1/1	0.94	0.54	70,70,70,70	0
55	MG	DA	3089	1/1	0.94	0.18	46,46,46,46	0
55	MG	DA	3216	1/1	0.94	0.27	47,47,47,47	0
55	MG	DA	3090	1/1	0.94	0.16	47,47,47,47	0
55	MG	CA	1649	1/1	0.94	0.17	70,70,70,70	0
55	MG	DA	3220	1/1	0.94	0.34	67,67,67,67	0
55	MG	AA	3097	1/1	0.94	0.18	65,65,65,65	0
55	MG	BQ	102	1/1	0.94	0.08	89,89,89,89	0
55	MG	DA	3095	1/1	0.94	0.35	45,45,45,45	0
55	MG	AE	301	1/1	0.94	0.13	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
55	MG	AA	3225	1/1	0.94	0.09	69,69,69,69	0
55	MG	BA	1780	1/1	0.94	0.29	58,58,58,58	0
55	MG	DA	3229	1/1	0.94	0.14	109,109,109,109	0
55	MG	DA	3231	1/1	0.94	0.23	55,55,55,55	0
55	MG	AA	3281	1/1	0.94	0.14	67,67,67,67	0
55	MG	DA	3233	1/1	0.94	0.49	84,84,84,84	0
55	MG	AA	3589	1/1	0.94	0.19	72,72,72,72	0
55	MG	AA	3316	1/1	0.94	0.28	87,87,87,87	0
55	MG	AA	3124	1/1	0.94	0.46	56,56,56,56	0
55	MG	AA	3356	1/1	0.94	0.08	72,72,72,72	0
55	MG	DA	3495	1/1	0.94	0.18	65,65,65,65	0
55	MG	AA	3527	1/1	0.94	0.21	77,77,77,77	0
55	MG	BA	1660	1/1	0.94	0.30	64,64,64,64	0
55	MG	DA	3363	1/1	0.94	0.26	73,73,73,73	0
55	MG	DA	3364	1/1	0.94	0.10	85,85,85,85	0
55	MG	BA	1725	1/1	0.94	0.27	82,82,82,82	0
55	MG	DA	3501	1/1	0.94	0.16	77,77,77,77	0
55	MG	AA	3395	1/1	0.94	0.07	57,57,57,57	0
55	MG	DA	3367	1/1	0.94	0.21	85,85,85,85	0
55	MG	DA	3005	1/1	0.94	0.33	83,83,83,83	0
55	MG	DA	3006	1/1	0.94	0.17	78,78,78,78	0
55	MG	AA	3228	1/1	0.94	0.14	89,89,89,89	0
55	MG	AA	3255	1/1	0.94	0.23	61,61,61,61	0
55	MG	CA	1751	1/1	0.94	0.19	102,102,102,102	0
55	MG	DA	3014	1/1	0.94	0.13	62,62,62,62	0
55	MG	DA	3510	1/1	0.94	0.24	67,67,67,67	0
55	MG	DA	3250	1/1	0.94	0.27	54,54,54,54	0
55	MG	AA	3320	1/1	0.94	0.28	70,70,70,70	0
55	MG	DA	3252	1/1	0.94	0.15	45,45,45,45	0
55	MG	AA	3321	1/1	0.94	0.34	68,68,68,68	0
55	MG	DA	3380	1/1	0.94	0.17	74,74,74,74	0
55	MG	AA	3033	1/1	0.94	0.26	46,46,46,46	0
55	MG	BA	1797	1/1	0.94	0.26	89,89,89,89	0
55	MG	DA	3122	1/1	0.94	0.11	71,71,71,71	0
55	MG	DA	3384	1/1	0.94	0.21	64,64,64,64	0
55	MG	AA	3142	1/1	0.94	0.13	61,61,61,61	0
55	MG	DA	3386	1/1	0.94	0.36	88,88,88,88	0
55	MG	AA	3605	1/1	0.94	0.30	45,45,45,45	0
55	MG	CA	1676	1/1	0.94	0.35	55,55,55,55	0
55	MG	AA	3365	1/1	0.94	0.20	83,83,83,83	0
55	MG	AA	3232	1/1	0.94	0.13	47,47,47,47	0
