wwPDB X-ray Structure Validation Summary Report (i)

Feb 10, 2025 – 10:07 PM EST

PDB ID	:	6BOH
Title	:	Antibiotic blasticidin S and E. coli release factor 1 (containing deletion 302-304) bound to the 70S ribosome
Authors	:	Svidritskiy, E.; Korostelev, A.A.
Deposited on	:	2017-11-20
Resolution	:	3.40 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 (i) 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 (i)) were used in the production of this report:

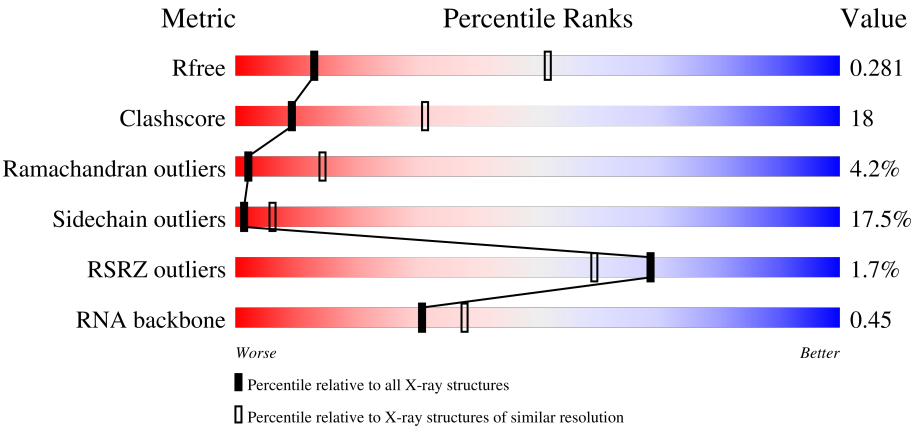
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)
RNA backbone	3690	1033 (3.80-3.00)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1507	34% 50% 15%
1	FB	1507	35% 50% 15%
2	B	2880	34% 45% 19%
2	GB	2880	37% 43% 18%

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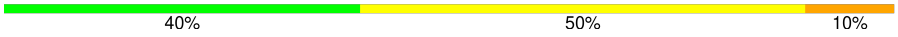
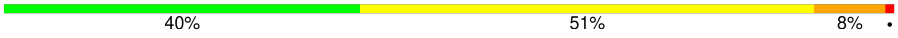
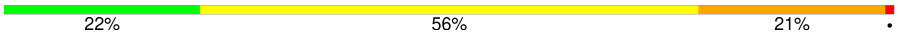
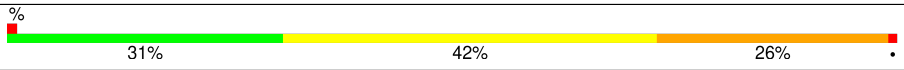
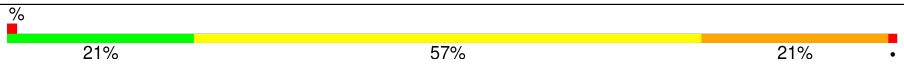
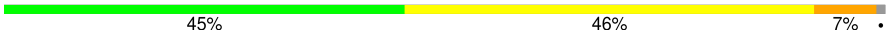
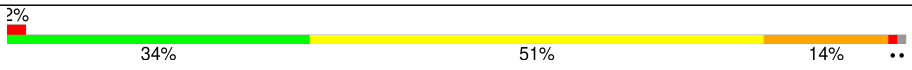
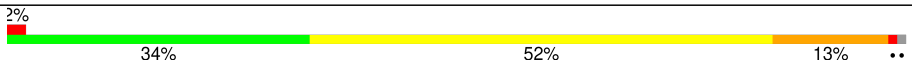
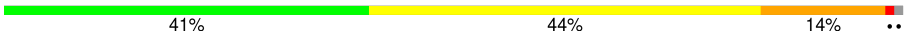
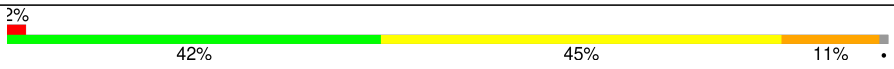
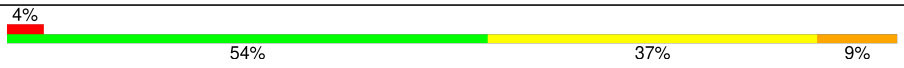
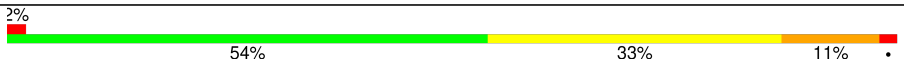
Mol	Chain	Length	Quality of chain
3	C	120	
3	HB	120	
4	D	77	
4	IA	77	
4	IB	77	
4	NC	77	
5	E	275	
5	JB	275	
6	F	206	
6	KB	206	
7	G	205	
7	LB	205	
8	H	182	
8	MB	182	
9	I	180	
9	NB	180	
10	J	148	
10	OB	148	
11	K	140	
11	PB	140	
12	L	122	
12	QB	122	
13	M	150	
13	RB	150	
14	N	141	

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Mol	Chain	Length	Quality of chain
14	SB	141	3% 56% 35% 8%
15	O	118	2% 49% 42% 9%
15	TB	118	4% 47% 43% 9%
16	P	112	8% 47% 39% 12%
16	UB	112	6% 47% 39% 12%
17	Q	146	% 39% 40% 14% 6%
17	VB	146	43% 38% 13% 6%
18	R	118	47% 46% 6%
18	WB	118	3% 48% 46% 5%
19	S	101	% 55% 37% 8%
19	XB	101	3% 56% 37% 7%
20	T	113	51% 39% 9%
20	YB	113	53% 38% 8%
21	U	96	50% 43% 6%
21	ZB	96	% 58% 32% 8%
22	AC	110	5% 46% 36% 15%
22	V	110	50% 33% 15%
23	BC	206	% 44% 38% 10% 8%
23	W	206	41% 40% 10% 8%
24	CC	85	8% 51% 41% 7%
24	X	85	8% 51% 39% 9%
25	DC	98	3% 44% 41% 14%
25	Y	98	% 52% 35% 12%
26	EC	72	% 53% 33% 11%
26	Z	72	51% 35% 11%

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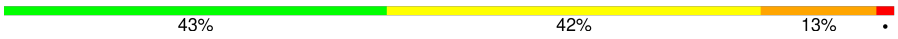
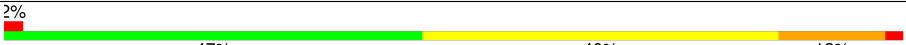
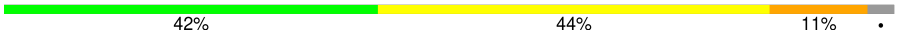
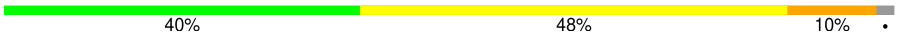
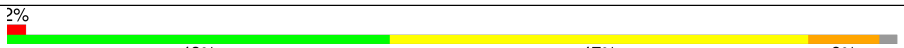
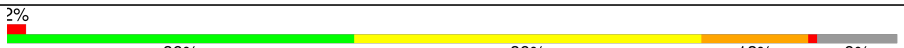
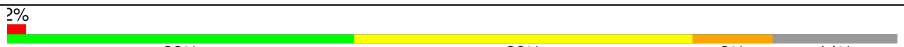
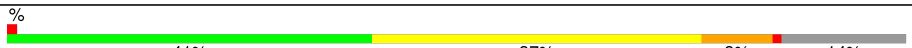
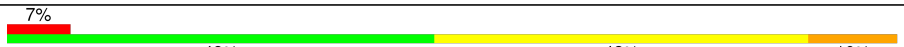
Mol	Chain	Length	Quality of chain
27	AA	60	
27	FC	60	
28	BA	71	
28	GC	71	
29	CA	60	
29	HC	60	
30	DA	54	
30	IC	54	
31	EA	49	
31	JC	49	
32	FA	65	
32	KC	65	
33	GA	37	
33	LC	37	
34	HA	27	
34	MC	27	
35	JA	365	
35	KA	365	
35	OC	365	
35	PC	365	
36	LA	256	
36	QC	256	
37	MA	239	
37	RC	239	
38	NA	209	

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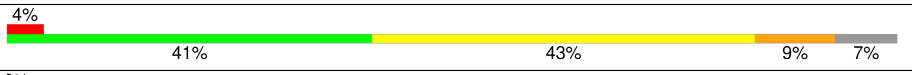
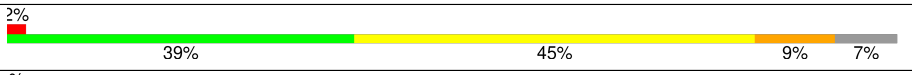
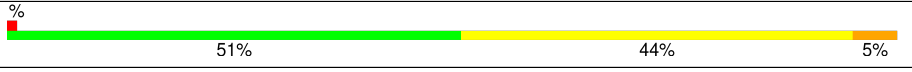
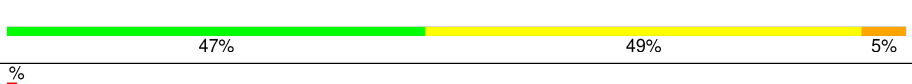
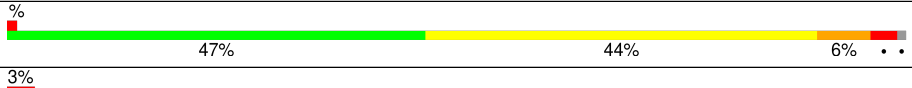
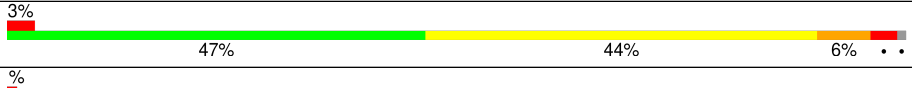
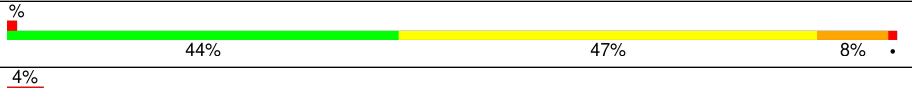
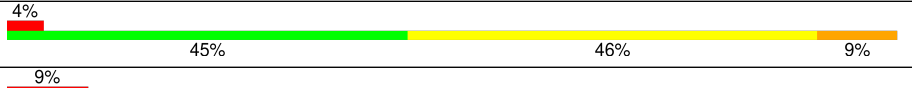
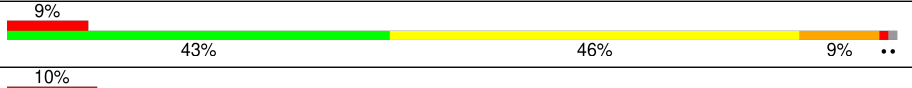
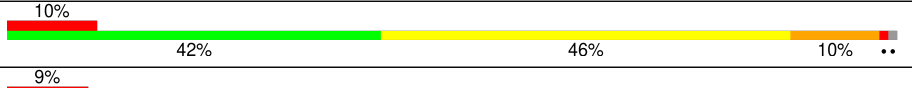
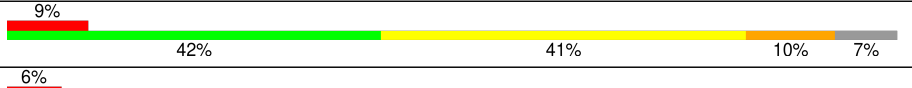
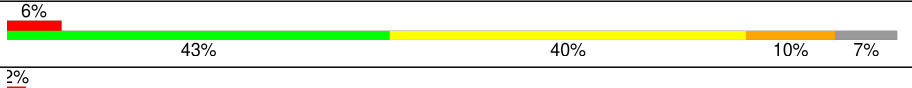
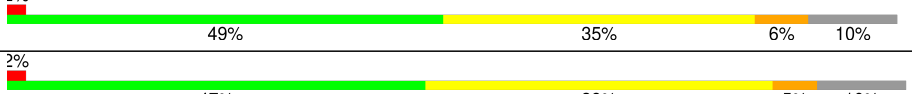
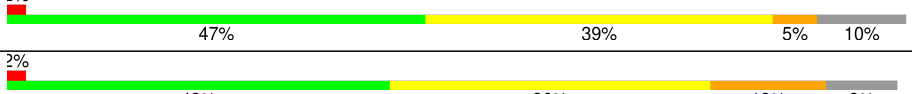
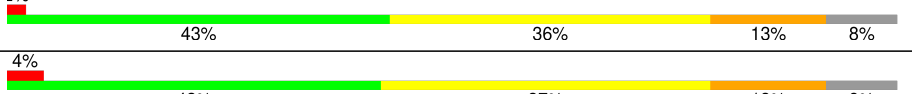
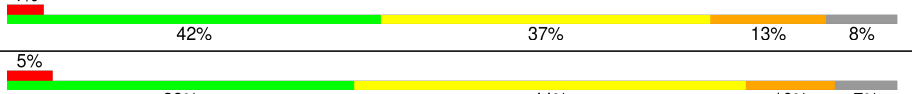
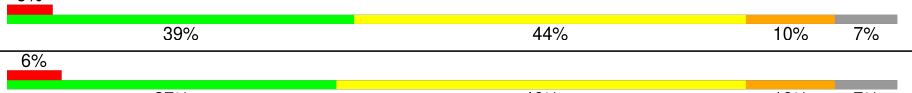
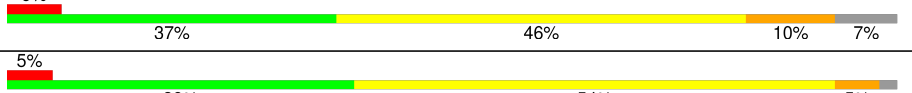
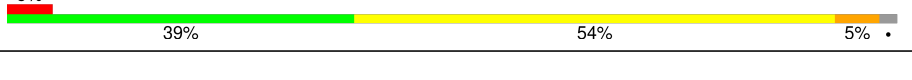
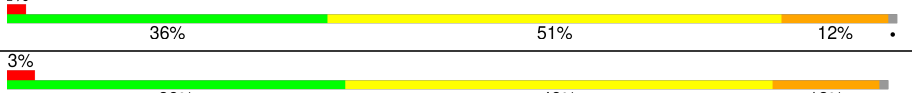
Mol	Chain	Length	Quality of chain
38	SC	209	
39	OA	162	
39	TC	162	
40	PA	101	
40	UC	101	
41	QA	156	
41	VC	156	
42	RA	138	
42	WC	138	
43	SA	128	
43	XC	128	
44	TA	105	
44	YC	105	
45	UA	129	
45	ZC	129	
46	AD	132	
46	VA	132	
47	BD	126	
47	WA	126	
48	CD	61	
48	XA	61	
49	DD	89	
49	YA	89	
50	ED	88	
50	ZA	88	

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Mol	Chain	Length	Quality of chain
51	AB	105	6% 43% 41% 10% 6%
51	FD	105	2% 45% 39% 10% • 6%
52	BB	88	38% 33% 9% 20%
52	GD	88	% 39% 32% 9% 20%
53	CB	93	3% 32% 42% 14% • 11%
53	HD	93	2% 37% 39% 14% 11%
54	DB	106	11% 46% 38% 9% 7%
54	ID	106	7% 50% 33% 10% 7%
55	EB	27	7% 30% 48% 11% 11%
55	JD	27	15% 33% 44% 11% 11%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 298186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			
1	FB	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			
2	GB	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	154A	C	UNK	conflict	GB 46197919
GB	154A	C	UNK	conflict	GB 46197919

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
3	HB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 4 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	IA	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	IB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	NC	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
5	JB	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
6	KB	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
7	LB	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			
8	MB	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
9	NB	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			
10	OB	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
11	PB	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
12	QB	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
13	RB	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	SB	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	TB	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	110	Total	C	N	O	0	0	0
			877	553	175	149			
16	UB	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
17	VB	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
18	WB	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
19	XB	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
20	YB	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	ZB	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			
22	AC	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			
23	BC	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
24	CC	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	11	ARG	LYS	conflict	UNP Q72HR3

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	11	ARG	LYS	conflict	UNP Q72HR3

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			
25	DC	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
26	EC	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AA	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
27	FC	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BA	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
28	GC	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CA	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			
29	HC	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DA	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	IC	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	EA	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	JC	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	FA	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	KC	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	GA	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	LC	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	HA	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			
34	MC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

- Molecule 35 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	JA	110	Total	C	N	O	S	0	0	0
			850	525	157	164	4			
35	KA	55	Total	C	N	O	S	0	0	0
			455	281	83	89	2			
35	OC	110	Total	C	N	O	S	0	0	0
			850	525	157	164	4			
35	PC	55	Total	C	N	O	S	0	0	0
			455	281	83	89	2			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	?	-	ASP	deletion	UNP B7MKB3
JA	?	-	ARG	deletion	UNP B7MKB3
JA	?	-	SER	deletion	UNP B7MKB3
JA	358	LEU	-	expression tag	UNP B7MKB3
JA	359	GLU	-	expression tag	UNP B7MKB3
JA	360	HIS	-	expression tag	UNP B7MKB3
JA	361	HIS	-	expression tag	UNP B7MKB3
JA	362	HIS	-	expression tag	UNP B7MKB3
JA	363	HIS	-	expression tag	UNP B7MKB3
JA	364	HIS	-	expression tag	UNP B7MKB3
JA	365	HIS	-	expression tag	UNP B7MKB3
KA	?	-	ASP	deletion	UNP B7MKB3
KA	?	-	ARG	deletion	UNP B7MKB3
KA	?	-	SER	deletion	UNP B7MKB3
KA	361	LEU	-	expression tag	UNP B7MKB3
KA	362	GLU	-	expression tag	UNP B7MKB3
KA	363	HIS	-	expression tag	UNP B7MKB3
KA	364	HIS	-	expression tag	UNP B7MKB3
KA	365	HIS	-	expression tag	UNP B7MKB3
KA	366	HIS	-	expression tag	UNP B7MKB3
KA	367	HIS	-	expression tag	UNP B7MKB3
KA	368	HIS	-	expression tag	UNP B7MKB3
OC	?	-	ASP	deletion	UNP B7MKB3
OC	?	-	ARG	deletion	UNP B7MKB3
OC	?	-	SER	deletion	UNP B7MKB3
OC	358	LEU	-	expression tag	UNP B7MKB3
OC	359	GLU	-	expression tag	UNP B7MKB3
OC	360	HIS	-	expression tag	UNP B7MKB3
OC	361	HIS	-	expression tag	UNP B7MKB3
OC	362	HIS	-	expression tag	UNP B7MKB3
OC	363	HIS	-	expression tag	UNP B7MKB3

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Chain	Residue	Modelled	Actual	Comment	Reference
OC	364	HIS	-	expression tag	UNP B7MKB3
OC	365	HIS	-	expression tag	UNP B7MKB3
PC	?	-	ASP	deletion	UNP B7MKB3
PC	?	-	ARG	deletion	UNP B7MKB3
PC	?	-	SER	deletion	UNP B7MKB3
PC	361	LEU	-	expression tag	UNP B7MKB3
PC	362	GLU	-	expression tag	UNP B7MKB3
PC	363	HIS	-	expression tag	UNP B7MKB3
PC	364	HIS	-	expression tag	UNP B7MKB3
PC	365	HIS	-	expression tag	UNP B7MKB3
PC	366	HIS	-	expression tag	UNP B7MKB3
PC	367	HIS	-	expression tag	UNP B7MKB3
PC	368	HIS	-	expression tag	UNP B7MKB3

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	LA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
36	QC	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	MA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
37	RC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 38 is a protein called 50S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	NA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
38	SC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	OA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
39	TC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	PA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
40	UC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	QA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
41	VC	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
42	WC	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	SA	127	Total	C	N	O	0	0	0
			1011	639	198	174			
43	XC	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	TA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	YC	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	UA	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
45	ZC	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	VA	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
46	AD	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	WA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
47	BD	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	XA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
48	CD	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	YA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
49	DD	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	ZA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
50	ED	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	AB	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
51	FD	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BB	70	Total	C	N	O	0	0	0
			574	367	112	95			
52	GD	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
53	HD	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
54	ID	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	EB	24	Total 208	C 128	N 50	O 30	0	0	0
55	JD	24	Total 208	C 128	N 50	O 30	0	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	A	183	Total 183	Mg 183	0	0
56	B	433	Total 433	Mg 433	0	0
56	C	22	Total 22	Mg 22	0	0
56	D	5	Total 5	Mg 5	0	0
56	E	6	Total 6	Mg 6	0	0
56	F	4	Total 4	Mg 4	0	0
56	G	2	Total 2	Mg 2	0	0
56	H	2	Total 2	Mg 2	0	0
56	J	1	Total 1	Mg 1	0	0
56	K	4	Total 4	Mg 4	0	0
56	L	3	Total 3	Mg 3	0	0
56	M	3	Total 3	Mg 3	0	0
56	O	2	Total 2	Mg 2	0	0
56	Q	1	Total 1	Mg 1	0	0
56	R	1	Total 1	Mg 1	0	0
56	S	1	Total 1	Mg 1	0	0
56	T	2	Total 2	Mg 2	0	0
56	U	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	V	2	Total Mg 2 2	0	0
56	Y	3	Total Mg 3 3	0	0
56	Z	1	Total Mg 1 1	0	0
56	AA	1	Total Mg 1 1	0	0
56	CA	1	Total Mg 1 1	0	0
56	EA	1	Total Mg 1 1	0	0
56	FA	1	Total Mg 1 1	0	0
56	HA	3	Total Mg 3 3	0	0
56	IA	9	Total Mg 9 9	0	0
56	JA	1	Total Mg 1 1	0	0
56	LA	1	Total Mg 1 1	0	0
56	MA	6	Total Mg 6 6	0	0
56	NA	2	Total Mg 2 2	0	0
56	OA	4	Total Mg 4 4	0	0
56	PA	3	Total Mg 3 3	0	0
56	QA	1	Total Mg 1 1	0	0
56	SA	1	Total Mg 1 1	0	0
56	UA	1	Total Mg 1 1	0	0
56	VA	2	Total Mg 2 2	0	0
56	YA	3	Total Mg 3 3	0	0
56	AB	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	BB	1	Total Mg 1 1	0	0
56	CB	1	Total Mg 1 1	0	0
56	FB	194	Total Mg 194 194	0	0
56	GB	402	Total Mg 402 402	0	0
56	HB	20	Total Mg 20 20	0	0
56	IB	2	Total Mg 2 2	0	0
56	JB	5	Total Mg 5 5	0	0
56	KB	2	Total Mg 2 2	0	0
56	LB	4	Total Mg 4 4	0	0
56	NB	1	Total Mg 1 1	0	0
56	OB	1	Total Mg 1 1	0	0
56	PB	2	Total Mg 2 2	0	0
56	QB	2	Total Mg 2 2	0	0
56	RB	3	Total Mg 3 3	0	0
56	SB	2	Total Mg 2 2	0	0
56	TB	1	Total Mg 1 1	0	0
56	UB	4	Total Mg 4 4	0	0
56	VB	3	Total Mg 3 3	0	0
56	XB	2	Total Mg 2 2	0	0
56	ZB	2	Total Mg 2 2	0	0
56	AC	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	BC	1	Total Mg 1 1	0	0
56	CC	1	Total Mg 1 1	0	0
56	DC	1	Total Mg 1 1	0	0
56	GC	1	Total Mg 1 1	0	0
56	IC	1	Total Mg 1 1	0	0
56	JC	1	Total Mg 1 1	0	0
56	KC	1	Total Mg 1 1	0	0
56	MC	3	Total Mg 3 3	0	0
56	NC	10	Total Mg 10 10	0	0
56	OC	1	Total Mg 1 1	0	0
56	PC	1	Total Mg 1 1	0	0
56	QC	3	Total Mg 3 3	0	0
56	RC	2	Total Mg 2 2	0	0
56	SC	4	Total Mg 4 4	0	0
56	TC	3	Total Mg 3 3	0	0
56	UC	3	Total Mg 3 3	0	0
56	VC	1	Total Mg 1 1	0	0
56	WC	1	Total Mg 1 1	0	0
56	ZC	1	Total Mg 1 1	0	0
56	AD	4	Total Mg 4 4	0	0
56	BD	1	Total Mg 1 1	0	0

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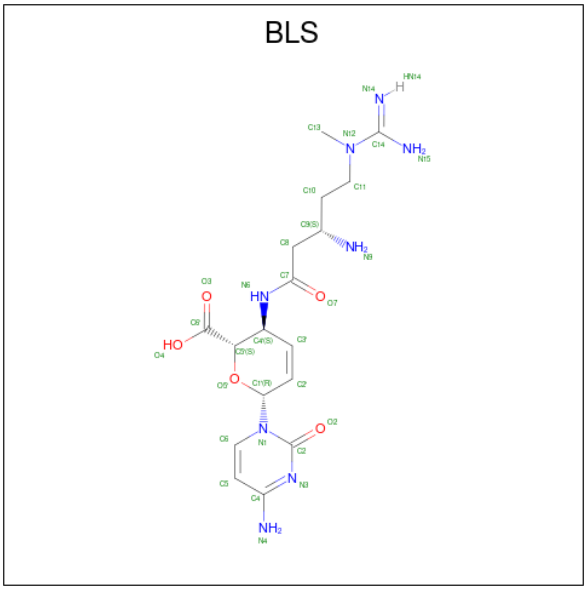
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DD	1	Total Mg 1 1	0	0
56	ED	1	Total Mg 1 1	0	0
56	HD	1	Total Mg 1 1	0	0

- Molecule 57 is BLASTICIDIN S (three-letter code: BLS) (formula: $C_{17}H_{26}N_8O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	B	1	Total C N O 30 17 8 5	0	0
57	GB	1	Total C N O 30 17 8 5	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	V	1	Total Zn 1 1	0	0
58	BA	1	Total Zn 1 1	0	0
58	CA	1	Total Zn 1 1	0	0
58	DA	1	Total Zn 1 1	0	0

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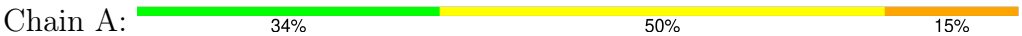
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	GA	1	Total Zn 1 1	0	0
58	AC	1	Total Zn 1 1	0	0
58	GC	1	Total Zn 1 1	0	0
58	HC	1	Total Zn 1 1	0	0
58	IC	1	Total Zn 1 1	0	0
58	LC	1	Total Zn 1 1	0	0

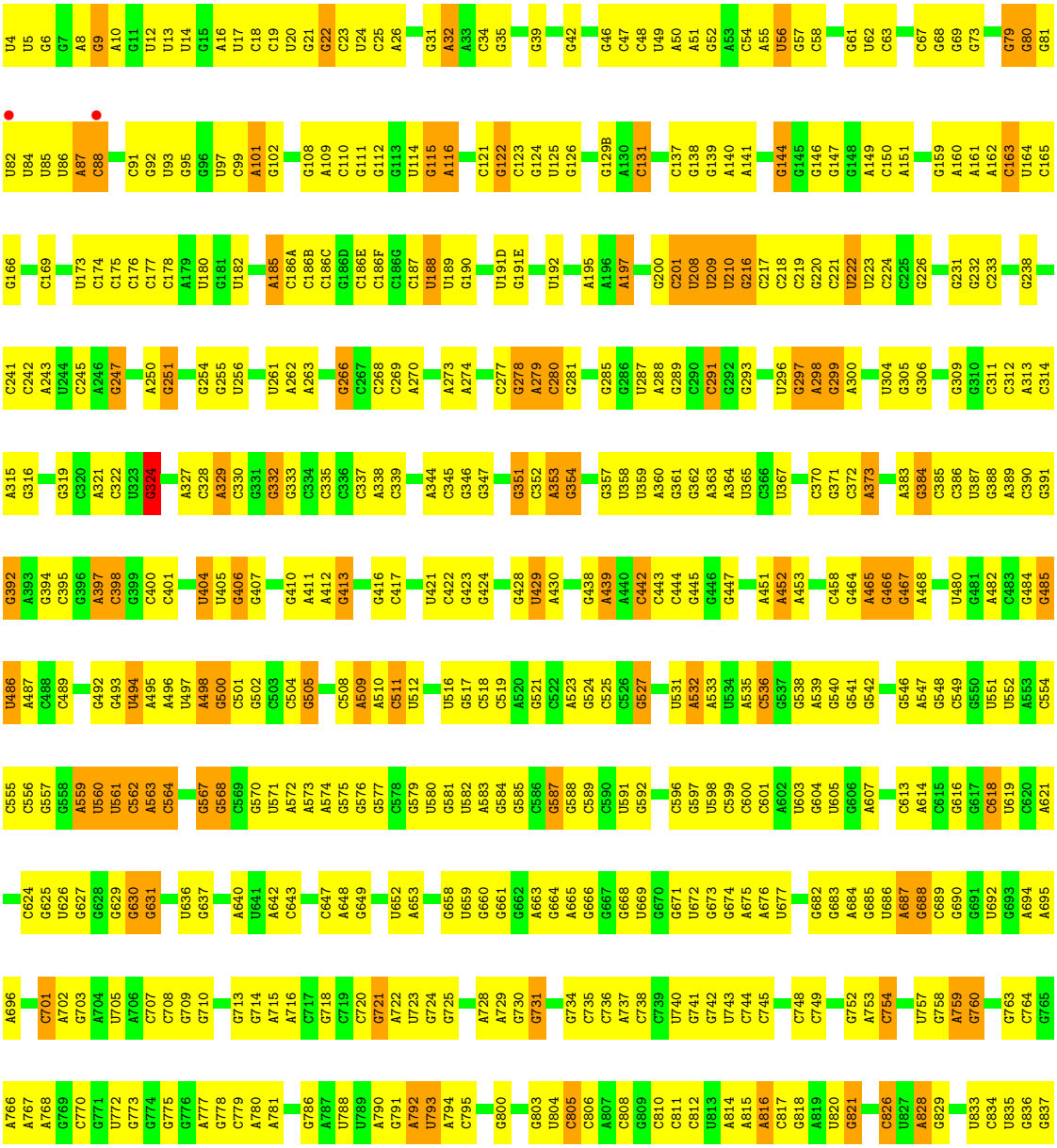
3 Residue-property plots (i)

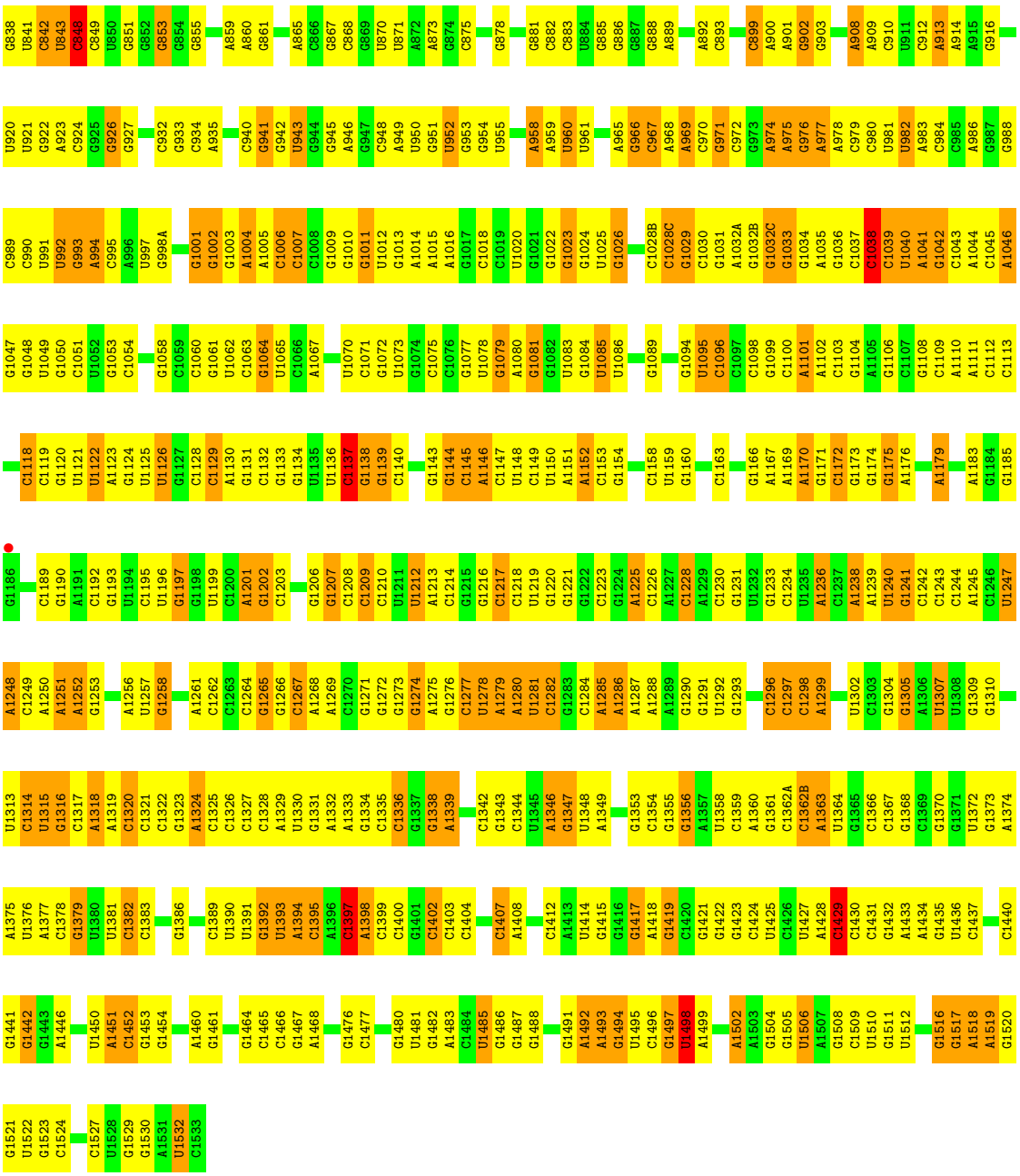
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S ribosomal RNA

Chain A:

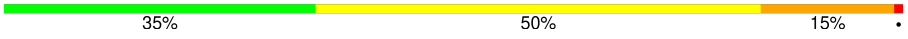


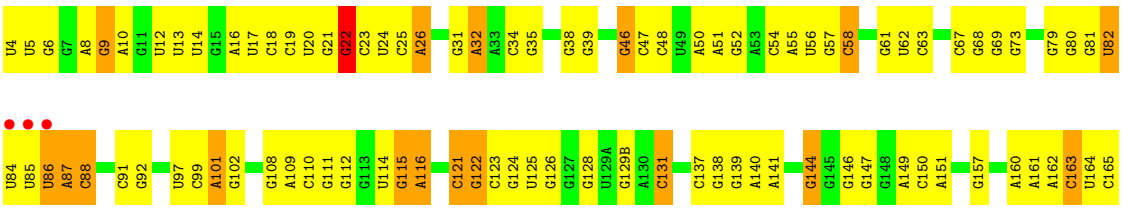


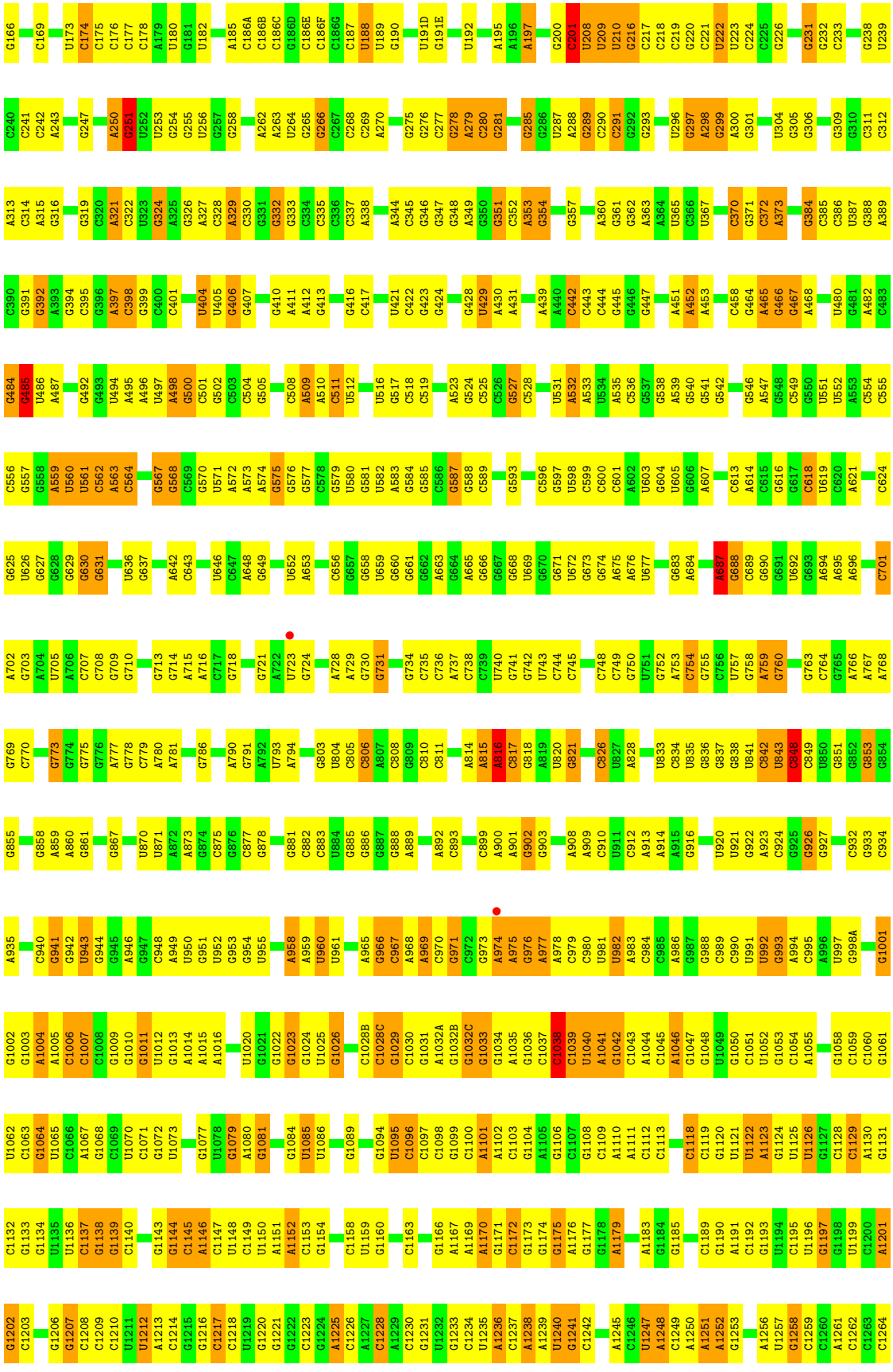


• Molecule 1: 16S ribosomal RNA

Chain FB:



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C240 C241 C242 A243 G247 A250 G251 U252 U253 G254 G255 U256 G257 G258 A262 A263 U264 G265 G266 C267 C268 C269 A270 G275 G276 C277 G278 A279 C280 G281 G285 G286 U287 A288 G289 C290 C291 G292 G293 U296 G297 A298 G299 A300 G301 U304 G305 G306 G309 G310 C311 C312
A313 C314 A315 G316 G319 C320 A321 G322 U323 G324 A325 G326 A327 C328 A329 C330 G331 G332 G333 C334 C335 C336 C337 A338 A344 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 G357 A360 G361 G362 A363 A364 U365 C366 U367 C370 G371 C372 A373 G384 C385 C386 U387 G388 A389
C390 G391 G392 A393 G394 C395 G396 A397 G398 G399 C400 C401 U404 U405 G406 G407 G410 A411 A412 G413 C416 C417 U421 C422 G423 G424 G428 U429 A430 A431 A439 A440 C442 C443 C444 G445 G446 G447 A451 A452 A453 C458 G464 A465 G466 G467 A468 U480 G481 A482 C483
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C556 G557 G558 A559 U560 U561 C562 A563 C564 G567 G568 C569 G570 U571 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 U582 A583 G584 G585 C586 G587 G588 C589 G593 C596 G597 U598 C599 C600 C601 A602 U603 G604 U605 G606 A607 C613 A614 G615 G616 G617 C618 U619 C620 A621 C624
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A702 G703 A704 U705 A706 C707 C708 G709 G710 G713 G714 A715 A716 C717 G718 G721 A722 U723 G724 A728 A729 G730 G731 G734 C735 C736 A737 C738 G739 U740 G741 G742 U743 C744 C745 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A759 G760 G763 C764 G765 A766 A767 A768
G769 C770 G773 G774 G775 G776 A777 G778 C779 A780 A781 G786 A790 G791 A792 U793 A794 G803 U804 C805 C806 A807 C808 G809 C810 C811 A814 A815 A816 C817 G818 A819 U820 G821 C826 U827 A828 U833 C834 U835 G836 G837 G838 U841 C842 U843 C848 C849 U850 G851 G852 G853 G854
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C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 C1158 U1159 G1160 C1163 G1166 A1167 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1183 G1184 G1185 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201
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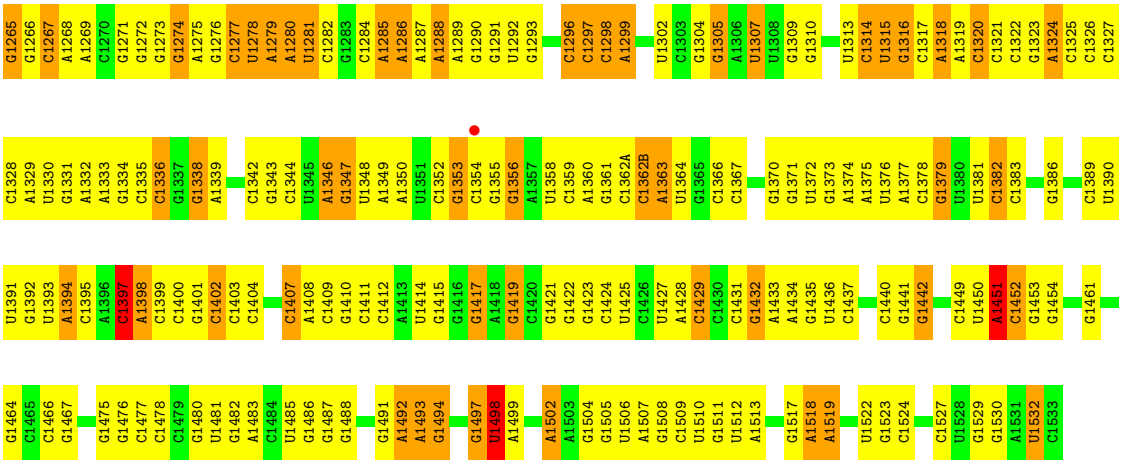
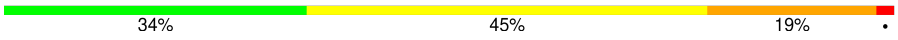
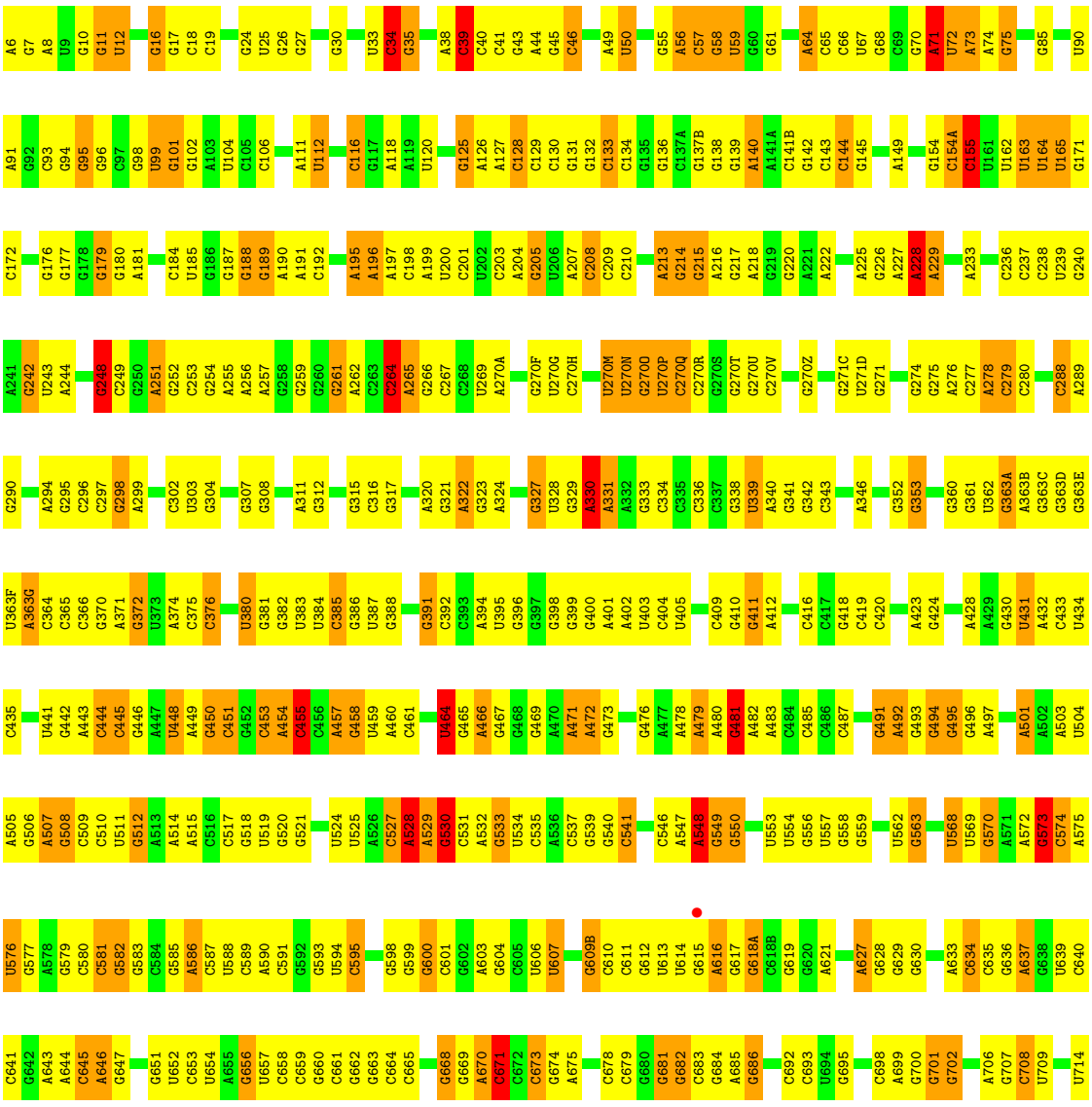
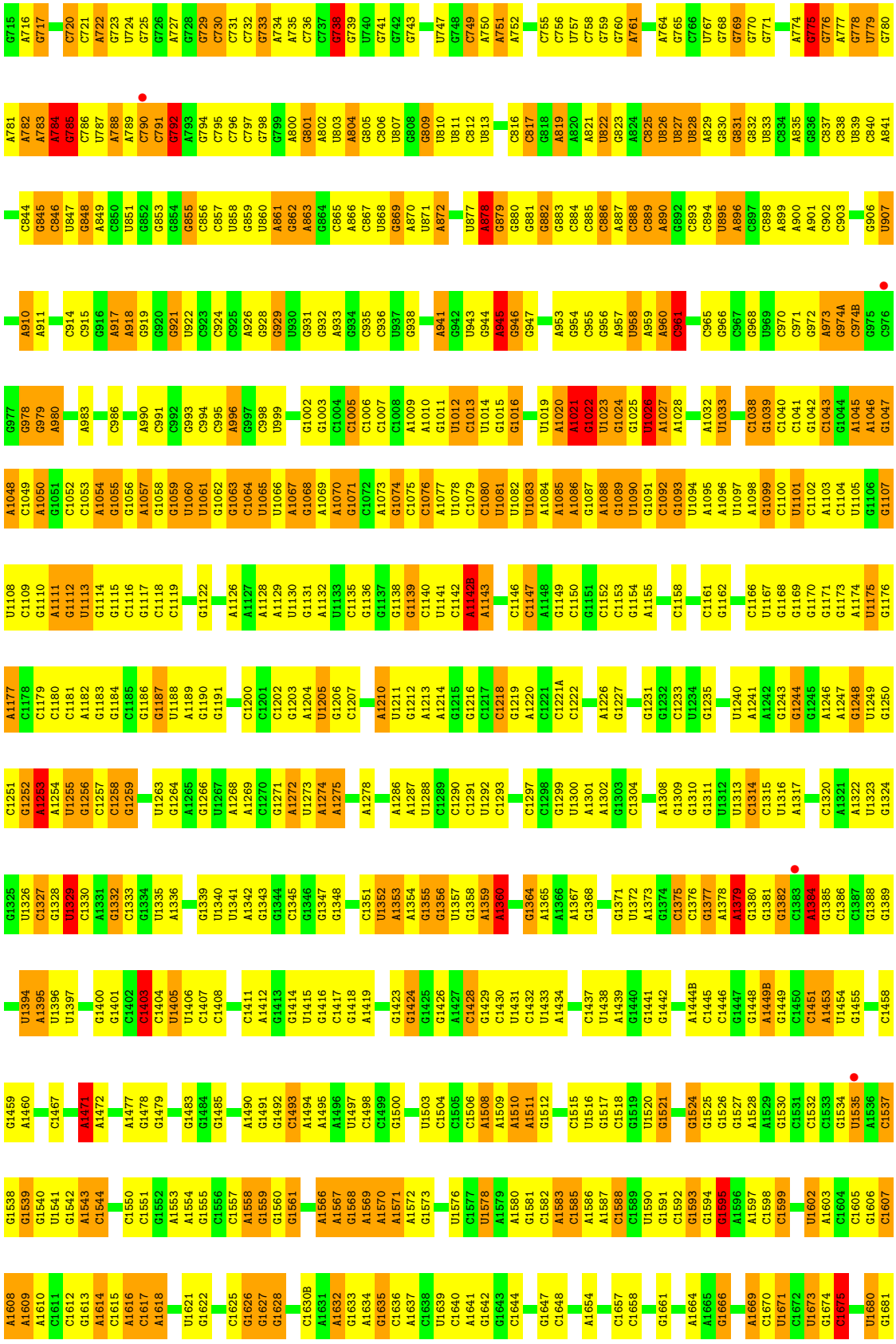