55	MG	AA	3144	1/1	0.94	0.30	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3409	1/1	0.94	0.21	98,98,98,98	0
55	MG	CA	1681	1/1	0.94	0.20	71,71,71,71	0
55	MG	AA	3544	1/1	0.94	0.22	67,67,67,67	0
55	MG	AA	3615	1/1	0.94	0.14	84,84,84,84	0
55	MG	BA	1809	1/1	0.94	0.29	88,88,88,88	0
55	MG	CA	1608	1/1	0.94	0.19	81,81,81,81	0
55	MG	AA	3291	1/1	0.94	0.24	70,70,70,70	0
55	MG	CA	1688	1/1	0.94	0.38	75,75,75,75	0
55	MG	AA	3327	1/1	0.94	0.13	82,82,82,82	0
55	MG	AA	3040	1/1	0.94	0.49	67,67,67,67	0
55	MG	AA	3551	1/1	0.94	0.25	73,73,73,73	0
55	MG	CA	1774	1/1	0.94	0.12	72,72,72,72	0
55	MG	AA	3552	1/1	0.94	0.32	75,75,75,75	0
55	MG	DE	301	1/1	0.94	0.17	43,43,43,43	0
55	MG	DE	302	1/1	0.94	0.24	75,75,75,75	0
55	MG	DA	3146	1/1	0.94	0.25	38,38,38,38	0
55	MG	DA	3149	1/1	0.94	0.23	60,60,60,60	0
55	MG	AA	3622	1/1	0.94	0.09	71,71,71,71	0
55	MG	AA	3454	1/1	0.94	0.15	78,78,78,78	0
55	MG	DA	3155	1/1	0.94	0.28	49,49,49,49	0
55	MG	CA	1778	1/1	0.94	0.11	69,69,69,69	0
56	ZN	BG	302	1/1	0.94	0.25	95,95,95,95	0
55	MG	AA	3090	1/1	0.95	0.27	68,68,68,68	0
55	MG	AA	3194	1/1	0.95	0.19	54,54,54,54	0
55	MG	DA	3119	1/1	0.95	0.31	80,80,80,80	0
55	MG	DA	3337	1/1	0.95	0.30	75,75,75,75	0
55	MG	DA	3338	1/1	0.95	0.30	75,75,75,75	0
55	MG	AA	3286	1/1	0.95	0.31	69,69,69,69	0
55	MG	AA	3063	1/1	0.95	0.11	64,64,64,64	0
55	MG	BA	1816	1/1	0.95	0.14	87,87,87,87	0
55	MG	AA	3092	1/1	0.95	0.28	59,59,59,59	0
55	MG	DA	3034	1/1	0.95	0.09	72,72,72,72	0
55	MG	AA	3198	1/1	0.95	0.30	57,57,57,57	0
55	MG	DA	3126	1/1	0.95	0.27	39,39,39,39	0
55	MG	DA	3127	1/1	0.95	0.27	44,44,44,44	0
55	MG	AA	3290	1/1	0.95	0.31	62,62,62,62	0
55	MG	DA	3129	1/1	0.95	0.34	55,55,55,55	0
55	MG	BA	1685	1/1	0.95	0.09	82,82,82,82	0
55	MG	BA	1821	1/1	0.95	0.24	78,78,78,78	0
55	MG	AA	3106	1/1	0.95	0.23	65,65,65,65	0
55	MG	AA	3328	1/1	0.95	0.29	71,71,71,71	0
55	MG	AA	3227	1/1	0.95	0.35	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1701	1/1	0.95	0.29	77,77,77,77	0
55	MG	DA	3044	1/1	0.95	0.15	66,66,66,66	0
55	MG	AA	3107	1/1	0.95	0.15	56,56,56,56	0
55	MG	AA	3332	1/1	0.95	0.40	82,82,82,82	0
55	MG	BA	1623	1/1	0.95	0.36	68,68,68,68	0
55	MG	AA	3003	1/1	0.95	0.21	43,43,43,43	0
55	MG	AA	3375	1/1	0.95	0.20	74,74,74,74	0
55	MG	AA	3566	1/1	0.95	0.33	73,73,73,73	0
55	MG	AA	3567	1/1	0.95	0.28	38,38,38,38	0