• Molecule 2: 23S ribosomal RNA

Chain B:



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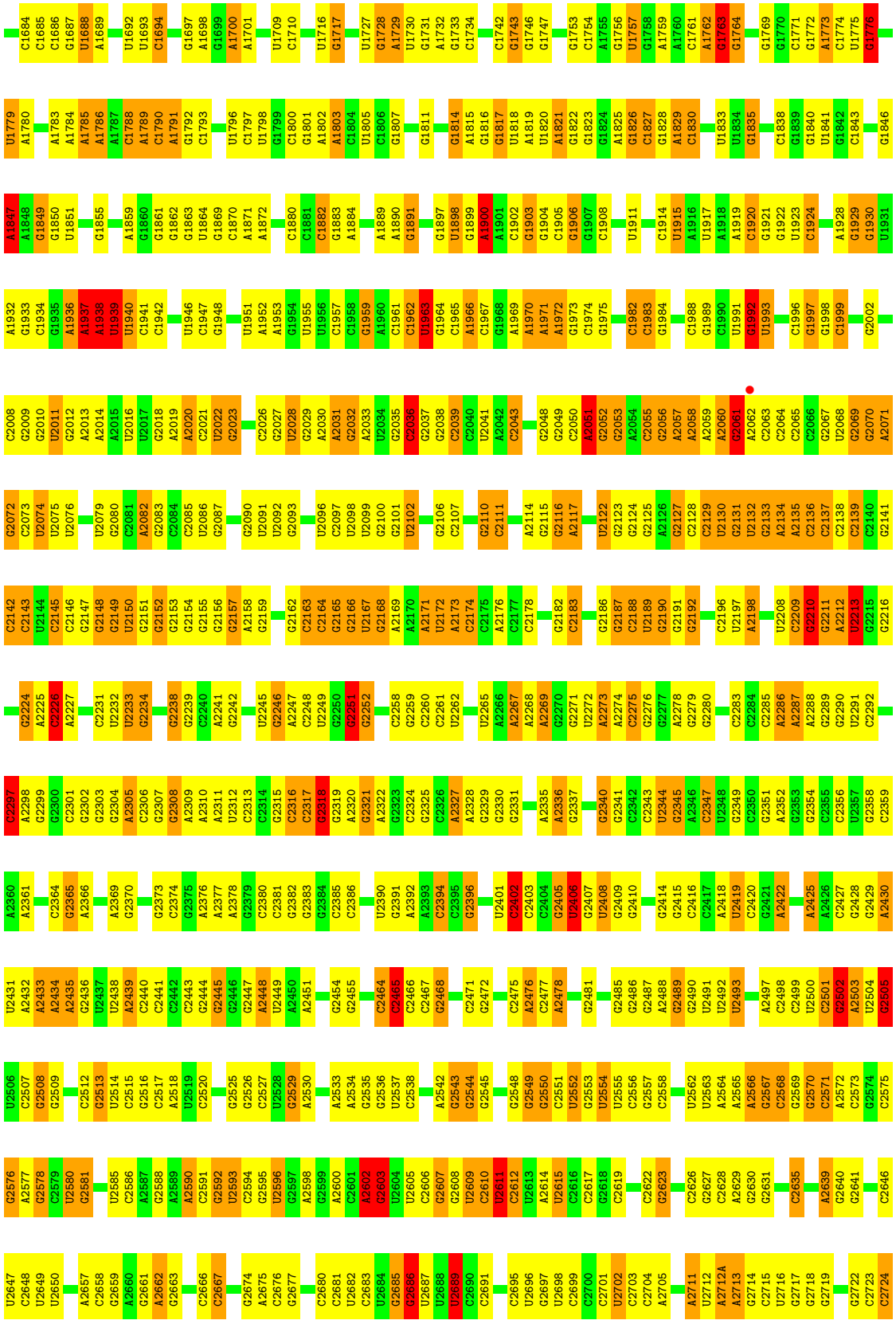
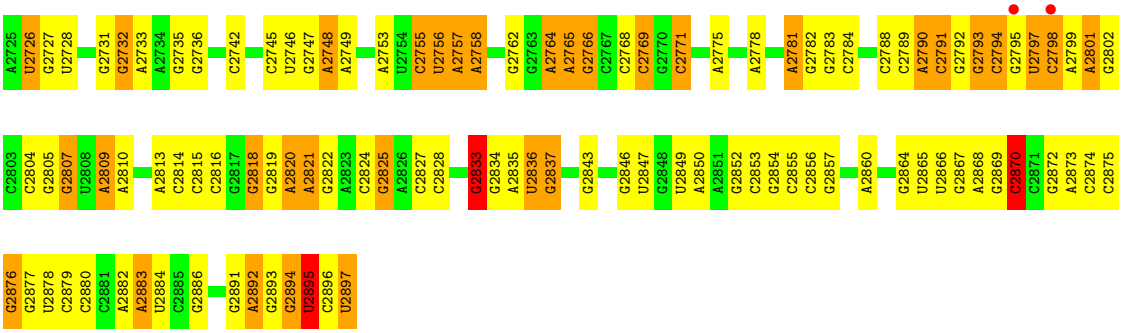
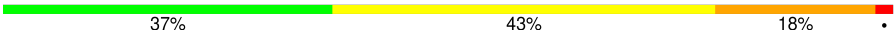
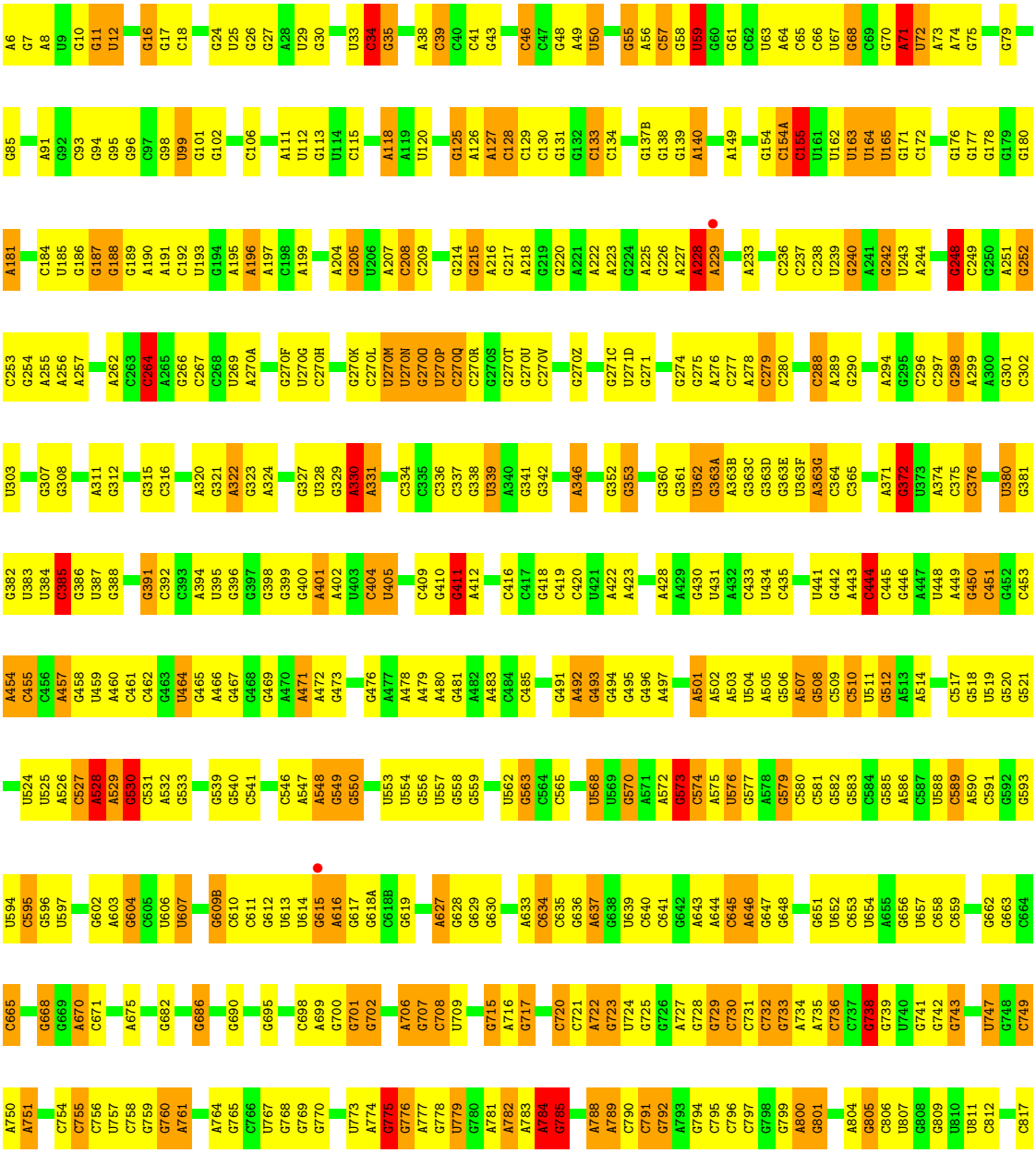


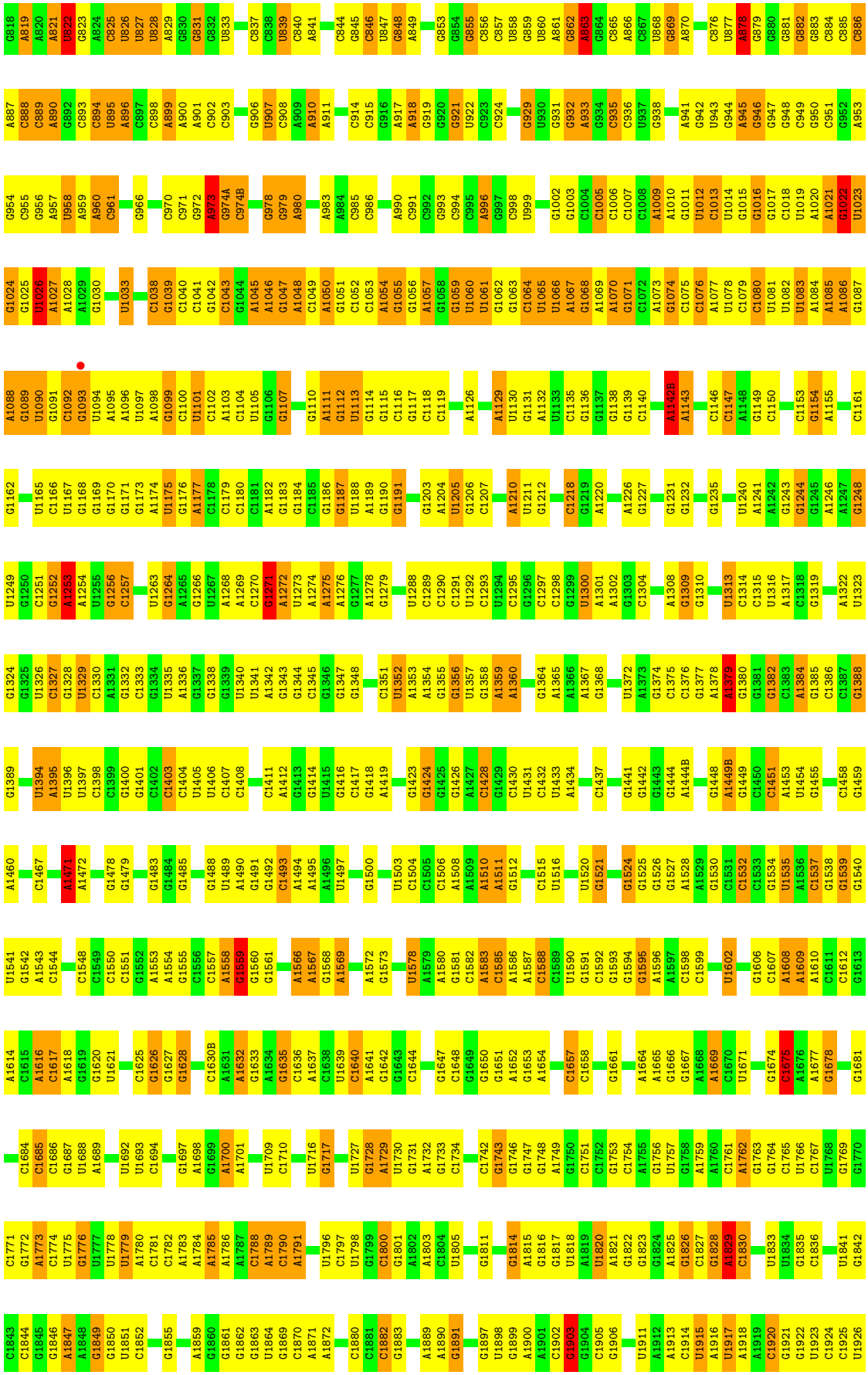


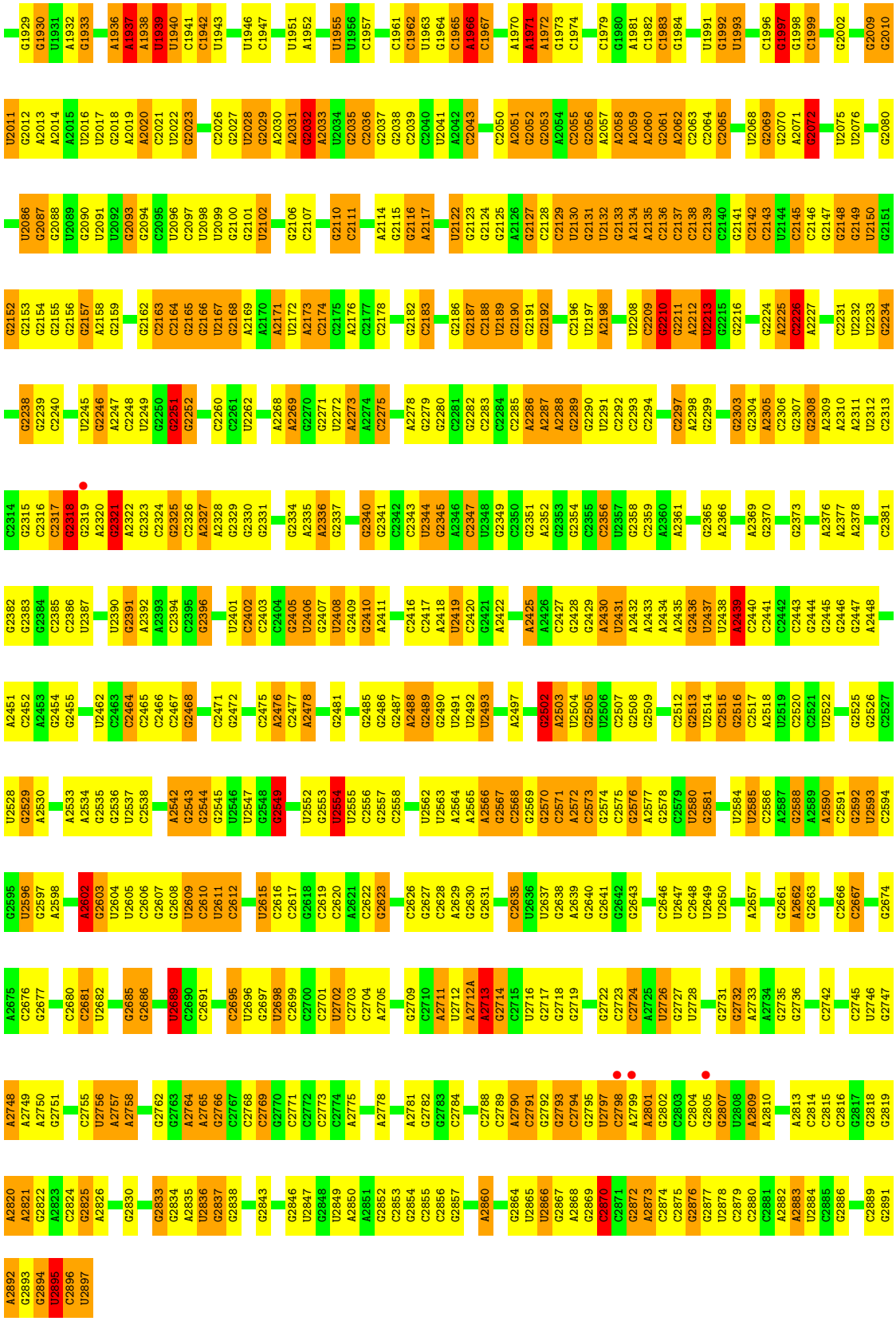
• Molecule 2: 23S ribosomal RNA

Chain GB:



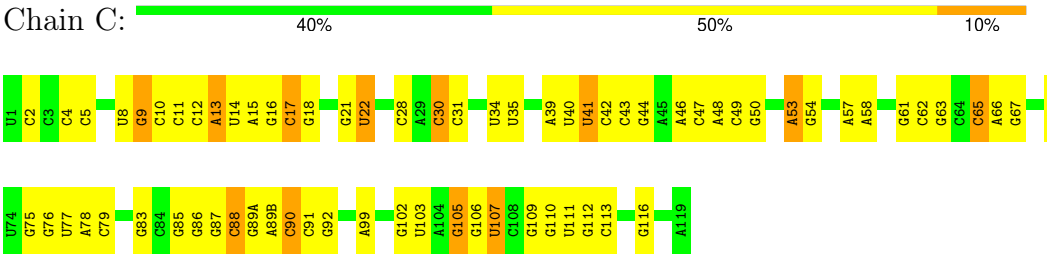






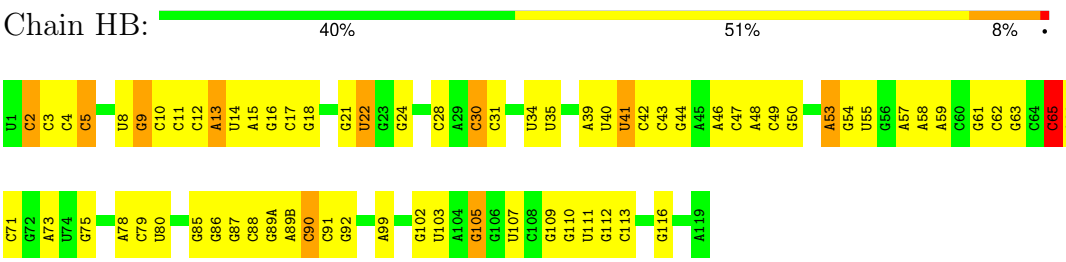
• Molecule 3: 5S ribosomal RNA

Chain C:



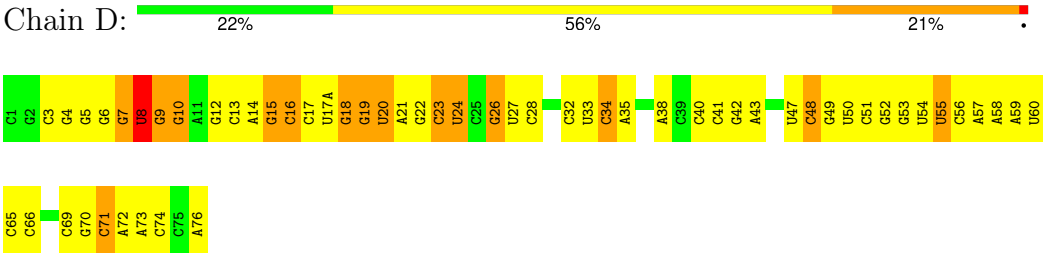
• Molecule 3: 5S ribosomal RNA

Chain HB:



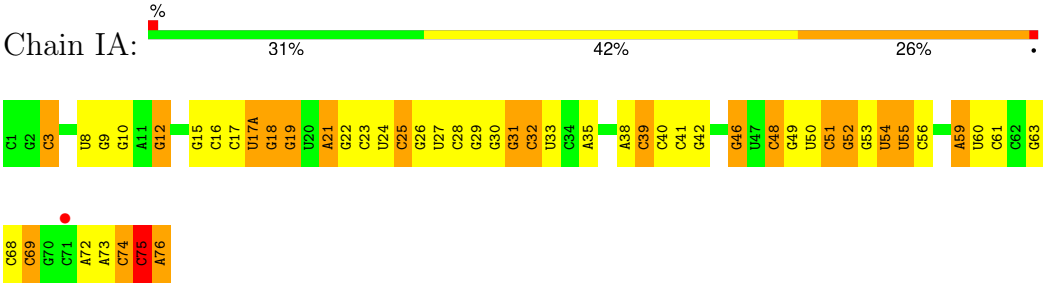
• Molecule 4: tRNA

Chain D:



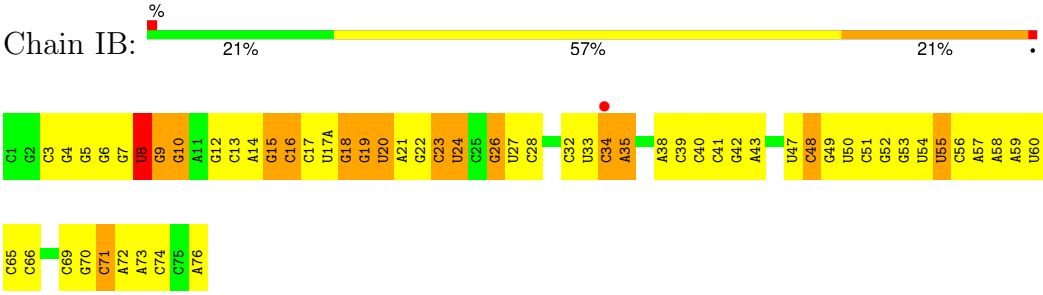
• Molecule 4: tRNA

Chain IA:



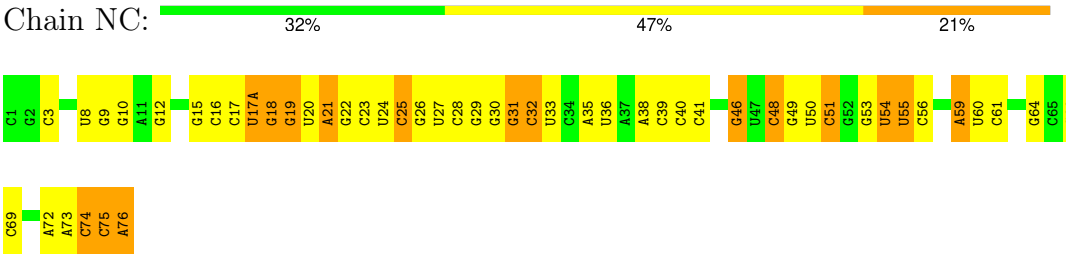
• Molecule 4: tRNA

Chain IB:



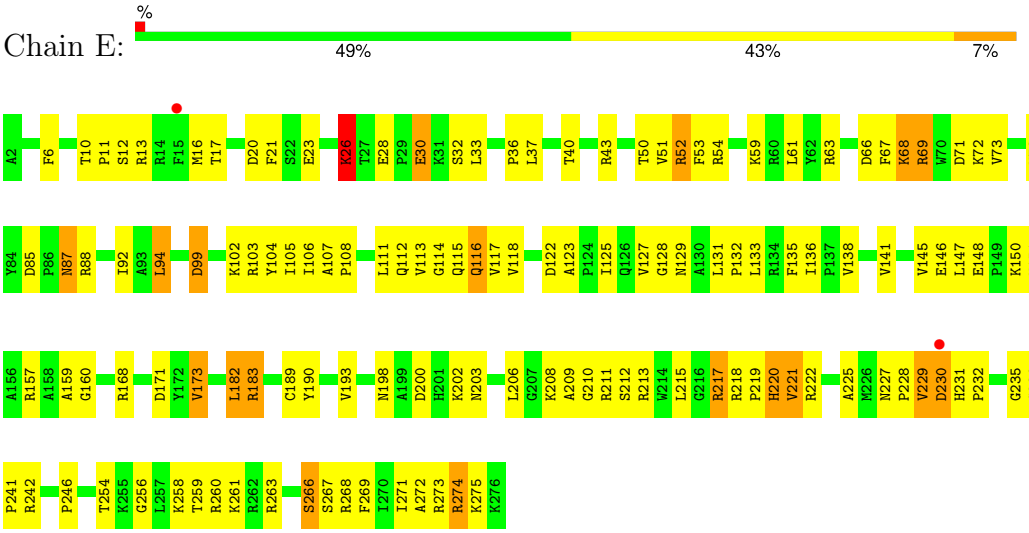
• Molecule 4: tRNA

Chain NC:



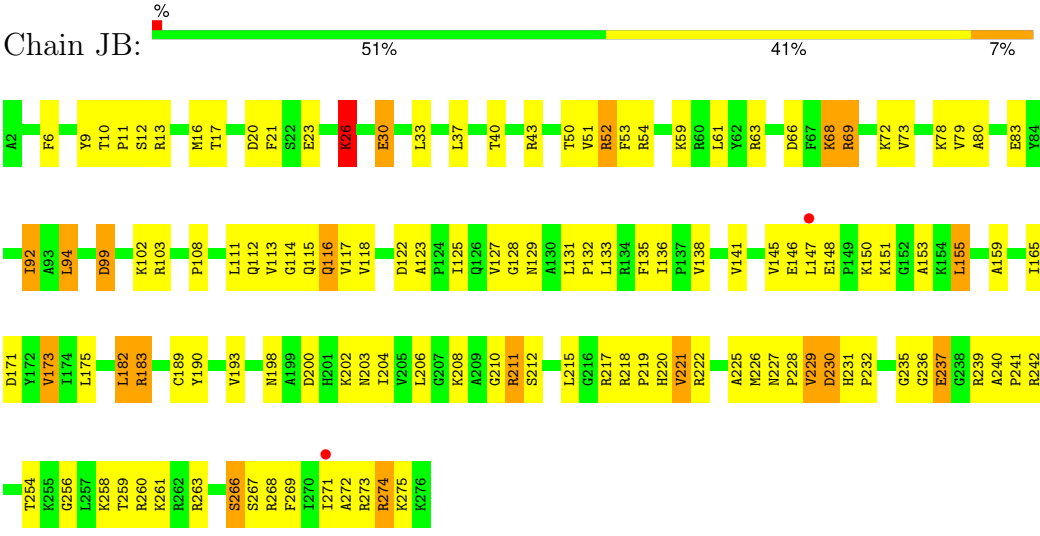
• Molecule 5: 50S ribosomal protein L2

Chain E:



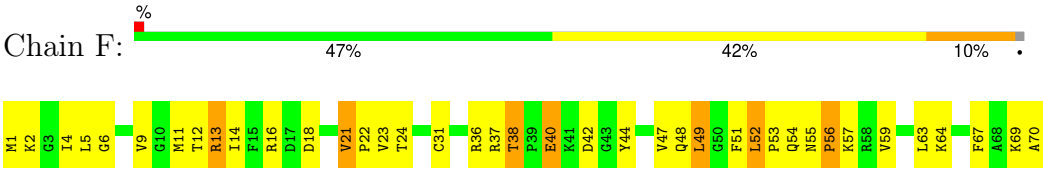
• Molecule 5: 50S ribosomal protein L2

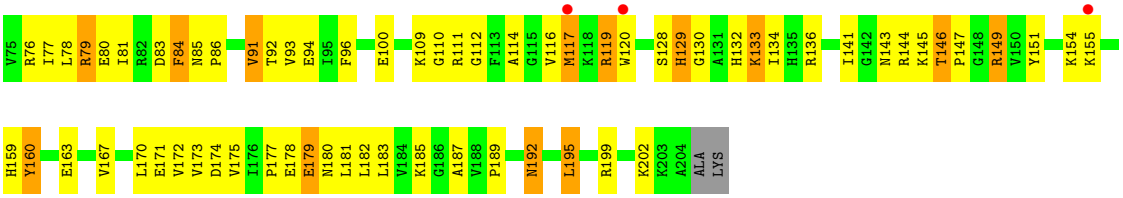
Chain JB:



• Molecule 6: 50S ribosomal protein L3

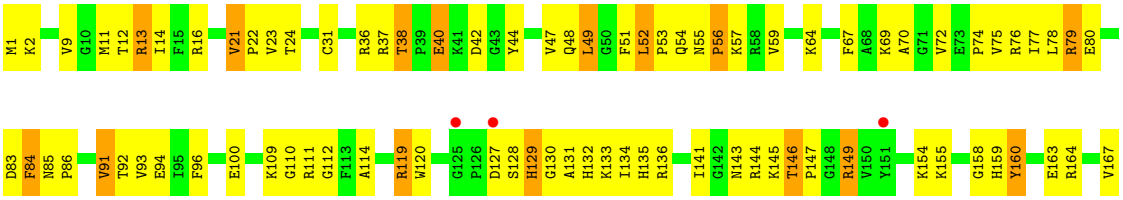
Chain F:

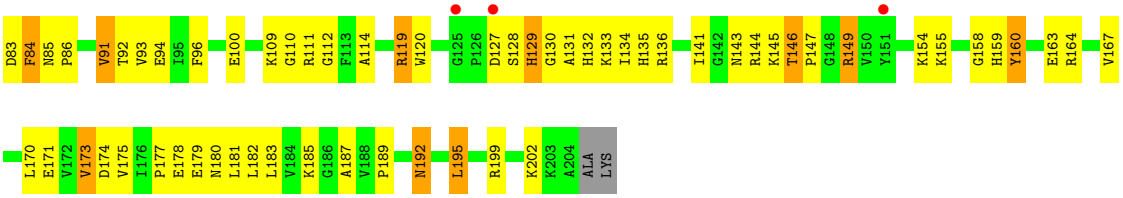




• Molecule 6: 50S ribosomal protein L3

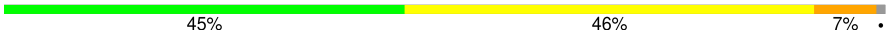
Chain KB:

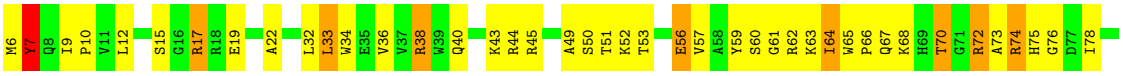


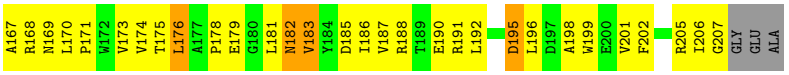


• Molecule 7: 50S ribosomal protein L4

Chain G:

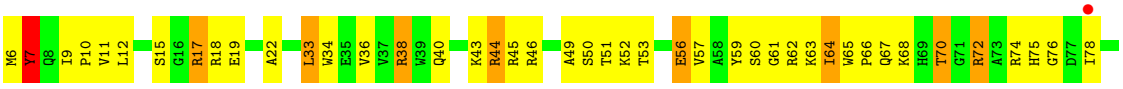


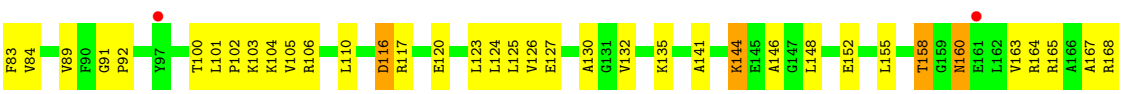




• Molecule 7: 50S ribosomal protein L4

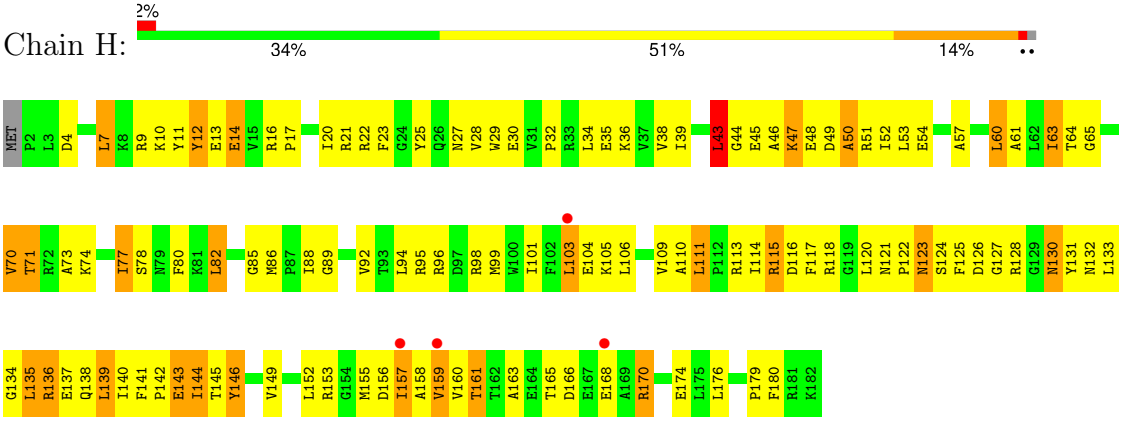
Chain LB:





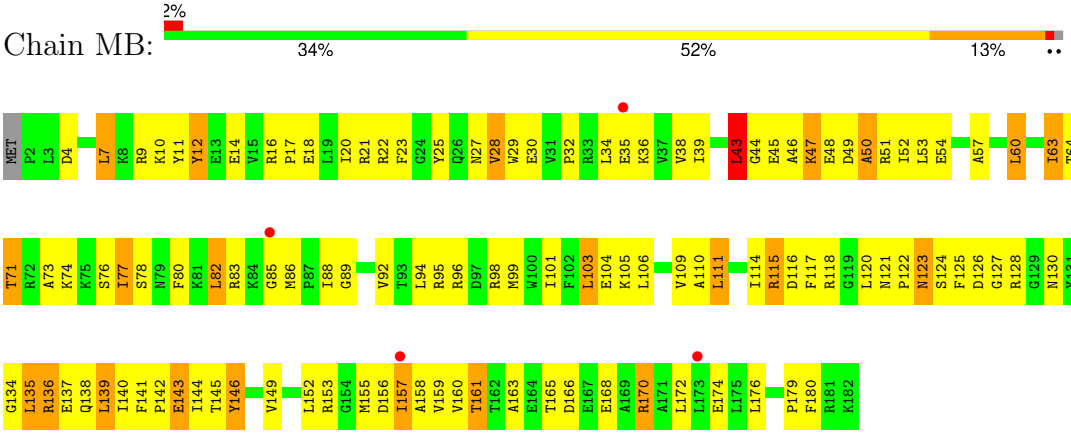
• Molecule 8: 50S ribosomal protein L5

Chain H:



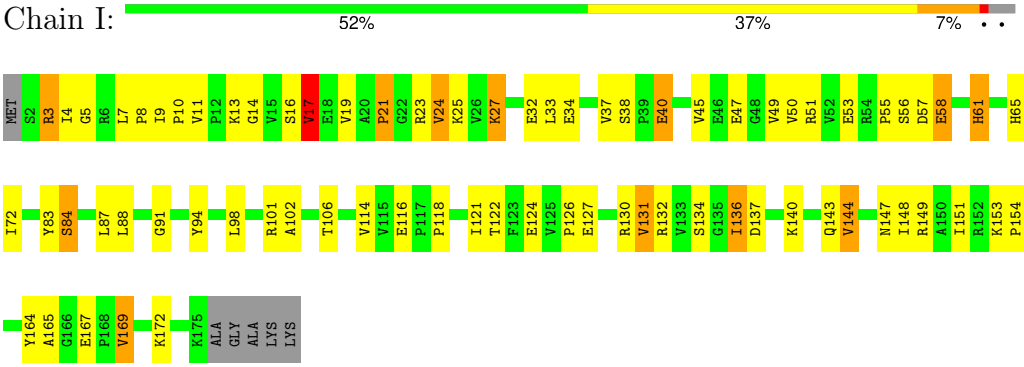
• Molecule 8: 50S ribosomal protein L5

Chain MB:



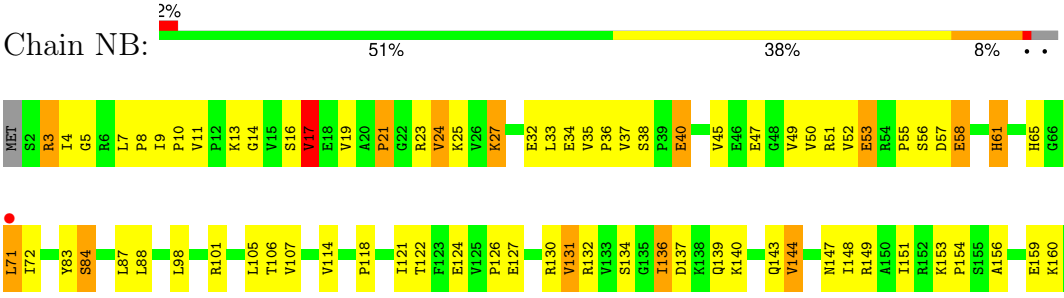
• Molecule 9: 50S ribosomal protein L6

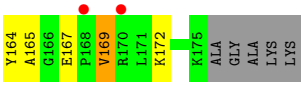
Chain I:



• Molecule 9: 50S ribosomal protein L6

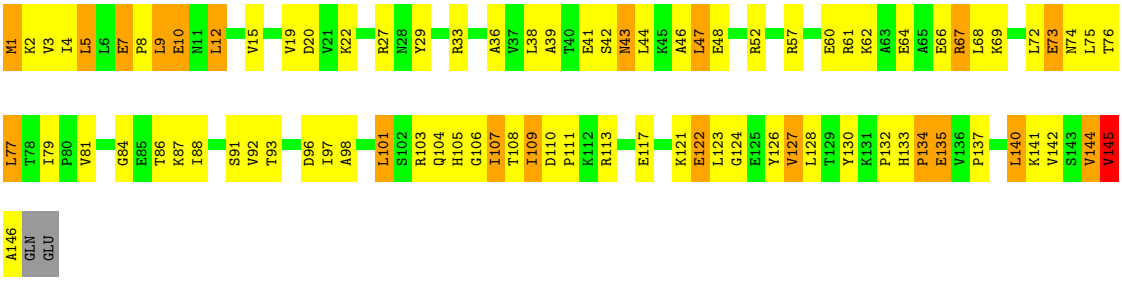
Chain NB:





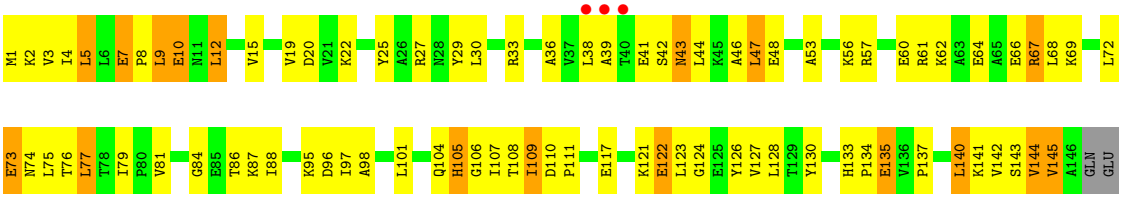
• Molecule 10: 50S ribosomal protein L9

Chain J:



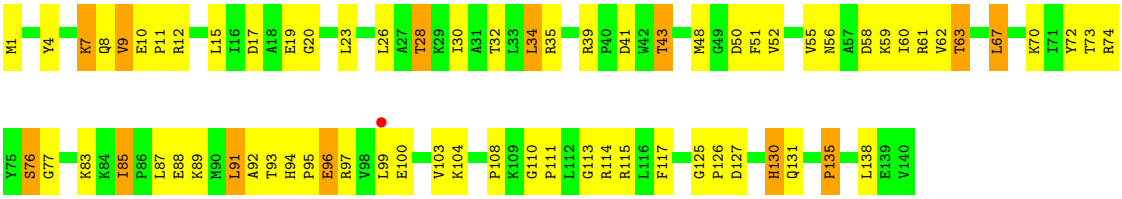
• Molecule 10: 50S ribosomal protein L9

Chain OB:



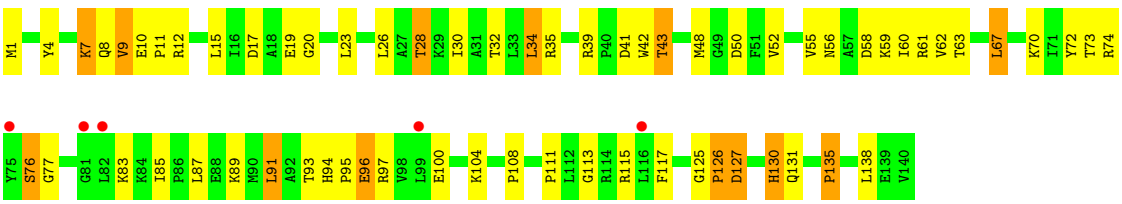
• Molecule 11: 50S ribosomal protein L13

Chain K:



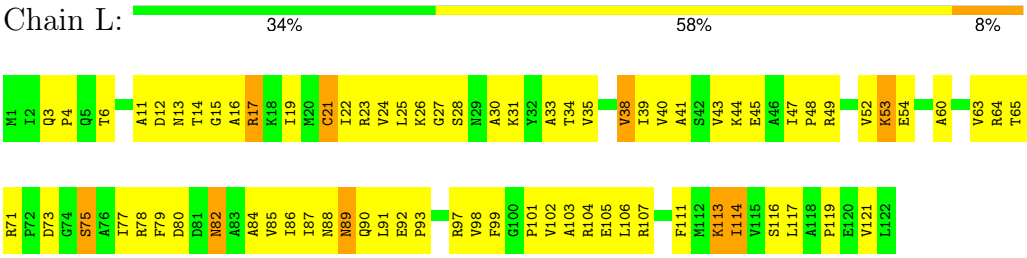
• Molecule 11: 50S ribosomal protein L13

Chain PB:



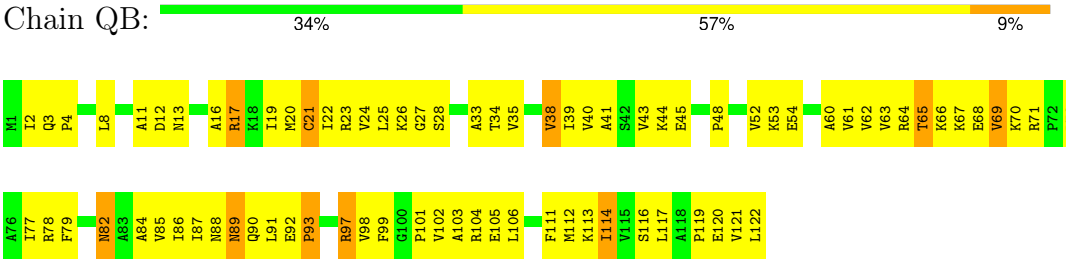
• Molecule 12: 50S ribosomal protein L14

Chain L:



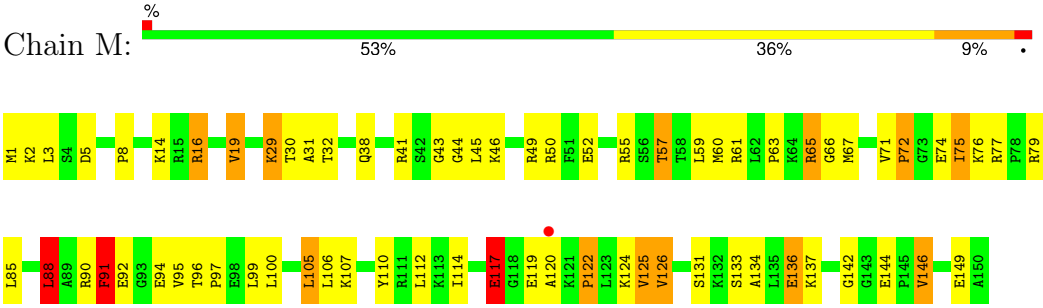
• Molecule 12: 50S ribosomal protein L14

Chain QB:



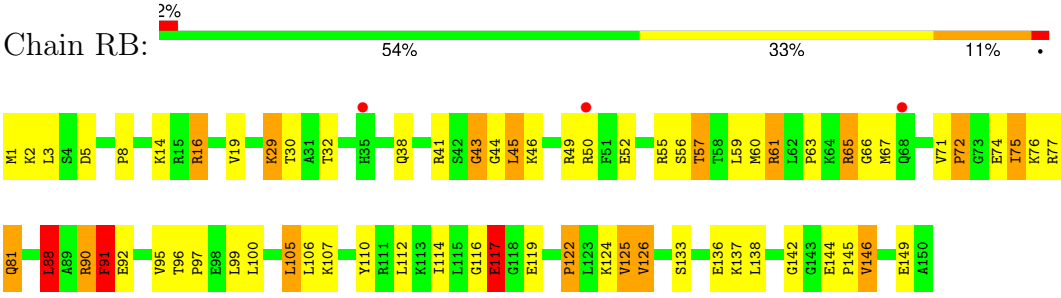
• Molecule 13: 50S ribosomal protein L15

Chain M:



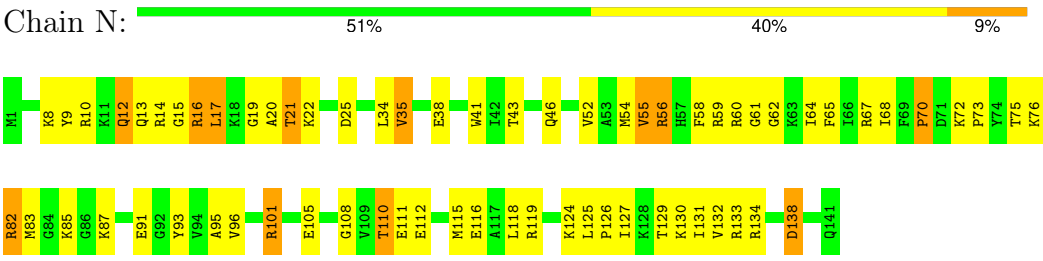
• Molecule 13: 50S ribosomal protein L15

Chain RB:



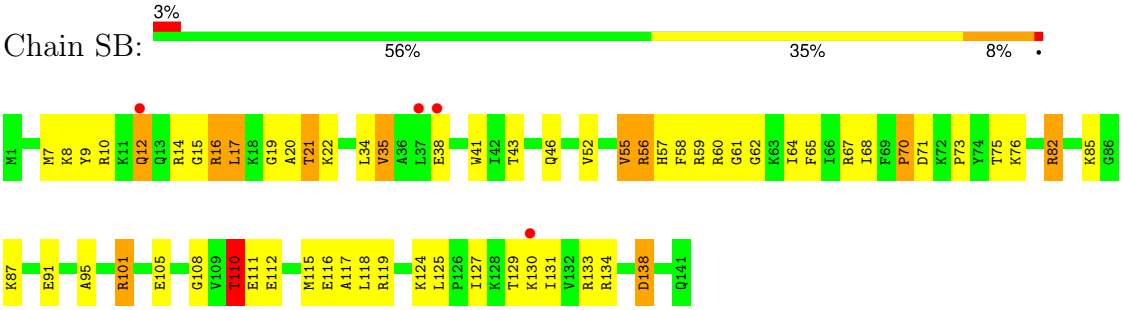
• Molecule 14: 50S ribosomal protein L16

Chain N:



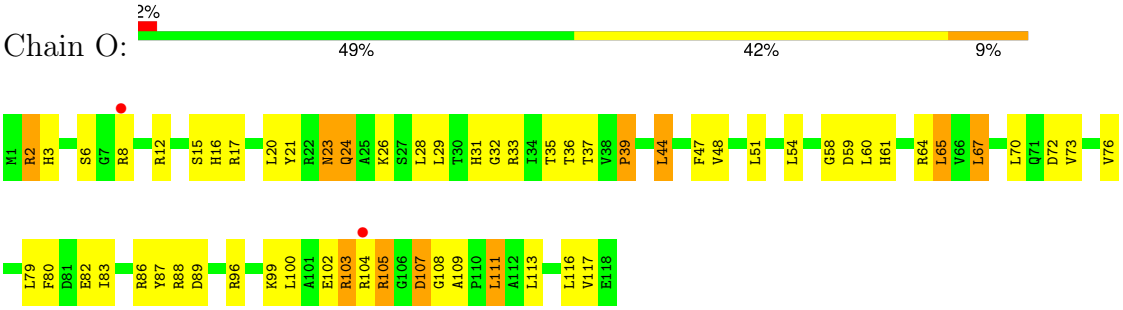
• Molecule 14: 50S ribosomal protein L16

Chain SB:



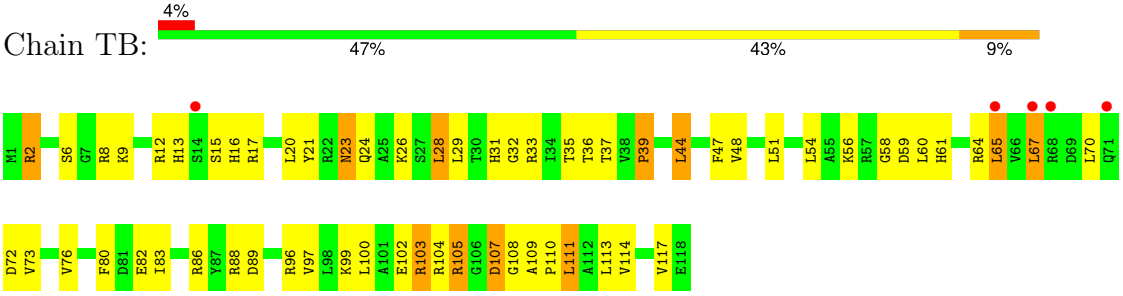
• Molecule 15: 50S ribosomal protein L17

Chain O:



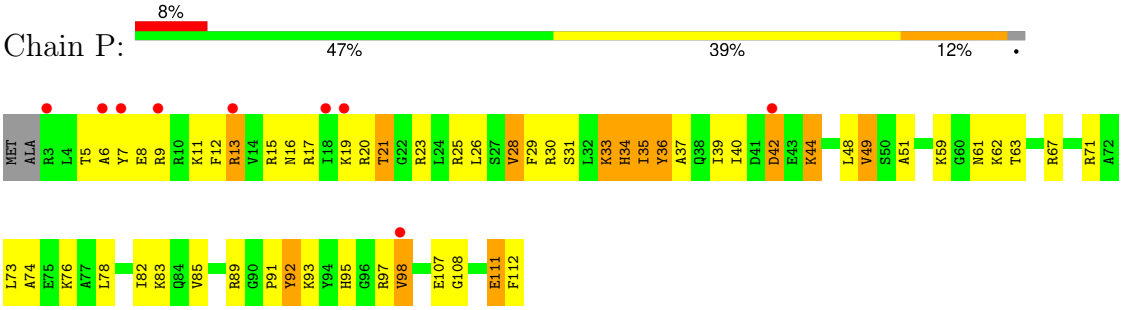
• Molecule 15: 50S ribosomal protein L17

Chain TB:



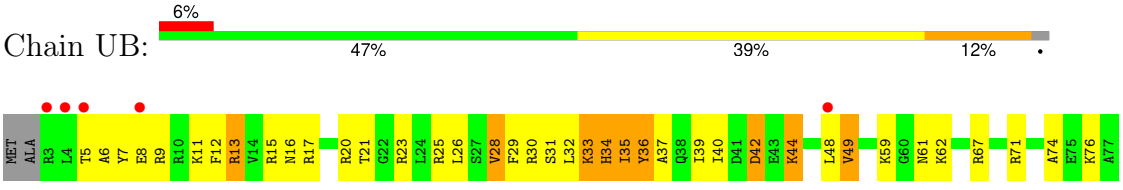
• Molecule 16: 50S ribosomal protein L18

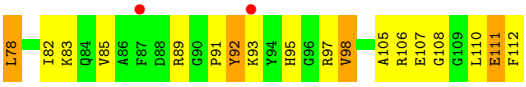
Chain P:



• Molecule 16: 50S ribosomal protein L18

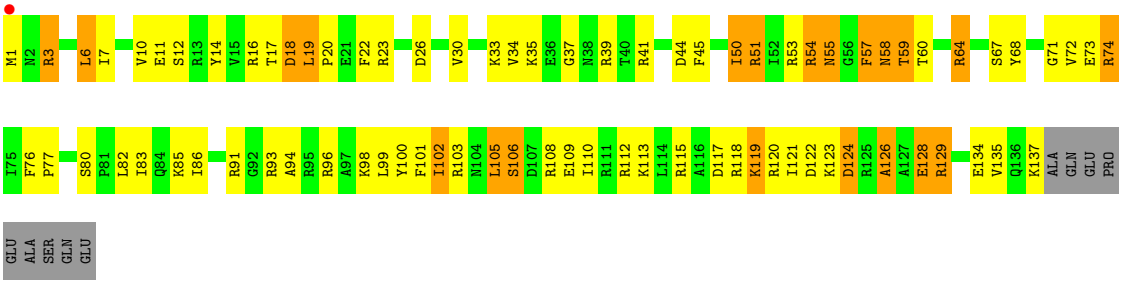
Chain UB:





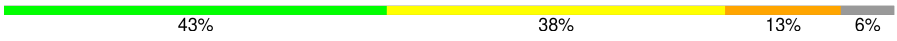
• Molecule 17: 50S ribosomal protein L19

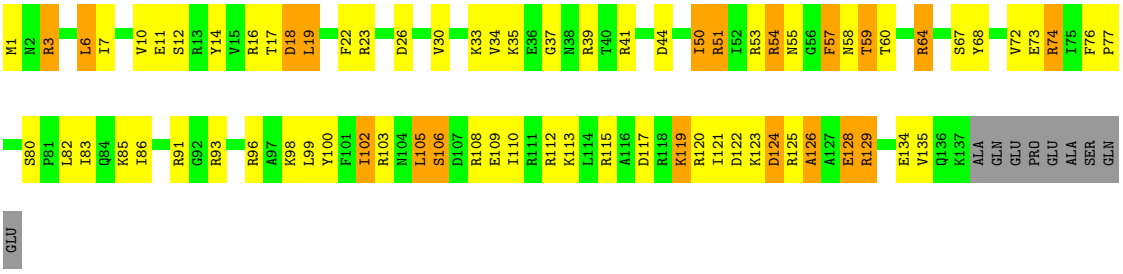
Chain Q:



• Molecule 17: 50S ribosomal protein L19

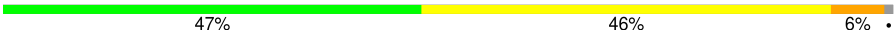
Chain VB:

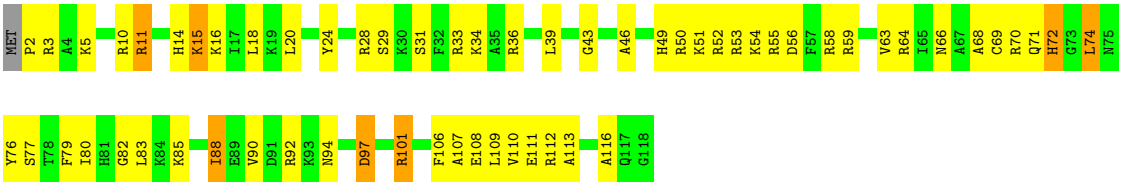




• Molecule 18: 50S ribosomal protein L20

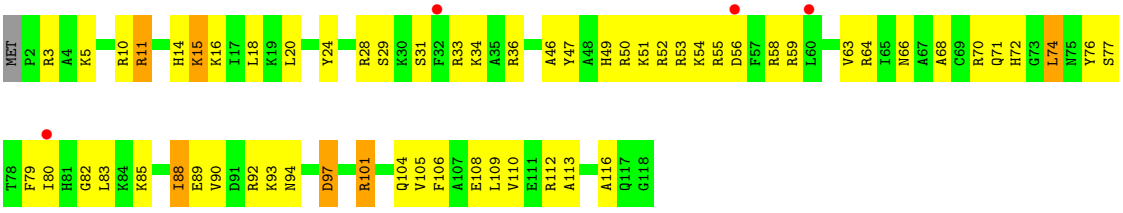
Chain R:





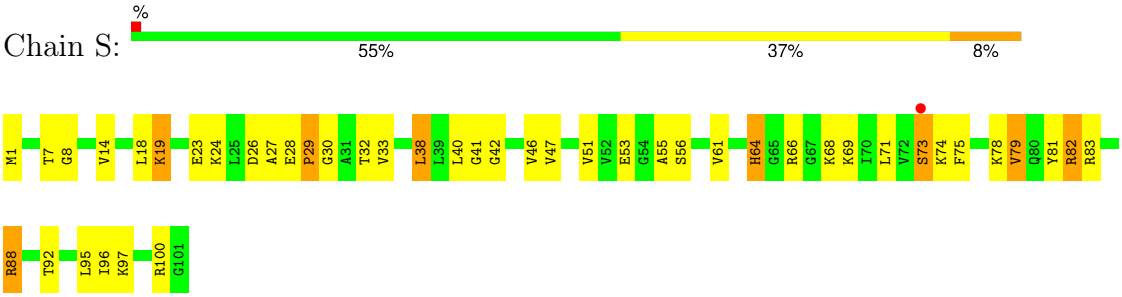
• Molecule 18: 50S ribosomal protein L20

Chain WB:



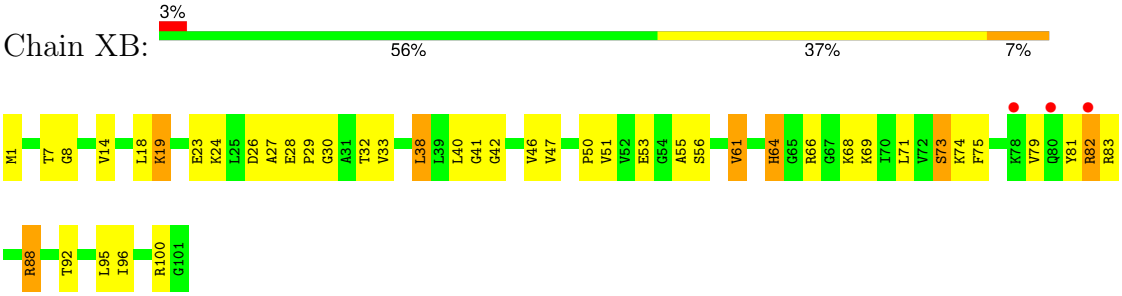
• Molecule 19: 50S ribosomal protein L21

Chain S:



• Molecule 19: 50S ribosomal protein L21

Chain XB:



• Molecule 20: 50S ribosomal protein L22

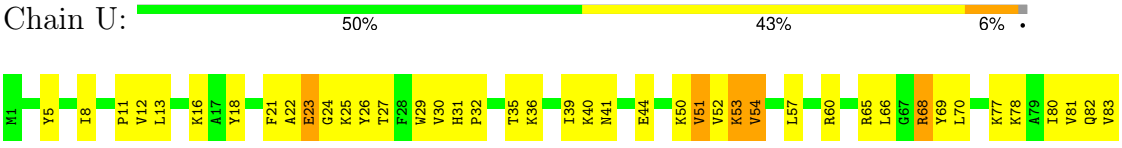
Chain T:

• Molecule 20: 50S ribosomal protein L22

Chain YB:

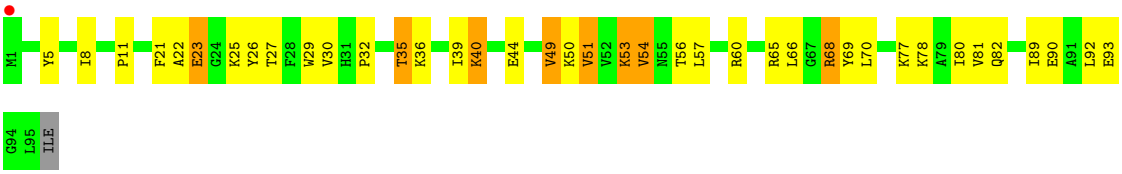
• Molecule 21: 50S ribosomal protein L23

Chain U:



• Molecule 21: 50S ribosomal protein L23

Chain ZB:

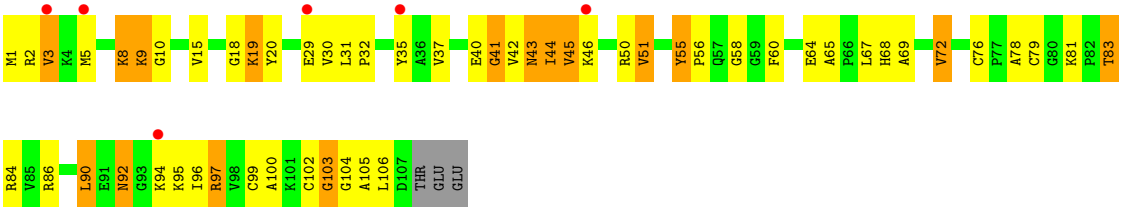


• Molecule 22: 50S ribosomal protein L24

Chain V:

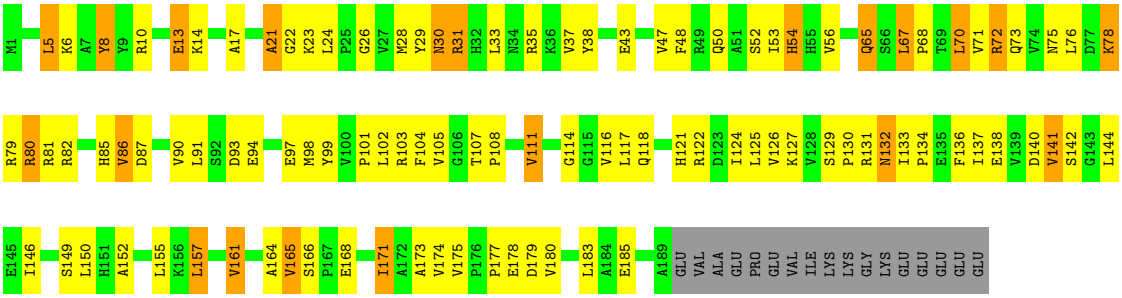
• Molecule 22: 50S ribosomal protein L24

Chain AC:



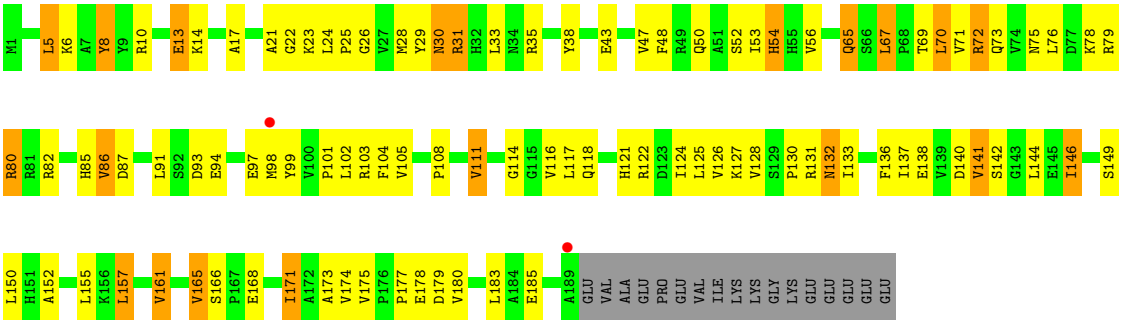
• Molecule 23: 50S ribosomal protein L25

Chain W:

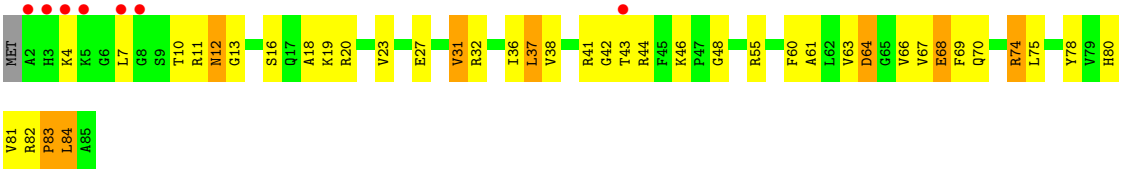


• Molecule 23: 50S ribosomal protein L25

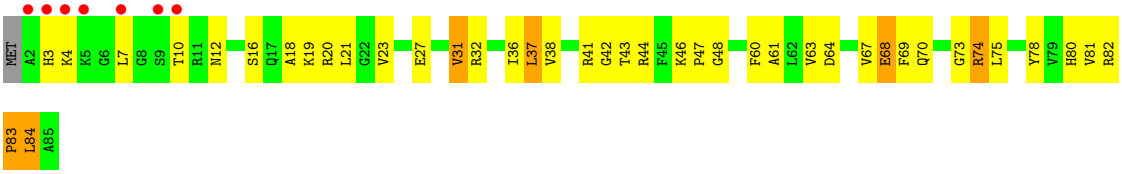
Chain BC:



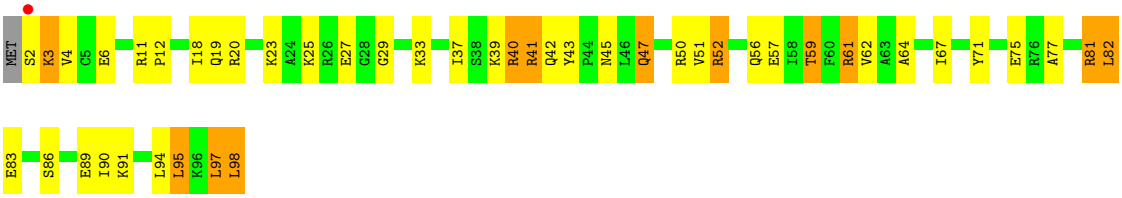
• Molecule 24: 50S ribosomal protein L27



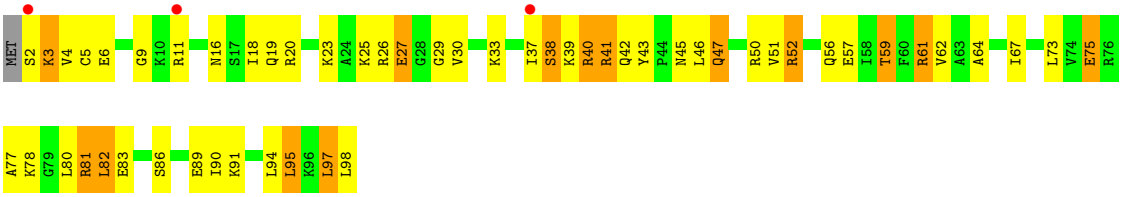
• Molecule 24: 50S ribosomal protein L27



• Molecule 25: 50S ribosomal protein L28

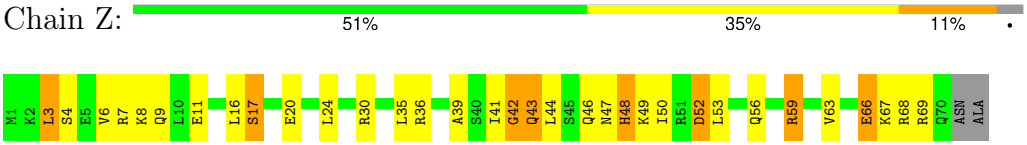


• Molecule 25: 50S ribosomal protein L28



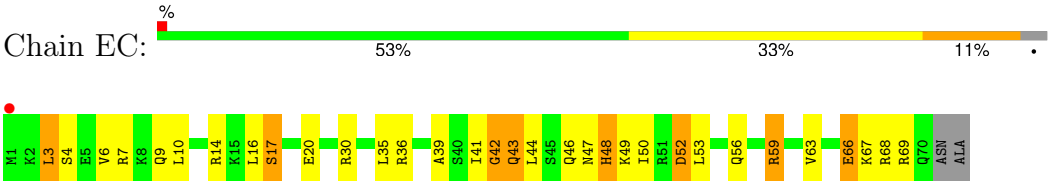
• Molecule 26: 50S ribosomal protein L29

Chain Z:



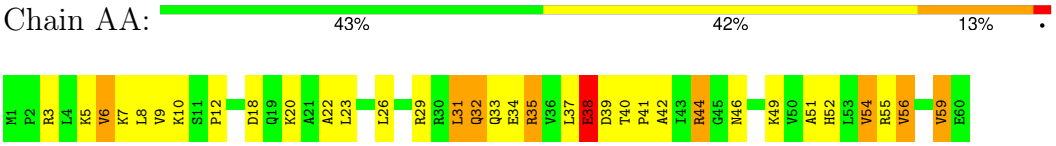
• Molecule 26: 50S ribosomal protein L29

Chain EC:



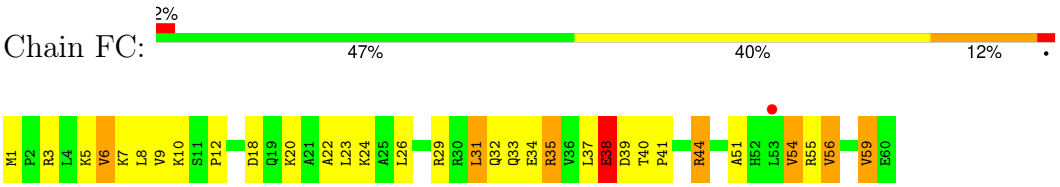
• Molecule 27: 50S ribosomal protein L30

Chain AA:



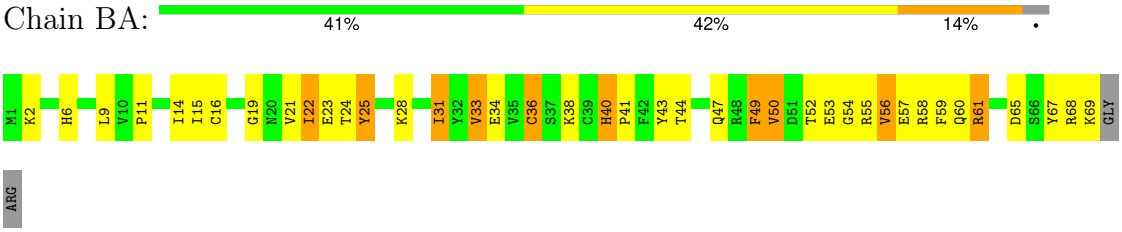
• Molecule 27: 50S ribosomal protein L30

Chain FC:



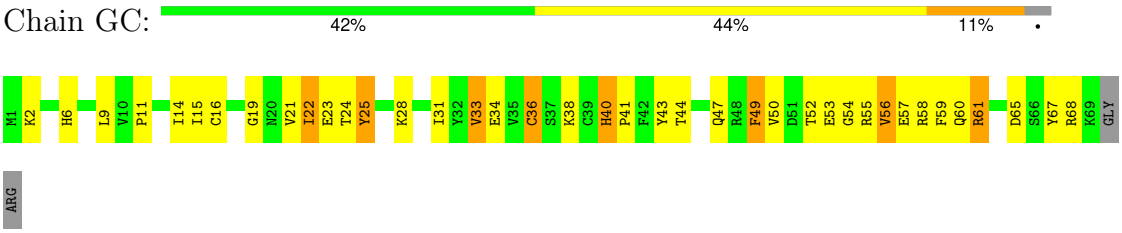
• Molecule 28: 50S ribosomal protein L31

Chain BA:



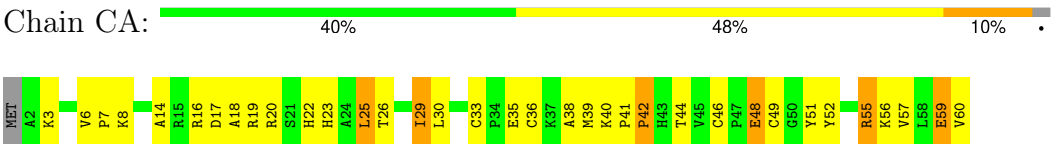
• Molecule 28: 50S ribosomal protein L31

Chain GC:



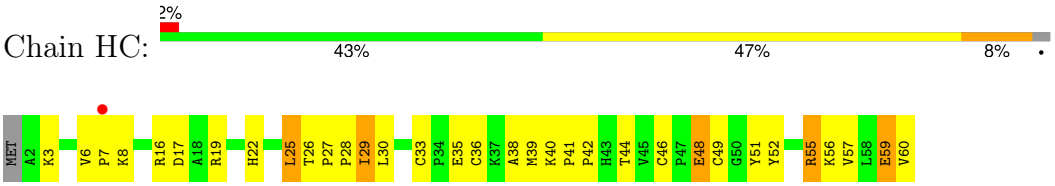
• Molecule 29: 50S ribosomal protein L32

Chain CA:



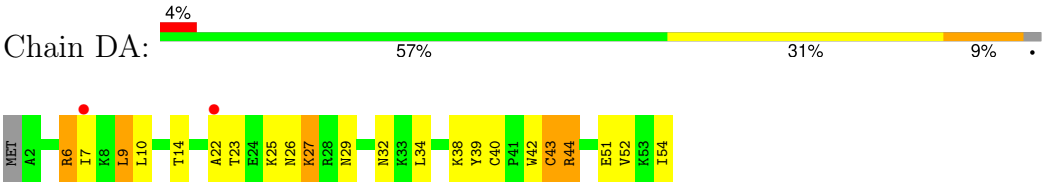
• Molecule 29: 50S ribosomal protein L32

Chain HC:



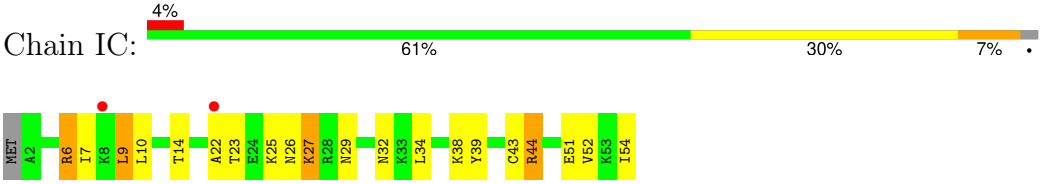
• Molecule 30: 50S ribosomal protein L33

Chain DA:



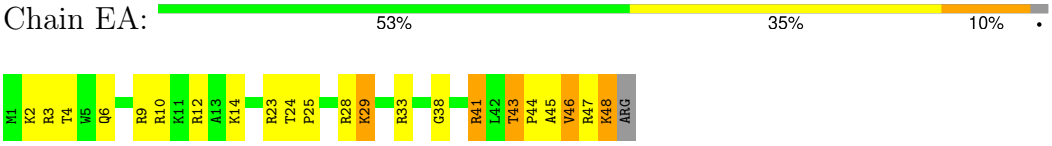
• Molecule 30: 50S ribosomal protein L33

Chain IC:



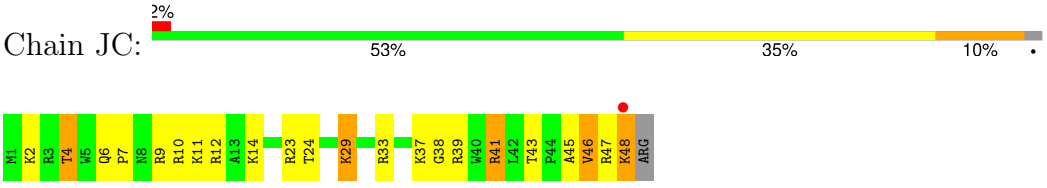
• Molecule 31: 50S ribosomal protein L34

Chain EA:



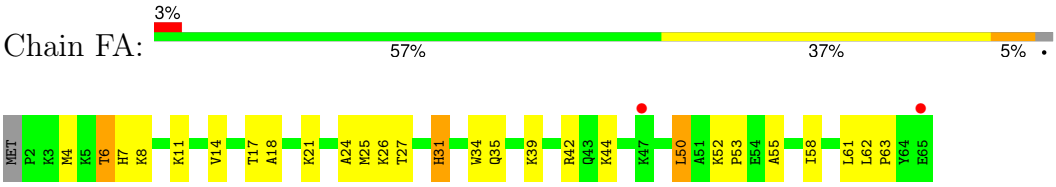
• Molecule 31: 50S ribosomal protein L34

Chain JC:



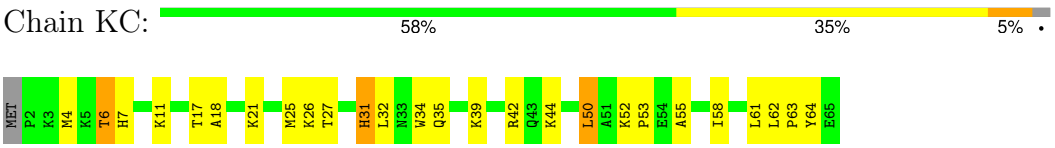
• Molecule 32: 50S ribosomal protein L35

Chain FA:



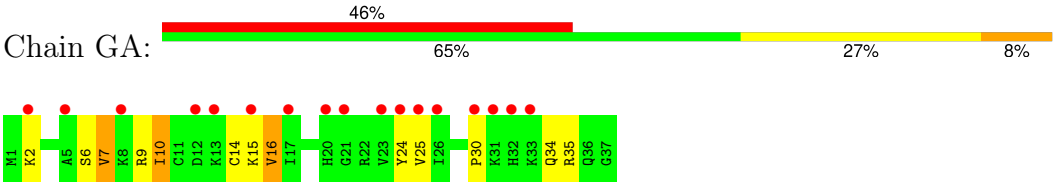
• Molecule 32: 50S ribosomal protein L35

Chain KC:



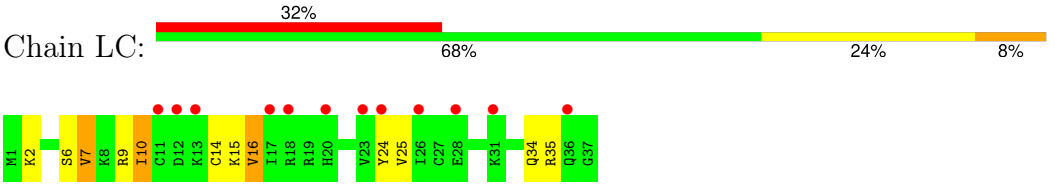
• Molecule 33: 50S ribosomal protein L36

Chain GA:



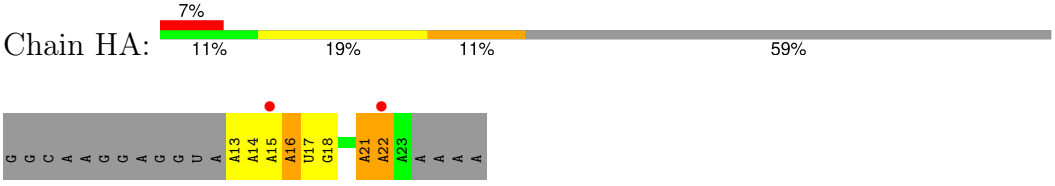
• Molecule 33: 50S ribosomal protein L36

Chain LC:



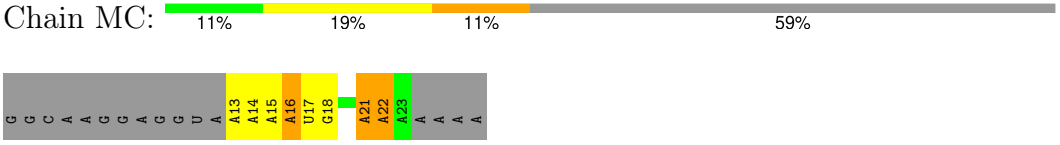
• Molecule 34: mRNA

Chain HA:



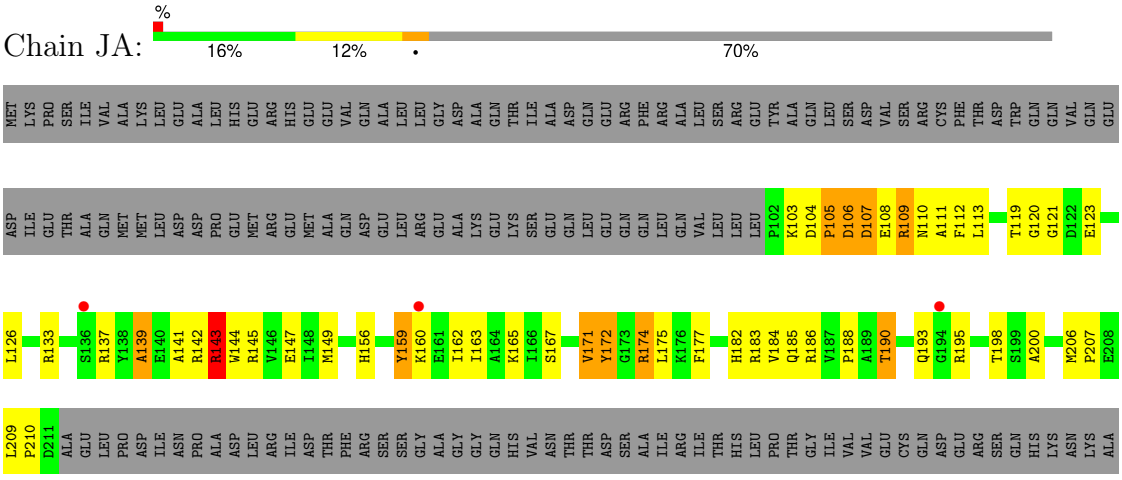
• Molecule 34: mRNA

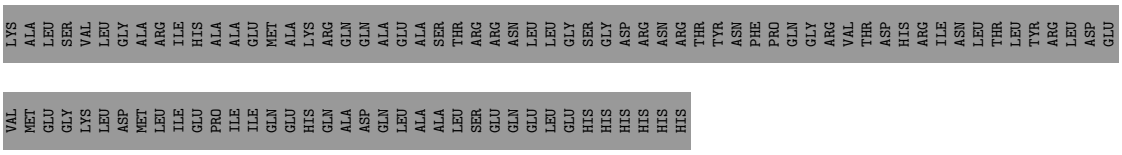
Chain MC:



• Molecule 35: Peptide chain release factor 1

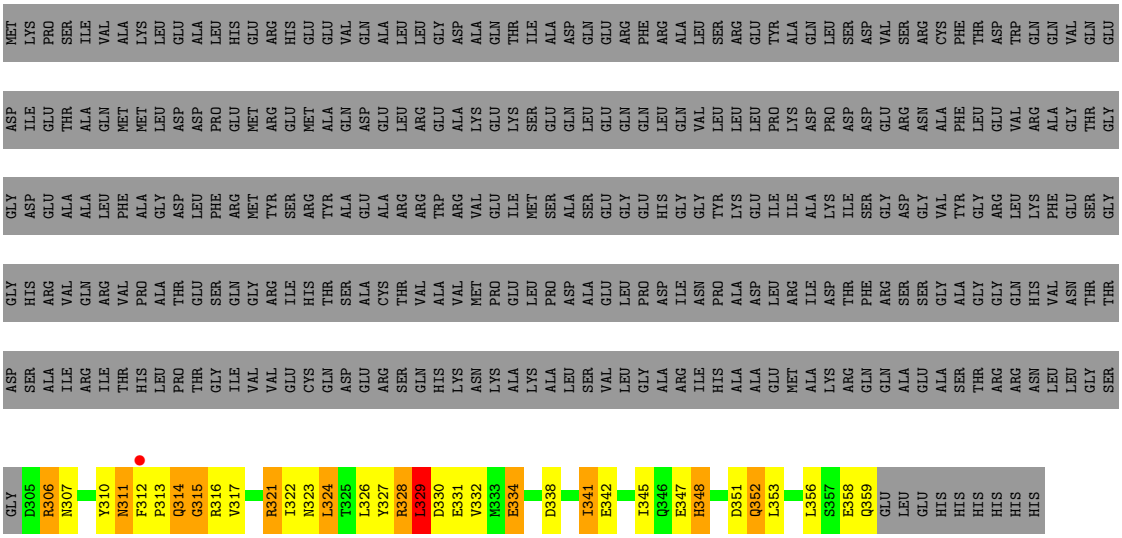
Chain JA:





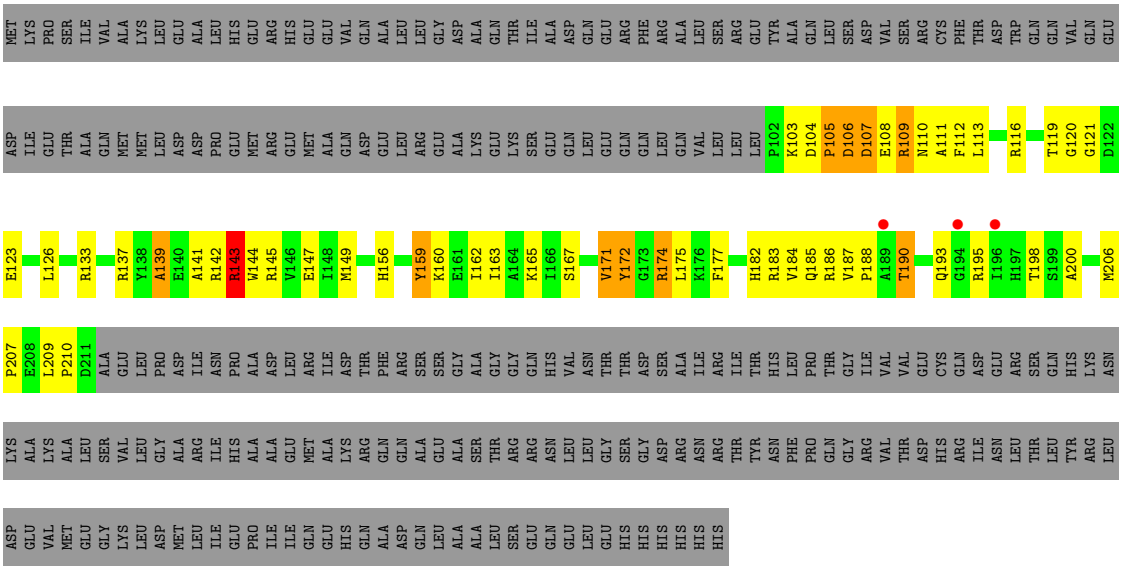
• Molecule 35: Peptide chain release factor 1