55	MG	CA	1709	1/1	0.95	0.39	81,81,81,81	0
55	MG	DA	3145	1/1	0.95	0.35	54,54,54,54	0
55	MG	DA	3258	1/1	0.95	0.22	56,56,56,56	0
55	MG	AA	3073	1/1	0.95	0.41	76,76,76,76	0
55	MG	BA	1697	1/1	0.95	0.12	84,84,84,84	0
55	MG	AA	3065	1/1	0.95	0.23	52,52,52,52	0
55	MG	BA	1836	1/1	0.95	0.19	73,73,73,73	0
55	MG	AA	3513	1/1	0.95	0.12	73,73,73,73	0
55	MG	AA	3206	1/1	0.95	0.30	53,53,53,53	0
55	MG	AA	3096	1/1	0.95	0.20	75,75,75,75	0
55	MG	DA	3482	1/1	0.95	0.18	56,56,56,56	0
55	MG	DA	3484	1/1	0.95	0.25	46,46,46,46	0
55	MG	BA	1840	1/1	0.95	0.25	80,80,80,80	0
55	MG	DA	3486	1/1	0.95	0.35	46,46,46,46	0
55	MG	CA	1796	1/1	0.95	0.20	81,81,81,81	0
55	MG	AA	3517	1/1	0.95	0.23	61,61,61,61	0
55	MG	AA	3266	1/1	0.95	0.14	47,47,47,47	0
55	MG	DA	3378	1/1	0.95	0.17	56,56,56,56	0
55	MG	AA	3341	1/1	0.95	0.16	63,63,63,63	0
55	MG	AA	3579	1/1	0.95	0.19	35,35,35,35	0
55	MG	AA	3580	1/1	0.95	0.21	44,44,44,44	0
55	MG	AA	3018	1/1	0.95	0.28	38,38,38,38	0
55	MG	AA	3427	1/1	0.95	0.26	78,78,78,78	0
55	MG	CA	1726	1/1	0.95	0.41	82,82,82,82	0
55	MG	AA	3160	1/1	0.95	0.21	31,31,31,31	0
55	MG	AA	3067	1/1	0.95	0.30	61,61,61,61	0
55	MG	CA	1652	1/1	0.95	0.27	70,70,70,70	0
55	MG	DA	3172	1/1	0.95	0.19	59,59,59,59	0
55	MG	DA	3174	1/1	0.95	0.16	49,49,49,49	0
55	MG	AA	3586	1/1	0.95	0.23	80,80,80,80	0
55	MG	AA	3305	1/1	0.95	0.22	62,62,62,62	0
55	MG	AA	3239	1/1	0.95	0.13	70,70,70,70	0
55	MG	BA	1645	1/1	0.95	0.31	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
55	MG	AA	3116	1/1	0.95	0.25	43,43,43,43	0
55	MG	AA	3308	1/1	0.95	0.14	58,58,58,58	0
55	MG	DA	3292	1/1	0.95	0.30	56,56,56,56	0
55	MG	AA	3099	1/1	0.95	0.27	64,64,64,64	0
55	MG	AA	3436	1/1	0.95	0.18	82,82,82,82	0
55	MG	CA	1738	1/1	0.95	0.41	75,75,75,75	0
55	MG	DA	3400	1/1	0.95	0.11	82,82,82,82	0
55	MG	DA	3515	1/1	0.95	0.19	52,52,52,52	0
55	MG	AF	302	1/1	0.95	0.14	80,80,80,80	0
55	MG	DA	3189	1/1	0.95	0.20	43,43,43,43	0
55	MG	AA	3014	1/1	0.95	0.33	41,41,41,41	0
55	MG	AA	3187	1/1	0.95	0.63	65,65,65,65	0
55	MG	AA	3313	1/1	0.95	0.40	62,62,62,62	0
55	MG	AA	3440	1/1	0.95	0.14	83,83,83,83	0
55	MG	A2	201	1/1	0.95	0.26	81,81,81,81	0
55	MG	DA	3523	1/1	0.95	0.31	86,86,86,86	0
55	MG	DA	3092	1/1	0.95	0.31	47,47,47,47	0
55	MG	AA	3119	1/1	0.95	0.25	64,64,64,64	0