Chain KA:



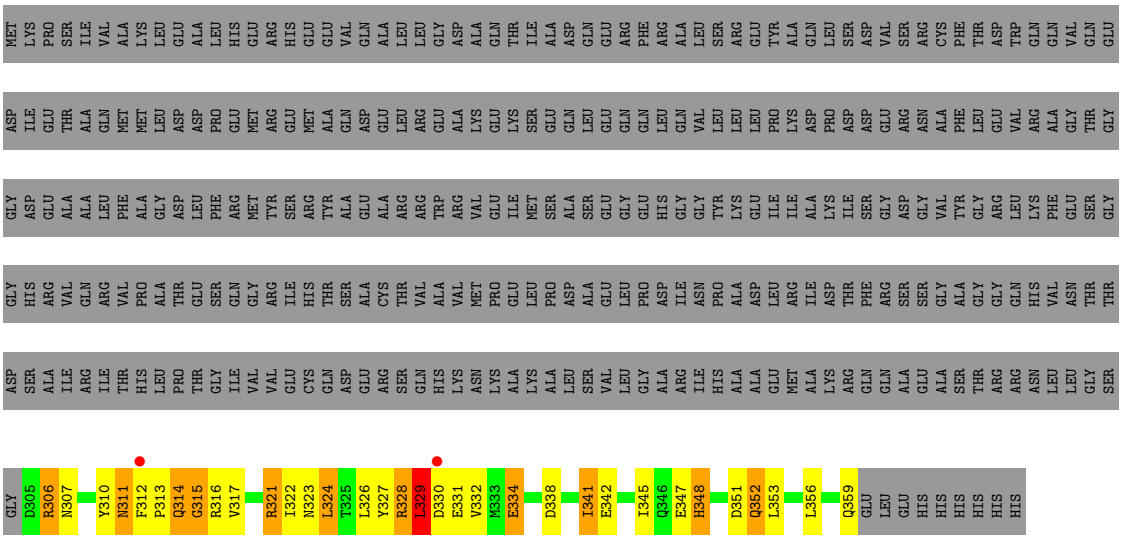
• Molecule 35: Peptide chain release factor 1

Chain OC:



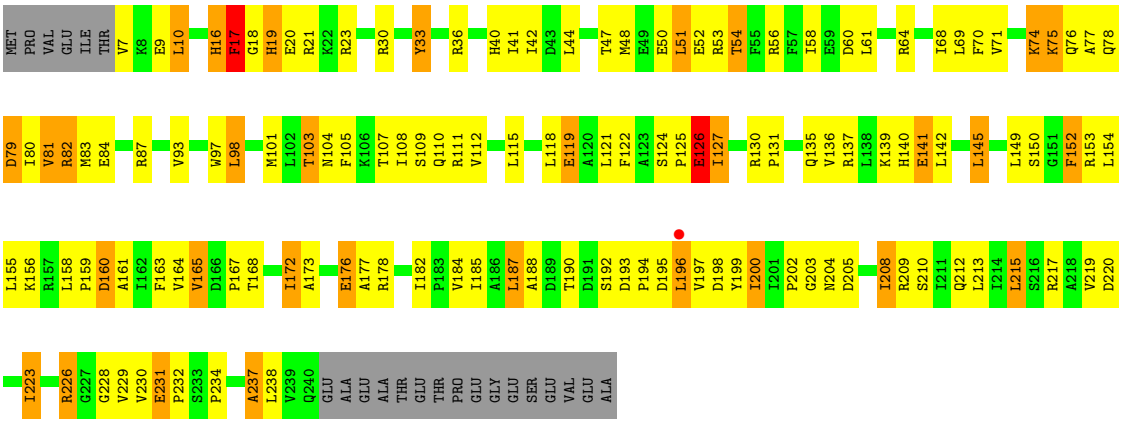
• Molecule 35: Peptide chain release factor 1

Chain PC:



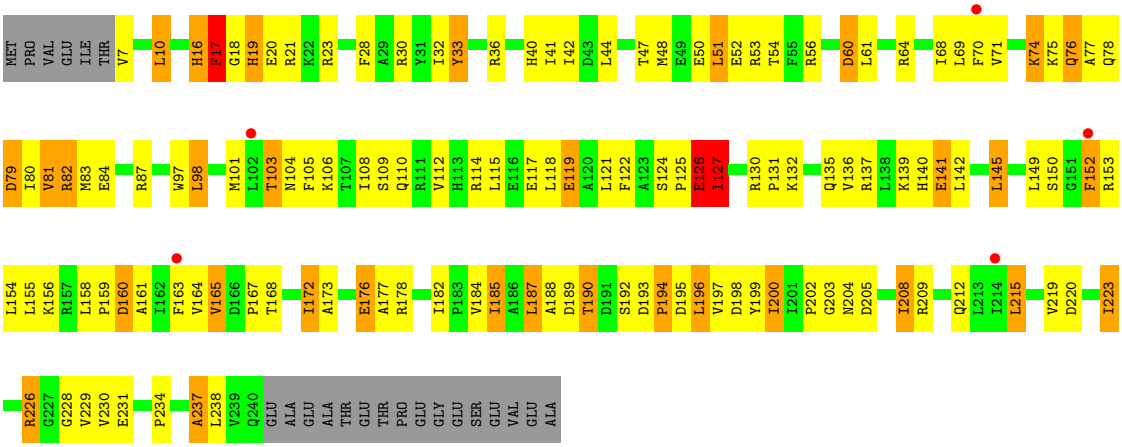
• Molecule 36: 30S ribosomal protein S2

Chain LA:



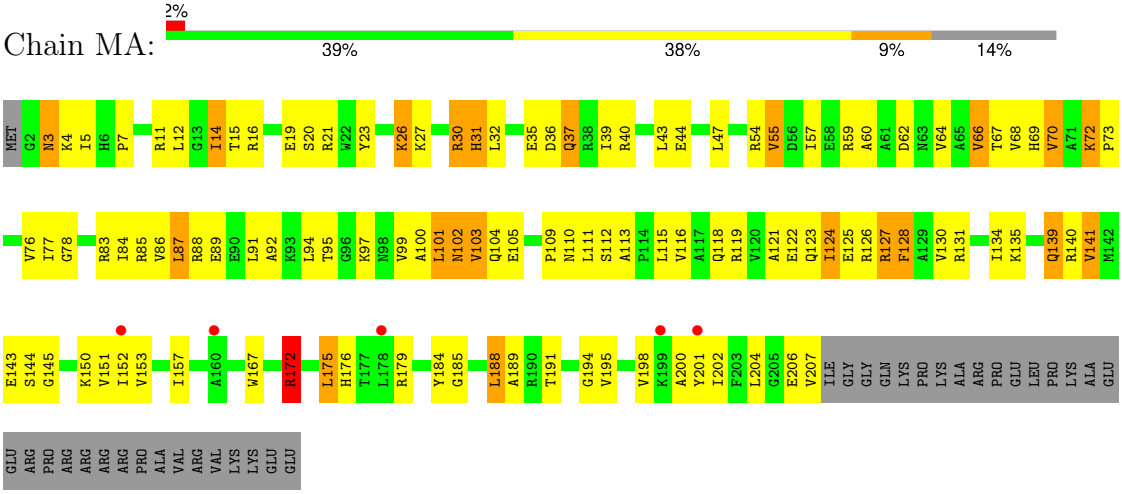
• Molecule 36: 30S ribosomal protein S2

Chain QC:



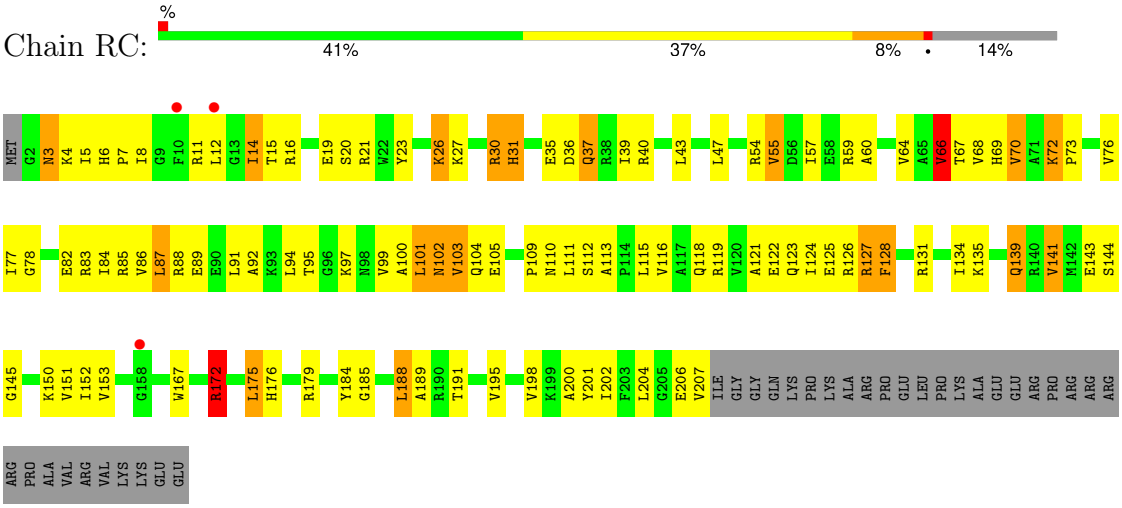
• Molecule 37: 30S ribosomal protein S3

Chain MA:



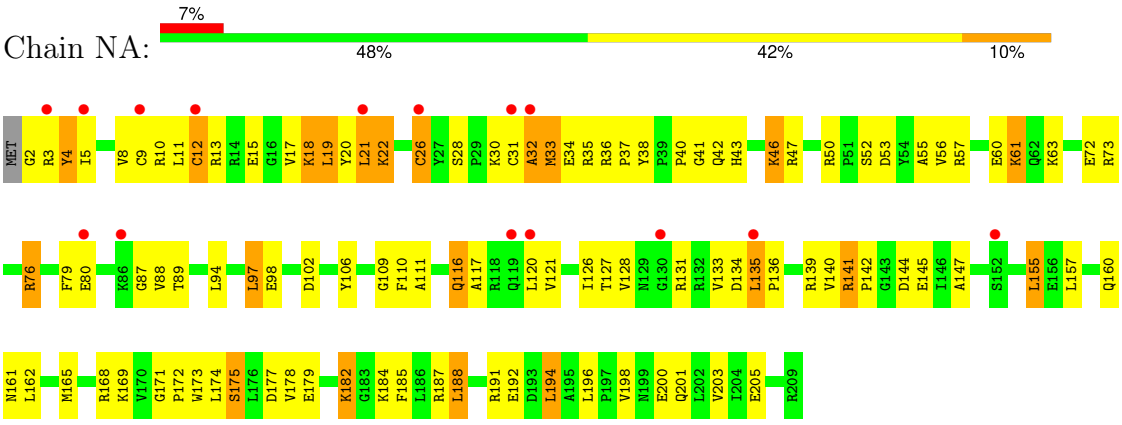
• Molecule 37: 30S ribosomal protein S3

Chain RC:



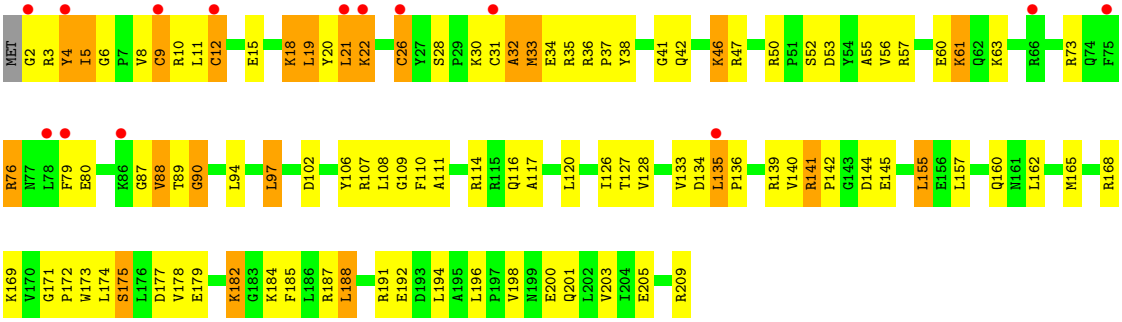
• Molecule 38: 50S ribosomal protein S4

Chain NA:



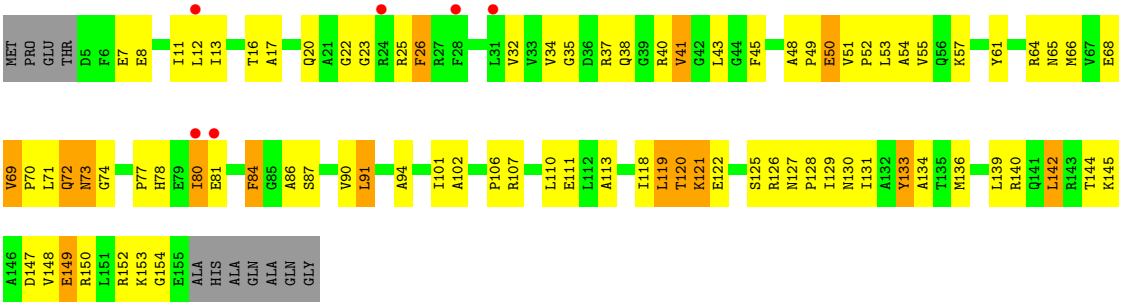
• Molecule 38: 50S ribosomal protein S4

Chain SC:



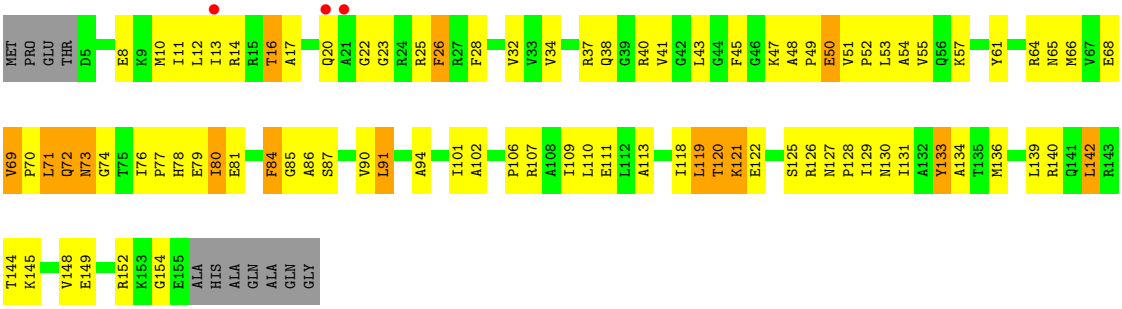
• Molecule 39: 30S ribosomal protein S5

Chain OA:



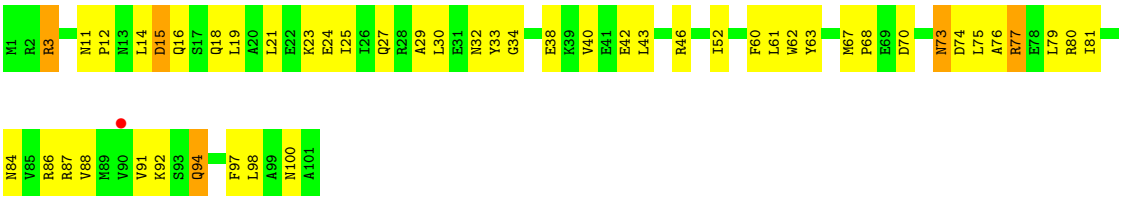
• Molecule 39: 30S ribosomal protein S5

Chain TC:



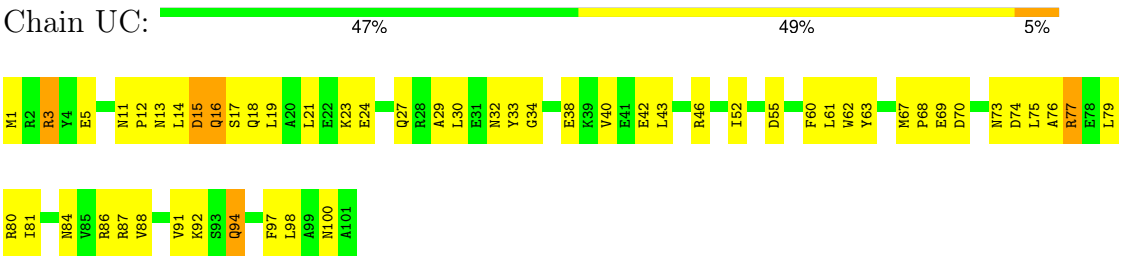
• Molecule 40: 30S ribosomal protein S6

Chain PA:



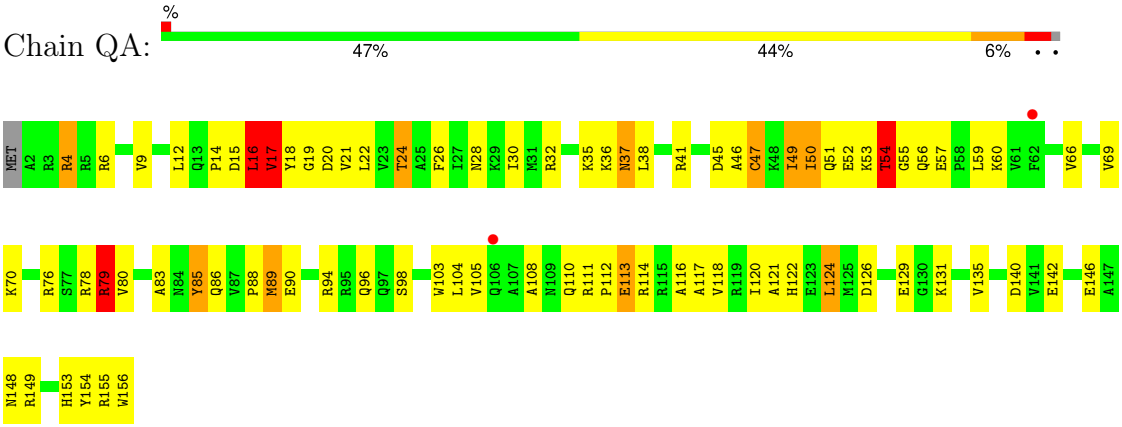
• Molecule 40: 30S ribosomal protein S6

Chain UC:



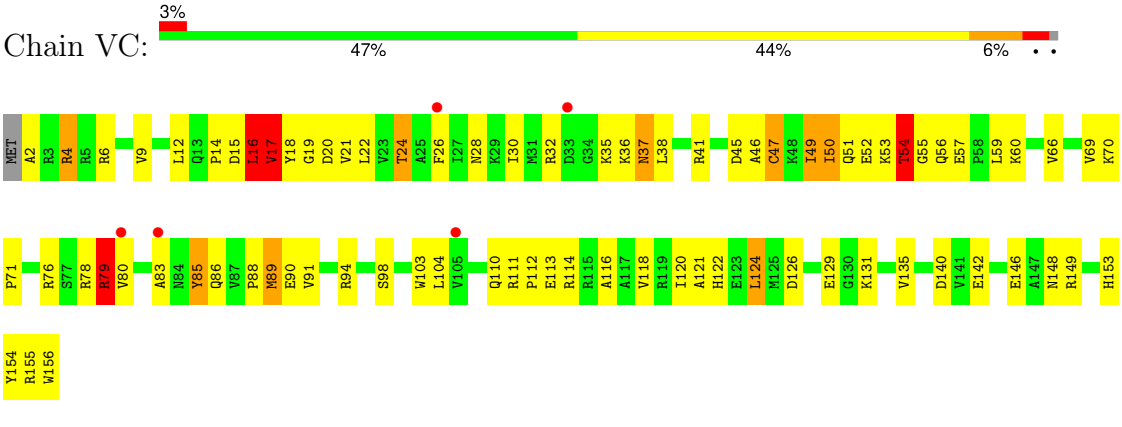
• Molecule 41: 30S ribosomal protein S7

Chain QA:



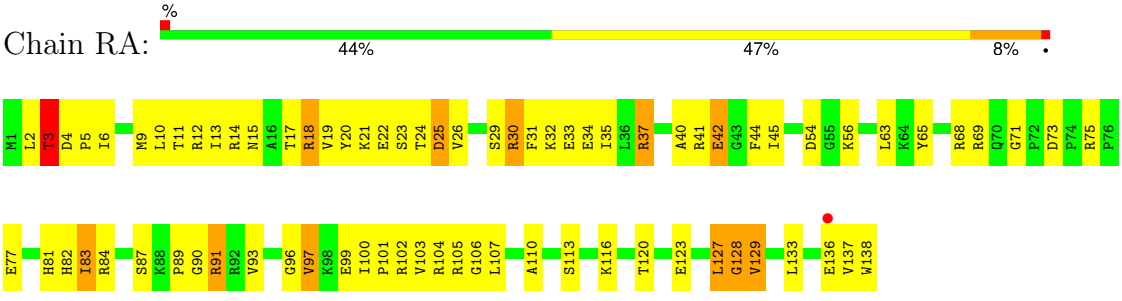
• Molecule 41: 30S ribosomal protein S7

Chain VC:



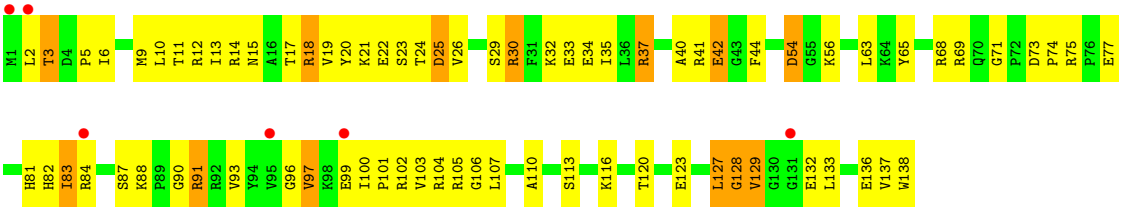
• Molecule 42: 30S ribosomal protein S8

Chain RA:



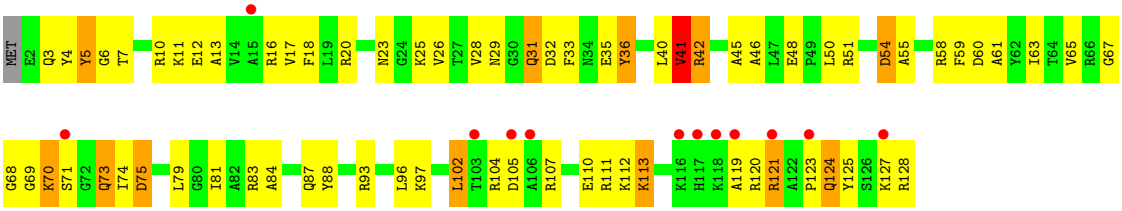
• Molecule 42: 30S ribosomal protein S8

Chain WC:



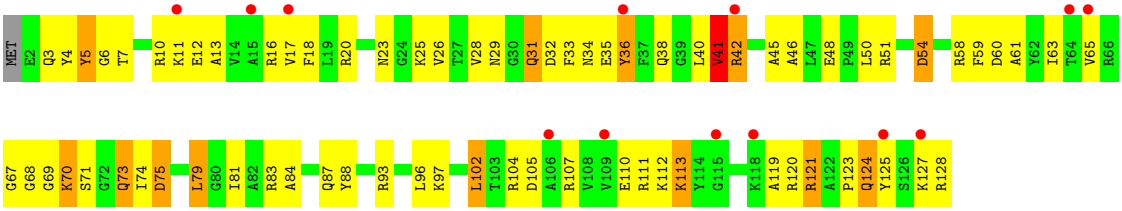
• Molecule 43: 30S ribosomal protein S9

Chain SA:



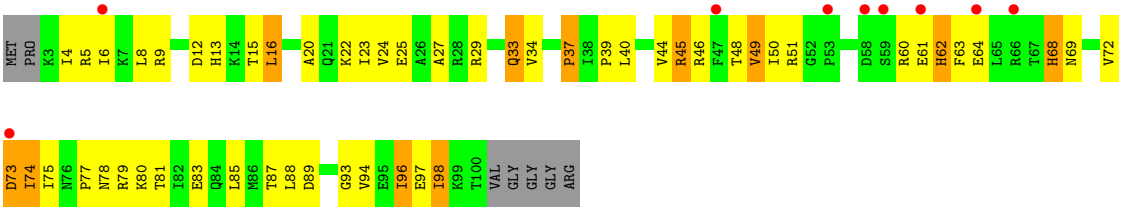
• Molecule 43: 30S ribosomal protein S9

Chain XC:



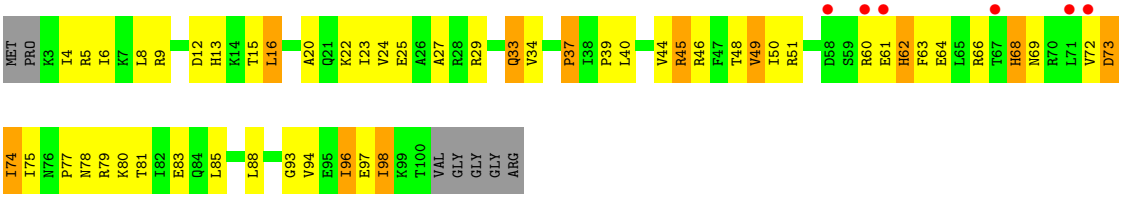
• Molecule 44: 30S ribosomal protein S10

Chain TA:



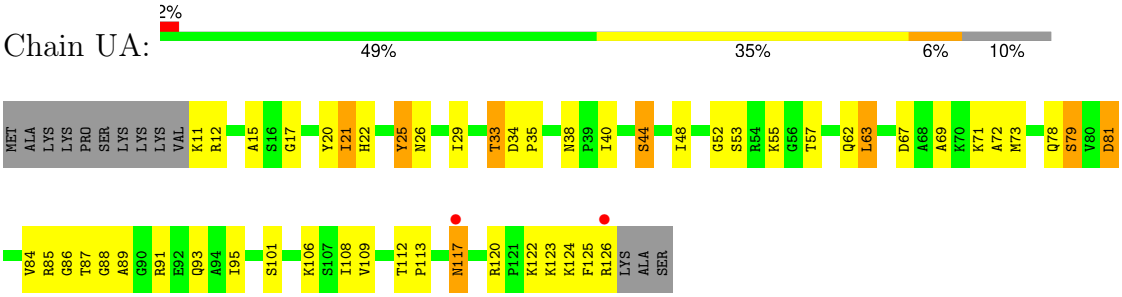
• Molecule 44: 30S ribosomal protein S10

Chain YC:



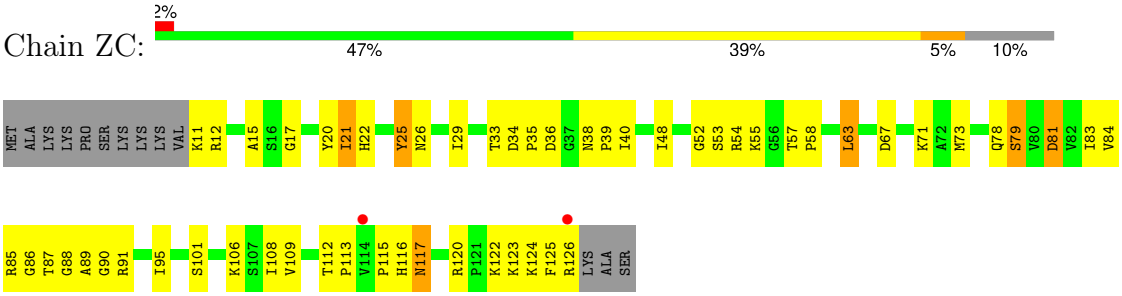
• Molecule 45: 30S ribosomal protein S11

Chain UA:



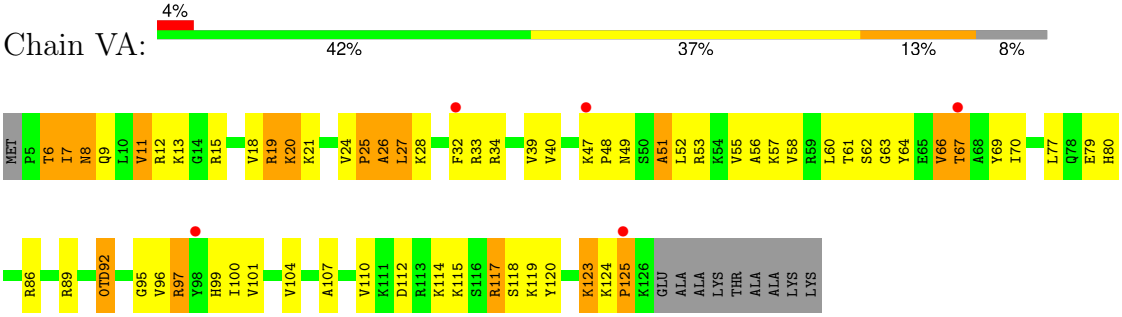
• Molecule 45: 30S ribosomal protein S11

Chain ZC:



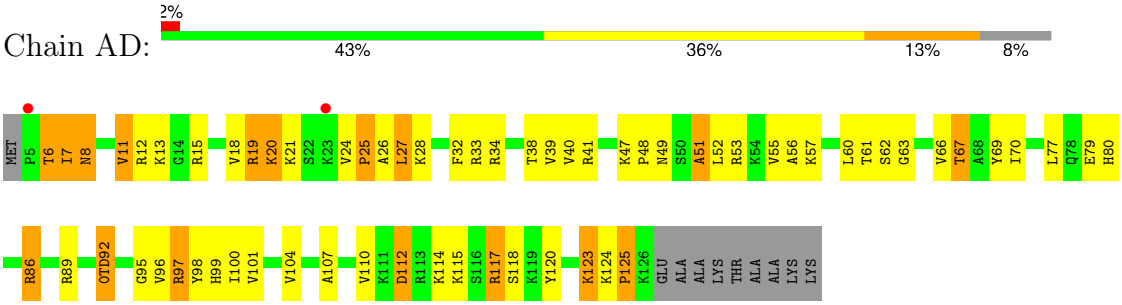
• Molecule 46: 30S ribosomal protein S12

Chain VA:



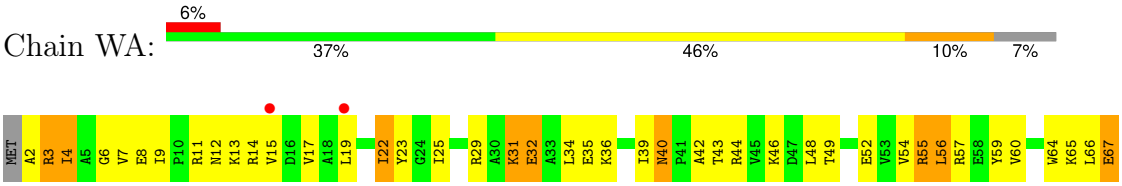
• Molecule 46: 30S ribosomal protein S12

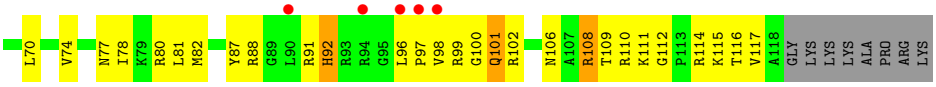
Chain AD:



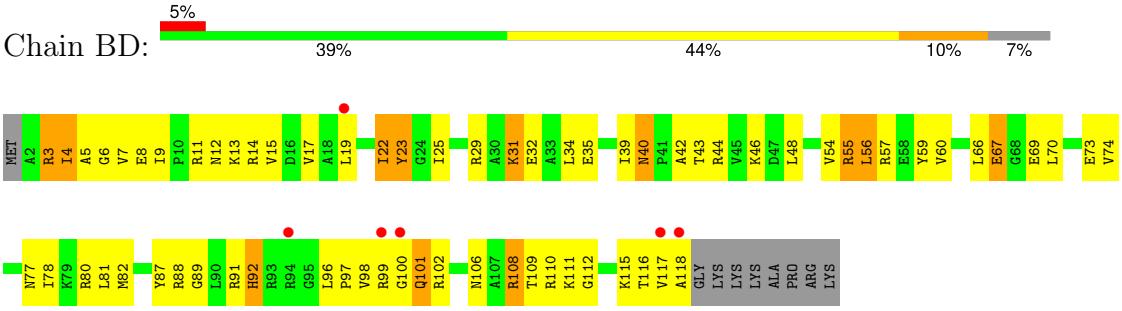
• Molecule 47: 30S ribosomal protein S13

Chain WA:

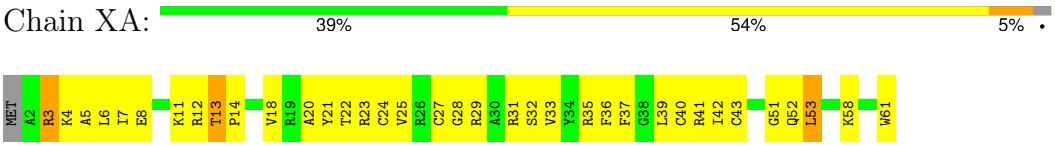




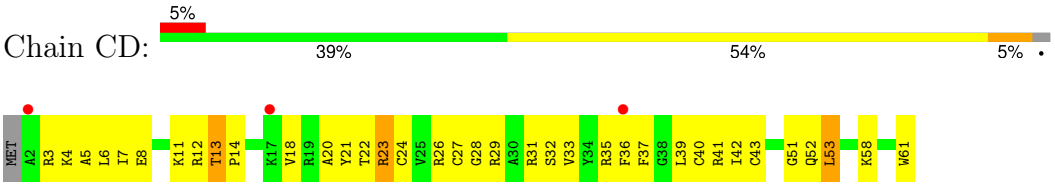
• Molecule 47: 30S ribosomal protein S13



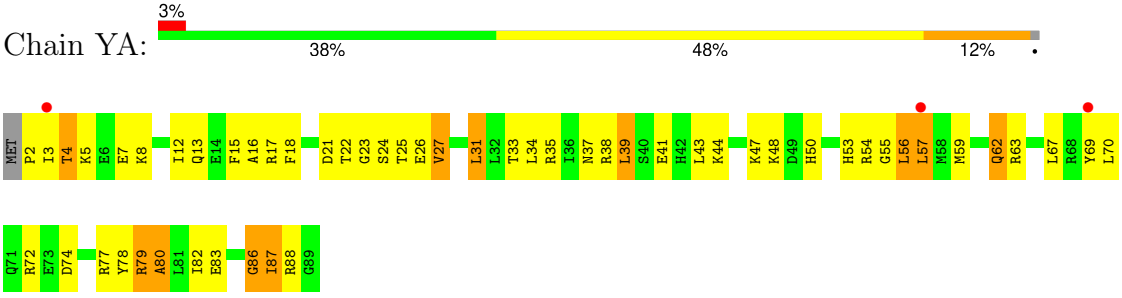
• Molecule 48: 30S ribosomal protein S14 type Z



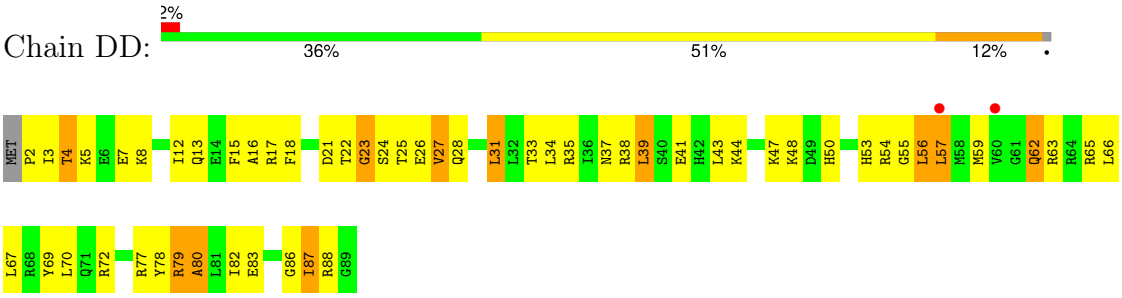
• Molecule 48: 30S ribosomal protein S14 type Z



• Molecule 49: 30S ribosomal protein S15

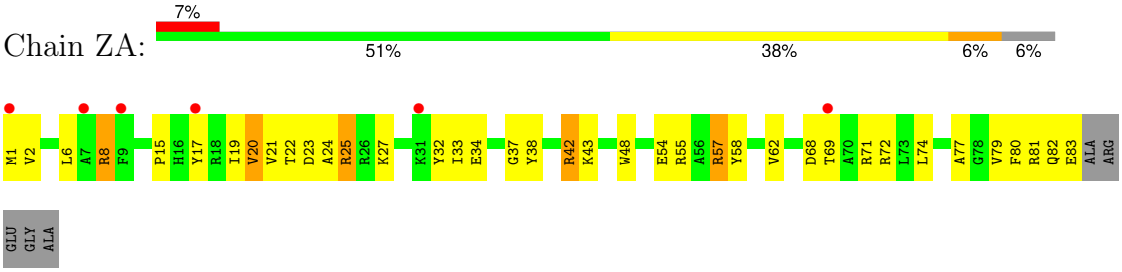


• Molecule 49: 30S ribosomal protein S15



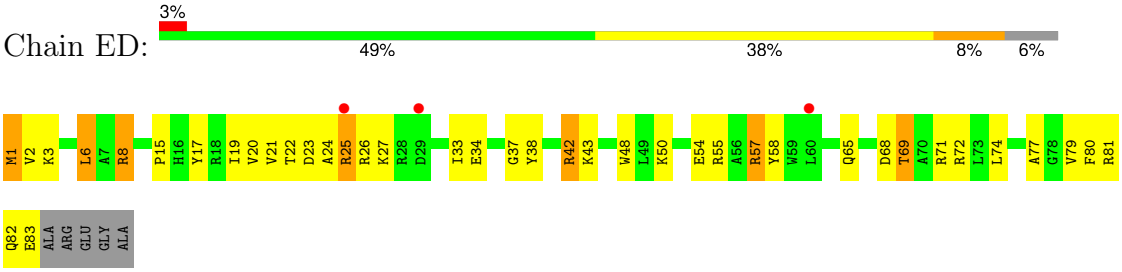
• Molecule 50: 30S ribosomal protein S16

Chain ZA:



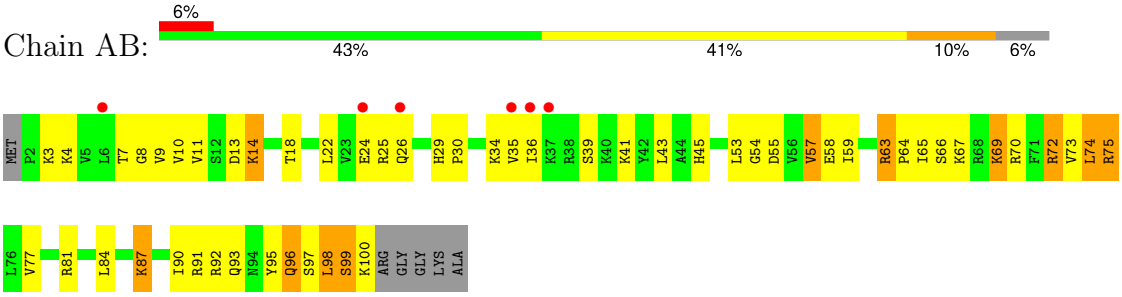
• Molecule 50: 30S ribosomal protein S16

Chain ED:



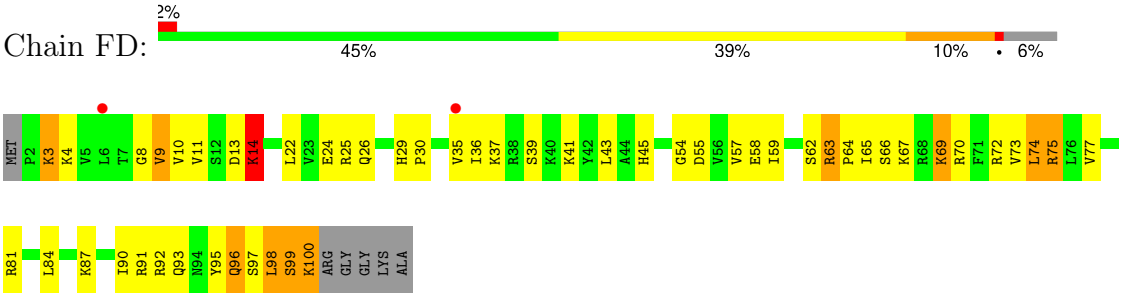
• Molecule 51: 30S ribosomal protein S17

Chain AB:



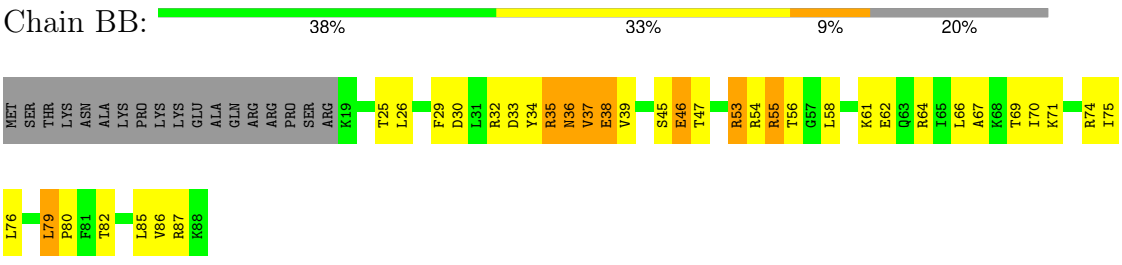
• Molecule 51: 30S ribosomal protein S17

Chain FD:



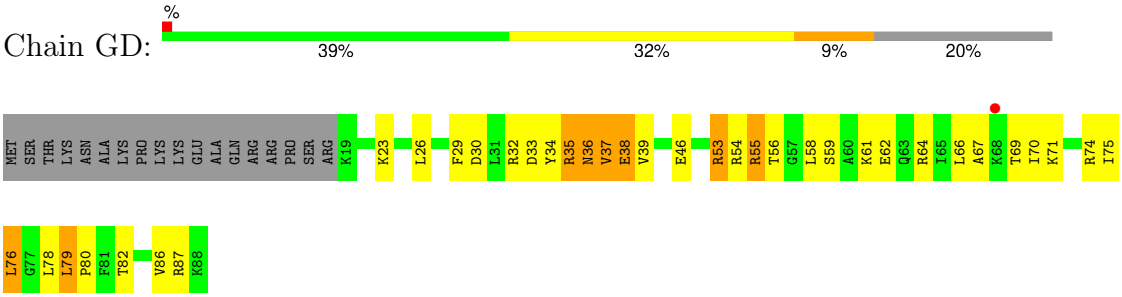
• Molecule 52: 30S ribosomal protein S18

Chain BB:



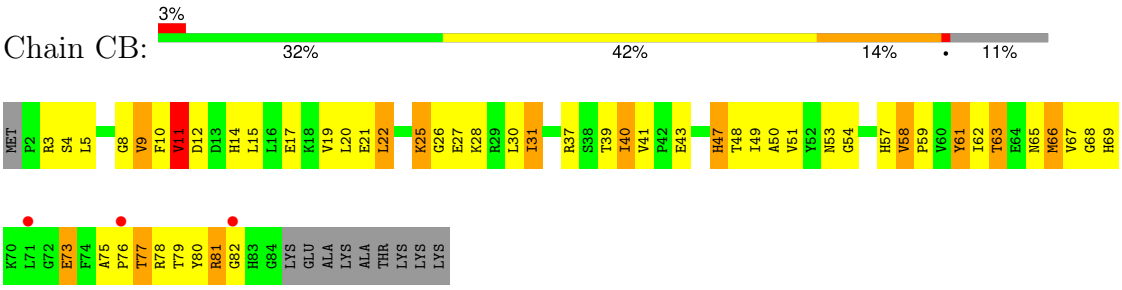
• Molecule 52: 30S ribosomal protein S18

Chain GD:



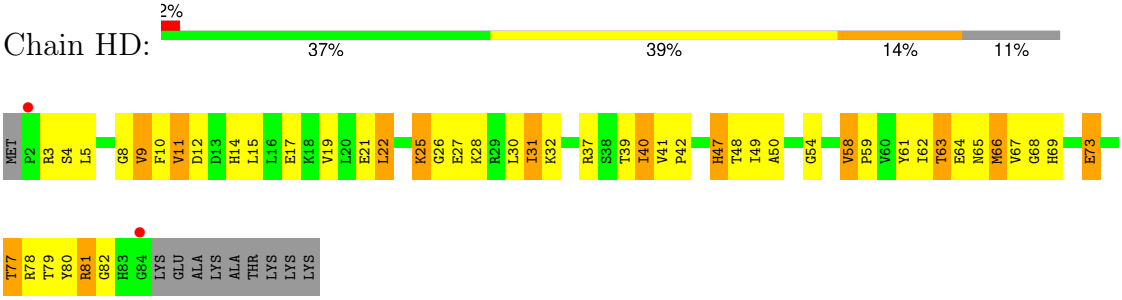
• Molecule 53: 30S ribosomal protein S19

Chain CB:



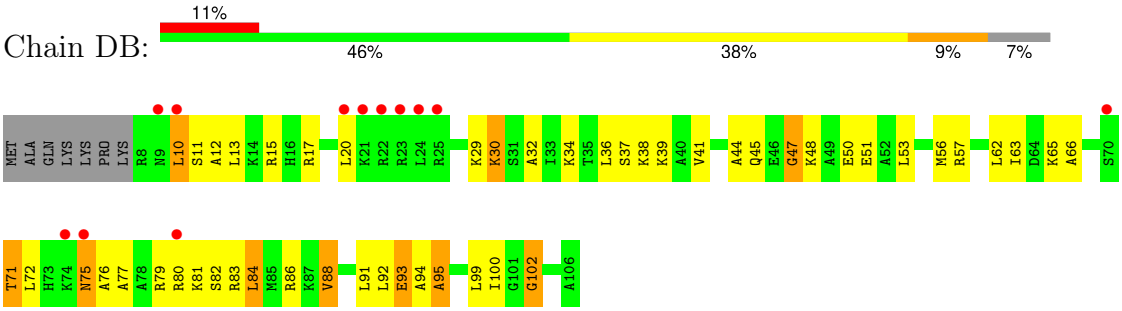
• Molecule 53: 30S ribosomal protein S19

Chain HD:



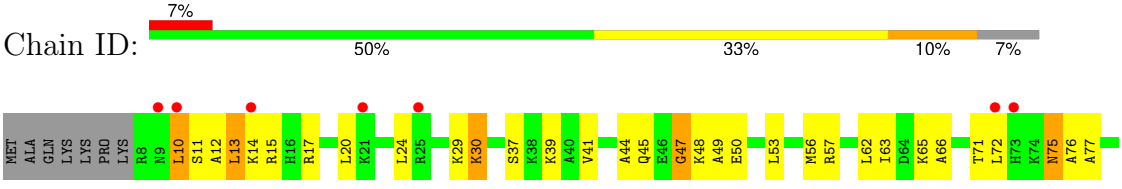
• Molecule 54: 30S ribosomal protein S20

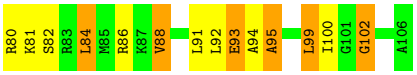
Chain DB:



• Molecule 54: 30S ribosomal protein S20

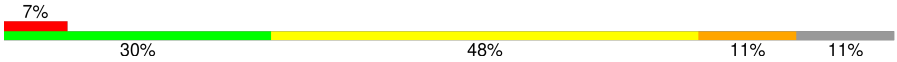
Chain ID:

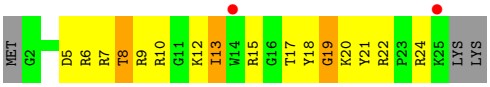




• Molecule 55: 30S ribosomal protein Thx

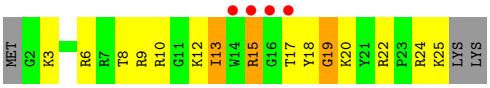
Chain EB:





• Molecule 55: 30S ribosomal protein Thx

Chain JD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.86Å 450.69Å 615.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 50.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 100.0 (50.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 3.41Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.243 , 0.281	Depositor DCC
R_{free} test set	784598 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	120.8	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	298186	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 7MG, UR3, 0TD, OMG, BLS, 5MU, 5MC, 4SU, 2MG, 4OC, M2G, MA6, 2MA, MG, ZN, PSU, 2MU

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	A	0.60	1/35961 (0.0%)	1.09	67/56125 (0.1%)
1	FB	0.59	1/35961 (0.0%)	1.09	73/56125 (0.1%)
2	B	0.94	58/69214 (0.1%)	1.41	808/108048 (0.7%)
2	GB	0.83	32/69214 (0.0%)	1.33	620/108048 (0.6%)
3	C	0.56	0/2881	1.05	3/4494 (0.1%)
3	HB	0.51	0/2881	1.02	2/4494 (0.0%)
4	D	0.40	0/1744	0.90	0/2719
4	IA	0.60	0/1744	1.06	4/2719 (0.1%)
4	IB	0.37	0/1744	0.90	0/2719
4	NC	0.50	0/1744	1.00	0/2719
5	E	0.80	4/2195 (0.2%)	0.80	1/2955 (0.0%)
5	JB	0.63	2/2195 (0.1%)	0.73	1/2955 (0.0%)
6	F	0.52	0/1596	0.69	1/2153 (0.0%)
6	KB	0.57	0/1596	0.70	1/2153 (0.0%)
7	G	0.61	0/1621	0.69	0/2194
7	LB	0.51	0/1621	0.65	0/2194
8	H	0.36	0/1496	0.57	0/2013
8	MB	0.33	0/1496	0.57	0/2013
9	I	0.43	0/1356	0.59	0/1834
9	NB	0.34	0/1356	0.55	0/1834
10	J	0.46	0/1152	0.62	0/1559
10	OB	0.42	0/1152	0.61	0/1559
11	K	0.49	0/1148	0.62	0/1547
11	PB	0.44	0/1148	0.59	0/1547
12	L	0.59	0/942	0.66	0/1268
12	QB	0.65	0/942	0.68	0/1268
13	M	0.54	0/1162	0.69	0/1544
13	RB	0.47	0/1162	0.65	0/1544
14	N	0.51	0/1142	0.62	0/1525
14	SB	0.49	0/1142	0.60	0/1525
15	O	0.51	0/982	0.63	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	TB	0.53	0/982	0.64	0/1312
16	P	0.42	0/887	0.56	0/1180
16	UB	0.40	0/887	0.56	0/1180
17	Q	0.48	0/1157	0.57	0/1544
17	VB	0.54	0/1157	0.59	0/1544
18	R	0.55	0/982	0.60	0/1306
18	WB	0.49	0/982	0.60	0/1306
19	S	0.49	0/790	0.65	0/1057
19	XB	0.44	0/790	0.61	0/1057
20	T	0.65	0/901	0.69	0/1209
20	YB	0.60	0/901	0.68	0/1209
21	U	0.71	0/764	0.68	0/1025
21	ZB	0.60	0/764	0.61	0/1025
22	AC	0.50	0/827	0.61	0/1103
22	V	0.58	0/827	0.64	0/1103
23	BC	0.40	0/1527	0.58	0/2073
23	W	0.44	0/1527	0.60	0/2073
24	CC	0.50	0/671	0.62	0/892
24	X	0.52	0/671	0.63	0/892
25	DC	0.57	0/768	0.69	0/1021
25	Y	0.63	0/768	0.68	0/1021
26	EC	0.50	0/594	0.64	0/785
26	Z	0.61	0/594	0.71	0/785
27	AA	0.50	0/482	0.63	0/646
27	FC	0.44	0/482	0.59	0/646
28	BA	0.39	0/565	0.53	0/761
28	GC	0.35	0/565	0.52	0/761
29	CA	0.54	0/474	0.66	0/640
29	HC	0.54	0/474	0.64	0/640
30	DA	0.34	0/460	0.51	0/613
30	IC	0.33	0/460	0.51	0/613
31	EA	0.77	0/426	0.76	0/561
31	JC	0.65	0/426	0.72	0/561
32	FA	0.60	0/525	0.64	0/691
32	KC	0.53	0/525	0.62	0/691
33	GA	0.41	0/310	0.58	0/407
33	LC	0.45	0/310	0.60	0/407
34	HA	0.72	0/247	0.92	0/382
34	MC	0.72	0/247	0.91	0/382
35	JA	0.37	0/867	0.51	0/1165
35	KA	0.39	0/461	0.56	0/622
35	OC	0.34	0/867	0.51	0/1165
35	PC	0.36	0/461	0.56	0/622

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
36	LA	0.39	0/1935	0.57	0/2609
36	QC	0.35	0/1935	0.55	0/2609
37	MA	0.37	0/1636	0.54	0/2205
37	RC	0.36	0/1636	0.54	0/2205
38	NA	0.47	1/1733 (0.1%)	0.59	1/2318 (0.0%)
38	SC	0.53	1/1733 (0.1%)	0.62	1/2318 (0.0%)
39	OA	0.45	0/1171	0.62	0/1576
39	TC	0.44	0/1171	0.61	0/1576
40	PA	0.51	0/856	0.62	0/1154
40	UC	0.43	0/856	0.60	0/1154
41	QA	0.36	0/1276	0.51	0/1709
41	VC	0.34	0/1276	0.50	0/1709
42	RA	0.37	0/1136	0.57	0/1527
42	WC	0.38	0/1136	0.56	0/1527
43	SA	0.34	0/1029	0.54	0/1378
43	XC	0.32	0/1029	0.53	1/1378 (0.1%)
44	TA	0.36	0/807	0.56	0/1085
44	YC	0.34	0/807	0.57	0/1085
45	UA	0.48	0/879	0.64	0/1187
45	ZC	0.41	0/879	0.59	0/1187
46	AD	0.52	0/963	0.62	0/1287
46	VA	0.50	0/963	0.61	0/1287
47	BD	0.33	0/943	0.51	0/1265
47	WA	0.36	0/943	0.52	0/1265
48	CD	0.35	0/501	0.48	0/664
48	XA	0.37	0/501	0.52	0/664
49	DD	0.42	0/745	0.55	0/992
49	YA	0.49	0/745	0.58	0/992
50	ED	0.40	0/716	0.59	0/963
50	ZA	0.34	0/716	0.56	0/963
51	AB	0.47	0/836	0.57	0/1117
51	FD	0.48	0/836	0.58	0/1117
52	BB	0.46	0/579	0.54	0/768
52	GD	0.41	0/579	0.52	0/768
53	CB	0.32	0/680	0.50	0/915
53	HD	0.30	0/680	0.51	0/915
54	DB	0.36	0/764	0.53	0/1006
54	ID	0.40	0/764	0.54	0/1006
55	EB	0.31	0/212	0.48	0/277
55	JD	0.31	0/212	0.46	0/277
All	All	0.71	100/320836 (0.0%)	1.12	1584/479388 (0.3%)

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
21	U	0	1

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	237	GLU	CG-CD	10.38	1.67	1.51
5	E	237	GLU	CB-CG	8.22	1.67	1.52
38	SC	12	CYS	CB-SG	8.17	1.96	1.82
38	NA	12	CYS	CB-SG	7.71	1.95	1.82
2	GB	1780	A	N9-C4	-7.60	1.33	1.37

The worst 5 of 1584 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	298	G	N1-C6-O6	16.25	129.65	119.90
2	B	2593	U	N3-C4-C5	-15.20	105.48	114.60
2	B	2593	U	C6-N1-C2	-14.08	112.55	121.00
2	GB	2593	U	N3-C4-C5	-13.88	106.27	114.60
2	B	2032	G	C4-C5-N7	13.65	116.26	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	U	84	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32394	0	16367	824	0
1	FB	32394	0	16367	817	0
2	B	62031	0	31273	1297	0
2	GB	62031	0	31275	1270	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2576	0	1305	62	0
3	HB	2576	0	1305	63	0
4	D	1642	0	841	47	0
4	IA	1642	0	841	44	0
4	IB	1642	0	841	46	0
4	NC	1642	0	841	41	0
5	E	2145	0	2234	111	0
5	JB	2145	0	2234	105	0
6	F	1563	0	1629	90	0
6	KB	1563	0	1629	88	0
7	G	1586	0	1632	110	0
7	LB	1586	0	1632	105	0
8	H	1471	0	1526	90	0
8	MB	1471	0	1526	86	1
9	I	1330	0	1407	63	0
9	NB	1330	0	1407	58	0
10	J	1137	0	1225	56	0
10	OB	1137	0	1225	55	0
11	K	1121	0	1195	57	0
11	PB	1121	0	1195	54	0
12	L	932	0	994	75	0
12	QB	932	0	994	72	0
13	M	1145	0	1228	56	0
13	RB	1145	0	1228	47	0
14	N	1121	0	1179	64	0
14	SB	1121	0	1179	59	0
15	O	968	0	1033	33	0
15	TB	968	0	1033	38	0
16	P	877	0	938	48	0
16	UB	877	0	938	48	0
17	Q	1143	0	1211	81	0
17	VB	1143	0	1211	67	0
18	R	964	0	1022	61	0
18	WB	964	0	1022	55	0
19	S	779	0	852	28	0
19	XB	779	0	852	25	0
20	T	890	0	951	37	0
20	YB	890	0	951	40	0
21	U	750	0	814	40	0
21	ZB	750	0	814	37	0
22	AC	814	0	907	40	0
22	V	814	0	907	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	BC	1495	0	1521	80	0
23	W	1495	0	1521	90	0
24	CC	662	0	688	40	0
24	X	662	0	688	38	0
25	DC	761	0	837	52	0
25	Y	761	0	837	46	0
26	EC	592	0	654	32	0
26	Z	592	0	654	33	0
27	AA	477	0	529	27	0
27	FC	477	0	529	25	0
28	BA	552	0	537	31	0
28	GC	552	0	537	30	0
29	CA	460	0	481	32	0
29	HC	460	0	482	30	0
30	DA	453	0	477	15	0
30	IC	453	0	477	13	0
31	EA	418	0	467	24	0
31	JC	418	0	467	30	0
32	FA	517	0	582	31	0
32	KC	517	0	582	28	0
33	GA	307	0	337	11	0
33	LC	307	0	337	9	0
34	HA	220	0	108	10	0
34	MC	220	0	108	10	0
35	JA	850	0	816	38	0
35	KA	455	0	444	24	0
35	OC	850	0	816	38	0
35	PC	455	0	444	26	0
36	LA	1900	0	1951	101	0
36	QC	1900	0	1951	96	0
37	MA	1612	0	1677	91	0
37	RC	1612	0	1677	80	0
38	NA	1703	0	1767	94	0
38	SC	1703	0	1767	91	0
39	OA	1155	0	1213	64	0
39	TC	1155	0	1213	75	0
40	PA	843	0	857	35	0
40	UC	843	0	857	37	0
41	QA	1257	0	1296	62	0
41	VC	1257	0	1296	61	0
42	RA	1116	0	1177	61	0
42	WC	1116	0	1177	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	SA	1011	0	1043	61	0
43	XC	1011	0	1043	59	0
44	TA	794	0	840	37	0
44	YC	794	0	840	38	0
45	UA	864	0	881	39	0
45	ZC	864	0	881	45	0
46	AD	958	0	1047	54	0
46	VA	958	0	1047	55	0
47	BD	933	0	992	62	0
47	WA	933	0	992	64	0
48	CD	492	0	533	37	0
48	XA	492	0	533	39	0
49	DD	734	0	771	41	0
49	YA	734	0	771	37	0
50	ED	700	0	720	33	0
50	ZA	700	0	720	28	0
51	AB	823	0	893	40	0
51	FD	823	0	893	40	0
52	BB	574	0	644	32	0
52	GD	574	0	644	31	0
53	CB	665	0	686	43	0
53	HD	665	0	686	43	0
54	DB	762	0	859	43	0
54	ID	762	0	859	41	0
55	EB	208	0	221	16	0
55	JD	208	0	221	16	0
56	A	183	0	0	0	0
56	AA	1	0	0	0	0
56	AB	2	0	0	0	0
56	AC	1	0	0	0	0
56	AD	4	0	0	0	0
56	B	433	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
56	C	22	0	0	0	0
56	CA	1	0	0	0	0
56	CB	1	0	0	0	0
56	CC	1	0	0	0	0
56	D	5	0	0	0	0
56	DC	1	0	0	0	0
56	DD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	E	6	0	0	0	0
56	EA	1	0	0	0	0
56	ED	1	0	0	0	0
56	F	4	0	0	0	0
56	FA	1	0	0	0	0
56	FB	194	0	0	0	0
56	G	2	0	0	0	0
56	GB	402	0	0	0	0
56	GC	1	0	0	0	0
56	H	2	0	0	0	0
56	HA	3	0	0	0	0
56	HB	20	0	0	0	0
56	HD	1	0	0	0	0
56	IA	9	0	0	0	0
56	IB	2	0	0	0	0
56	IC	1	0	0	0	0
56	J	1	0	0	0	0
56	JA	1	0	0	0	0
56	JB	5	0	0	0	0
56	JC	1	0	0	0	0
56	K	4	0	0	0	0
56	KB	2	0	0	0	0
56	KC	1	0	0	0	0
56	L	3	0	0	0	0
56	LA	1	0	0	0	0
56	LB	4	0	0	0	0
56	M	3	0	0	0	0
56	MA	6	0	0	0	0
56	MC	3	0	0	0	0
56	NA	2	0	0	0	0
56	NB	1	0	0	0	0
56	NC	10	0	0	0	0
56	O	2	0	0	0	0
56	OA	4	0	0	0	0
56	OB	1	0	0	0	0
56	OC	1	0	0	0	0
56	PA	3	0	0	0	0
56	PB	2	0	0	0	0
56	PC	1	0	0	0	0
56	Q	1	0	0	0	0
56	QA	1	0	0	0	0
56	QB	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QC	3	0	0	0	0
56	R	1	0	0	0	0
56	RB	3	0	0	0	0
56	RC	2	0	0	0	0
56	S	1	0	0	0	0
56	SA	1	0	0	0	0
56	SB	2	0	0	0	0
56	SC	4	0	0	0	0
56	T	2	0	0	0	0
56	TB	1	0	0	0	0
56	TC	3	0	0	0	0
56	U	1	0	0	0	0
56	UA	1	0	0	0	0
56	UB	4	0	0	0	0
56	UC	3	0	0	0	0
56	V	2	0	0	0	0
56	VA	2	0	0	0	0
56	VB	3	0	0	0	0
56	VC	1	0	0	0	0
56	WC	1	0	0	0	0
56	XB	2	0	0	0	0
56	Y	3	0	0	0	0
56	YA	3	0	0	0	0
56	Z	1	0	0	0	0
56	ZB	2	0	0	0	0
56	ZC	1	0	0	0	0
57	B	30	0	24	4	0
57	GB	30	0	24	7	0
58	AC	1	0	0	0	0
58	BA	1	0	0	0	0
58	CA	1	0	0	0	0
58	DA	1	0	0	0	0
58	GA	1	0	0	0	0
58	GC	1	0	0	0	0
58	HC	1	0	0	0	0
58	IC	1	0	0	0	0
58	LC	1	0	0	0	0
58	V	1	0	0	0	0
All	All	298186	0	202351	8489	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8489 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)
38:SC:18:LYS:NZ	38:SC:26:CYS:SG	2.02	1.33
38:SC:18:LYS:NZ	38:SC:31:CYS:SG	2.07	1.27
38:NA:18:LYS:NZ	38:NA:26:CYS:SG	2.09	1.26
3:C:90:C:OP2	14:N:16:ARG:NH1	1.77	1.18
1:FB:9:G:OP2	39:TC:121:LYS:NZ	1.76	1.16

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1412:A:O2'	8:MB:9:ARG:NH1[1_655]	1.99	0.21

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	273/275 (99%)	243 (89%)	24 (9%)	6 (2%)	5 24
5	JB	273/275 (99%)	245 (90%)	22 (8%)	6 (2%)	5 24
6	F	202/206 (98%)	166 (82%)	28 (14%)	8 (4%)	2 15
6	KB	202/206 (98%)	167 (83%)	29 (14%)	6 (3%)	3 19
7	G	200/205 (98%)	173 (86%)	24 (12%)	3 (2%)	8 30
7	LB	200/205 (98%)	172 (86%)	25 (12%)	3 (2%)	8 30
8	H	179/182 (98%)	134 (75%)	37 (21%)	8 (4%)	2 13
8	MB	179/182 (98%)	134 (75%)	37 (21%)	8 (4%)	2 13
9	I	172/180 (96%)	134 (78%)	32 (19%)	6 (4%)	3 17
9	NB	172/180 (96%)	134 (78%)	32 (19%)	6 (4%)	3 17
10	J	144/148 (97%)	111 (77%)	23 (16%)	10 (7%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	OB	144/148 (97%)	111 (77%)	24 (17%)	9 (6%)	1 7
11	K	138/140 (99%)	115 (83%)	17 (12%)	6 (4%)	2 14
11	PB	138/140 (99%)	118 (86%)	15 (11%)	5 (4%)	3 16
12	L	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16 44
12	QB	120/122 (98%)	108 (90%)	9 (8%)	3 (2%)	4 22
13	M	148/150 (99%)	126 (85%)	12 (8%)	10 (7%)	1 6
13	RB	148/150 (99%)	124 (84%)	14 (10%)	10 (7%)	1 6
14	N	139/141 (99%)	120 (86%)	17 (12%)	2 (1%)	9 31
14	SB	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	5 24
15	O	116/118 (98%)	99 (85%)	12 (10%)	5 (4%)	2 14
15	TB	116/118 (98%)	97 (84%)	13 (11%)	6 (5%)	1 10
16	P	108/112 (96%)	82 (76%)	23 (21%)	3 (3%)	4 20
16	UB	108/112 (96%)	83 (77%)	22 (20%)	3 (3%)	4 20
17	Q	135/146 (92%)	118 (87%)	13 (10%)	4 (3%)	3 19
17	VB	135/146 (92%)	117 (87%)	15 (11%)	3 (2%)	5 24
18	R	115/118 (98%)	106 (92%)	9 (8%)	0	100 100
18	WB	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14 41
19	S	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	2 15
19	XB	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	3 19
20	T	110/113 (97%)	97 (88%)	11 (10%)	2 (2%)	7 27
20	YB	110/113 (97%)	98 (89%)	12 (11%)	0	100 100
21	U	93/96 (97%)	83 (89%)	8 (9%)	2 (2%)	5 24
21	ZB	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	5 24
22	AC	105/110 (96%)	83 (79%)	16 (15%)	6 (6%)	1 9
22	V	105/110 (96%)	83 (79%)	14 (13%)	8 (8%)	1 5
23	BC	187/206 (91%)	137 (73%)	43 (23%)	7 (4%)	2 16
23	W	187/206 (91%)	139 (74%)	41 (22%)	7 (4%)	2 16
24	CC	82/85 (96%)	70 (85%)	8 (10%)	4 (5%)	2 11
24	X	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	2 16
25	DC	95/98 (97%)	87 (92%)	7 (7%)	1 (1%)	12 37
25	Y	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	12 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	EC	68/72 (94%)	61 (90%)	4 (6%)	3 (4%)	2 13
26	Z	68/72 (94%)	59 (87%)	6 (9%)	3 (4%)	2 13
27	AA	58/60 (97%)	44 (76%)	12 (21%)	2 (3%)	3 17
27	FC	58/60 (97%)	45 (78%)	11 (19%)	2 (3%)	3 17
28	BA	67/71 (94%)	43 (64%)	16 (24%)	8 (12%)	0 2
28	GC	67/71 (94%)	44 (66%)	15 (22%)	8 (12%)	0 2
29	CA	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	7 27
29	HC	57/60 (95%)	49 (86%)	8 (14%)	0	100 100
30	DA	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	6 25
30	IC	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	6 25
31	EA	46/49 (94%)	41 (89%)	5 (11%)	0	100 100
31	JC	46/49 (94%)	38 (83%)	8 (17%)	0	100 100
32	FA	62/65 (95%)	53 (86%)	9 (14%)	0	100 100
32	KC	62/65 (95%)	53 (86%)	9 (14%)	0	100 100
33	GA	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	0 4
33	LC	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	0 4
35	JA	108/365 (30%)	84 (78%)	18 (17%)	6 (6%)	1 10
35	KA	53/365 (14%)	31 (58%)	13 (24%)	9 (17%)	0 0
35	OC	108/365 (30%)	83 (77%)	19 (18%)	6 (6%)	1 10
35	PC	53/365 (14%)	31 (58%)	14 (26%)	8 (15%)	0 0
36	LA	232/256 (91%)	176 (76%)	40 (17%)	16 (7%)	1 6
36	QC	232/256 (91%)	174 (75%)	41 (18%)	17 (7%)	1 5
37	MA	204/239 (85%)	166 (81%)	28 (14%)	10 (5%)	2 11
37	RC	204/239 (85%)	167 (82%)	25 (12%)	12 (6%)	1 8
38	NA	206/209 (99%)	162 (79%)	35 (17%)	9 (4%)	2 13
38	SC	206/209 (99%)	158 (77%)	39 (19%)	9 (4%)	2 13
39	OA	149/162 (92%)	126 (85%)	19 (13%)	4 (3%)	4 21
39	TC	149/162 (92%)	124 (83%)	20 (13%)	5 (3%)	3 17
40	PA	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	2 15
40	UC	99/101 (98%)	82 (83%)	13 (13%)	4 (4%)	2 15
41	QA	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	VC	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	1 10
42	RA	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	2 16
42	WC	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	2 16
43	SA	125/128 (98%)	91 (73%)	28 (22%)	6 (5%)	2 12
43	XC	125/128 (98%)	93 (74%)	25 (20%)	7 (6%)	1 10
44	TA	96/105 (91%)	72 (75%)	15 (16%)	9 (9%)	0 3
44	YC	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	0 3
45	UA	114/129 (88%)	87 (76%)	23 (20%)	4 (4%)	3 17
45	ZC	114/129 (88%)	87 (76%)	24 (21%)	3 (3%)	4 22
46	AD	119/132 (90%)	91 (76%)	20 (17%)	8 (7%)	1 7
46	VA	119/132 (90%)	89 (75%)	22 (18%)	8 (7%)	1 7
47	BD	115/126 (91%)	90 (78%)	18 (16%)	7 (6%)	1 8
47	WA	115/126 (91%)	91 (79%)	18 (16%)	6 (5%)	1 10
48	CD	58/61 (95%)	45 (78%)	12 (21%)	1 (2%)	7 28
48	XA	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	7 28
49	DD	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3 17
49	YA	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	2 12
50	ED	81/88 (92%)	72 (89%)	8 (10%)	1 (1%)	11 35
50	ZA	81/88 (92%)	71 (88%)	9 (11%)	1 (1%)	11 35
51	AB	97/105 (92%)	78 (80%)	15 (16%)	4 (4%)	2 15
51	FD	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	1 10
52	BB	68/88 (77%)	63 (93%)	4 (6%)	1 (2%)	8 30
52	GD	68/88 (77%)	61 (90%)	5 (7%)	2 (3%)	3 19
53	CB	81/93 (87%)	58 (72%)	16 (20%)	7 (9%)	0 4
53	HD	81/93 (87%)	58 (72%)	17 (21%)	6 (7%)	1 5
54	DB	97/106 (92%)	79 (81%)	11 (11%)	7 (7%)	1 6
54	ID	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	1 8
55	EB	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	0 4
55	JD	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	0 4
All	All	11806/13576 (87%)	9599 (81%)	1713 (14%)	494 (4%)	2 14

5 of 494 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	122	ASP
7	G	130	ALA
8	H	12	TYR
8	H	43	LEU
8	H	47	LYS

5.3.2 Protein sidechains (i)

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	
5	E	217/217 (100%)	177 (82%)	40 (18%)	1	5
5	JB	217/217 (100%)	176 (81%)	41 (19%)	1	4
6	F	165/166 (99%)	139 (84%)	26 (16%)	2	8
6	KB	165/166 (99%)	139 (84%)	26 (16%)	2	8
7	G	161/162 (99%)	136 (84%)	25 (16%)	2	9
7	LB	161/162 (99%)	134 (83%)	27 (17%)	1	7
8	H	154/156 (99%)	121 (79%)	33 (21%)	1	2
8	MB	154/156 (99%)	121 (79%)	33 (21%)	1	2
9	I	144/148 (97%)	123 (85%)	21 (15%)	2	10
9	NB	144/148 (97%)	122 (85%)	22 (15%)	2	9
10	J	122/124 (98%)	95 (78%)	27 (22%)	1	2
10	OB	122/124 (98%)	94 (77%)	28 (23%)	0	2
11	K	119/119 (100%)	99 (83%)	20 (17%)	1	7
11	PB	119/119 (100%)	98 (82%)	21 (18%)	1	6
12	L	100/100 (100%)	88 (88%)	12 (12%)	4	16
12	QB	100/100 (100%)	87 (87%)	13 (13%)	3	13
13	M	116/116 (100%)	86 (74%)	30 (26%)	0	1
13	RB	116/116 (100%)	86 (74%)	30 (26%)	0	1
14	N	111/111 (100%)	94 (85%)	17 (15%)	2	9
14	SB	111/111 (100%)	94 (85%)	17 (15%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	O	101/101 (100%)	83 (82%)	18 (18%)	1 5
15	TB	101/101 (100%)	84 (83%)	17 (17%)	1 7
16	P	87/88 (99%)	72 (83%)	15 (17%)	1 6
16	UB	87/88 (99%)	73 (84%)	14 (16%)	2 8
17	Q	121/128 (94%)	97 (80%)	24 (20%)	1 3
17	VB	121/128 (94%)	96 (79%)	25 (21%)	1 2
18	R	93/94 (99%)	82 (88%)	11 (12%)	4 16
18	WB	93/94 (99%)	82 (88%)	11 (12%)	4 16
19	S	82/82 (100%)	64 (78%)	18 (22%)	1 2
19	XB	82/82 (100%)	64 (78%)	18 (22%)	1 2
20	T	91/92 (99%)	78 (86%)	13 (14%)	2 10
20	YB	91/92 (99%)	79 (87%)	12 (13%)	3 13
21	U	77/78 (99%)	70 (91%)	7 (9%)	7 26
21	ZB	77/78 (99%)	68 (88%)	9 (12%)	4 16
22	AC	87/91 (96%)	71 (82%)	16 (18%)	1 5
22	V	87/91 (96%)	71 (82%)	16 (18%)	1 5
23	BC	163/179 (91%)	133 (82%)	30 (18%)	1 5
23	W	163/179 (91%)	133 (82%)	30 (18%)	1 5
24	CC	66/67 (98%)	54 (82%)	12 (18%)	1 5
24	X	66/67 (98%)	53 (80%)	13 (20%)	1 3
25	DC	81/83 (98%)	64 (79%)	17 (21%)	1 2
25	Y	81/83 (98%)	67 (83%)	14 (17%)	1 6
26	EC	66/67 (98%)	60 (91%)	6 (9%)	7 26
26	Z	66/67 (98%)	59 (89%)	7 (11%)	5 20
27	AA	52/52 (100%)	38 (73%)	14 (27%)	0 1
27	FC	52/52 (100%)	37 (71%)	15 (29%)	0 1
28	BA	59/63 (94%)	44 (75%)	15 (25%)	0 1
28	GC	59/63 (94%)	44 (75%)	15 (25%)	0 1
29	CA	51/52 (98%)	43 (84%)	8 (16%)	2 8
29	HC	51/52 (98%)	43 (84%)	8 (16%)	2 8
30	DA	51/52 (98%)	41 (80%)	10 (20%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	IC	51/52 (98%)	41 (80%)	10 (20%)	1 3
31	EA	41/42 (98%)	33 (80%)	8 (20%)	1 3
31	JC	41/42 (98%)	33 (80%)	8 (20%)	1 3
32	FA	54/55 (98%)	50 (93%)	4 (7%)	11 35
32	KC	54/55 (98%)	49 (91%)	5 (9%)	7 25
33	GA	34/34 (100%)	33 (97%)	1 (3%)	37 61
33	LC	34/34 (100%)	33 (97%)	1 (3%)	37 61
35	JA	85/305 (28%)	68 (80%)	17 (20%)	1 3
35	KA	50/305 (16%)	38 (76%)	12 (24%)	0 1
35	OC	85/305 (28%)	68 (80%)	17 (20%)	1 3
35	PC	50/305 (16%)	38 (76%)	12 (24%)	0 1
36	LA	202/220 (92%)	156 (77%)	46 (23%)	0 2
36	QC	202/220 (92%)	154 (76%)	48 (24%)	0 1
37	MA	160/188 (85%)	137 (86%)	23 (14%)	2 10
37	RC	160/188 (85%)	138 (86%)	22 (14%)	3 11
38	NA	180/181 (99%)	155 (86%)	25 (14%)	3 11
38	SC	180/181 (99%)	155 (86%)	25 (14%)	3 11
39	OA	116/123 (94%)	93 (80%)	23 (20%)	1 3
39	TC	116/123 (94%)	94 (81%)	22 (19%)	1 4
40	PA	90/90 (100%)	79 (88%)	11 (12%)	4 15
40	UC	90/90 (100%)	78 (87%)	12 (13%)	3 12
41	QA	126/127 (99%)	105 (83%)	21 (17%)	2 7
41	VC	126/127 (99%)	105 (83%)	21 (17%)	2 7
42	RA	119/119 (100%)	105 (88%)	14 (12%)	4 16
42	WC	119/119 (100%)	106 (89%)	13 (11%)	5 19
43	SA	98/99 (99%)	79 (81%)	19 (19%)	1 3
43	XC	98/99 (99%)	79 (81%)	19 (19%)	1 3
44	TA	88/92 (96%)	72 (82%)	16 (18%)	1 5
44	YC	88/92 (96%)	71 (81%)	17 (19%)	1 3
45	UA	88/99 (89%)	77 (88%)	11 (12%)	3 14
45	ZC	88/99 (89%)	77 (88%)	11 (12%)	3 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	AD	102/108 (94%)	84 (82%)	18 (18%)	1 6
46	VA	102/108 (94%)	84 (82%)	18 (18%)	1 6
47	BD	94/101 (93%)	74 (79%)	20 (21%)	1 2
47	WA	94/101 (93%)	74 (79%)	20 (21%)	1 2
48	CD	49/50 (98%)	42 (86%)	7 (14%)	2 10
48	XA	49/50 (98%)	42 (86%)	7 (14%)	2 10
49	DD	79/80 (99%)	62 (78%)	17 (22%)	1 2
49	YA	79/80 (99%)	62 (78%)	17 (22%)	1 2
50	ED	72/74 (97%)	60 (83%)	12 (17%)	2 7
50	ZA	72/74 (97%)	61 (85%)	11 (15%)	2 9
51	AB	94/97 (97%)	77 (82%)	17 (18%)	1 5
51	FD	94/97 (97%)	76 (81%)	18 (19%)	1 4
52	BB	61/77 (79%)	49 (80%)	12 (20%)	1 3
52	GD	61/77 (79%)	50 (82%)	11 (18%)	1 5
53	CB	72/80 (90%)	57 (79%)	15 (21%)	1 2
53	HD	72/80 (90%)	58 (81%)	14 (19%)	1 3
54	DB	76/82 (93%)	66 (87%)	10 (13%)	3 13
54	ID	76/82 (93%)	66 (87%)	10 (13%)	3 13
55	EB	19/22 (86%)	15 (79%)	4 (21%)	1 2
55	JD	19/22 (86%)	15 (79%)	4 (21%)	1 2
All	All	9972/11276 (88%)	8229 (82%)	1743 (18%)	1 6

5 of 1743 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	KB	160	TYR
16	UB	42	ASP
44	YC	96	ILE
7	LB	158	THR
6	KB	154	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
12	QB	82	ASN
15	TB	24	GLN
45	ZC	22	HIS
12	QB	90	GLN
16	UB	16	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	347 (23%)	12 (0%)
1	FB	1502/1507 (99%)	343 (22%)	12 (0%)
2	B	2876/2880 (99%)	658 (22%)	22 (0%)
2	GB	2876/2880 (99%)	658 (22%)	22 (0%)
3	C	119/120 (99%)	19 (15%)	0
3	HB	119/120 (99%)	20 (16%)	0
34	HA	9/27 (33%)	3 (33%)	0
34	MC	9/27 (33%)	3 (33%)	0
4	D	76/77 (98%)	27 (35%)	0
4	IA	76/77 (98%)	20 (26%)	0
4	IB	76/77 (98%)	26 (34%)	0
4	NC	76/77 (98%)	19 (25%)	0
All	All	9316/9376 (99%)	2143 (23%)	68 (0%)

5 of 2143 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	13	U
1	A	22	G
1	A	26	A
1	A	31	G

5 of 68 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	GB	1558	A
2	GB	1939	5MU
2	GB	2439	A
2	B	1608	A
2	B	1558	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	1404	1	19,22,23	2.84	5 (26%)	26,32,35	1.27	5 (19%)
1	UR3	A	1498	1	19,22,23	1.78	1 (5%)	26,32,35	1.43	2 (7%)
2	5MU	B	1915	2	19,22,23	2.01	3 (15%)	27,32,35	2.30	9 (33%)
2	5MC	B	1942	2	19,22,23	2.57	4 (21%)	26,32,35	1.41	3 (11%)
2	5MC	GB	1942	2	19,22,23	2.35	4 (21%)	26,32,35	1.55	3 (11%)
4	PSU	NC	55	4	18,21,22	1.72	2 (11%)	21,30,33	1.82	4 (19%)
1	PSU	FB	516	1	18,21,22	1.78	3 (16%)	21,30,33	1.40	3 (14%)
2	2MU	B	2552	2	19,22,24	2.69	6 (31%)	25,31,36	2.27	7 (28%)
2	2MU	GB	2552	2	19,22,24	2.54	5 (26%)	25,31,36	2.31	7 (28%)
4	PSU	IA	55	4	18,21,22	1.64	2 (11%)	21,30,33	1.88	4 (19%)
1	5MC	A	1407	1	19,22,23	2.71	4 (21%)	26,32,35	1.17	3 (11%)
1	5MC	FB	1400	1	19,22,23	2.66	5 (26%)	26,32,35	1.16	2 (7%)
1	UR3	FB	1498	1	19,22,23	1.80	1 (5%)	26,32,35	1.51	3 (11%)
2	5MU	GB	1915	2	19,22,23	2.01	3 (15%)	27,32,35	2.19	8 (29%)
4	4SU	IB	8	4	18,21,22	4.57	7 (38%)	25,30,33	5.95	11 (44%)
2	5MU	B	1939	2	19,22,23	2.08	4 (21%)	27,32,35	2.60	8 (29%)
4	5MC	IB	32	4	19,22,23	2.50	4 (21%)	26,32,35	1.10	2 (7%)
2	PSU	GB	1911	2	18,21,22	1.59	3 (16%)	21,30,33	2.19	7 (33%)
4	5MU	IA	54	4	19,22,23	2.07	3 (15%)	27,32,35	2.05	8 (29%)
2	OMG	B	2251	2	19,26,27	2.00	4 (21%)	21,38,41	1.66	5 (23%)
1	2MG	A	1207	1	18,26,27	2.22	4 (22%)	16,38,41	1.47	3 (18%)
4	5MC	NC	32	4	19,22,23	2.64	4 (21%)	26,32,35	1.08	2 (7%)
4	PSU	D	55	4	18,21,22	1.69	2 (11%)	21,30,33	1.76	5 (23%)
4	5MU	IB	54	4	19,22,23	2.06	3 (15%)	27,32,35	2.12	7 (25%)
1	4OC	A	1402	1	20,23,24	1.08	2 (10%)	25,32,35	1.20	1 (4%)
1	5MC	FB	1404	1	19,22,23	3.02	4 (21%)	26,32,35	1.14	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	A	967	1	19,22,23	2.47	5 (26%)	26,32,35	1.43	4 (15%)
1	7MG	FB	527	1	23,26,27	3.15	7 (30%)	27,39,42	2.29	8 (29%)
2	4OC	B	1920	56,2	19,22,24	1.13	1 (5%)	25,31,35	1.55	2 (8%)
1	7MG	A	527	1	23,26,27	3.02	7 (30%)	27,39,42	2.18	8 (29%)
4	5MU	NC	54	4	19,22,23	2.09	3 (15%)	27,32,35	2.03	7 (25%)
4	4SU	NC	8	4	18,21,22	4.65	7 (38%)	25,30,33	6.26	10 (40%)
2	PSU	B	1917	2	18,21,22	1.77	2 (11%)	21,30,33	1.79	4 (19%)
4	5MC	D	32	4	19,22,23	2.69	4 (21%)	26,32,35	1.11	3 (11%)
4	4SU	IA	8	4	18,21,22	4.94	7 (38%)	25,30,33	5.95	10 (40%)
1	MA6	A	1518	1	19,26,27	2.15	4 (21%)	18,38,41	1.73	4 (22%)
1	5MC	FB	1407	1	19,22,23	2.56	4 (21%)	26,32,35	1.11	3 (11%)
2	PSU	GB	1917	2	18,21,22	1.81	2 (11%)	21,30,33	1.83	5 (23%)
1	PSU	A	516	1	18,21,22	1.61	3 (16%)	21,30,33	1.44	2 (9%)
2	PSU	B	2605	2	18,21,22	1.53	2 (11%)	21,30,33	2.13	5 (23%)
46	0TD	AD	92	46	8,9,10	1.98	2 (25%)	6,11,13	3.12	4 (66%)
4	4SU	D	8	4	18,21,22	4.71	7 (38%)	25,30,33	5.99	10 (40%)
4	5MU	D	54	4	19,22,23	2.09	3 (15%)	27,32,35	2.11	6 (22%)
1	5MC	FB	967	1	19,22,23	2.54	5 (26%)	26,32,35	1.40	5 (19%)
2	OMG	GB	2251	2	19,26,27	2.07	5 (26%)	21,38,41	1.60	5 (23%)
2	4OC	GB	1920	2	19,22,24	1.07	1 (5%)	25,31,35	1.46	1 (4%)
2	PSU	B	1911	2	18,21,22	1.35	1 (5%)	21,30,33	2.13	7 (33%)
1	5MC	A	1400	1	19,22,23	2.61	5 (26%)	26,32,35	1.34	4 (15%)
1	MA6	A	1519	1	19,26,27	1.93	5 (26%)	18,38,41	2.05	2 (11%)
2	2MA	B	2503	2	17,25,26	1.42	2 (11%)	16,37,40	1.92	3 (18%)
2	2MA	GB	2503	2	17,25,26	1.45	2 (11%)	16,37,40	1.84	3 (18%)
1	4OC	FB	1402	1	20,23,24	1.02	2 (10%)	25,32,35	1.30	2 (8%)
2	PSU	GB	2605	2	18,21,22	1.72	3 (16%)	21,30,33	2.34	6 (28%)
4	5MC	IA	32	4	19,22,23	2.69	4 (21%)	26,32,35	0.98	2 (7%)
1	2MG	FB	1207	1	18,26,27	2.16	3 (16%)	16,38,41	1.50	3 (18%)
4	PSU	IB	55	4	18,21,22	1.66	2 (11%)	21,30,33	1.74	5 (23%)
1	M2G	A	966	1	20,27,28	2.33	4 (20%)	19,40,43	1.43	3 (15%)
2	5MC	B	1962	2	19,22,23	2.82	5 (26%)	26,32,35	1.48	4 (15%)
2	5MC	GB	1962	2	19,22,23	2.50	5 (26%)	26,32,35	1.36	2 (7%)
46	0TD	VA	92	46	8,9,10	2.40	2 (25%)	6,11,13	3.17	4 (66%)
1	M2G	FB	966	1	20,27,28	2.29	5 (25%)	19,40,43	1.30	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MA6	FB	1519	1	19,26,27	2.24	5 (26%)	18,38,41	1.92	3 (16%)
2	5MU	GB	1939	2	19,22,23	2.24	4 (21%)	27,32,35	2.43	8 (29%)
1	MA6	FB	1518	1	19,26,27	2.09	5 (26%)	18,38,41	1.86	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
2	5MU	B	1915	2	-	0/7/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/7/25/26	0/2/2/2
2	5MC	GB	1942	2	-	0/7/25/26	0/2/2/2
4	PSU	NC	55	4	-	1/7/25/26	0/2/2/2
1	PSU	FB	516	1	-	0/7/25/26	0/2/2/2
2	2MU	B	2552	2	-	1/9/27/28	0/2/2/2
2	2MU	GB	2552	2	-	1/9/27/28	0/2/2/2
4	PSU	IA	55	4	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	FB	1400	1	-	0/7/25/26	0/2/2/2
1	UR3	FB	1498	1	-	2/7/25/26	0/2/2/2
2	5MU	GB	1915	2	-	0/7/25/26	0/2/2/2
4	4SU	IB	8	4	-	1/7/25/26	0/2/2/2
2	5MU	B	1939	2	-	1/7/25/26	0/2/2/2
4	5MC	IB	32	4	-	0/7/25/26	0/2/2/2
2	PSU	GB	1911	2	-	0/7/25/26	0/2/2/2
4	5MU	IA	54	4	-	0/7/25/26	0/2/2/2
2	OMG	B	2251	2	-	3/5/27/28	0/3/3/3
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
4	5MC	NC	32	4	-	0/7/25/26	0/2/2/2
4	PSU	D	55	4	-	1/7/25/26	0/2/2/2
4	5MU	IB	54	4	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	1/9/29/30	0/2/2/2
1	5MC	FB	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	7MG	FB	527	1	-	2/7/37/38	0/3/3/3
2	4OC	B	1920	56,2	-	1/9/27/30	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
4	5MU	NC	54	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4SU	NC	8	4	-	2/7/25/26	0/2/2/2
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	2/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
1	5MC	FB	1407	1	-	0/7/25/26	0/2/2/2
2	PSU	GB	1917	2	-	1/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
46	0TD	AD	92	46	-	2/7/12/14	-
4	4SU	D	8	4	-	1/7/25/26	0/2/2/2
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
1	5MC	FB	967	1	-	0/7/25/26	0/2/2/2
2	OMG	GB	2251	2	-	3/5/27/28	0/3/3/3
2	4OC	GB	1920	2	-	1/9/27/30	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	4/7/29/30	0/3/3/3
2	2MA	B	2503	2	-	1/3/25/26	0/3/3/3
2	2MA	GB	2503	2	-	1/3/25/26	0/3/3/3
1	4OC	FB	1402	1	-	2/9/29/30	0/2/2/2
2	PSU	GB	2605	2	-	0/7/25/26	0/2/2/2
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
1	2MG	FB	1207	1	-	0/5/27/28	0/3/3/3
4	PSU	IB	55	4	-	1/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
2	5MC	B	1962	2	-	2/7/25/26	0/2/2/2
2	5MC	GB	1962	2	-	2/7/25/26	0/2/2/2
46	0TD	VA	92	46	-	3/7/12/14	-
1	M2G	FB	966	1	-	0/7/29/30	0/3/3/3
1	MA6	FB	1519	1	-	4/7/29/30	0/3/3/3
2	5MU	GB	1939	2	-	0/7/25/26	0/2/2/2
1	MA6	FB	1518	1	-	2/7/29/30	0/3/3/3

The worst 5 of 237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	IA	8	4SU	C4-N3	13.44	1.51	1.37
4	D	8	4SU	C4-N3	12.49	1.50	1.37
4	NC	8	4SU	C4-N3	12.20	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	IB	8	4SU	C4-N3	11.78	1.49	1.37
4	IA	8	4SU	O2-C2	11.75	1.43	1.23

The worst 5 of 298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	IB	8	4SU	S4-C4-N3	-15.25	104.25	120.20
4	NC	8	4SU	C4-N3-C2	-15.06	112.88	127.31
4	IA	8	4SU	C4-N3-C2	-14.45	113.47	127.31
4	IB	8	4SU	C5-C4-S4	-13.95	108.37	124.31
4	D	8	4SU	C4-N3-C2	-13.80	114.09	127.31

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	C1'-C2'-O2'-CM2
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	1519	MA6	O4'-C4'-C5'-O5'
2	B	1920	4OC	C3'-C2'-O2'-CM2

There are no ring outliers.