55	MG	DA	3197	1/1	0.95	0.32	52,52,52,52	0
55	MG	DA	3411	1/1	0.95	0.24	77,77,77,77	0
55	MG	AA	3601	1/1	0.95	0.32	79,79,79,79	0
55	MG	AA	3189	1/1	0.95	0.23	57,57,57,57	0
55	MG	DA	3001	1/1	0.95	0.18	58,58,58,58	0
55	MG	DB	203	1/1	0.95	0.21	71,71,71,71	0
55	MG	DA	3201	1/1	0.95	0.26	75,75,75,75	0
55	MG	DA	3203	1/1	0.95	0.40	52,52,52,52	0
55	MG	CA	1670	1/1	0.95	0.32	54,54,54,54	0
55	MG	AA	3139	1/1	0.95	0.24	42,42,42,42	0
55	MG	AA	3218	1/1	0.95	0.29	77,77,77,77	0
55	MG	AA	3359	1/1	0.95	0.17	60,60,60,60	0
55	MG	BA	1603	1/1	0.95	0.26	63,63,63,63	0
55	MG	DA	3009	1/1	0.95	0.14	88,88,88,88	0
55	MG	AA	3492	1/1	0.95	0.24	84,84,84,84	0
55	MG	AA	3401	1/1	0.95	0.10	98,98,98,98	0
55	MG	BA	1606	1/1	0.95	0.09	88,88,88,88	0
55	MG	BA	1807	1/1	0.95	0.18	70,70,70,70	0
55	MG	CA	1758	1/1	0.95	0.28	64,64,64,64	0
55	MG	AA	3140	1/1	0.95	0.15	53,53,53,53	0
55	MG	AA	3002	1/1	0.95	0.26	40,40,40,40	0
55	MG	CA	1683	1/1	0.95	0.26	84,84,84,84	0
55	MG	AA	3612	1/1	0.95	0.09	38,38,38,38	0
55	MG	AA	3549	1/1	0.95	0.26	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3223	1/1	0.95	0.09	83,83,83,83	0
55	MG	CA	1610	1/1	0.95	0.12	75,75,75,75	0
56	ZN	CG	304	1/1	0.95	0.22	112,112,112,112	0
55	MG	AA	3163	1/1	0.96	0.12	48,48,48,48	0
55	MG	DA	3179	1/1	0.96	0.27	56,56,56,56	0
55	MG	AA	3104	1/1	0.96	0.24	54,54,54,54	0
55	MG	DA	3181	1/1	0.96	0.22	48,48,48,48	0
55	MG	DA	3270	1/1	0.96	0.32	73,73,73,73	0
55	MG	DA	3182	1/1	0.96	0.30	72,72,72,72	0
55	MG	DA	3460	1/1	0.96	0.29	45,45,45,45	0
55	MG	AA	3595	1/1	0.96	0.10	90,90,90,90	0
55	MG	DA	3463	1/1	0.96	0.26	44,44,44,44	0
55	MG	DA	3464	1/1	0.96	0.25	55,55,55,55	0
55	MG	DA	3030	1/1	0.96	0.11	66,66,66,66	0
55	MG	DA	3104	1/1	0.96	0.23	38,38,38,38	0
55	MG	AA	3016	1/1	0.96	0.26	53,53,53,53	0
55	MG	DA	3187	1/1	0.96	0.21	40,40,40,40	0
55	MG	BA	1663	1/1	0.96	0.12	47,47,47,47	0
55	MG	DA	3470	1/1	0.96	0.15	75,75,75,75	0
55	MG	AA	3597	1/1	0.96	0.11	67,67,67,67	0
55	MG	CA	1791	1/1	0.96	0.25	70,70,70,70	0
55	MG	AA	3152	1/1	0.96	0.29	53,53,53,53	0
55	MG	BA	1715	1/1	0.96	0.24	69,69,69,69	0
55	MG	AA	3408	1/1	0.96	0.18	70,70,70,70	0
55	MG	DA	3040	1/1	0.96	0.26	92,92,92,92	0
55	MG	AA	3265	1/1	0.96	0.30	42,42,42,42	0
55	MG	BA	1827	1/1	0.96	0.19	85,85,85,85	0
55	MG	CA	1674	1/1	0.96	0.15	76,76,76,76	0
55	MG	AA	3385	1/1	0.96	0.19	75,75,75,75	0
55	MG	AA	3153	1/1	0.96	0.18	33,33,33,33	0
55	MG	DA	3289	1/1	0.96	0.07	47,47,47,47	0
55	MG	DA	3483	1/1	0.96	0.30	45,45,45,45	0
55	MG	AA	3138	1/1	0.96	0.27	41,41,41,41	0
55	MG	BA	1671	1/1	0.96	0.08	74,74,74,74	0
55	MG	DA	3202	1/1	0.96	0.23	65,65,65,65	0
55	MG	DA	3048	1/1	0.96	0.09	84,84,84,84	0
55	MG	DA	3488	1/1	0.96	0.17	45,45,45,45	0
55	MG	DA	3049	1/1	0.96	0.27	72,72,72,72	0
55	MG	DA	3296	1/1	0.96	0.18	56,56,56,56	0
55	MG	CA	1618	1/1	0.96	0.22	89,89,89,89	0
55	MG	CA	1619	1/1	0.96	0.14	62,62,62,62	0
55	MG	DA	3493	1/1	0.96	0.29	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3052	1/1	0.96	0.07	84,84,84,84	0
55	MG	DA	3208	1/1	0.96	0.24	40,40,40,40	0
55	MG	CA	1804	1/1	0.96	0.12	81,81,81,81	0
55	MG	AA	3564	1/1	0.96	0.20	54,54,54,54	0
55	MG	AA	3146	1/1	0.96	0.16	62,62,62,62	0
55	MG	AA	3469	1/1	0.96	0.47	76,76,76,76	0
55	MG	AA	3253	1/1	0.96	0.19	82,82,82,82	0
55	MG	AA	3609	1/1	0.96	0.14	39,39,39,39	0
55	MG	AE	302	1/1	0.96	0.23	38,38,38,38	0
55	MG	AA	3238	1/1	0.96	0.26	48,48,48,48	0
55	MG	AA	3156	1/1	0.96	0.14	87,87,87,87	0
55	MG	BA	1680	1/1	0.96	0.26	71,71,71,71	0
55	MG	AA	3571	1/1	0.96	0.19	48,48,48,48	0
55	MG	AA	3309	1/1	0.96	0.32	64,64,64,64	0
55	MG	AA	3614	1/1	0.96	0.22	91,91,91,91	0
55	MG	DA	3224	1/1	0.96	0.32	59,59,59,59	0
55	MG	AA	3474	1/1	0.96	0.29	93,93,93,93	0
55	MG	AA	3616	1/1	0.96	0.25	69,69,69,69	0
55	MG	AA	3536	1/1	0.96	0.12	102,102,102,102	0
55	MG	AA	3159	1/1	0.96	0.14	30,30,30,30	0
55	MG	AA	3540	1/1	0.96	0.18	44,44,44,44	0
55	MG	DA	3230	1/1	0.96	0.13	68,68,68,68	0
55	MG	A5	101	1/1	0.96	0.16	49,49,49,49	0
55	MG	CA	1639	1/1	0.96	0.22	64,64,64,64	0
55	MG	BA	1795	1/1	0.96	0.18	66,66,66,66	0
55	MG	DA	3418	1/1	0.96	0.29	81,81,81,81	0
55	MG	DA	3148	1/1	0.96	0.22	42,42,42,42	0
55	MG	DA	3235	1/1	0.96	0.17	53,53,53,53	0
55	MG	AA	3329	1/1	0.96	0.29	77,77,77,77	0
55	MG	DA	3150	1/1	0.96	0.24	76,76,76,76	0
55	MG	AA	3019	1/1	0.96	0.13	35,35,35,35	0
55	MG	DA	3330	1/1	0.96	0.10	74,74,74,74	0
55	MG	AA	3396	1/1	0.96	0.21	58,58,58,58	0
55	MG	AA	3397	1/1	0.96	0.22	40,40,40,40	0
55	MG	AA	3293	1/1	0.96	0.26	87,87,87,87	0
55	MG	AA	3200	1/1	0.96	0.09	80,80,80,80	0
55	MG	AA	3425	1/1	0.96	0.43	70,70,70,70	0