43 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	2	0
2	B	1915	5MU	1	0
2	GB	1942	5MC	1	0
4	NC	55	PSU	1	0
2	B	2552	2MU	1	0
4	IA	55	PSU	1	0
1	A	1407	5MC	1	0
1	FB	1498	UR3	3	0
2	GB	1915	5MU	1	0
4	IB	8	4SU	2	0
2	B	1939	5MU	1	0
4	IA	54	5MU	4	0
2	B	2251	OMG	3	0
1	A	1207	2MG	3	0
4	NC	32	5MC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
1	A	967	5MC	4	0
1	FB	527	7MG	1	0
2	B	1920	4OC	4	0
1	A	527	7MG	1	0
4	NC	54	5MU	4	0
1	A	1518	MA6	1	0
1	FB	1407	5MC	1	0
2	GB	1917	PSU	2	0
46	AD	92	0TD	1	0
4	D	8	4SU	3	0
1	FB	967	5MC	4	0
2	GB	2251	OMG	3	0
2	GB	1920	4OC	1	0
1	A	1519	MA6	1	0
2	B	2503	2MA	3	0
2	GB	2503	2MA	3	0
1	FB	1402	4OC	2	0
4	IA	32	5MC	3	0
1	FB	1207	2MG	3	0
1	A	966	M2G	2	0
2	B	1962	5MC	1	0
2	GB	1962	5MC	1	0
46	VA	92	0TD	1	0
1	FB	966	M2G	1	0
1	FB	1519	MA6	1	0
2	GB	1939	5MU	2	0
1	FB	1518	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1440 ligands modelled in this entry, 1438 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	BLS	GB	9001	-	28,31,31	3.11	10 (35%)	26,43,43	2.19	8 (30%)
57	BLS	B	9001	-	28,31,31	3.12	10 (35%)	26,43,43	2.68	9 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	BLS	GB	9001	-	-	7/21/38/38	0/2/2/2
57	BLS	B	9001	-	-	6/21/38/38	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	9001	BLS	C14-N12	9.09	1.54	1.35
57	GB	9001	BLS	C14-N12	8.65	1.53	1.35
57	GB	9001	BLS	C7-N6	7.71	1.50	1.34
57	B	9001	BLS	C7-N6	6.83	1.48	1.34
57	B	9001	BLS	C11-N12	4.89	1.57	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	B	9001	BLS	C1'-C2'-C3'	-9.47	110.80	122.45
57	GB	9001	BLS	C1'-C2'-C3'	-7.62	113.08	122.45
57	B	9001	BLS	C4-N3-C2	3.95	120.34	116.34
57	B	9001	BLS	N15-C14-N12	3.71	122.71	118.64
57	B	9001	BLS	O4-C6'-O3	3.27	131.49	124.08

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	B	9001	BLS	C11-C10-C9-C8
57	B	9001	BLS	C11-C10-C9-N9
57	B	9001	BLS	C10-C11-N12-C13
57	B	9001	BLS	C10-C11-N12-C14

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Mol	Chain	Res	Type	Atoms
57	GB	9001	BLS	C11-C10-C9-C8

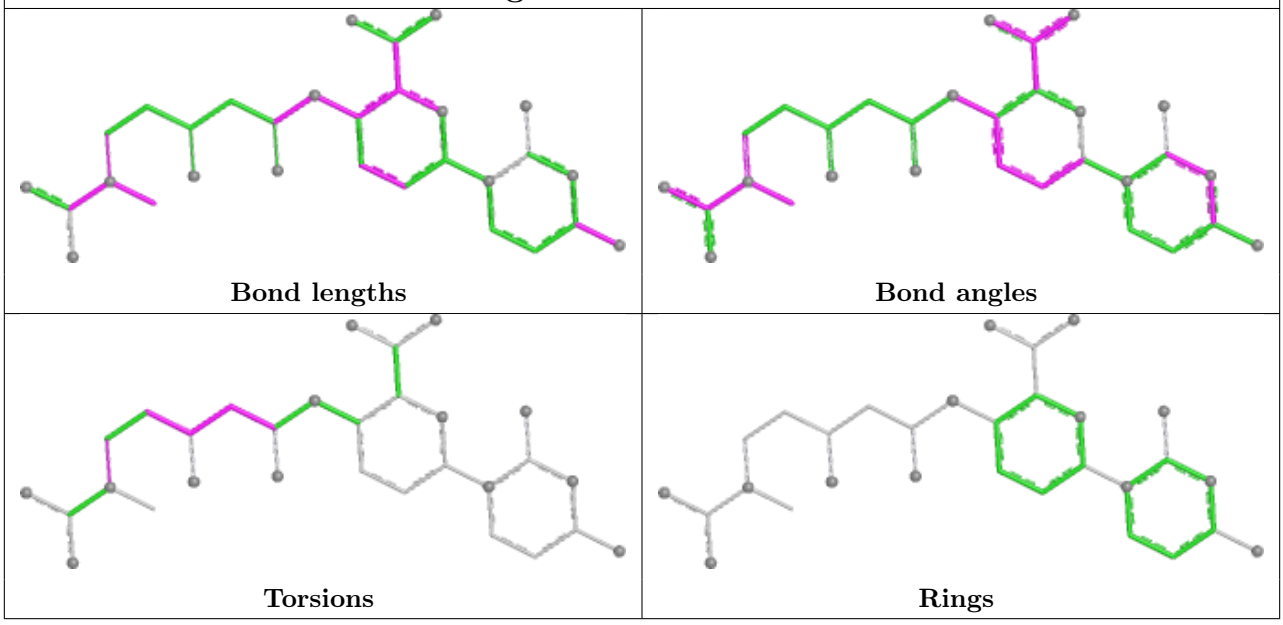
There are no ring outliers.

2 monomers are involved in 11 short contacts:

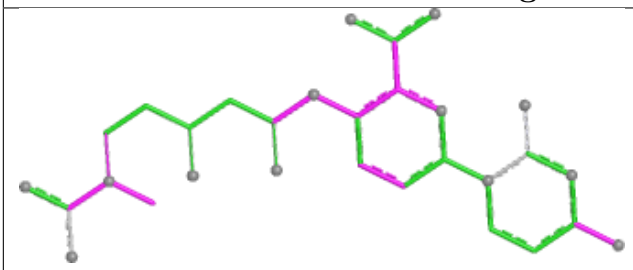
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	GB	9001	BLS	7	0
57	B	9001	BLS	4	0

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

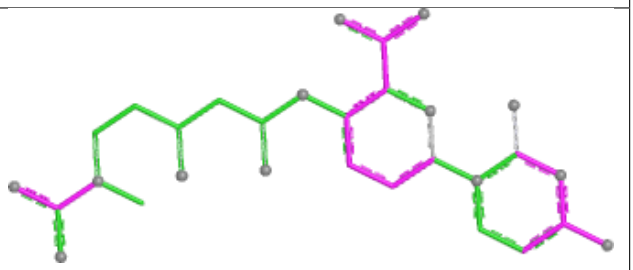
Ligand BLS GB 9001



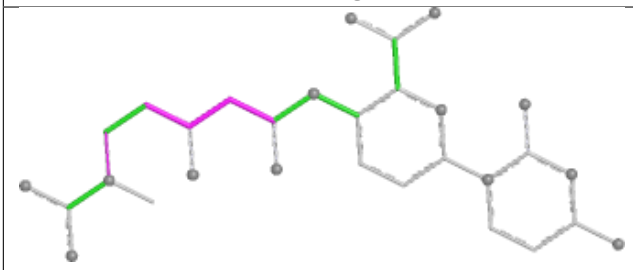
Ligand BLS B 9001



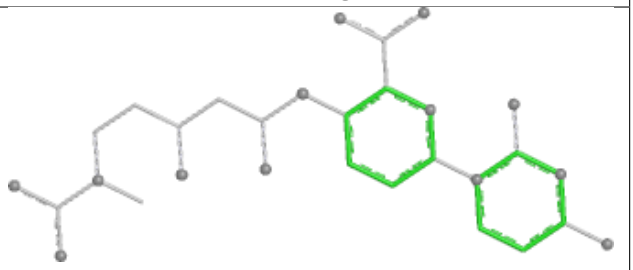
Bond lengths



Bond angles



Torsions



Rings

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

Warning: The R factor obtained from EDS is 0.2476, which does not match the depositor's R factor of 0.0. Please interpret the results in this section carefully.

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	A	1495/1507 (99%)	-0.73	3 (0%) 92 92	92, 150, 224, 269	0
1	FB	1495/1507 (99%)	-0.52	6 (0%) 89 86	99, 138, 232, 276	0
2	B	2869/2880 (99%)	-0.77	8 (0%) 90 89	73, 105, 203, 272	0
2	GB	2869/2880 (99%)	-0.65	7 (0%) 92 92	81, 114, 229, 316	0
3	C	120/120 (100%)	-0.78	0 100 100	129, 165, 182, 187	0
3	HB	120/120 (100%)	-0.40	0 100 100	139, 177, 198, 207	0
4	D	73/77 (94%)	-0.53	0 100 100	135, 221, 238, 244	0
4	IA	73/77 (94%)	-0.49	1 (1%) 73 64	130, 161, 182, 190	0
4	IB	73/77 (94%)	-0.35	1 (1%) 73 64	158, 256, 274, 283	0
4	NC	73/77 (94%)	-0.43	0 100 100	148, 189, 217, 220	0
5	E	275/275 (100%)	-0.38	3 (1%) 77 70	69, 83, 95, 102	0
5	JB	275/275 (100%)	-0.12	4 (1%) 71 62	84, 104, 121, 128	0
6	F	204/206 (99%)	-0.23	3 (1%) 71 62	82, 119, 139, 147	0
6	KB	204/206 (99%)	-0.17	3 (1%) 71 62	81, 107, 132, 144	0
7	G	202/205 (98%)	-0.45	0 100 100	77, 107, 121, 133	0
7	LB	202/205 (98%)	-0.24	3 (1%) 71 62	82, 126, 141, 150	0
8	H	181/182 (99%)	-0.05	4 (2%) 62 53	165, 174, 184, 186	0
8	MB	181/182 (99%)	-0.09	4 (2%) 62 53	181, 188, 199, 202	0
9	I	174/180 (96%)	-0.28	0 100 100	116, 131, 138, 155	0
9	NB	174/180 (96%)	-0.01	4 (2%) 61 51	149, 188, 215, 222	0
10	J	146/148 (98%)	-0.39	0 100 100	107, 130, 149, 153	0
10	OB	146/148 (98%)	-0.21	3 (2%) 63 53	124, 155, 159, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
11	K	140/140 (100%)	-0.05	1 (0%) 84 78	100, 121, 133, 138	0
11	PB	140/140 (100%)	0.07	5 (3%) 46 39	100, 129, 143, 147	0
12	L	122/122 (100%)	-0.34	0 100 100	94, 108, 119, 123	0
12	QB	122/122 (100%)	-0.43	0 100 100	88, 96, 103, 107	0
13	M	150/150 (100%)	-0.05	2 (1%) 74 66	82, 110, 137, 139	0
13	RB	150/150 (100%)	-0.01	3 (2%) 64 55	104, 124, 140, 142	0
14	N	141/141 (100%)	0.01	0 100 100	100, 123, 140, 148	0
14	SB	141/141 (100%)	0.06	4 (2%) 55 47	106, 137, 154, 160	0
15	O	118/118 (100%)	-0.04	2 (1%) 69 59	93, 111, 126, 130	0
15	TB	118/118 (100%)	0.10	5 (4%) 41 36	90, 106, 116, 121	0
16	P	110/112 (98%)	0.40	9 (8%) 19 20	147, 157, 163, 164	0
16	UB	110/112 (98%)	0.28	7 (6%) 27 26	153, 169, 181, 188	0
17	Q	137/146 (93%)	-0.22	1 (0%) 84 78	111, 125, 174, 192	0
17	VB	137/146 (93%)	-0.47	0 100 100	93, 108, 139, 148	0
18	R	117/118 (99%)	-0.10	0 100 100	83, 116, 131, 132	0
18	WB	117/118 (99%)	-0.09	4 (3%) 48 41	98, 129, 143, 146	0
19	S	101/101 (100%)	-0.34	1 (0%) 79 71	86, 126, 132, 136	0
19	XB	101/101 (100%)	-0.35	3 (2%) 52 45	96, 141, 148, 150	0
20	T	112/113 (99%)	-0.42	0 100 100	78, 97, 113, 122	0
20	YB	112/113 (99%)	-0.19	0 100 100	83, 101, 121, 127	0
21	U	95/96 (98%)	-0.24	0 100 100	86, 92, 102, 109	0
21	ZB	95/96 (98%)	0.03	1 (1%) 77 70	109, 120, 129, 135	0
22	AC	107/110 (97%)	0.22	6 (5%) 31 29	120, 125, 139, 143	0
22	V	107/110 (97%)	-0.39	0 100 100	101, 108, 120, 126	0
23	BC	189/206 (91%)	-0.18	2 (1%) 77 70	143, 165, 176, 180	0
23	W	189/206 (91%)	-0.25	0 100 100	131, 152, 162, 164	0
24	CC	84/85 (98%)	0.35	7 (8%) 19 20	128, 134, 146, 154	0
24	X	84/85 (98%)	0.41	7 (8%) 19 20	119, 125, 139, 146	0
25	DC	97/98 (98%)	0.05	3 (3%) 51 44	94, 114, 137, 145	0
25	Y	97/98 (98%)	-0.05	1 (1%) 79 71	83, 105, 132, 140	0
26	EC	70/72 (97%)	-0.10	1 (1%) 73 64	123, 129, 136, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
26	Z	70/72 (97%)	-0.38	0 100 100	95, 101, 107, 116	0
27	AA	60/60 (100%)	-0.20	0 100 100	104, 117, 128, 134	0
27	FC	60/60 (100%)	-0.01	1 (1%) 69 59	118, 131, 141, 142	0
28	BA	69/71 (97%)	-0.44	0 100 100	186, 191, 204, 206	0
28	GC	69/71 (97%)	-0.33	0 100 100	200, 207, 212, 213	0
29	CA	59/60 (98%)	-0.34	0 100 100	90, 115, 125, 130	0
29	HC	59/60 (98%)	-0.50	1 (1%) 69 59	81, 113, 123, 124	0
30	DA	53/54 (98%)	0.06	2 (3%) 44 38	184, 184, 185, 185	0
30	IC	53/54 (98%)	0.34	2 (3%) 44 38	207, 213, 217, 219	0
31	EA	48/49 (97%)	-0.39	0 100 100	72, 77, 83, 88	0
31	JC	48/49 (97%)	-0.01	1 (2%) 63 53	89, 91, 100, 110	0
32	FA	64/65 (98%)	0.32	2 (3%) 51 44	93, 102, 119, 127	0
32	KC	64/65 (98%)	0.20	0 100 100	101, 112, 128, 135	0
33	GA	37/37 (100%)	1.91	17 (45%) 1 1	185, 186, 188, 188	0
33	LC	37/37 (100%)	1.79	12 (32%) 1 2	187, 189, 190, 191	0
34	HA	11/27 (40%)	0.51	2 (18%) 4 6	127, 142, 152, 153	0
34	MC	11/27 (40%)	-0.05	0 100 100	143, 154, 164, 168	0
35	JA	110/365 (30%)	-0.19	3 (2%) 56 48	158, 176, 196, 210	0
35	KA	55/365 (15%)	-0.19	1 (1%) 67 58	172, 187, 214, 219	0
35	OC	110/365 (30%)	-0.10	3 (2%) 56 48	186, 196, 207, 214	0
35	PC	55/365 (15%)	-0.21	2 (3%) 46 39	195, 202, 215, 219	0
36	LA	234/256 (91%)	-0.32	1 (0%) 89 86	148, 161, 170, 174	0
36	QC	234/256 (91%)	-0.15	5 (2%) 63 53	167, 184, 197, 202	0
37	MA	206/239 (86%)	-0.27	5 (2%) 59 51	153, 163, 175, 182	0
37	RC	206/239 (86%)	-0.22	3 (1%) 71 62	159, 177, 193, 200	0
38	NA	208/209 (99%)	0.39	15 (7%) 23 22	135, 159, 171, 177	0
38	SC	208/209 (99%)	0.07	14 (6%) 25 25	117, 126, 133, 137	0
39	OA	151/162 (93%)	-0.13	6 (3%) 43 37	128, 140, 147, 155	0
39	TC	151/162 (93%)	-0.24	3 (1%) 64 55	124, 140, 150, 152	0
40	PA	101/101 (100%)	-0.37	1 (0%) 79 71	119, 128, 134, 146	0
40	UC	101/101 (100%)	-0.40	0 100 100	141, 149, 156, 163	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
41	QA	155/156 (99%)	-0.18	2 (1%) 74 66	146, 168, 177, 181	0
41	VC	155/156 (99%)	0.03	5 (3%) 50 42	167, 185, 197, 201	0
42	RA	138/138 (100%)	-0.18	1 (0%) 84 78	130, 145, 149, 153	0
42	WC	138/138 (100%)	0.07	6 (4%) 40 35	128, 144, 156, 163	0
43	SA	127/128 (99%)	0.43	12 (9%) 15 17	167, 190, 195, 199	0
43	XC	127/128 (99%)	0.50	13 (10%) 13 15	176, 212, 221, 227	0
44	TA	98/105 (93%)	0.37	9 (9%) 16 17	166, 189, 198, 201	0
44	YC	98/105 (93%)	0.42	6 (6%) 28 27	176, 197, 211, 213	0
45	UA	116/129 (89%)	-0.21	2 (1%) 69 59	104, 128, 135, 139	0
45	ZC	116/129 (89%)	-0.16	2 (1%) 69 59	126, 154, 160, 162	0
46	AD	121/132 (91%)	-0.07	2 (1%) 69 59	109, 116, 124, 136	0
46	VA	121/132 (91%)	0.13	5 (4%) 42 36	115, 124, 134, 139	0
47	BD	117/126 (92%)	0.18	6 (5%) 34 30	179, 210, 214, 215	0
47	WA	117/126 (92%)	0.03	7 (5%) 29 27	161, 193, 196, 198	0
48	CD	60/61 (98%)	0.59	3 (5%) 35 31	180, 189, 208, 209	0
48	XA	60/61 (98%)	0.41	0 100 100	164, 171, 193, 194	0
49	DD	88/89 (98%)	-0.11	2 (2%) 61 51	126, 142, 153, 155	0
49	YA	88/89 (98%)	-0.19	3 (3%) 48 41	106, 126, 136, 137	0
50	ED	83/88 (94%)	0.04	3 (3%) 46 39	112, 120, 133, 148	0
50	ZA	83/88 (94%)	0.18	6 (7%) 23 22	150, 160, 174, 183	0
51	AB	99/105 (94%)	0.01	6 (6%) 28 27	116, 138, 144, 148	0
51	FD	99/105 (94%)	-0.19	2 (2%) 64 55	115, 124, 130, 132	0
52	BB	70/88 (79%)	-0.48	0 100 100	119, 132, 140, 147	0
52	GD	70/88 (79%)	-0.12	1 (1%) 73 64	145, 156, 163, 165	0
53	CB	83/93 (89%)	0.33	3 (3%) 46 39	171, 198, 201, 203	0
53	HD	83/93 (89%)	0.18	2 (2%) 59 51	179, 212, 217, 221	0
54	DB	99/106 (93%)	0.50	12 (12%) 10 12	152, 164, 174, 175	0
54	ID	99/106 (93%)	0.21	7 (7%) 23 23	115, 133, 145, 146	0
55	EB	24/27 (88%)	0.77	2 (8%) 19 20	179, 189, 195, 198	0
55	JD	24/27 (88%)	0.97	4 (16%) 5 7	202, 210, 219, 223	0
All	All	21292/22952 (92%)	-0.33	368 (1%) 69 59	69, 131, 210, 316	0