55	MG	BA	1803	1/1	0.96	0.07	81,81,81,81	0
55	MG	DA	3245	1/1	0.96	0.25	80,80,80,80	0
55	MG	AA	3585	1/1	0.96	0.10	46,46,46,46	0
55	MG	BA	1805	1/1	0.96	0.28	62,62,62,62	0
55	MG	AA	3548	1/1	0.96	0.10	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3013	1/1	0.96	0.17	55,55,55,55	0
55	MG	AA	3112	1/1	0.96	0.30	48,48,48,48	0
55	MG	DA	3165	1/1	0.96	0.27	73,73,73,73	0
55	MG	AA	3021	1/1	0.96	0.28	38,38,38,38	0
55	MG	BA	1701	1/1	0.96	0.20	73,73,73,73	0
55	MG	AA	3335	1/1	0.96	0.29	90,90,90,90	0
55	MG	AA	3457	1/1	0.96	0.18	73,73,73,73	0
55	MG	DA	3020	1/1	0.96	0.24	51,51,51,51	0
55	MG	AA	3358	1/1	0.96	0.20	79,79,79,79	0
55	MG	BA	1655	1/1	0.96	0.31	89,89,89,89	0
55	MG	DP	201	1/1	0.96	0.11	63,63,63,63	0
55	MG	DA	3259	1/1	0.96	0.24	56,56,56,56	0
55	MG	DA	3173	1/1	0.96	0.44	59,59,59,59	0
55	MG	BA	1706	1/1	0.96	0.28	55,55,55,55	0
55	MG	BA	1657	1/1	0.96	0.24	44,44,44,44	0
55	MG	CA	1722	1/1	0.96	0.34	63,63,63,63	0
55	MG	BA	1760	1/1	0.96	0.26	67,67,67,67	0
56	ZN	BQ	103	1/1	0.96	0.08	129,129,129,129	0
55	MG	DA	3265	1/1	0.96	0.14	63,63,63,63	0
55	MG	AA	3528	1/1	0.97	0.34	88,88,88,88	0
55	MG	AA	3229	1/1	0.97	0.04	18,18,18,18	0
55	MG	AA	3068	1/1	0.97	0.11	49,49,49,49	0
55	MG	CA	1671	1/1	0.97	0.28	51,51,51,51	0
55	MG	DA	3459	1/1	0.97	0.16	49,49,49,49	0
55	MG	BA	1656	1/1	0.97	0.29	78,78,78,78	0
55	MG	DA	3461	1/1	0.97	0.19	50,50,50,50	0
55	MG	DA	3098	1/1	0.97	0.19	41,41,41,41	0
55	MG	AA	3020	1/1	0.97	0.19	31,31,31,31	0
55	MG	AA	3278	1/1	0.97	0.19	81,81,81,81	0
55	MG	BA	1659	1/1	0.97	0.26	70,70,70,70	0
55	MG	AA	3296	1/1	0.97	0.17	75,75,75,75	0
55	MG	AA	3170	1/1	0.97	0.19	34,34,34,34	0
55	MG	DA	3369	1/1	0.97	0.23	61,61,61,61	0
55	MG	AA	3280	1/1	0.97	0.23	65,65,65,65	0
55	MG	AA	3143	1/1	0.97	0.24	40,40,40,40	0
55	MG	AA	3537	1/1	0.97	0.25	39,39,39,39	0
55	MG	AA	3538	1/1	0.97	0.18	37,37,37,37	0
55	MG	DA	3031	1/1	0.97	0.16	69,69,69,69	0
55	MG	AA	3432	1/1	0.97	0.31	41,41,41,41	0
55	MG	DA	3071	1/1	0.97	0.21	74,74,74,74	0
55	MG	DA	3152	1/1	0.97	0.13	44,44,44,44	0
55	MG	AA	3515	1/1	0.97	0.28	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3154	1/1	0.97	0.25	59,59,59,59	0
55	MG	DA	3112	1/1	0.97	0.22	70,70,70,70	0
55	MG	AA	3336	1/1	0.97	0.19	48,48,48,48	0
55	MG	DA	3333	1/1	0.97	0.13	85,85,85,85	0