The worst 5 of 368 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	NA	120	LEU	7.2
24	X	4	LYS	6.6
42	WC	1	MET	6.0
49	DD	57	LEU	5.7
33	LC	12	ASP	5.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	4SU	D	8	20/21	0.63	0.09	223,225,227,227	0
4	PSU	D	55	20/21	0.66	0.07	239,243,246,247	0
4	PSU	IB	55	20/21	0.68	0.08	276,281,283,284	0
4	5MU	IB	54	21/22	0.73	0.09	275,277,280,281	0
4	5MU	D	54	21/22	0.74	0.07	237,240,244,246	0
4	PSU	NC	55	20/21	0.75	0.08	211,216,222,223	0
4	4SU	IA	8	20/21	0.78	0.08	158,160,162,163	0
4	5MC	IB	32	21/22	0.79	0.10	204,204,204,204	0
2	PSU	GB	1911	20/21	0.81	0.09	127,133,134,135	0
4	4SU	IB	8	20/21	0.81	0.09	254,257,259,260	0
4	4SU	NC	8	20/21	0.82	0.07	185,190,192,193	0
2	5MU	B	1915	21/22	0.84	0.06	129,131,133,134	0
4	5MC	D	32	21/22	0.86	0.07	212,212,212,212	0
4	5MC	NC	32	21/22	0.87	0.10	156,157,157,157	0
1	5MC	FB	967	21/22	0.87	0.12	160,163,166,168	0
1	PSU	A	516	20/21	0.87	0.07	139,142,145,146	0
2	5MU	GB	1915	21/22	0.88	0.05	143,146,149,150	0
4	5MU	NC	54	21/22	0.88	0.10	213,217,223,226	0
1	2MG	FB	1207	24/25	0.88	0.08	171,174,176,178	0
4	PSU	IA	55	20/21	0.88	0.07	185,189,193,195	0
2	5MU	B	1939	21/22	0.88	0.11	83,84,84,84	0
4	5MU	IA	54	21/22	0.88	0.07	184,188,192,194	0
1	PSU	FB	516	20/21	0.89	0.06	132,134,138,138	0
2	OMG	GB	2251	24/25	0.90	0.11	95,97,100,100	0
2	4OC	GB	1920	21/23	0.90	0.11	123,127,129,131	0
1	5MC	A	967	21/22	0.91	0.09	139,142,145,147	0
4	5MC	IA	32	21/22	0.91	0.10	138,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	4OC	A	1402	22/23	0.92	0.11	117,118,120,120	0
1	4OC	FB	1402	22/23	0.92	0.09	134,136,138,138	0
2	5MC	B	1942	21/22	0.92	0.07	90,92,93,94	0
2	5MC	B	1962	21/22	0.92	0.10	90,92,94,95	0
2	PSU	GB	1917	20/21	0.92	0.06	129,132,136,137	0
2	PSU	B	1911	20/21	0.92	0.06	113,117,119,120	0
2	5MU	GB	1939	21/22	0.92	0.10	86,88,89,89	0
1	2MG	A	1207	24/25	0.92	0.08	163,164,166,167	0
1	5MC	A	1400	21/22	0.93	0.10	125,127,130,132	0
2	5MC	GB	1962	21/22	0.93	0.08	93,96,98,99	0
2	2MA	B	2503	23/24	0.93	0.11	76,78,79,80	0
2	2MA	GB	2503	23/24	0.93	0.13	83,84,86,86	0
46	0TD	AD	92	10/11	0.93	0.20	122,122,123,123	0
1	5MC	FB	1400	21/22	0.93	0.13	141,145,148,150	0
2	PSU	B	1917	20/21	0.93	0.06	111,113,117,118	0
1	UR3	FB	1498	21/22	0.94	0.14	130,130,132,132	0
2	4OC	B	1920	21/23	0.94	0.08	106,109,111,113	0
1	7MG	FB	527	24/25	0.94	0.09	122,124,126,127	0
2	5MC	GB	1942	21/22	0.94	0.06	90,93,94,95	0
1	5MC	FB	1404	21/22	0.95	0.09	123,125,126,126	0
1	UR3	A	1498	21/22	0.95	0.09	109,109,110,110	0
2	PSU	GB	2605	20/21	0.95	0.07	85,85,86,87	0
1	M2G	FB	966	25/26	0.95	0.14	157,160,164,165	0
1	M2G	A	966	25/26	0.96	0.09	137,140,143,144	0
1	5MC	FB	1407	21/22	0.96	0.08	121,124,125,126	0
2	OMG	B	2251	24/25	0.96	0.07	87,89,92,92	0
1	7MG	A	527	24/25	0.96	0.09	125,127,129,130	0
2	2MU	B	2552	21/23	0.96	0.10	86,87,88,89	0
2	2MU	GB	2552	21/23	0.96	0.06	86,87,88,89	0
2	PSU	B	2605	20/21	0.96	0.07	78,79,80,81	0
1	MA6	A	1518	24/25	0.96	0.10	98,102,104,104	0
1	5MC	A	1404	21/22	0.97	0.07	105,107,108,108	0
1	MA6	FB	1519	24/25	0.97	0.12	117,121,123,123	0
1	5MC	A	1407	21/22	0.97	0.06	108,110,112,112	0
46	0TD	VA	92	10/11	0.97	0.12	125,126,126,126	0
1	MA6	A	1519	24/25	0.97	0.11	98,101,103,103	0
1	MA6	FB	1518	24/25	0.98	0.09	116,119,122,123	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9272	1/1	-0.51	0.24	194,194,194,194	0
56	MG	FB	1638	1/1	-0.50	0.50	198,198,198,198	0
56	MG	B	9072	1/1	-0.41	0.18	248,248,248,248	0
56	MG	B	9207	1/1	-0.30	0.24	185,185,185,185	0
56	MG	FB	1644	1/1	-0.29	0.18	239,239,239,239	0
56	MG	GB	9320	1/1	-0.29	0.14	223,223,223,223	0
56	MG	FB	1612	1/1	-0.28	0.26	201,201,201,201	0
56	MG	HB	208	1/1	-0.24	0.31	177,177,177,177	0
56	MG	A	1747	1/1	-0.22	0.18	215,215,215,215	0
56	MG	GB	9298	1/1	-0.20	0.20	250,250,250,250	0
56	MG	FB	1765	1/1	-0.18	0.15	234,234,234,234	0
56	MG	GB	9247	1/1	-0.18	0.11	278,278,278,278	0
56	MG	B	9378	1/1	-0.18	0.19	254,254,254,254	0
56	MG	A	1764	1/1	-0.14	0.29	204,204,204,204	0
56	MG	A	1778	1/1	-0.14	0.22	156,156,156,156	0
56	MG	GB	9136	1/1	-0.12	0.21	154,154,154,154	0
56	MG	IB	101	1/1	-0.07	0.14	243,243,243,243	0
56	MG	A	1641	1/1	-0.06	0.23	154,154,154,154	0
56	MG	A	1634	1/1	-0.06	0.29	165,165,165,165	0
56	MG	FB	1646	1/1	-0.05	0.29	170,170,170,170	0
56	MG	A	1652	1/1	-0.05	0.18	232,232,232,232	0
56	MG	A	1650	1/1	-0.05	0.34	170,170,170,170	0
56	MG	A	1620	1/1	-0.04	0.30	201,201,201,201	0
56	MG	A	1660	1/1	-0.02	0.19	252,252,252,252	0
56	MG	A	1686	1/1	-0.01	0.38	169,169,169,169	0
56	MG	GB	9278	1/1	-0.00	0.27	149,149,149,149	0
56	MG	HB	209	1/1	0.01	0.22	183,183,183,183	0
56	MG	B	9305	1/1	0.02	0.27	207,207,207,207	0
56	MG	GB	9269	1/1	0.02	0.16	146,146,146,146	0
56	MG	H	202	1/1	0.02	0.14	161,161,161,161	0
56	MG	B	9285	1/1	0.03	0.17	164,164,164,164	0
56	MG	GB	9118	1/1	0.03	0.17	144,144,144,144	0
56	MG	IA	102	1/1	0.03	0.31	162,162,162,162	0
56	MG	GC	102	1/1	0.03	0.21	205,205,205,205	0
56	MG	GB	9066	1/1	0.04	0.25	176,176,176,176	0
56	MG	A	1653	1/1	0.06	0.11	260,260,260,260	0
56	MG	FB	1671	1/1	0.06	0.15	255,255,255,255	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B	9157	1/1	0.07	0.33	128,128,128,128	0
56	MG	FB	1705	1/1	0.07	0.17	200,200,200,200	0
56	MG	HB	215	1/1	0.08	0.14	189,189,189,189	0
56	MG	GB	9121	1/1	0.08	0.24	186,186,186,186	0
56	MG	C	213	1/1	0.08	0.23	156,156,156,156	0
56	MG	A	1638	1/1	0.10	0.17	188,188,188,188	0
56	MG	GB	9106	1/1	0.10	0.24	142,142,142,142	0
56	MG	IA	101	1/1	0.11	0.35	152,152,152,152	0
56	MG	GB	9117	1/1	0.11	0.32	160,160,160,160	0
56	MG	HB	201	1/1	0.13	0.42	130,130,130,130	0
56	MG	FB	1623	1/1	0.13	0.31	136,136,136,136	0
56	MG	HB	202	1/1	0.14	0.29	149,149,149,149	0
56	MG	GB	9057	1/1	0.14	0.26	145,145,145,145	0
56	MG	NA	302	1/1	0.14	0.12	163,163,163,163	0
56	MG	HB	204	1/1	0.15	0.33	138,138,138,138	0
56	MG	GB	9301	1/1	0.15	0.25	252,252,252,252	0
56	MG	A	1717	1/1	0.16	0.29	154,154,154,154	0
56	MG	GB	9391	1/1	0.16	0.17	172,172,172,172	0
56	MG	GB	9167	1/1	0.16	0.24	166,166,166,166	0
56	MG	A	1635	1/1	0.16	0.28	168,168,168,168	0
56	MG	NA	301	1/1	0.16	0.30	159,159,159,159	0
56	MG	A	1642	1/1	0.17	0.41	143,143,143,143	0
56	MG	FB	1601	1/1	0.17	0.37	117,117,117,117	0
56	MG	HB	220	1/1	0.17	0.18	159,159,159,159	0
56	MG	A	1664	1/1	0.17	0.20	172,172,172,172	0
56	MG	GB	9208	1/1	0.17	0.14	210,210,210,210	0
56	MG	FB	1710	1/1	0.18	0.17	155,155,155,155	0
56	MG	FB	1643	1/1	0.19	0.44	138,138,138,138	0
56	MG	HB	205	1/1	0.19	0.36	140,140,140,140	0
56	MG	GB	9195	1/1	0.20	0.10	172,172,172,172	0
56	MG	GB	9224	1/1	0.20	0.18	152,152,152,152	0
56	MG	B	9256	1/1	0.21	0.24	157,157,157,157	0
56	MG	A	1644	1/1	0.21	0.24	159,159,159,159	0
56	MG	GB	9306	1/1	0.21	0.16	151,151,151,151	0
56	MG	GB	9335	1/1	0.22	0.21	141,141,141,141	0
56	MG	HB	210	1/1	0.22	0.26	166,166,166,166	0
56	MG	NB	201	1/1	0.23	0.16	189,189,189,189	0
56	MG	A	1631	1/1	0.23	0.29	142,142,142,142	0
56	MG	FB	1684	1/1	0.24	0.16	140,140,140,140	0
56	MG	FB	1730	1/1	0.24	0.19	167,167,167,167	0
56	MG	A	1657	1/1	0.24	0.24	155,155,155,155	0
56	MG	B	9302	1/1	0.25	0.18	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1634	1/1	0.25	0.35	128,128,128,128	0
56	MG	FB	1615	1/1	0.25	0.17	209,209,209,209	0
56	MG	NC	101	1/1	0.25	0.22	189,189,189,189	0
56	MG	RC	302	1/1	0.25	0.16	161,161,161,161	0
56	MG	GB	9139	1/1	0.26	0.21	166,166,166,166	0
56	MG	A	1782	1/1	0.27	0.15	159,159,159,159	0
56	MG	A	1742	1/1	0.27	0.14	160,160,160,160	0
56	MG	FB	1665	1/1	0.27	0.22	188,188,188,188	0
56	MG	A	1643	1/1	0.28	0.34	170,170,170,170	0
56	MG	GB	9181	1/1	0.29	0.22	135,135,135,135	0
56	MG	FB	1618	1/1	0.29	0.49	111,111,111,111	0
56	MG	A	1618	1/1	0.29	0.38	141,141,141,141	0
56	MG	GB	9052	1/1	0.29	0.27	132,132,132,132	0
56	MG	IB	102	1/1	0.30	0.09	246,246,246,246	0
56	MG	GB	9383	1/1	0.30	0.16	137,137,137,137	0
56	MG	GB	9093	1/1	0.30	0.25	116,116,116,116	0
56	MG	FB	1716	1/1	0.30	0.38	197,197,197,197	0
56	MG	B	9280	1/1	0.30	0.17	183,183,183,183	0
56	MG	FB	1630	1/1	0.31	0.30	128,128,128,128	0
56	MG	A	1760	1/1	0.31	0.16	178,178,178,178	0
56	MG	GB	9373	1/1	0.31	0.16	157,157,157,157	0
56	MG	B	9024	1/1	0.31	0.30	120,120,120,120	0
56	MG	FB	1720	1/1	0.31	0.18	164,164,164,164	0
56	MG	FB	1635	1/1	0.32	0.17	151,151,151,151	0
56	MG	D	102	1/1	0.32	0.18	185,185,185,185	0
56	MG	GB	9028	1/1	0.32	0.27	112,112,112,112	0
56	MG	A	1683	1/1	0.32	0.16	166,166,166,166	0
56	MG	IA	108	1/1	0.32	0.11	165,165,165,165	0
56	MG	A	1714	1/1	0.33	0.20	111,111,111,111	0
56	MG	GB	9288	1/1	0.33	0.23	202,202,202,202	0
56	MG	A	1612	1/1	0.33	0.37	125,125,125,125	0
56	MG	FB	1659	1/1	0.33	0.22	122,122,122,122	0
56	MG	FB	1662	1/1	0.33	0.28	139,139,139,139	0
56	MG	B	9399	1/1	0.34	0.22	175,175,175,175	0
56	MG	C	201	1/1	0.34	0.42	132,132,132,132	0
56	MG	FB	1675	1/1	0.34	0.28	197,197,197,197	0
56	MG	HB	207	1/1	0.35	0.30	146,146,146,146	0
56	MG	A	1674	1/1	0.35	0.30	133,133,133,133	0
56	MG	GB	9140	1/1	0.36	0.24	102,102,102,102	0
56	MG	GB	9166	1/1	0.36	0.20	129,129,129,129	0
56	MG	A	1617	1/1	0.36	0.19	193,193,193,193	0
56	MG	FB	1777	1/1	0.36	0.32	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B	9066	1/1	0.36	0.23	130,130,130,130	0
56	MG	B	9183	1/1	0.36	0.17	172,172,172,172	0
56	MG	SB	201	1/1	0.36	0.29	143,143,143,143	0
56	MG	FB	1653	1/1	0.36	0.30	146,146,146,146	0
56	MG	FB	1606	1/1	0.36	0.22	137,137,137,137	0
56	MG	GB	9078	1/1	0.36	0.20	185,185,185,185	0
56	MG	TC	201	1/1	0.36	0.37	120,120,120,120	0
56	MG	B	9174	1/1	0.37	0.35	113,113,113,113	0
56	MG	LB	302	1/1	0.37	0.12	137,137,137,137	0
56	MG	D	103	1/1	0.37	0.20	147,147,147,147	0
56	MG	B	9119	1/1	0.37	0.33	114,114,114,114	0
56	MG	GB	9228	1/1	0.38	0.18	226,226,226,226	0
56	MG	GB	9337	1/1	0.38	0.19	147,147,147,147	0
56	MG	FB	1686	1/1	0.38	0.23	139,139,139,139	0
56	MG	A	1672	1/1	0.38	0.17	158,158,158,158	0
56	MG	FB	1708	1/1	0.38	0.15	152,152,152,152	0
56	MG	LA	5800	1/1	0.38	0.20	163,163,163,163	0
56	MG	A	1640	1/1	0.39	0.23	140,140,140,140	0
56	MG	A	1692	1/1	0.39	0.31	149,149,149,149	0
56	MG	GB	9024	1/1	0.39	0.22	151,151,151,151	0
56	MG	B	9282	1/1	0.39	0.15	153,153,153,153	0
56	MG	A	1685	1/1	0.39	0.13	154,154,154,154	0
56	MG	B	9237	1/1	0.39	0.16	165,165,165,165	0
56	MG	FB	1691	1/1	0.39	0.18	144,144,144,144	0
56	MG	GB	9183	1/1	0.40	0.20	169,169,169,169	0
56	MG	UB	204	1/1	0.40	0.18	161,161,161,161	0
56	MG	B	9131	1/1	0.40	0.23	92,92,92,92	0
56	MG	A	1719	1/1	0.40	0.27	170,170,170,170	0
56	MG	GB	9132	1/1	0.40	0.29	151,151,151,151	0
56	MG	HB	217	1/1	0.40	0.23	135,135,135,135	0
56	MG	B	9116	1/1	0.41	0.25	127,127,127,127	0
56	MG	QA	201	1/1	0.41	0.33	144,144,144,144	0
56	MG	GB	9229	1/1	0.41	0.17	135,135,135,135	0
56	MG	GB	9235	1/1	0.41	0.18	156,156,156,156	0
56	MG	GB	9381	1/1	0.41	0.16	132,132,132,132	0
56	MG	FB	1780	1/1	0.41	0.15	184,184,184,184	0
56	MG	A	1677	1/1	0.41	0.12	237,237,237,237	0
56	MG	FB	1648	1/1	0.42	0.33	108,108,108,108	0
56	MG	FB	1651	1/1	0.42	0.20	186,186,186,186	0
56	MG	A	1622	1/1	0.42	0.29	125,125,125,125	0
56	MG	FB	1622	1/1	0.43	0.25	128,128,128,128	0
56	MG	FB	1688	1/1	0.43	0.25	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	A	1702	1/1	0.43	0.15	211,211,211,211	0
56	MG	FB	1757	1/1	0.43	0.17	170,170,170,170	0
56	MG	JA	401	1/1	0.44	0.09	169,169,169,169	0
56	MG	FB	1633	1/1	0.44	0.18	153,153,153,153	0
56	MG	GB	9303	1/1	0.44	0.16	165,165,165,165	0
56	MG	FB	1751	1/1	0.44	0.14	174,174,174,174	0
56	MG	GB	9027	1/1	0.44	0.25	140,140,140,140	0
56	MG	MC	101	1/1	0.44	0.38	130,130,130,130	0
56	MG	B	9177	1/1	0.44	0.28	126,126,126,126	0
56	MG	NC	102	1/1	0.44	0.14	165,165,165,165	0
56	MG	GB	9115	1/1	0.44	0.28	109,109,109,109	0
56	MG	A	1602	1/1	0.44	0.34	124,124,124,124	0
56	MG	IA	104	1/1	0.45	0.14	140,140,140,140	0
56	MG	GB	9257	1/1	0.45	0.19	124,124,124,124	0
56	MG	GB	9205	1/1	0.45	0.13	158,158,158,158	0
56	MG	GB	9017	1/1	0.45	0.19	132,132,132,132	0
56	MG	GB	9018	1/1	0.45	0.24	136,136,136,136	0
56	MG	C	215	1/1	0.45	0.10	137,137,137,137	0
56	MG	A	1639	1/1	0.45	0.15	166,166,166,166	0
56	MG	A	1721	1/1	0.45	0.44	169,169,169,169	0
56	MG	B	9139	1/1	0.46	0.24	147,147,147,147	0
56	MG	B	9088	1/1	0.46	0.35	108,108,108,108	0
56	MG	FB	1699	1/1	0.46	0.25	120,120,120,120	0
56	MG	B	9036	1/1	0.46	0.22	75,75,75,75	0
56	MG	A	1739	1/1	0.46	0.19	161,161,161,161	0
56	MG	A	1689	1/1	0.46	0.17	184,184,184,184	0
56	MG	A	1656	1/1	0.47	0.18	161,161,161,161	0
56	MG	FB	1641	1/1	0.47	0.28	131,131,131,131	0
56	MG	GB	9013	1/1	0.47	0.29	111,111,111,111	0
56	MG	XB	202	1/1	0.47	0.14	140,140,140,140	0
56	MG	B	9201	1/1	0.47	0.17	159,159,159,159	0
56	MG	GB	9398	1/1	0.48	0.17	165,165,165,165	0
56	MG	HB	214	1/1	0.48	0.15	163,163,163,163	0
56	MG	A	1636	1/1	0.48	0.23	138,138,138,138	0
56	MG	C	214	1/1	0.48	0.14	170,170,170,170	0
56	MG	GB	9295	1/1	0.48	0.12	182,182,182,182	0
56	MG	GB	9248	1/1	0.48	0.12	158,158,158,158	0
56	MG	B	9102	1/1	0.48	0.28	107,107,107,107	0
56	MG	A	1754	1/1	0.48	0.11	201,201,201,201	0
56	MG	B	9144	1/1	0.48	0.24	117,117,117,117	0
56	MG	BD	201	1/1	0.48	0.11	182,182,182,182	0
56	MG	FB	1624	1/1	0.49	0.19	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9114	1/1	0.49	0.22	134,134,134,134	0
56	MG	GB	9350	1/1	0.49	0.11	143,143,143,143	0
56	MG	GB	9390	1/1	0.49	0.13	238,238,238,238	0
56	MG	B	9349	1/1	0.50	0.13	163,163,163,163	0
56	MG	GB	9097	1/1	0.50	0.24	134,134,134,134	0
56	MG	MA	304	1/1	0.50	0.15	165,165,165,165	0
56	MG	OB	201	1/1	0.50	0.17	148,148,148,148	0
56	MG	A	1768	1/1	0.50	0.11	151,151,151,151	0
56	MG	B	9042	1/1	0.50	0.33	120,120,120,120	0
56	MG	VC	201	1/1	0.50	0.11	145,145,145,145	0
56	MG	GB	9138	1/1	0.50	0.35	122,122,122,122	0
56	MG	B	9233	1/1	0.51	0.19	207,207,207,207	0
56	MG	B	9135	1/1	0.51	0.20	142,142,142,142	0
56	MG	GB	9354	1/1	0.51	0.14	164,164,164,164	0
56	MG	FB	1627	1/1	0.51	0.19	123,123,123,123	0
56	MG	B	9385	1/1	0.51	0.16	173,173,173,173	0
56	MG	B	9392	1/1	0.51	0.16	140,140,140,140	0
56	MG	GB	9158	1/1	0.51	0.28	136,136,136,136	0
56	MG	HB	216	1/1	0.51	0.10	184,184,184,184	0
56	MG	FB	1672	1/1	0.51	0.30	131,131,131,131	0
56	MG	GB	9055	1/1	0.51	0.25	123,123,123,123	0
56	MG	V	502	1/1	0.51	0.17	109,109,109,109	0
56	MG	GB	9256	1/1	0.51	0.18	138,138,138,138	0
56	MG	CB	101	1/1	0.51	0.15	191,191,191,191	0
56	MG	B	9057	1/1	0.52	0.29	85,85,85,85	0
56	MG	IA	109	1/1	0.52	0.12	140,140,140,140	0
56	MG	FB	1772	1/1	0.52	0.25	165,165,165,165	0
56	MG	MC	102	1/1	0.52	0.18	145,145,145,145	0
56	MG	C	218	1/1	0.52	0.11	166,166,166,166	0
56	MG	C	219	1/1	0.52	0.15	155,155,155,155	0
56	MG	GB	9212	1/1	0.52	0.12	210,210,210,210	0
56	MG	A	1762	1/1	0.52	0.13	153,153,153,153	0
56	MG	FB	1732	1/1	0.52	0.12	164,164,164,164	0
56	MG	A	1687	1/1	0.52	0.12	247,247,247,247	0
56	MG	FB	1756	1/1	0.53	0.14	123,123,123,123	0
56	MG	A	1722	1/1	0.53	0.24	132,132,132,132	0
56	MG	FB	1762	1/1	0.53	0.09	256,256,256,256	0
56	MG	B	9222	1/1	0.53	0.29	126,126,126,126	0
56	MG	GB	9238	1/1	0.53	0.33	120,120,120,120	0
56	MG	GB	9355	1/1	0.53	0.16	131,131,131,131	0
56	MG	B	9138	1/1	0.53	0.14	158,158,158,158	0
56	MG	NC	109	1/1	0.53	0.24	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B	9199	1/1	0.53	0.17	94,94,94,94	0
56	MG	FB	1680	1/1	0.53	0.16	139,139,139,139	0
56	MG	A	1609	1/1	0.53	0.31	112,112,112,112	0
56	MG	HB	211	1/1	0.53	0.26	147,147,147,147	0
56	MG	FB	1642	1/1	0.54	0.18	121,121,121,121	0
56	MG	GB	9034	1/1	0.54	0.24	139,139,139,139	0
56	MG	FB	1702	1/1	0.54	0.22	171,171,171,171	0
56	MG	FB	1604	1/1	0.54	0.45	103,103,103,103	0
56	MG	FB	1752	1/1	0.54	0.22	132,132,132,132	0
56	MG	B	9109	1/1	0.54	0.23	70,70,70,70	0
56	MG	A	1713	1/1	0.54	0.20	151,151,151,151	0
56	MG	GB	9184	1/1	0.54	0.26	130,130,130,130	0
56	MG	A	1623	1/1	0.54	0.28	119,119,119,119	0
56	MG	A	1671	1/1	0.54	0.35	114,114,114,114	0
56	MG	GB	9313	1/1	0.54	0.11	127,127,127,127	0
56	MG	GB	9116	1/1	0.55	0.20	124,124,124,124	0
56	MG	B	9277	1/1	0.55	0.19	131,131,131,131	0
56	MG	OA	201	1/1	0.55	0.34	118,118,118,118	0
56	MG	IA	103	1/1	0.55	0.17	149,149,149,149	0
56	MG	FB	1735	1/1	0.55	0.18	131,131,131,131	0
56	MG	B	9324	1/1	0.55	0.17	182,182,182,182	0
56	MG	GB	9174	1/1	0.55	0.19	136,136,136,136	0
56	MG	LB	303	1/1	0.56	0.19	123,123,123,123	0
56	MG	GB	9331	1/1	0.56	0.10	143,143,143,143	0
56	MG	A	1720	1/1	0.56	0.26	126,126,126,126	0
56	MG	GB	9075	1/1	0.56	0.20	129,129,129,129	0
56	MG	VA	201	1/1	0.56	0.11	120,120,120,120	0
56	MG	GB	9022	1/1	0.56	0.40	99,99,99,99	0
56	MG	FB	1714	1/1	0.56	0.17	202,202,202,202	0
56	MG	B	9311	1/1	0.56	0.18	136,136,136,136	0
56	MG	GB	9112	1/1	0.56	0.18	139,139,139,139	0
56	MG	B	9219	1/1	0.56	0.18	138,138,138,138	0
56	MG	GB	9386	1/1	0.56	0.20	135,135,135,135	0
56	MG	GB	9230	1/1	0.56	0.25	137,137,137,137	0
56	MG	B	9396	1/1	0.56	0.17	120,120,120,120	0
56	MG	SC	302	1/1	0.56	0.29	129,129,129,129	0
56	MG	B	9330	1/1	0.56	0.21	125,125,125,125	0
56	MG	B	9430	1/1	0.56	0.14	159,159,159,159	0
56	MG	B	9220	1/1	0.56	0.18	112,112,112,112	0
56	MG	GB	9041	1/1	0.57	0.32	111,111,111,111	0
56	MG	GB	9169	1/1	0.57	0.16	142,142,142,142	0
56	MG	B	9418	1/1	0.57	0.19	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1725	1/1	0.57	0.11	138,138,138,138	0
56	MG	B	9111	1/1	0.57	0.27	104,104,104,104	0
56	MG	FB	1697	1/1	0.57	0.16	149,149,149,149	0
56	MG	GB	9349	1/1	0.57	0.12	134,134,134,134	0
56	MG	GB	9262	1/1	0.57	0.25	119,119,119,119	0
56	MG	A	1663	1/1	0.57	0.20	135,135,135,135	0
56	MG	B	9382	1/1	0.57	0.08	135,135,135,135	0
56	MG	GB	9137	1/1	0.57	0.32	134,134,134,134	0
56	MG	B	9098	1/1	0.57	0.25	114,114,114,114	0
56	MG	A	1624	1/1	0.57	0.20	144,144,144,144	0
56	MG	GB	9297	1/1	0.57	0.15	132,132,132,132	0
56	MG	B	9327	1/1	0.57	0.19	139,139,139,139	0
56	MG	FB	1614	1/1	0.57	0.31	125,125,125,125	0
56	MG	A	1758	1/1	0.57	0.11	98,98,98,98	0
56	MG	FB	1703	1/1	0.58	0.18	116,116,116,116	0
56	MG	GB	9325	1/1	0.58	0.17	105,105,105,105	0
56	MG	FB	1609	1/1	0.58	0.37	110,110,110,110	0
56	MG	A	1715	1/1	0.58	0.22	121,121,121,121	0
56	MG	A	1751	1/1	0.58	0.17	159,159,159,159	0
56	MG	B	9105	1/1	0.58	0.32	111,111,111,111	0
56	MG	A	1770	1/1	0.58	0.13	163,163,163,163	0
56	MG	B	9321	1/1	0.58	0.13	132,132,132,132	0
56	MG	GB	9035	1/1	0.58	0.22	104,104,104,104	0
56	MG	GB	9275	1/1	0.58	0.25	149,149,149,149	0
56	MG	B	9428	1/1	0.59	0.15	138,138,138,138	0
56	MG	GB	9401	1/1	0.59	0.23	106,106,106,106	0
56	MG	C	221	1/1	0.59	0.23	157,157,157,157	0
56	MG	GB	9172	1/1	0.59	0.17	135,135,135,135	0
56	MG	B	9238	1/1	0.59	0.23	95,95,95,95	0
56	MG	UB	201	1/1	0.59	0.14	149,149,149,149	0
56	MG	B	9015	1/1	0.59	0.28	84,84,84,84	0
56	MG	GB	9019	1/1	0.59	0.19	130,130,130,130	0
56	MG	GB	9127	1/1	0.59	0.17	119,119,119,119	0
56	MG	A	1756	1/1	0.59	0.20	102,102,102,102	0
56	MG	A	1745	1/1	0.59	0.14	172,172,172,172	0
56	MG	FB	1603	1/1	0.59	0.29	118,118,118,118	0
56	MG	GB	9279	1/1	0.59	0.13	140,140,140,140	0
56	MG	GB	9095	1/1	0.59	0.36	108,108,108,108	0
56	MG	B	9351	1/1	0.59	0.13	147,147,147,147	0
56	MG	GB	9033	1/1	0.59	0.26	131,131,131,131	0
56	MG	GB	9152	1/1	0.59	0.21	119,119,119,119	0
56	MG	FB	1728	1/1	0.59	0.17	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	A	1606	1/1	0.59	0.20	109,109,109,109	0
56	MG	B	9267	1/1	0.60	0.11	164,164,164,164	0
56	MG	FB	1620	1/1	0.60	0.18	126,126,126,126	0
56	MG	GB	9234	1/1	0.60	0.19	132,132,132,132	0
56	MG	B	9112	1/1	0.60	0.22	138,138,138,138	0
56	MG	B	9232	1/1	0.60	0.22	111,111,111,111	0
56	MG	A	1605	1/1	0.60	0.25	119,119,119,119	0
56	MG	A	1726	1/1	0.60	0.14	140,140,140,140	0
56	MG	GB	9043	1/1	0.60	0.24	112,112,112,112	0
56	MG	GB	9200	1/1	0.60	0.15	152,152,152,152	0
56	MG	A	1699	1/1	0.60	0.18	136,136,136,136	0
56	MG	GB	9207	1/1	0.60	0.23	119,119,119,119	0
56	MG	B	9243	1/1	0.60	0.13	153,153,153,153	0
56	MG	SA	201	1/1	0.60	0.13	169,169,169,169	0
56	MG	GB	9058	1/1	0.60	0.29	117,117,117,117	0
56	MG	B	9190	1/1	0.60	0.17	110,110,110,110	0
56	MG	GB	9108	1/1	0.61	0.47	116,116,116,116	0
56	MG	GB	9375	1/1	0.61	0.09	152,152,152,152	0
56	MG	GB	9308	1/1	0.61	0.31	102,102,102,102	0
56	MG	B	9076	1/1	0.61	0.23	104,104,104,104	0
56	MG	FB	1650	1/1	0.61	0.25	135,135,135,135	0
56	MG	A	1780	1/1	0.61	0.17	163,163,163,163	0
56	MG	GB	9328	1/1	0.61	0.10	152,152,152,152	0
56	MG	A	1693	1/1	0.61	0.11	154,154,154,154	0
56	MG	F	303	1/1	0.61	0.12	131,131,131,131	0
56	MG	H	201	1/1	0.61	0.23	146,146,146,146	0
56	MG	B	9156	1/1	0.61	0.16	145,145,145,145	0
56	MG	HB	203	1/1	0.61	0.27	137,137,137,137	0
56	MG	GB	9123	1/1	0.61	0.27	109,109,109,109	0
56	MG	J	201	1/1	0.61	0.13	157,157,157,157	0
56	MG	A	1729	1/1	0.61	0.17	141,141,141,141	0
56	MG	B	9084	1/1	0.62	0.25	101,101,101,101	0
56	MG	B	9307	1/1	0.62	0.14	142,142,142,142	0
56	MG	A	1748	1/1	0.62	0.19	116,116,116,116	0
56	MG	B	9254	1/1	0.62	0.13	188,188,188,188	0
56	MG	UA	201	1/1	0.62	0.09	139,139,139,139	0
56	MG	FB	1613	1/1	0.62	0.37	105,105,105,105	0
56	MG	B	9171	1/1	0.62	0.17	150,150,150,150	0
56	MG	B	9043	1/1	0.62	0.24	95,95,95,95	0
56	MG	GB	9190	1/1	0.62	0.23	112,112,112,112	0
56	MG	GB	9067	1/1	0.62	0.19	105,105,105,105	0
56	MG	B	9303	1/1	0.62	0.24	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1791	1/1	0.62	0.13	138,138,138,138	0
56	MG	A	1688	1/1	0.63	0.13	170,170,170,170	0
56	MG	GB	9385	1/1	0.63	0.19	105,105,105,105	0
56	MG	GB	9039	1/1	0.63	0.29	130,130,130,130	0
56	MG	B	9310	1/1	0.63	0.08	162,162,162,162	0
56	MG	A	1665	1/1	0.63	0.17	134,134,134,134	0
56	MG	GB	9395	1/1	0.63	0.09	158,158,158,158	0
56	MG	GB	9051	1/1	0.63	0.33	106,106,106,106	0
56	MG	GB	9246	1/1	0.63	0.14	133,133,133,133	0
56	MG	YA	101	1/1	0.63	0.23	126,126,126,126	0
56	MG	B	9234	1/1	0.63	0.18	130,130,130,130	0
56	MG	GB	9119	1/1	0.63	0.34	126,126,126,126	0
56	MG	B	9055	1/1	0.63	0.18	127,127,127,127	0
56	MG	FB	1731	1/1	0.63	0.18	156,156,156,156	0
56	MG	B	9284	1/1	0.63	0.17	128,128,128,128	0
56	MG	A	1783	1/1	0.63	0.16	160,160,160,160	0
56	MG	FB	1744	1/1	0.63	0.16	135,135,135,135	0
56	MG	B	9348	1/1	0.63	0.12	151,151,151,151	0
56	MG	A	1613	1/1	0.63	0.33	121,121,121,121	0
56	MG	C	202	1/1	0.63	0.29	126,126,126,126	0
56	MG	A	1604	1/1	0.63	0.20	125,125,125,125	0
56	MG	GB	9377	1/1	0.63	0.40	114,114,114,114	0
56	MG	A	1738	1/1	0.63	0.19	127,127,127,127	0
56	MG	B	9265	1/1	0.64	0.13	136,136,136,136	0
56	MG	B	9235	1/1	0.64	0.12	165,165,165,165	0
56	MG	A	1700	1/1	0.64	0.16	97,97,97,97	0
56	MG	FB	1729	1/1	0.64	0.19	134,134,134,134	0
56	MG	GB	9077	1/1	0.64	0.35	84,84,84,84	0
56	MG	B	9025	1/1	0.64	0.42	87,87,87,87	0
56	MG	GB	9083	1/1	0.64	0.23	125,125,125,125	0
56	MG	B	9080	1/1	0.64	0.26	117,117,117,117	0
56	MG	B	9129	1/1	0.64	0.20	108,108,108,108	0
56	MG	GB	9010	1/1	0.64	0.30	92,92,92,92	0
56	MG	B	9101	1/1	0.64	0.19	102,102,102,102	0
56	MG	B	9289	1/1	0.64	0.23	138,138,138,138	0
56	MG	FB	1647	1/1	0.64	0.23	136,136,136,136	0
56	MG	GB	9271	1/1	0.64	0.29	126,126,126,126	0
56	MG	GB	9146	1/1	0.64	0.16	116,116,116,116	0
56	MG	IA	107	1/1	0.64	0.13	109,109,109,109	0
56	MG	C	207	1/1	0.64	0.12	152,152,152,152	0
56	MG	GB	9380	1/1	0.65	0.12	120,120,120,120	0
56	MG	B	9180	1/1	0.65	0.14	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9092	1/1	0.65	0.22	110,110,110,110	0
56	MG	B	9210	1/1	0.65	0.17	133,133,133,133	0
56	MG	FB	1723	1/1	0.65	0.26	181,181,181,181	0
56	MG	GB	9128	1/1	0.65	0.21	136,136,136,136	0
56	MG	B	9260	1/1	0.65	0.23	103,103,103,103	0
56	MG	B	9423	1/1	0.65	0.26	117,117,117,117	0
56	MG	A	1718	1/1	0.65	0.20	133,133,133,133	0
56	MG	FB	1771	1/1	0.65	0.17	138,138,138,138	0
56	MG	A	1707	1/1	0.65	0.22	164,164,164,164	0
56	MG	FB	1706	1/1	0.65	0.26	117,117,117,117	0
56	MG	JB	303	1/1	0.65	0.10	102,102,102,102	0
56	MG	B	9133	1/1	0.65	0.18	89,89,89,89	0
56	MG	FB	1658	1/1	0.65	0.37	119,119,119,119	0
56	MG	A	1776	1/1	0.65	0.23	144,144,144,144	0
56	MG	HD	101	1/1	0.65	0.22	150,150,150,150	0
56	MG	C	208	1/1	0.66	0.15	164,164,164,164	0
56	MG	FB	1605	1/1	0.66	0.38	103,103,103,103	0
56	MG	FB	1685	1/1	0.66	0.13	141,141,141,141	0
56	MG	GB	9151	1/1	0.66	0.23	104,104,104,104	0
56	MG	B	9023	1/1	0.66	0.32	92,92,92,92	0
56	MG	GB	9153	1/1	0.66	0.15	110,110,110,110	0
56	MG	B	9186	1/1	0.66	0.16	116,116,116,116	0
56	MG	GB	9008	1/1	0.66	0.27	83,83,83,83	0
56	MG	GB	9270	1/1	0.66	0.17	123,123,123,123	0
56	MG	MC	103	1/1	0.66	0.20	140,140,140,140	0
56	MG	GB	9103	1/1	0.66	0.20	126,126,126,126	0
56	MG	GB	9388	1/1	0.66	0.19	108,108,108,108	0
56	MG	NC	105	1/1	0.66	0.05	174,174,174,174	0
56	MG	GB	9063	1/1	0.66	0.18	115,115,115,115	0
56	MG	QC	302	1/1	0.66	0.19	143,143,143,143	0
56	MG	B	9373	1/1	0.66	0.13	160,160,160,160	0
56	MG	FB	1759	1/1	0.66	0.29	134,134,134,134	0
56	MG	FB	1673	1/1	0.66	0.21	133,133,133,133	0
56	MG	GB	9343	1/1	0.66	0.09	133,133,133,133	0
56	MG	B	9045	1/1	0.66	0.40	105,105,105,105	0
56	MG	GB	9290	1/1	0.66	0.14	146,146,146,146	0
56	MG	BC	301	1/1	0.67	0.19	136,136,136,136	0
56	MG	B	9140	1/1	0.67	0.20	111,111,111,111	0
56	MG	HB	219	1/1	0.67	0.16	141,141,141,141	0
56	MG	B	9078	1/1	0.67	0.24	88,88,88,88	0
56	MG	GB	9090	1/1	0.67	0.25	129,129,129,129	0
56	MG	B	9052	1/1	0.67	0.26	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1645	1/1	0.67	0.17	144,144,144,144	0
56	MG	B	9038	1/1	0.67	0.31	85,85,85,85	0
56	MG	GB	9060	1/1	0.67	0.25	124,124,124,124	0
56	MG	PC	401	1/1	0.67	0.15	167,167,167,167	0
56	MG	A	1727	1/1	0.67	0.18	161,161,161,161	0
56	MG	B	9092	1/1	0.67	0.13	140,140,140,140	0
56	MG	GB	9129	1/1	0.67	0.10	103,103,103,103	0
56	MG	SB	202	1/1	0.67	0.21	137,137,137,137	0
56	MG	GB	9040	1/1	0.67	0.25	113,113,113,113	0
56	MG	FB	1639	1/1	0.67	0.15	123,123,123,123	0
56	MG	OA	204	1/1	0.67	0.10	134,134,134,134	0
56	MG	A	1759	1/1	0.68	0.38	175,175,175,175	0
56	MG	B	9040	1/1	0.68	0.37	98,98,98,98	0
56	MG	B	9401	1/1	0.68	0.08	139,139,139,139	0
56	MG	FB	1670	1/1	0.68	0.18	197,197,197,197	0
56	MG	UB	202	1/1	0.68	0.34	164,164,164,164	0
56	MG	GB	9020	1/1	0.68	0.48	94,94,94,94	0
56	MG	FB	1607	1/1	0.68	0.33	99,99,99,99	0
56	MG	GB	9110	1/1	0.68	0.16	98,98,98,98	0
56	MG	A	1698	1/1	0.68	0.13	171,171,171,171	0
56	MG	GB	9218	1/1	0.68	0.15	108,108,108,108	0
56	MG	GB	9113	1/1	0.68	0.24	99,99,99,99	0
56	MG	HB	212	1/1	0.68	0.30	130,130,130,130	0
56	MG	GB	9026	1/1	0.68	0.27	88,88,88,88	0
56	MG	K	204	1/1	0.68	0.10	133,133,133,133	0
56	MG	A	1676	1/1	0.68	0.25	133,133,133,133	0
56	MG	D	101	1/1	0.68	0.13	231,231,231,231	0
56	MG	FB	1781	1/1	0.68	0.39	179,179,179,179	0
56	MG	MA	306	1/1	0.68	0.11	149,149,149,149	0
56	MG	GB	9244	1/1	0.68	0.20	132,132,132,132	0
56	MG	GB	9004	1/1	0.68	0.40	88,88,88,88	0
56	MG	GB	9084	1/1	0.68	0.26	111,111,111,111	0
56	MG	C	209	1/1	0.68	0.29	130,130,130,130	0
56	MG	WC	201	1/1	0.68	0.11	134,134,134,134	0
56	MG	GB	9254	1/1	0.68	0.10	109,109,109,109	0
56	MG	A	1696	1/1	0.68	0.11	106,106,106,106	0
56	MG	GB	9201	1/1	0.69	0.22	107,107,107,107	0
56	MG	A	1755	1/1	0.69	0.26	110,110,110,110	0
56	MG	B	9013	1/1	0.69	0.22	96,96,96,96	0
56	MG	B	9253	1/1	0.69	0.12	107,107,107,107	0
56	MG	GB	9155	1/1	0.69	0.14	150,150,150,150	0
56	MG	A	1710	1/1	0.69	0.28	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9102	1/1	0.69	0.26	81,81,81,81	0
56	MG	B	9044	1/1	0.69	0.37	73,73,73,73	0
56	MG	FB	1753	1/1	0.69	0.22	132,132,132,132	0
56	MG	MA	301	1/1	0.69	0.16	152,152,152,152	0
56	MG	GB	9109	1/1	0.69	0.17	111,111,111,111	0
56	MG	GB	9175	1/1	0.69	0.19	92,92,92,92	0
56	MG	A	1777	1/1	0.69	0.18	152,152,152,152	0
56	MG	LB	304	1/1	0.69	0.12	127,127,127,127	0
56	MG	A	1763	1/1	0.69	0.12	104,104,104,104	0
56	MG	A	1666	1/1	0.69	0.25	123,123,123,123	0
56	MG	PB	201	1/1	0.69	0.10	134,134,134,134	0
56	MG	RB	201	1/1	0.69	0.27	87,87,87,87	0
56	MG	B	9375	1/1	0.69	0.08	95,95,95,95	0
56	MG	A	1781	1/1	0.69	0.11	149,149,149,149	0
56	MG	A	1690	1/1	0.69	0.31	105,105,105,105	0
56	MG	GB	9227	1/1	0.70	0.25	116,116,116,116	0
56	MG	B	9070	1/1	0.70	0.12	83,83,83,83	0
56	MG	O	202	1/1	0.70	0.28	102,102,102,102	0
56	MG	FB	1663	1/1	0.70	0.14	110,110,110,110	0
56	MG	B	9182	1/1	0.70	0.11	116,116,116,116	0
56	MG	AB	201	1/1	0.70	0.15	135,135,135,135	0
56	MG	GB	9292	1/1	0.70	0.22	122,122,122,122	0
56	MG	FB	1766	1/1	0.70	0.28	110,110,110,110	0
56	MG	GB	9243	1/1	0.70	0.15	127,127,127,127	0
56	MG	HB	213	1/1	0.70	0.06	187,187,187,187	0
56	MG	GB	9120	1/1	0.70	0.11	101,101,101,101	0
56	MG	GB	9038	1/1	0.70	0.30	98,98,98,98	0
56	MG	G	301	1/1	0.70	0.15	101,101,101,101	0
56	MG	GB	9203	1/1	0.70	0.17	100,100,100,100	0
56	MG	FB	1696	1/1	0.70	0.18	191,191,191,191	0
56	MG	A	1732	1/1	0.70	0.22	139,139,139,139	0
56	MG	GB	9319	1/1	0.70	0.27	104,104,104,104	0
56	MG	C	203	1/1	0.70	0.17	161,161,161,161	0
56	MG	GB	9392	1/1	0.70	0.20	147,147,147,147	0
56	MG	GB	9321	1/1	0.70	0.12	147,147,147,147	0
56	MG	SC	304	1/1	0.70	0.11	116,116,116,116	0
56	MG	GB	9168	1/1	0.70	0.15	115,115,115,115	0
56	MG	GB	9400	1/1	0.70	0.09	150,150,150,150	0
56	MG	GB	9044	1/1	0.70	0.23	119,119,119,119	0
56	MG	A	1658	1/1	0.70	0.30	177,177,177,177	0
56	MG	GB	9225	1/1	0.70	0.13	93,93,93,93	0
56	MG	B	9258	1/1	0.71	0.09	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B	9224	1/1	0.71	0.16	120,120,120,120	0
56	MG	FB	1637	1/1	0.71	0.37	109,109,109,109	0
56	MG	B	9308	1/1	0.71	0.11	125,125,125,125	0
56	MG	B	9231	1/1	0.71	0.15	85,85,85,85	0
56	MG	GB	9088	1/1	0.71	0.21	115,115,115,115	0
56	MG	GB	9339	1/1	0.71	0.24	102,102,102,102	0
56	MG	GB	9056	1/1	0.71	0.25	93,93,93,93	0
56	MG	GB	9015	1/1	0.71	0.24	86,86,86,86	0
56	MG	B	9335	1/1	0.71	0.13	126,126,126,126	0
56	MG	A	1645	1/1	0.71	0.42	131,131,131,131	0
56	MG	FB	1616	1/1	0.71	0.40	108,108,108,108	0
56	MG	GB	9149	1/1	0.71	0.11	108,108,108,108	0
56	MG	FB	1678	1/1	0.71	0.23	115,115,115,115	0
56	MG	FB	1617	1/1	0.71	0.25	110,110,110,110	0
56	MG	DC	101	1/1	0.71	0.20	122,122,122,122	0
56	MG	GB	9104	1/1	0.71	0.18	103,103,103,103	0
56	MG	FB	1767	1/1	0.72	0.15	137,137,137,137	0
56	MG	B	9175	1/1	0.72	0.19	102,102,102,102	0
56	MG	K	201	1/1	0.72	0.08	128,128,128,128	0
56	MG	GB	9130	1/1	0.72	0.20	116,116,116,116	0
56	MG	B	9204	1/1	0.72	0.21	113,113,113,113	0
56	MG	A	1734	1/1	0.72	0.16	143,143,143,143	0
56	MG	B	9121	1/1	0.72	0.22	142,142,142,142	0
56	MG	FB	1738	1/1	0.72	0.22	143,143,143,143	0
56	MG	GB	9241	1/1	0.72	0.26	113,113,113,113	0
56	MG	GB	9185	1/1	0.72	0.16	120,120,120,120	0
56	MG	A	1607	1/1	0.72	0.27	122,122,122,122	0
56	MG	A	1749	1/1	0.72	0.10	129,129,129,129	0
56	MG	GB	9197	1/1	0.72	0.19	91,91,91,91	0
56	MG	NC	106	1/1	0.72	0.17	108,108,108,108	0
56	MG	NC	107	1/1	0.72	0.19	122,122,122,122	0
56	MG	D	104	1/1	0.72	0.12	131,131,131,131	0
56	MG	D	105	1/1	0.72	0.09	129,129,129,129	0
56	MG	A	1728	1/1	0.72	0.07	183,183,183,183	0
56	MG	GB	9089	1/1	0.72	0.30	113,113,113,113	0
56	MG	A	1603	1/1	0.72	0.24	102,102,102,102	0
56	MG	A	1704	1/1	0.72	0.14	106,106,106,106	0
56	MG	B	9314	1/1	0.72	0.14	131,131,131,131	0
56	MG	YA	102	1/1	0.72	0.16	134,134,134,134	0
56	MG	GB	9219	1/1	0.72	0.16	143,143,143,143	0
56	MG	GB	9220	1/1	0.72	0.21	122,122,122,122	0
56	MG	FB	1692	1/1	0.72	0.18	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1776	1/1	0.73	0.10	214,214,214,214	0
56	MG	RB	202	1/1	0.73	0.10	134,134,134,134	0
56	MG	FB	1724	1/1	0.73	0.34	162,162,162,162	0
56	MG	A	1669	1/1	0.73	0.17	132,132,132,132	0
56	MG	GB	9188	1/1	0.73	0.23	90,90,90,90	0
56	MG	FB	1682	1/1	0.73	0.17	130,130,130,130	0
56	MG	GB	9133	1/1	0.73	0.22	107,107,107,107	0
56	MG	B	9429	1/1	0.73	0.17	100,100,100,100	0
56	MG	B	9181	1/1	0.73	0.12	97,97,97,97	0
56	MG	B	9212	1/1	0.73	0.21	108,108,108,108	0
56	MG	GB	9259	1/1	0.73	0.15	91,91,91,91	0
56	MG	B	9213	1/1	0.73	0.21	105,105,105,105	0
56	MG	GB	9107	1/1	0.73	0.15	88,88,88,88	0
56	MG	B	9125	1/1	0.73	0.32	100,100,100,100	0
56	MG	B	9383	1/1	0.73	0.18	116,116,116,116	0
56	MG	B	9058	1/1	0.73	0.16	151,151,151,151	0
56	MG	B	9037	1/1	0.73	0.24	89,89,89,89	0
56	MG	C	211	1/1	0.73	0.14	149,149,149,149	0
56	MG	B	9067	1/1	0.73	0.19	89,89,89,89	0
56	MG	A	1633	1/1	0.73	0.30	112,112,112,112	0
56	MG	B	9338	1/1	0.73	0.39	112,112,112,112	0
56	MG	C	217	1/1	0.73	0.13	140,140,140,140	0
56	MG	A	1725	1/1	0.73	0.29	126,126,126,126	0
56	MG	PA	201	1/1	0.73	0.07	109,109,109,109	0
56	MG	FB	1674	1/1	0.73	0.24	107,107,107,107	0
56	MG	Y	102	1/1	0.73	0.09	126,126,126,126	0
56	MG	FB	1677	1/1	0.73	0.21	119,119,119,119	0
56	MG	A	1682	1/1	0.73	0.19	136,136,136,136	0
56	MG	ZC	201	1/1	0.73	0.28	126,126,126,126	0
56	MG	GB	9240	1/1	0.73	0.14	113,113,113,113	0
56	MG	GB	9310	1/1	0.73	0.21	124,124,124,124	0
56	MG	B	9124	1/1	0.74	0.28	94,94,94,94	0
56	MG	A	1712	1/1	0.74	0.12	198,198,198,198	0
56	MG	GB	9206	1/1	0.74	0.25	113,113,113,113	0
56	MG	GB	9323	1/1	0.74	0.23	98,98,98,98	0
56	MG	GB	9324	1/1	0.74	0.11	153,153,153,153	0
56	MG	A	1730	1/1	0.74	0.15	115,115,115,115	0
56	MG	B	9062	1/1	0.74	0.19	109,109,109,109	0
56	MG	GB	9280	1/1	0.74	0.16	104,104,104,104	0
56	MG	GB	9287	1/1	0.74	0.08	164,164,164,164	0
56	MG	B	9269	1/1	0.74	0.12	153,153,153,153	0
56	MG	MA	303	1/1	0.74	0.10	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B	9169	1/1	0.74	0.24	110,110,110,110	0
56	MG	B	9115	1/1	0.74	0.27	119,119,119,119	0
56	MG	GB	9296	1/1	0.74	0.14	133,133,133,133	0
56	MG	GB	9250	1/1	0.74	0.20	132,132,132,132	0
56	MG	HB	206	1/1	0.74	0.17	141,141,141,141	0
56	MG	B	9221	1/1	0.74	0.15	161,161,161,161	0
56	MG	GB	9086	1/1	0.74	0.13	123,123,123,123	0
56	MG	UC	202	1/1	0.74	0.11	138,138,138,138	0
56	MG	GB	9154	1/1	0.74	0.25	114,114,114,114	0
56	MG	B	9064	1/1	0.74	0.20	107,107,107,107	0
56	MG	FB	1727	1/1	0.74	0.23	119,119,119,119	0
56	MG	B	9054	1/1	0.74	0.26	115,115,115,115	0
56	MG	A	1701	1/1	0.74	0.20	160,160,160,160	0
56	MG	GB	9011	1/1	0.75	0.27	88,88,88,88	0
56	MG	A	1654	1/1	0.75	0.27	98,98,98,98	0
56	MG	GB	9326	1/1	0.75	0.11	180,180,180,180	0
56	MG	B	9422	1/1	0.75	0.10	148,148,148,148	0
56	MG	GB	9126	1/1	0.75	0.21	109,109,109,109	0
56	MG	B	9301	1/1	0.75	0.11	119,119,119,119	0
56	MG	GB	9276	1/1	0.75	0.18	94,94,94,94	0
56	MG	A	1630	1/1	0.75	0.30	112,112,112,112	0
56	MG	A	1615	1/1	0.75	0.28	101,101,101,101	0
56	MG	B	9136	1/1	0.75	0.17	121,121,121,121	0