55	MG	AA	3082	1/1	0.97	0.20	39,39,39,39	0
55	MG	BA	1793	1/1	0.97	0.15	82,82,82,82	0
55	MG	AA	3569	1/1	0.97	0.29	40,40,40,40	0
55	MG	DA	3290	1/1	0.97	0.23	59,59,59,59	0
55	MG	AA	3137	1/1	0.97	0.12	43,43,43,43	0
55	MG	AA	3174	1/1	0.97	0.30	43,43,43,43	0
55	MG	AA	3197	1/1	0.97	0.30	63,63,63,63	0
55	MG	DA	3002	1/1	0.97	0.15	91,91,91,91	0
55	MG	AA	3499	1/1	0.97	0.23	79,79,79,79	0
55	MG	CA	1692	1/1	0.97	0.22	75,75,75,75	0
55	MG	AA	3042	1/1	0.97	0.15	67,67,67,67	0
55	MG	BA	1646	1/1	0.97	0.17	70,70,70,70	0
55	MG	AA	3088	1/1	0.97	0.26	60,60,60,60	0
55	MG	DA	3300	1/1	0.97	0.21	71,71,71,71	0
55	MG	AA	3089	1/1	0.97	0.19	44,44,44,44	0
55	MG	DA	3212	1/1	0.97	0.14	70,70,70,70	0
55	MG	AA	3201	1/1	0.97	0.16	42,42,42,42	0
55	MG	AA	3158	1/1	0.97	0.22	66,66,66,66	0
55	MG	AA	3243	1/1	0.97	0.25	52,52,52,52	0
55	MG	BA	1774	1/1	0.97	0.22	98,98,98,98	0
55	MG	DA	3217	1/1	0.97	0.29	51,51,51,51	0
55	MG	AB	205	1/1	0.97	0.18	75,75,75,75	0
55	MG	DA	3016	1/1	0.97	0.19	105,105,105,105	0
55	MG	AA	3157	1/1	0.98	0.27	41,41,41,41	0
55	MG	AA	3136	1/1	0.98	0.13	40,40,40,40	0
55	MG	CC	103	1/1	0.98	0.25	72,72,72,72	0
55	MG	AA	3110	1/1	0.98	0.08	39,39,39,39	0
55	MG	AA	3456	1/1	0.98	0.16	70,70,70,70	0
55	MG	AO	201	1/1	0.98	0.27	39,39,39,39	0
55	MG	AA	3607	1/1	0.98	0.17	54,54,54,54	0
55	MG	DA	3336	1/1	0.98	0.15	68,68,68,68	0
55	MG	BA	1748	1/1	0.98	0.27	61,61,61,61	0
55	MG	AA	3268	1/1	0.98	0.31	47,47,47,47	0
55	MG	AA	3590	1/1	0.98	0.08	56,56,56,56	0
55	MG	CA	1632	1/1	0.98	0.13	77,77,77,77	0
55	MG	A1	201	1/1	0.98	0.20	49,49,49,49	0
55	MG	CA	1746	1/1	0.98	0.34	59,59,59,59	0
55	MG	AA	3060	1/1	0.98	0.05	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1738	1/1	0.98	0.10	73,73,73,73	0
55	MG	DA	3008	1/1	0.98	0.20	76,76,76,76	0
55	MG	AU	201	1/1	0.98	0.17	74,74,74,74	0
55	MG	AA	3550	1/1	0.98	0.25	52,52,52,52	0
55	MG	DA	3436	1/1	0.98	0.07	69,69,69,69	0
55	MG	D5	101	1/1	0.98	0.17	50,50,50,50	0
55	MG	DA	3011	1/1	0.98	0.07	68,68,68,68	0
55	MG	DA	3032	1/1	0.98	0.19	73,73,73,73	0
55	MG	AA	3350	1/1	0.98	0.29	59,59,59,59	0
55	MG	AA	3031	1/1	0.99	0.27	44,44,44,44	0
55	MG	AA	3574	1/1	0.99	0.17	29,29,29,29	0
55	MG	DA	3147	1/1	0.99	0.05	16,16,16,16	0
56	ZN	CQ	101	1/1	0.99	0.09	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.