56	MG	GB	9176	1/1	0.75	0.18	104,104,104,104	0
56	MG	FB	1770	1/1	0.75	0.11	133,133,133,133	0
56	MG	GB	9182	1/1	0.75	0.17	125,125,125,125	0
56	MG	GB	9368	1/1	0.75	0.07	139,139,139,139	0
56	MG	Z	101	1/1	0.75	0.20	105,105,105,105	0
56	MG	GB	9293	1/1	0.75	0.10	90,90,90,90	0
56	MG	GB	9061	1/1	0.75	0.16	108,108,108,108	0
56	MG	NC	108	1/1	0.75	0.13	136,136,136,136	0
56	MG	E	306	1/1	0.75	0.07	88,88,88,88	0
56	MG	FB	1737	1/1	0.75	0.11	114,114,114,114	0
56	MG	FB	1660	1/1	0.75	0.33	102,102,102,102	0
56	MG	GB	9191	1/1	0.75	0.17	116,116,116,116	0
56	MG	GB	9031	1/1	0.75	0.32	96,96,96,96	0
56	MG	B	9352	1/1	0.75	0.12	121,121,121,121	0
56	MG	GB	9147	1/1	0.75	0.29	114,114,114,114	0
56	MG	FB	1745	1/1	0.75	0.22	138,138,138,138	0
56	MG	A	1649	1/1	0.75	0.19	88,88,88,88	0
56	MG	A	1737	1/1	0.75	0.20	131,131,131,131	0
56	MG	GB	9007	1/1	0.75	0.28	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	IA	105	1/1	0.75	0.24	135,135,135,135	0
56	MG	C	204	1/1	0.75	0.27	113,113,113,113	0
56	MG	FB	1695	1/1	0.76	0.24	118,118,118,118	0
56	MG	B	9193	1/1	0.76	0.25	96,96,96,96	0
56	MG	C	205	1/1	0.76	0.17	101,101,101,101	0
56	MG	FB	1778	1/1	0.76	0.13	121,121,121,121	0
56	MG	B	9229	1/1	0.76	0.15	100,100,100,100	0
56	MG	B	9241	1/1	0.76	0.08	118,118,118,118	0
56	MG	FB	1782	1/1	0.76	0.17	175,175,175,175	0
56	MG	B	9272	1/1	0.76	0.15	116,116,116,116	0
56	MG	B	9417	1/1	0.76	0.14	113,113,113,113	0
56	MG	GB	9389	1/1	0.76	0.23	107,107,107,107	0
56	MG	B	9230	1/1	0.76	0.14	129,129,129,129	0
56	MG	FB	1707	1/1	0.76	0.35	113,113,113,113	0
56	MG	B	9419	1/1	0.76	0.11	102,102,102,102	0
56	MG	A	1648	1/1	0.76	0.13	130,130,130,130	0
56	MG	B	9007	1/1	0.76	0.55	75,75,75,75	0
56	MG	GB	9101	1/1	0.76	0.27	84,84,84,84	0
56	MG	GB	9054	1/1	0.76	0.31	105,105,105,105	0
56	MG	A	1711	1/1	0.76	0.20	110,110,110,110	0
56	MG	GB	9135	1/1	0.76	0.24	105,105,105,105	0
56	MG	FB	1625	1/1	0.76	0.23	99,99,99,99	0
56	MG	B	9316	1/1	0.76	0.11	126,126,126,126	0
56	MG	FB	1629	1/1	0.76	0.12	101,101,101,101	0
56	MG	B	9319	1/1	0.76	0.08	110,110,110,110	0
56	MG	B	9050	1/1	0.76	0.45	105,105,105,105	0
56	MG	B	9192	1/1	0.76	0.13	132,132,132,132	0
56	MG	B	9262	1/1	0.76	0.24	110,110,110,110	0
56	MG	B	9288	1/1	0.77	0.12	153,153,153,153	0
56	MG	GB	9177	1/1	0.77	0.26	124,124,124,124	0
56	MG	GB	9180	1/1	0.77	0.34	104,104,104,104	0
56	MG	MA	302	1/1	0.77	0.11	157,157,157,157	0
56	MG	GB	9215	1/1	0.77	0.20	145,145,145,145	0
56	MG	B	9158	1/1	0.77	0.20	90,90,90,90	0
56	MG	GB	9030	1/1	0.77	0.34	80,80,80,80	0
56	MG	B	9100	1/1	0.77	0.18	100,100,100,100	0
56	MG	FB	1774	1/1	0.77	0.24	118,118,118,118	0
56	MG	QC	301	1/1	0.77	0.19	133,133,133,133	0
56	MG	B	9248	1/1	0.77	0.22	104,104,104,104	0
56	MG	B	9376	1/1	0.77	0.17	94,94,94,94	0
56	MG	B	9089	1/1	0.77	0.14	126,126,126,126	0
56	MG	FB	1636	1/1	0.77	0.23	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1736	1/1	0.77	0.16	120,120,120,120	0
56	MG	TC	202	1/1	0.77	0.14	135,135,135,135	0
56	MG	GB	9304	1/1	0.77	0.17	102,102,102,102	0
56	MG	CC	101	1/1	0.77	0.52	111,111,111,111	0
56	MG	A	1621	1/1	0.77	0.17	105,105,105,105	0
56	MG	GB	9072	1/1	0.77	0.16	113,113,113,113	0
56	MG	FB	1788	1/1	0.77	0.11	127,127,127,127	0
56	MG	A	1668	1/1	0.77	0.14	147,147,147,147	0
56	MG	FB	1632	1/1	0.78	0.18	104,104,104,104	0
56	MG	GB	9374	1/1	0.78	0.27	117,117,117,117	0
56	MG	GB	9105	1/1	0.78	0.20	116,116,116,116	0
56	MG	GB	9150	1/1	0.78	0.24	143,143,143,143	0
56	MG	GB	9053	1/1	0.78	0.36	88,88,88,88	0
56	MG	B	9203	1/1	0.78	0.13	128,128,128,128	0
56	MG	B	9061	1/1	0.78	0.27	104,104,104,104	0
56	MG	B	9206	1/1	0.78	0.19	96,96,96,96	0
56	MG	B	9432	1/1	0.78	0.24	119,119,119,119	0
56	MG	GB	9294	1/1	0.78	0.17	131,131,131,131	0
56	MG	GB	9157	1/1	0.78	0.10	143,143,143,143	0
56	MG	FB	1666	1/1	0.78	0.13	128,128,128,128	0
56	MG	A	1706	1/1	0.78	0.11	147,147,147,147	0
56	MG	A	1614	1/1	0.78	0.23	116,116,116,116	0
56	MG	B	9002	1/1	0.78	0.54	64,64,64,64	0
56	MG	GB	9231	1/1	0.78	0.16	96,96,96,96	0
56	MG	FB	1640	1/1	0.78	0.17	103,103,103,103	0
56	MG	B	9239	1/1	0.78	0.16	86,86,86,86	0
56	MG	GB	9068	1/1	0.78	0.25	100,100,100,100	0
56	MG	B	9033	1/1	0.78	0.29	78,78,78,78	0
56	MG	A	1694	1/1	0.78	0.19	100,100,100,100	0
56	MG	FB	1619	1/1	0.78	0.18	125,125,125,125	0
56	MG	B	9122	1/1	0.78	0.18	106,106,106,106	0
56	MG	GB	9125	1/1	0.78	0.28	89,89,89,89	0
56	MG	B	9146	1/1	0.78	0.26	78,78,78,78	0
56	MG	A	1752	1/1	0.78	0.23	112,112,112,112	0
56	MG	FB	1726	1/1	0.78	0.19	107,107,107,107	0
56	MG	B	9014	1/1	0.78	0.24	60,60,60,60	0
56	MG	A	1628	1/1	0.78	0.19	101,101,101,101	0
56	MG	GB	9329	1/1	0.78	0.18	91,91,91,91	0
56	MG	B	9130	1/1	0.78	0.15	115,115,115,115	0
56	MG	GB	9091	1/1	0.78	0.19	107,107,107,107	0
56	MG	FB	1689	1/1	0.78	0.32	109,109,109,109	0
56	MG	GB	9263	1/1	0.78	0.11	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1690	1/1	0.78	0.22	107,107,107,107	0
56	MG	B	9020	1/1	0.78	0.26	83,83,83,83	0
56	MG	UC	203	1/1	0.78	0.08	120,120,120,120	0
56	MG	FB	1783	1/1	0.78	0.14	160,160,160,160	0
56	MG	MA	305	1/1	0.78	0.08	156,156,156,156	0
56	MG	FB	1790	1/1	0.78	0.10	138,138,138,138	0
56	MG	GB	9360	1/1	0.78	0.14	101,101,101,101	0
56	MG	FB	1693	1/1	0.78	0.17	160,160,160,160	0
56	MG	GB	9371	1/1	0.79	0.13	92,92,92,92	0
56	MG	FB	1794	1/1	0.79	0.20	125,125,125,125	0
56	MG	GB	9213	1/1	0.79	0.13	92,92,92,92	0
56	MG	B	9403	1/1	0.79	0.16	132,132,132,132	0
56	MG	FB	1739	1/1	0.79	0.17	115,115,115,115	0
56	MG	B	9346	1/1	0.79	0.09	109,109,109,109	0
56	MG	B	9347	1/1	0.79	0.09	115,115,115,115	0
56	MG	AB	202	1/1	0.79	0.13	133,133,133,133	0
56	MG	B	9150	1/1	0.79	0.15	101,101,101,101	0
56	MG	GB	9111	1/1	0.79	0.25	102,102,102,102	0
56	MG	GB	9014	1/1	0.79	0.29	88,88,88,88	0
56	MG	A	1675	1/1	0.79	0.20	96,96,96,96	0
56	MG	B	9073	1/1	0.79	0.20	79,79,79,79	0
56	MG	B	9245	1/1	0.79	0.41	103,103,103,103	0
56	MG	B	9368	1/1	0.79	0.21	92,92,92,92	0
56	MG	A	1740	1/1	0.79	0.20	108,108,108,108	0
56	MG	GB	9021	1/1	0.79	0.39	109,109,109,109	0
56	MG	GB	9309	1/1	0.79	0.11	109,109,109,109	0
56	MG	A	1691	1/1	0.79	0.08	145,145,145,145	0
56	MG	GB	9311	1/1	0.79	0.11	132,132,132,132	0
56	MG	GB	9076	1/1	0.79	0.18	104,104,104,104	0
56	MG	B	9060	1/1	0.79	0.33	91,91,91,91	0
56	MG	GB	9178	1/1	0.79	0.16	115,115,115,115	0
56	MG	B	9255	1/1	0.79	0.16	100,100,100,100	0
56	MG	GB	9081	1/1	0.79	0.22	97,97,97,97	0
56	MG	FB	1679	1/1	0.79	0.08	244,244,244,244	0
56	MG	B	9380	1/1	0.79	0.18	100,100,100,100	0
56	MG	B	9142	1/1	0.79	0.18	116,116,116,116	0
56	MG	B	9068	1/1	0.79	0.29	93,93,93,93	0
56	MG	B	9291	1/1	0.79	0.14	77,77,77,77	0
56	MG	GB	9131	1/1	0.79	0.21	90,90,90,90	0
56	MG	SC	301	1/1	0.79	0.25	102,102,102,102	0
56	MG	B	9194	1/1	0.79	0.09	151,151,151,151	0
56	MG	B	9393	1/1	0.79	0.10	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	R	201	1/1	0.79	0.11	119,119,119,119	0
56	MG	B	9334	1/1	0.79	0.23	91,91,91,91	0
56	MG	B	9032	1/1	0.79	0.28	73,73,73,73	0
56	MG	FB	1733	1/1	0.79	0.08	92,92,92,92	0
56	MG	GB	9098	1/1	0.79	0.11	122,122,122,122	0
56	MG	B	9200	1/1	0.79	0.14	109,109,109,109	0
56	MG	AA	101	1/1	0.79	0.20	106,106,106,106	0
56	MG	GB	9364	1/1	0.79	0.14	122,122,122,122	0
56	MG	ED	101	1/1	0.79	0.10	120,120,120,120	0
56	MG	B	9402	1/1	0.79	0.21	104,104,104,104	0
56	MG	GB	9122	1/1	0.80	0.16	88,88,88,88	0
56	MG	B	9075	1/1	0.80	0.31	106,106,106,106	0
56	MG	B	9021	1/1	0.80	0.45	79,79,79,79	0
56	MG	FB	1793	1/1	0.80	0.07	138,138,138,138	0
56	MG	B	9345	1/1	0.80	0.10	85,85,85,85	0
56	MG	FB	1652	1/1	0.80	0.14	111,111,111,111	0
56	MG	B	9431	1/1	0.80	0.11	89,89,89,89	0
56	MG	GB	9253	1/1	0.80	0.23	104,104,104,104	0
56	MG	FB	1621	1/1	0.80	0.32	97,97,97,97	0
56	MG	B	9276	1/1	0.80	0.28	105,105,105,105	0
56	MG	GB	9173	1/1	0.80	0.10	108,108,108,108	0
56	MG	B	9104	1/1	0.80	0.14	78,78,78,78	0
56	MG	FB	1683	1/1	0.80	0.19	104,104,104,104	0
56	MG	A	1601	1/1	0.80	0.31	75,75,75,75	0
56	MG	GB	9268	1/1	0.80	0.17	109,109,109,109	0
56	MG	GB	9080	1/1	0.80	0.29	84,84,84,84	0
56	MG	GB	9314	1/1	0.80	0.33	98,98,98,98	0
56	MG	GB	9316	1/1	0.80	0.12	157,157,157,157	0
56	MG	FB	1611	1/1	0.80	0.26	112,112,112,112	0
56	MG	FB	1664	1/1	0.80	0.16	98,98,98,98	0
56	MG	GB	9047	1/1	0.80	0.49	99,99,99,99	0
56	MG	SC	303	1/1	0.80	0.08	114,114,114,114	0
56	MG	GB	9322	1/1	0.80	0.13	112,112,112,112	0
56	MG	A	1616	1/1	0.80	0.24	101,101,101,101	0
56	MG	B	9188	1/1	0.80	0.20	95,95,95,95	0
56	MG	TC	203	1/1	0.80	0.09	134,134,134,134	0
56	MG	FB	1668	1/1	0.80	0.29	105,105,105,105	0
56	MG	GB	9397	1/1	0.80	0.16	104,104,104,104	0
56	MG	C	220	1/1	0.80	0.14	161,161,161,161	0
56	MG	B	9099	1/1	0.80	0.28	83,83,83,83	0
56	MG	FB	1787	1/1	0.80	0.08	127,127,127,127	0
56	MG	AD	201	1/1	0.80	0.20	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9025	1/1	0.80	0.33	88,88,88,88	0
56	MG	GB	9289	1/1	0.80	0.12	95,95,95,95	0
56	MG	B	9056	1/1	0.80	0.40	94,94,94,94	0
56	MG	B	9362	1/1	0.81	0.12	97,97,97,97	0
56	MG	IC	102	1/1	0.81	0.21	131,131,131,131	0
56	MG	A	1750	1/1	0.81	0.15	157,157,157,157	0
56	MG	B	9328	1/1	0.81	0.09	105,105,105,105	0
56	MG	B	9149	1/1	0.81	0.19	104,104,104,104	0
56	MG	B	9079	1/1	0.81	0.09	73,73,73,73	0
56	MG	B	9215	1/1	0.81	0.14	92,92,92,92	0
56	MG	B	9155	1/1	0.81	0.10	97,97,97,97	0
56	MG	GB	9096	1/1	0.81	0.24	114,114,114,114	0
56	MG	B	9342	1/1	0.81	0.24	104,104,104,104	0
56	MG	A	1697	1/1	0.81	0.14	135,135,135,135	0
56	MG	FB	1649	1/1	0.81	0.31	119,119,119,119	0
56	MG	FB	1704	1/1	0.81	0.24	129,129,129,129	0
56	MG	A	1766	1/1	0.81	0.21	133,133,133,133	0
56	MG	B	9005	1/1	0.81	0.34	79,79,79,79	0
56	MG	B	9433	1/1	0.81	0.13	99,99,99,99	0
56	MG	B	9434	1/1	0.81	0.12	133,133,133,133	0
56	MG	FB	1785	1/1	0.81	0.19	123,123,123,123	0
56	MG	FB	1709	1/1	0.81	0.12	116,116,116,116	0
56	MG	B	9161	1/1	0.81	0.21	94,94,94,94	0
56	MG	A	1667	1/1	0.81	0.39	112,112,112,112	0
56	MG	B	9350	1/1	0.81	0.16	115,115,115,115	0
56	MG	GB	9330	1/1	0.81	0.13	95,95,95,95	0
56	MG	UC	201	1/1	0.81	0.13	130,130,130,130	0
56	MG	GB	9143	1/1	0.81	0.15	94,94,94,94	0
56	MG	FB	1792	1/1	0.81	0.11	134,134,134,134	0
56	MG	FB	1754	1/1	0.81	0.14	155,155,155,155	0
56	MG	B	9296	1/1	0.81	0.13	84,84,84,84	0
56	MG	GB	9194	1/1	0.81	0.07	119,119,119,119	0
56	MG	A	1757	1/1	0.81	0.09	169,169,169,169	0
56	MG	F	301	1/1	0.81	0.10	114,114,114,114	0
56	MG	FB	1760	1/1	0.81	0.08	112,112,112,112	0
56	MG	GB	9300	1/1	0.81	0.23	107,107,107,107	0
56	MG	B	9145	1/1	0.82	0.17	78,78,78,78	0
56	MG	B	9030	1/1	0.82	0.41	87,87,87,87	0
56	MG	FB	1657	1/1	0.82	0.17	166,166,166,166	0
56	MG	B	9266	1/1	0.82	0.12	82,82,82,82	0
56	MG	GB	9363	1/1	0.82	0.29	97,97,97,97	0
56	MG	FB	1722	1/1	0.82	0.16	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B	9355	1/1	0.82	0.07	158,158,158,158	0
56	MG	FB	1761	1/1	0.82	0.18	125,125,125,125	0
56	MG	FB	1687	1/1	0.82	0.15	116,116,116,116	0
56	MG	FB	1763	1/1	0.82	0.08	108,108,108,108	0
56	MG	EA	101	1/1	0.82	0.15	85,85,85,85	0
56	MG	FB	1661	1/1	0.82	0.14	90,90,90,90	0
56	MG	B	9356	1/1	0.82	0.11	96,96,96,96	0
56	MG	GB	9216	1/1	0.82	0.28	90,90,90,90	0
56	MG	B	9117	1/1	0.82	0.28	79,79,79,79	0
56	MG	B	9367	1/1	0.82	0.13	102,102,102,102	0
56	MG	B	9009	1/1	0.82	0.30	82,82,82,82	0
56	MG	JB	305	1/1	0.82	0.15	112,112,112,112	0
56	MG	LB	301	1/1	0.82	0.06	118,118,118,118	0
56	MG	GB	9100	1/1	0.82	0.28	112,112,112,112	0
56	MG	F	302	1/1	0.82	0.08	119,119,119,119	0
56	MG	IA	106	1/1	0.82	0.10	135,135,135,135	0
56	MG	B	9270	1/1	0.82	0.14	93,93,93,93	0
56	MG	B	9134	1/1	0.82	0.24	80,80,80,80	0
56	MG	GB	9286	1/1	0.82	0.28	105,105,105,105	0
56	MG	QB	201	1/1	0.82	0.27	104,104,104,104	0
56	MG	B	9120	1/1	0.82	0.33	91,91,91,91	0
56	MG	B	9095	1/1	0.82	0.17	99,99,99,99	0
56	MG	B	9059	1/1	0.82	0.24	95,95,95,95	0
56	MG	GB	9071	1/1	0.82	0.29	105,105,105,105	0
56	MG	A	1679	1/1	0.82	0.11	125,125,125,125	0
56	MG	B	9086	1/1	0.82	0.30	93,93,93,93	0
56	MG	B	9127	1/1	0.82	0.34	104,104,104,104	0
56	MG	FB	1628	1/1	0.82	0.23	98,98,98,98	0
56	MG	A	1610	1/1	0.82	0.15	152,152,152,152	0
56	MG	VB	201	1/1	0.83	0.14	105,105,105,105	0
56	MG	B	9069	1/1	0.83	0.20	111,111,111,111	0
56	MG	B	9083	1/1	0.83	0.28	100,100,100,100	0
56	MG	FB	1713	1/1	0.83	0.11	163,163,163,163	0
56	MG	FB	1784	1/1	0.83	0.12	137,137,137,137	0
56	MG	A	1632	1/1	0.83	0.40	89,89,89,89	0
56	MG	B	9400	1/1	0.83	0.08	136,136,136,136	0
56	MG	C	222	1/1	0.83	0.13	164,164,164,164	0
56	MG	B	9343	1/1	0.83	0.23	110,110,110,110	0
56	MG	GB	9074	1/1	0.83	0.26	101,101,101,101	0
56	MG	GB	9032	1/1	0.83	0.33	86,86,86,86	0
56	MG	B	9114	1/1	0.83	0.18	88,88,88,88	0
56	MG	B	9159	1/1	0.83	0.10	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1669	1/1	0.83	0.23	105,105,105,105	0
56	MG	GB	9036	1/1	0.83	0.23	85,85,85,85	0
56	MG	GB	9367	1/1	0.83	0.12	118,118,118,118	0
56	MG	FB	1626	1/1	0.83	0.41	103,103,103,103	0
56	MG	NC	110	1/1	0.83	0.29	100,100,100,100	0
56	MG	GB	9249	1/1	0.83	0.07	107,107,107,107	0
56	MG	B	9406	1/1	0.83	0.11	130,130,130,130	0
56	MG	B	9411	1/1	0.83	0.08	139,139,139,139	0
56	MG	B	9320	1/1	0.83	0.17	86,86,86,86	0
56	MG	B	9211	1/1	0.83	0.09	169,169,169,169	0
56	MG	FB	1701	1/1	0.83	0.24	114,114,114,114	0
56	MG	GB	9012	1/1	0.83	0.45	77,77,77,77	0
56	MG	GB	9261	1/1	0.83	0.23	104,104,104,104	0
56	MG	GB	9164	1/1	0.83	0.28	85,85,85,85	0
56	MG	B	9240	1/1	0.83	0.06	88,88,88,88	0
56	MG	GB	9267	1/1	0.83	0.09	118,118,118,118	0
56	MG	B	9304	1/1	0.83	0.08	86,86,86,86	0
56	MG	B	9018	1/1	0.83	0.24	82,82,82,82	0
56	MG	FB	1654	1/1	0.83	0.17	111,111,111,111	0
56	MG	GB	9170	1/1	0.83	0.15	101,101,101,101	0
56	MG	B	9049	1/1	0.83	0.26	69,69,69,69	0
56	MG	GB	9274	1/1	0.83	0.31	103,103,103,103	0
56	MG	B	9389	1/1	0.83	0.17	112,112,112,112	0
56	MG	AD	202	1/1	0.83	0.23	103,103,103,103	0
56	MG	B	9151	1/1	0.83	0.16	95,95,95,95	0
56	MG	GB	9327	1/1	0.83	0.10	171,171,171,171	0
56	MG	FB	1741	1/1	0.83	0.22	106,106,106,106	0
56	MG	B	9331	1/1	0.84	0.07	118,118,118,118	0
56	MG	A	1735	1/1	0.84	0.12	106,106,106,106	0
56	MG	B	9264	1/1	0.84	0.07	98,98,98,98	0
56	MG	FB	1715	1/1	0.84	0.19	121,121,121,121	0
56	MG	B	9143	1/1	0.84	0.22	102,102,102,102	0
56	MG	GB	9160	1/1	0.84	0.15	97,97,97,97	0
56	MG	GB	9162	1/1	0.84	0.10	97,97,97,97	0
56	MG	FB	1718	1/1	0.84	0.12	133,133,133,133	0
56	MG	A	1673	1/1	0.84	0.14	121,121,121,121	0
56	MG	B	9165	1/1	0.84	0.09	104,104,104,104	0
56	MG	FB	1655	1/1	0.84	0.24	103,103,103,103	0
56	MG	B	9387	1/1	0.84	0.14	124,124,124,124	0
56	MG	B	9167	1/1	0.84	0.21	95,95,95,95	0
56	MG	GB	9094	1/1	0.84	0.39	89,89,89,89	0
56	MG	B	9391	1/1	0.84	0.14	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9332	1/1	0.84	0.08	102,102,102,102	0
56	MG	GB	9334	1/1	0.84	0.32	89,89,89,89	0
56	MG	GB	9285	1/1	0.84	0.20	108,108,108,108	0
56	MG	B	9006	1/1	0.84	0.29	61,61,61,61	0
56	MG	B	9197	1/1	0.84	0.22	73,73,73,73	0
56	MG	B	9071	1/1	0.84	0.21	85,85,85,85	0
56	MG	B	9148	1/1	0.84	0.25	99,99,99,99	0
56	MG	A	1743	1/1	0.84	0.17	121,121,121,121	0
56	MG	GB	9237	1/1	0.84	0.14	117,117,117,117	0
56	MG	GB	9134	1/1	0.84	0.15	111,111,111,111	0
56	MG	GB	9358	1/1	0.84	0.09	94,94,94,94	0
56	MG	B	9315	1/1	0.84	0.25	91,91,91,91	0
56	MG	GB	9361	1/1	0.84	0.14	86,86,86,86	0
56	MG	A	1765	1/1	0.84	0.08	134,134,134,134	0
56	MG	GB	9065	1/1	0.84	0.36	81,81,81,81	0
56	MG	B	9283	1/1	0.84	0.21	105,105,105,105	0
56	MG	K	202	1/1	0.84	0.10	105,105,105,105	0
56	MG	GB	9369	1/1	0.84	0.19	95,95,95,95	0
56	MG	B	9074	1/1	0.84	0.13	109,109,109,109	0
56	MG	GB	9141	1/1	0.84	0.21	101,101,101,101	0
56	MG	L	203	1/1	0.84	0.09	89,89,89,89	0
56	MG	A	1655	1/1	0.84	0.15	232,232,232,232	0
56	MG	GB	9252	1/1	0.84	0.19	94,94,94,94	0
56	MG	A	1746	1/1	0.84	0.14	116,116,116,116	0
56	MG	B	9259	1/1	0.84	0.13	100,100,100,100	0
56	MG	B	9290	1/1	0.84	0.27	107,107,107,107	0
56	MG	PA	203	1/1	0.84	0.09	127,127,127,127	0
56	MG	A	1647	1/1	0.84	0.24	127,127,127,127	0
56	MG	GB	9387	1/1	0.84	0.14	131,131,131,131	0
56	MG	B	9271	1/1	0.85	0.09	76,76,76,76	0
56	MG	B	9323	1/1	0.85	0.09	68,68,68,68	0
56	MG	UB	203	1/1	0.85	0.08	130,130,130,130	0
56	MG	B	9012	1/1	0.85	0.33	70,70,70,70	0
56	MG	GB	9283	1/1	0.85	0.31	99,99,99,99	0
56	MG	GB	9232	1/1	0.85	0.18	106,106,106,106	0
56	MG	AC	202	1/1	0.85	0.22	124,124,124,124	0
56	MG	GB	9006	1/1	0.85	0.51	87,87,87,87	0
56	MG	GB	9402	1/1	0.85	0.12	122,122,122,122	0
56	MG	B	9103	1/1	0.85	0.13	87,87,87,87	0
56	MG	GB	9144	1/1	0.85	0.16	80,80,80,80	0
56	MG	K	203	1/1	0.85	0.07	130,130,130,130	0
56	MG	B	9077	1/1	0.85	0.13	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9148	1/1	0.85	0.19	86,86,86,86	0
56	MG	B	9195	1/1	0.85	0.09	85,85,85,85	0
56	MG	A	1637	1/1	0.85	0.20	102,102,102,102	0
56	MG	GB	9245	1/1	0.85	0.09	107,107,107,107	0
56	MG	GB	9045	1/1	0.85	0.12	89,89,89,89	0
56	MG	GB	9357	1/1	0.85	0.07	125,125,125,125	0
56	MG	Q	201	1/1	0.85	0.14	121,121,121,121	0
56	MG	GB	9196	1/1	0.85	0.09	82,82,82,82	0
56	MG	B	9118	1/1	0.85	0.23	117,117,117,117	0
56	MG	GB	9199	1/1	0.85	0.16	98,98,98,98	0
56	MG	FB	1773	1/1	0.85	0.14	106,106,106,106	0
56	MG	GB	9366	1/1	0.85	0.11	92,92,92,92	0
56	MG	B	9309	1/1	0.85	0.09	159,159,159,159	0
56	MG	QC	303	1/1	0.85	0.19	155,155,155,155	0
56	MG	RC	301	1/1	0.85	0.11	151,151,151,151	0
56	MG	B	9372	1/1	0.85	0.09	102,102,102,102	0
56	MG	FB	1631	1/1	0.85	0.21	104,104,104,104	0
56	MG	FB	1681	1/1	0.85	0.13	126,126,126,126	0
56	MG	FB	1608	1/1	0.85	0.28	86,86,86,86	0
56	MG	B	9337	1/1	0.85	0.08	96,96,96,96	0
56	MG	GB	9165	1/1	0.85	0.22	83,83,83,83	0
56	MG	KB	302	1/1	0.85	0.14	99,99,99,99	0
56	MG	GB	9059	1/1	0.85	0.31	91,91,91,91	0
56	MG	B	9162	1/1	0.85	0.10	85,85,85,85	0
56	MG	GB	9318	1/1	0.85	0.07	112,112,112,112	0
56	MG	GB	9382	1/1	0.85	0.30	107,107,107,107	0
56	MG	B	9087	1/1	0.85	0.13	80,80,80,80	0
56	MG	HA	101	1/1	0.85	0.17	129,129,129,129	0
56	MG	B	9184	1/1	0.85	0.24	77,77,77,77	0
56	MG	FB	1717	1/1	0.85	0.08	129,129,129,129	0
56	MG	B	9004	1/1	0.85	0.36	70,70,70,70	0
56	MG	B	9152	1/1	0.85	0.14	89,89,89,89	0
56	MG	A	1627	1/1	0.85	0.21	101,101,101,101	0
56	MG	B	9208	1/1	0.85	0.09	104,104,104,104	0
56	MG	B	9244	1/1	0.86	0.23	101,101,101,101	0
56	MG	FB	1602	1/1	0.86	0.40	87,87,87,87	0
56	MG	GB	9029	1/1	0.86	0.21	71,71,71,71	0
56	MG	VB	203	1/1	0.86	0.15	112,112,112,112	0
56	MG	B	9364	1/1	0.86	0.12	95,95,95,95	0
56	MG	FB	1748	1/1	0.86	0.09	119,119,119,119	0
56	MG	GB	9242	1/1	0.86	0.10	122,122,122,122	0
56	MG	FB	1712	1/1	0.86	0.07	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9346	1/1	0.86	0.08	118,118,118,118	0
56	MG	GB	9348	1/1	0.86	0.07	112,112,112,112	0
56	MG	GB	9192	1/1	0.86	0.18	123,123,123,123	0
56	MG	A	1695	1/1	0.86	0.27	101,101,101,101	0
56	MG	A	1772	1/1	0.86	0.10	91,91,91,91	0
56	MG	B	9370	1/1	0.86	0.08	108,108,108,108	0
56	MG	B	9326	1/1	0.86	0.08	79,79,79,79	0
56	MG	S	201	1/1	0.86	0.07	111,111,111,111	0
56	MG	GB	9359	1/1	0.86	0.12	123,123,123,123	0
56	MG	T	202	1/1	0.86	0.10	105,105,105,105	0
56	MG	B	9294	1/1	0.86	0.17	82,82,82,82	0
56	MG	A	1709	1/1	0.86	0.15	107,107,107,107	0
56	MG	B	9329	1/1	0.86	0.12	91,91,91,91	0
56	MG	E	303	1/1	0.86	0.16	76,76,76,76	0
56	MG	GB	9087	1/1	0.86	0.20	81,81,81,81	0
56	MG	GB	9258	1/1	0.86	0.19	104,104,104,104	0
56	MG	B	9016	1/1	0.86	0.28	79,79,79,79	0
56	MG	GB	9046	1/1	0.86	0.24	91,91,91,91	0
56	MG	GB	9312	1/1	0.86	0.24	93,93,93,93	0
56	MG	JB	302	1/1	0.86	0.09	117,117,117,117	0
56	MG	FB	1694	1/1	0.86	0.08	143,143,143,143	0
56	MG	GB	9048	1/1	0.86	0.26	92,92,92,92	0
56	MG	GB	9265	1/1	0.86	0.17	106,106,106,106	0
56	MG	GB	9049	1/1	0.86	0.15	79,79,79,79	0
56	MG	B	9132	1/1	0.86	0.13	93,93,93,93	0
56	MG	B	9381	1/1	0.86	0.20	84,84,84,84	0
56	MG	B	9094	1/1	0.86	0.21	93,93,93,93	0
56	MG	F	304	1/1	0.86	0.06	119,119,119,119	0
56	MG	FB	1700	1/1	0.86	0.15	120,120,120,120	0
56	MG	A	1731	1/1	0.86	0.09	130,130,130,130	0
56	MG	B	9336	1/1	0.86	0.06	94,94,94,94	0
56	MG	B	9029	1/1	0.86	0.32	81,81,81,81	0
56	MG	YA	103	1/1	0.86	0.12	125,125,125,125	0
56	MG	B	9426	1/1	0.86	0.09	99,99,99,99	0
56	MG	B	9388	1/1	0.86	0.13	100,100,100,100	0
56	MG	TB	201	1/1	0.86	0.29	101,101,101,101	0
56	MG	GB	9394	1/1	0.86	0.09	88,88,88,88	0
56	MG	B	9359	1/1	0.86	0.13	78,78,78,78	0
56	MG	B	9317	1/1	0.87	0.04	137,137,137,137	0
56	MG	B	9295	1/1	0.87	0.06	108,108,108,108	0
56	MG	A	1646	1/1	0.87	0.17	120,120,120,120	0
56	MG	L	202	1/1	0.87	0.06	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9187	1/1	0.87	0.37	92,92,92,92	0
56	MG	B	9273	1/1	0.87	0.13	130,130,130,130	0
56	MG	A	1774	1/1	0.87	0.04	176,176,176,176	0
56	MG	FB	1749	1/1	0.87	0.16	110,110,110,110	0
56	MG	GB	9239	1/1	0.87	0.15	96,96,96,96	0
56	MG	B	9141	1/1	0.87	0.20	130,130,130,130	0
56	MG	B	9011	1/1	0.87	0.37	61,61,61,61	0
56	MG	B	9093	1/1	0.87	0.15	95,95,95,95	0
56	MG	B	9082	1/1	0.87	0.24	98,98,98,98	0
56	MG	FB	1610	1/1	0.87	0.38	87,87,87,87	0
56	MG	KB	301	1/1	0.87	0.46	90,90,90,90	0
56	MG	GB	9062	1/1	0.87	0.12	110,110,110,110	0
56	MG	GB	9163	1/1	0.87	0.10	94,94,94,94	0
56	MG	U	101	1/1	0.87	0.07	91,91,91,91	0
56	MG	B	9404	1/1	0.87	0.08	157,157,157,157	0
56	MG	B	9017	1/1	0.87	0.25	78,78,78,78	0
56	MG	GB	9393	1/1	0.87	0.08	84,84,84,84	0
56	MG	B	9407	1/1	0.87	0.12	114,114,114,114	0
56	MG	B	9028	1/1	0.87	0.37	90,90,90,90	0
56	MG	C	206	1/1	0.87	0.14	149,149,149,149	0
56	MG	GB	9211	1/1	0.87	0.17	123,123,123,123	0
56	MG	B	9413	1/1	0.87	0.10	100,100,100,100	0
56	MG	GB	9352	1/1	0.87	0.11	85,85,85,85	0
56	MG	HA	103	1/1	0.87	0.23	111,111,111,111	0
56	MG	B	9414	1/1	0.87	0.14	77,77,77,77	0
56	MG	B	9249	1/1	0.87	0.10	123,123,123,123	0
56	MG	B	9268	1/1	0.87	0.19	94,94,94,94	0
56	MG	A	1775	1/1	0.87	0.05	208,208,208,208	0
56	MG	GB	9079	1/1	0.87	0.22	86,86,86,86	0
56	MG	GB	9222	1/1	0.87	0.28	93,93,93,93	0
56	MG	B	9113	1/1	0.87	0.15	98,98,98,98	0
56	MG	XB	201	1/1	0.87	0.12	117,117,117,117	0
56	MG	GB	9179	1/1	0.87	0.20	87,87,87,87	0
56	MG	A	1779	1/1	0.87	0.08	152,152,152,152	0
56	MG	C	216	1/1	0.87	0.09	167,167,167,167	0
56	MG	VB	202	1/1	0.88	0.13	97,97,97,97	0
56	MG	B	9397	1/1	0.88	0.12	96,96,96,96	0
56	MG	B	9179	1/1	0.88	0.09	158,158,158,158	0
56	MG	GB	9002	1/1	0.88	0.57	75,75,75,75	0
56	MG	B	9106	1/1	0.88	0.15	72,72,72,72	0
56	MG	A	1678	1/1	0.88	0.12	97,97,97,97	0
56	MG	B	9281	1/1	0.88	0.23	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	C	210	1/1	0.88	0.12	125,125,125,125	0
56	MG	B	9110	1/1	0.88	0.30	71,71,71,71	0
56	MG	A	1716	1/1	0.88	0.20	112,112,112,112	0
56	MG	GB	9362	1/1	0.88	0.11	147,147,147,147	0
56	MG	GB	9214	1/1	0.88	0.06	99,99,99,99	0
56	MG	B	9154	1/1	0.88	0.37	76,76,76,76	0
56	MG	A	1733	1/1	0.88	0.07	143,143,143,143	0
56	MG	B	9091	1/1	0.88	0.23	78,78,78,78	0
56	MG	NC	104	1/1	0.88	0.13	134,134,134,134	0
56	MG	GB	9264	1/1	0.88	0.09	126,126,126,126	0
56	MG	OA	202	1/1	0.88	0.09	131,131,131,131	0
56	MG	OA	203	1/1	0.88	0.12	123,123,123,123	0
56	MG	B	9369	1/1	0.88	0.16	90,90,90,90	0
56	MG	A	1744	1/1	0.88	0.17	123,123,123,123	0
56	MG	A	1611	1/1	0.88	0.26	84,84,84,84	0
56	MG	A	1662	1/1	0.88	0.11	105,105,105,105	0
56	MG	B	9225	1/1	0.88	0.12	147,147,147,147	0
56	MG	JB	304	1/1	0.88	0.18	101,101,101,101	0
56	MG	B	9228	1/1	0.88	0.14	76,76,76,76	0
56	MG	A	1767	1/1	0.88	0.15	93,93,93,93	0
56	MG	B	9297	1/1	0.88	0.13	100,100,100,100	0
56	MG	B	9263	1/1	0.88	0.13	77,77,77,77	0
56	MG	B	9026	1/1	0.88	0.26	92,92,92,92	0
56	MG	A	1705	1/1	0.88	0.19	105,105,105,105	0
56	MG	GB	9282	1/1	0.88	0.11	107,107,107,107	0
56	MG	FB	1698	1/1	0.88	0.08	120,120,120,120	0
56	MG	GB	9189	1/1	0.88	0.11	154,154,154,154	0
56	MG	B	9198	1/1	0.88	0.15	92,92,92,92	0
56	MG	B	9046	1/1	0.88	0.26	70,70,70,70	0
56	MG	B	9081	1/1	0.88	0.13	98,98,98,98	0
56	MG	A	1626	1/1	0.88	0.24	98,98,98,98	0
56	MG	FB	1740	1/1	0.88	0.08	156,156,156,156	0
56	MG	GB	9341	1/1	0.88	0.21	96,96,96,96	0
56	MG	A	1771	1/1	0.88	0.18	99,99,99,99	0
56	MG	GB	9345	1/1	0.88	0.28	106,106,106,106	0
56	MG	B	9031	1/1	0.88	0.34	78,78,78,78	0
56	MG	B	9176	1/1	0.88	0.21	90,90,90,90	0
56	MG	DD	101	1/1	0.88	0.14	144,144,144,144	0
56	MG	GB	9403	1/1	0.88	0.10	89,89,89,89	0
56	MG	A	1659	1/1	0.88	0.16	124,124,124,124	0
56	MG	T	201	1/1	0.89	0.08	101,101,101,101	0
56	MG	E	302	1/1	0.89	0.16	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9069	1/1	0.89	0.30	82,82,82,82	0
56	MG	GB	9171	1/1	0.89	0.24	88,88,88,88	0
56	MG	GB	9209	1/1	0.89	0.14	89,89,89,89	0
56	MG	FB	1764	1/1	0.89	0.24	136,136,136,136	0
56	MG	GB	9333	1/1	0.89	0.14	82,82,82,82	0
56	MG	B	9363	1/1	0.89	0.16	103,103,103,103	0
56	MG	A	1608	1/1	0.89	0.22	96,96,96,96	0
56	MG	B	9341	1/1	0.89	0.08	121,121,121,121	0
56	MG	GB	9338	1/1	0.89	0.05	136,136,136,136	0
56	MG	GB	9255	1/1	0.89	0.09	107,107,107,107	0
56	MG	B	9209	1/1	0.89	0.18	90,90,90,90	0
56	MG	B	9322	1/1	0.89	0.06	85,85,85,85	0
56	MG	CA	102	1/1	0.89	0.05	116,116,116,116	0
56	MG	B	9424	1/1	0.89	0.10	112,112,112,112	0
56	MG	B	9287	1/1	0.89	0.15	82,82,82,82	0
56	MG	GB	9016	1/1	0.89	0.28	98,98,98,98	0
56	MG	B	9166	1/1	0.89	0.14	82,82,82,82	0
56	MG	B	9178	1/1	0.89	0.07	125,125,125,125	0
56	MG	GB	9353	1/1	0.89	0.28	100,100,100,100	0
56	MG	B	9189	1/1	0.89	0.29	102,102,102,102	0
56	MG	A	1684	1/1	0.89	0.08	111,111,111,111	0
56	MG	B	9107	1/1	0.89	0.17	91,91,91,91	0
56	MG	B	9313	1/1	0.89	0.10	91,91,91,91	0
56	MG	GB	9023	1/1	0.89	0.37	79,79,79,79	0
56	MG	FB	1750	1/1	0.89	0.16	105,105,105,105	0
56	MG	GB	9156	1/1	0.89	0.23	86,86,86,86	0
56	MG	GB	9317	1/1	0.89	0.11	116,116,116,116	0
56	MG	B	9218	1/1	0.89	0.10	78,78,78,78	0
56	MG	FB	1721	1/1	0.89	0.10	118,118,118,118	0
56	MG	A	1736	1/1	0.89	0.07	169,169,169,169	0
56	MG	A	1723	1/1	0.89	0.13	170,170,170,170	0
56	MG	M	203	1/1	0.89	0.21	82,82,82,82	0
56	MG	ZB	102	1/1	0.89	0.05	100,100,100,100	0
56	MG	AD	203	1/1	0.89	0.09	99,99,99,99	0
56	MG	AD	204	1/1	0.89	0.07	96,96,96,96	0
56	MG	B	9408	1/1	0.89	0.22	85,85,85,85	0
56	MG	B	9384	1/1	0.89	0.09	98,98,98,98	0
56	MG	B	9251	1/1	0.89	0.20	106,106,106,106	0
56	MG	B	9164	1/1	0.89	0.24	90,90,90,90	0
56	MG	GB	9356	1/1	0.90	0.17	90,90,90,90	0
56	MG	B	9357	1/1	0.90	0.11	94,94,94,94	0
56	MG	GB	9085	1/1	0.90	0.16	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9226	1/1	0.90	0.09	91,91,91,91	0
56	MG	B	9358	1/1	0.90	0.10	121,121,121,121	0
56	MG	GB	9315	1/1	0.90	0.05	151,151,151,151	0
56	MG	B	9298	1/1	0.90	0.13	92,92,92,92	0
56	MG	B	9318	1/1	0.90	0.12	137,137,137,137	0
56	MG	A	1708	1/1	0.90	0.06	134,134,134,134	0
56	MG	A	1619	1/1	0.90	0.27	82,82,82,82	0
56	MG	GB	9273	1/1	0.90	0.09	96,96,96,96	0
56	MG	A	1773	1/1	0.90	0.12	116,116,116,116	0
56	MG	HB	218	1/1	0.90	0.14	129,129,129,129	0
56	MG	B	9286	1/1	0.90	0.08	84,84,84,84	0
56	MG	B	9257	1/1	0.90	0.20	92,92,92,92	0
56	MG	GB	9124	1/1	0.90	0.14	104,104,104,104	0
56	MG	B	9395	1/1	0.90	0.25	76,76,76,76	0
56	MG	FB	1734	1/1	0.90	0.14	109,109,109,109	0
56	MG	B	9191	1/1	0.90	0.19	90,90,90,90	0
56	MG	V	503	1/1	0.90	0.06	93,93,93,93	0
56	MG	Y	101	1/1	0.90	0.17	97,97,97,97	0
56	MG	GB	9099	1/1	0.90	0.13	93,93,93,93	0
56	MG	GB	9202	1/1	0.90	0.09	86,86,86,86	0
56	MG	B	9053	1/1	0.90	0.15	84,84,84,84	0
56	MG	Y	103	1/1	0.90	0.11	101,101,101,101	0
56	MG	B	9398	1/1	0.90	0.06	96,96,96,96	0
56	MG	GB	9042	1/1	0.90	0.24	78,78,78,78	0
56	MG	GB	9336	1/1	0.90	0.17	121,121,121,121	0
56	MG	B	9223	1/1	0.90	0.15	74,74,74,74	0
56	MG	B	9185	1/1	0.90	0.12	61,61,61,61	0
56	MG	GB	9251	1/1	0.90	0.27	87,87,87,87	0
56	MG	QB	202	1/1	0.90	0.10	100,100,100,100	0
56	MG	B	9292	1/1	0.90	0.08	98,98,98,98	0
56	MG	GB	9342	1/1	0.90	0.08	111,111,111,111	0
56	MG	B	9236	1/1	0.90	0.12	77,77,77,77	0
56	MG	HA	102	1/1	0.90	0.36	133,133,133,133	0
56	MG	B	9108	1/1	0.90	0.16	84,84,84,84	0
56	MG	GB	9347	1/1	0.90	0.07	126,126,126,126	0
56	MG	B	9252	1/1	0.90	0.13	98,98,98,98	0
56	MG	GB	9142	1/1	0.90	0.18	96,96,96,96	0
56	MG	GB	9217	1/1	0.90	0.07	141,141,141,141	0
56	MG	GB	9351	1/1	0.90	0.15	113,113,113,113	0
56	MG	B	9187	1/1	0.90	0.25	101,101,101,101	0
56	MG	GB	9082	1/1	0.90	0.27	105,105,105,105	0
56	MG	GB	9145	1/1	0.90	0.14	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	L	201	1/1	0.90	0.10	114,114,114,114	0
56	MG	O	201	1/1	0.91	0.26	83,83,83,83	0
56	MG	B	9293	1/1	0.91	0.21	94,94,94,94	0
56	MG	GB	9070	1/1	0.91	0.27	81,81,81,81	0
56	MG	B	9090	1/1	0.91	0.17	77,77,77,77	0
56	MG	A	1625	1/1	0.91	0.11	94,94,94,94	0
56	MG	GB	9073	1/1	0.91	0.17	77,77,77,77	0
56	MG	B	9250	1/1	0.91	0.21	99,99,99,99	0
56	MG	A	1661	1/1	0.91	0.10	103,103,103,103	0
56	MG	GB	9050	1/1	0.91	0.22	76,76,76,76	0
56	MG	B	9022	1/1	0.91	0.24	78,78,78,78	0
56	MG	FB	1747	1/1	0.91	0.07	116,116,116,116	0
56	MG	B	9196	1/1	0.91	0.09	93,93,93,93	0
56	MG	B	9008	1/1	0.91	0.27	61,61,61,61	0
56	MG	GB	9281	1/1	0.91	0.14	97,97,97,97	0
56	MG	GB	9159	1/1	0.91	0.26	94,94,94,94	0
56	MG	PA	202	1/1	0.91	0.08	125,125,125,125	0
56	MG	B	9153	1/1	0.91	0.20	66,66,66,66	0
56	MG	B	9126	1/1	0.91	0.33	116,116,116,116	0
56	MG	A	1670	1/1	0.91	0.07	91,91,91,91	0
56	MG	FB	1779	1/1	0.91	0.09	115,115,115,115	0
56	MG	B	9063	1/1	0.91	0.19	90,90,90,90	0
56	MG	FB	1755	1/1	0.91	0.17	104,104,104,104	0
56	MG	JB	301	1/1	0.91	0.15	75,75,75,75	0
56	MG	GB	9291	1/1	0.91	0.09	124,124,124,124	0
56	MG	B	9217	1/1	0.91	0.12	98,98,98,98	0
56	MG	B	9274	1/1	0.91	0.05	84,84,84,84	0
56	MG	GB	9064	1/1	0.91	0.20	80,80,80,80	0
56	MG	JC	101	1/1	0.91	0.14	87,87,87,87	0
56	MG	GB	9399	1/1	0.91	0.19	129,129,129,129	0
56	MG	B	9405	1/1	0.91	0.11	103,103,103,103	0
56	MG	GB	9233	1/1	0.91	0.14	83,83,83,83	0
56	MG	B	9168	1/1	0.91	0.15	91,91,91,91	0
56	MG	FA	101	1/1	0.91	0.15	98,98,98,98	0
56	MG	NC	103	1/1	0.91	0.19	112,112,112,112	0
56	MG	B	9227	1/1	0.92	0.13	93,93,93,93	0
56	MG	B	9354	1/1	0.92	0.12	103,103,103,103	0
56	MG	GB	9305	1/1	0.92	0.07	80,80,80,80	0
56	MG	B	9048	1/1	0.92	0.19	70,70,70,70	0
56	MG	C	212	1/1	0.92	0.13	138,138,138,138	0
56	MG	PB	202	1/1	0.92	0.05	127,127,127,127	0
56	MG	GB	9186	1/1	0.92	0.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GB	9372	1/1	0.92	0.07	101,101,101,101	0
56	MG	A	1680	1/1	0.92	0.17	84,84,84,84	0
56	MG	OC	401	1/1	0.92	0.14	171,171,171,171	0
56	MG	GB	9340	1/1	0.92	0.11	111,111,111,111	0
56	MG	RB	203	1/1	0.92	0.09	103,103,103,103	0
56	MG	B	9163	1/1	0.92	0.11	85,85,85,85	0
56	MG	GB	9037	1/1	0.92	0.22	82,82,82,82	0
56	MG	GB	9378	1/1	0.92	0.07	134,134,134,134	0
56	MG	B	9010	1/1	0.92	0.32	69,69,69,69	0
56	MG	B	9065	1/1	0.92	0.14	69,69,69,69	0
56	MG	G	302	1/1	0.92	0.14	90,90,90,90	0
56	MG	B	9361	1/1	0.92	0.10	91,91,91,91	0
56	MG	GB	9384	1/1	0.92	0.13	131,131,131,131	0
56	MG	B	9051	1/1	0.92	0.11	93,93,93,93	0
56	MG	A	1703	1/1	0.92	0.16	101,101,101,101	0
56	MG	B	9128	1/1	0.92	0.18	106,106,106,106	0
56	MG	B	9366	1/1	0.92	0.09	76,76,76,76	0
56	MG	ZB	101	1/1	0.92	0.11	103,103,103,103	0
56	MG	FB	1786	1/1	0.92	0.09	96,96,96,96	0
56	MG	A	1761	1/1	0.92	0.11	106,106,106,106	0
56	MG	B	9170	1/1	0.92	0.11	78,78,78,78	0
56	MG	FB	1711	1/1	0.92	0.10	118,118,118,118	0
56	MG	B	9047	1/1	0.92	0.28	89,89,89,89	0
56	MG	FB	1667	1/1	0.92	0.20	103,103,103,103	0
56	MG	B	9172	1/1	0.92	0.14	87,87,87,87	0
56	MG	GB	9266	1/1	0.92	0.08	118,118,118,118	0
56	MG	B	9299	1/1	0.92	0.10	101,101,101,101	0
56	MG	M	201	1/1	0.92	0.07	104,104,104,104	0
56	MG	GB	9210	1/1	0.92	0.15	99,99,99,99	0
56	MG	B	9333	1/1	0.92	0.10	85,85,85,85	0
58	ZN	IC	101	1/1	0.92	0.13	158,158,158,158	0
56	MG	B	9147	1/1	0.93	0.08	103,103,103,103	0
56	MG	B	9410	1/1	0.93	0.08	84,84,84,84	0
56	MG	VA	202	1/1	0.93	0.13	127,127,127,127	0
56	MG	GB	9260	1/1	0.93	0.13	109,109,109,109	0
56	MG	B	9247	1/1	0.93	0.10	93,93,93,93	0
56	MG	E	301	1/1	0.93	0.23	68,68,68,68	0
56	MG	B	9412	1/1	0.93	0.08	82,82,82,82	0
56	MG	B	9390	1/1	0.93	0.10	89,89,89,89	0
56	MG	E	305	1/1	0.93	0.05	85,85,85,85	0
56	MG	GB	9009	1/1	0.93	0.30	78,78,78,78	0
56	MG	FB	1768	1/1	0.93	0.16	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1769	1/1	0.93	0.11	109,109,109,109	0
56	MG	GB	9376	1/1	0.93	0.06	143,143,143,143	0
56	MG	BB	101	1/1	0.93	0.13	118,118,118,118	0
56	MG	B	9034	1/1	0.93	0.15	69,69,69,69	0
56	MG	GB	9379	1/1	0.93	0.22	89,89,89,89	0
56	MG	B	9415	1/1	0.93	0.11	97,97,97,97	0
56	MG	B	9332	1/1	0.93	0.09	96,96,96,96	0
56	MG	GB	9344	1/1	0.93	0.14	100,100,100,100	0
56	MG	B	9035	1/1	0.93	0.28	69,69,69,69	0
56	MG	B	9275	1/1	0.93	0.12	76,76,76,76	0
56	MG	B	9420	1/1	0.93	0.20	94,94,94,94	0
56	MG	A	1629	1/1	0.93	0.26	85,85,85,85	0
56	MG	B	9160	1/1	0.93	0.18	103,103,103,103	0
56	MG	B	9214	1/1	0.93	0.07	93,93,93,93	0
56	MG	B	9377	1/1	0.93	0.07	92,92,92,92	0
56	MG	A	1753	1/1	0.93	0.07	132,132,132,132	0
56	MG	B	9340	1/1	0.93	0.06	85,85,85,85	0
56	MG	B	9097	1/1	0.93	0.12	73,73,73,73	0
56	MG	B	9360	1/1	0.93	0.04	106,106,106,106	0
56	MG	B	9325	1/1	0.93	0.19	92,92,92,92	0
56	MG	A	1724	1/1	0.93	0.07	100,100,100,100	0
56	MG	B	9137	1/1	0.93	0.12	83,83,83,83	0
56	MG	FB	1758	1/1	0.93	0.06	104,104,104,104	0
56	MG	GB	9221	1/1	0.93	0.13	80,80,80,80	0
58	ZN	BA	101	1/1	0.93	0.04	194,194,194,194	0
56	MG	B	9123	1/1	0.93	0.15	88,88,88,88	0
56	MG	GB	9299	1/1	0.94	0.06	162,162,162,162	0
56	MG	GB	9277	1/1	0.94	0.08	82,82,82,82	0
56	MG	GB	9198	1/1	0.94	0.07	89,89,89,89	0
56	MG	GB	9003	1/1	0.94	0.30	67,67,67,67	0
56	MG	B	9427	1/1	0.94	0.19	84,84,84,84	0
56	MG	B	9278	1/1	0.94	0.10	101,101,101,101	0
56	MG	E	304	1/1	0.94	0.08	85,85,85,85	0
56	MG	GB	9307	1/1	0.94	0.07	109,109,109,109	0
56	MG	B	9019	1/1	0.94	0.37	79,79,79,79	0
56	MG	GB	9223	1/1	0.94	0.06	85,85,85,85	0
56	MG	B	9353	1/1	0.94	0.13	92,92,92,92	0
56	MG	B	9003	1/1	0.94	0.40	64,64,64,64	0
56	MG	B	9386	1/1	0.94	0.08	114,114,114,114	0
56	MG	FB	1656	1/1	0.94	0.09	120,120,120,120	0
56	MG	FB	1789	1/1	0.94	0.19	107,107,107,107	0
56	MG	B	9312	1/1	0.94	0.04	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B	9242	1/1	0.94	0.18	93,93,93,93	0
56	MG	GB	9193	1/1	0.94	0.13	95,95,95,95	0
56	MG	B	9205	1/1	0.94	0.12	120,120,120,120	0
56	MG	B	9027	1/1	0.94	0.33	68,68,68,68	0
56	MG	B	9425	1/1	0.94	0.08	83,83,83,83	0
56	MG	A	1769	1/1	0.94	0.13	117,117,117,117	0
58	ZN	GC	101	1/1	0.94	0.05	206,206,206,206	0
56	MG	GB	9236	1/1	0.94	0.06	87,87,87,87	0
56	MG	GB	9365	1/1	0.95	0.11	87,87,87,87	0
56	MG	B	9039	1/1	0.95	0.07	68,68,68,68	0
56	MG	B	9279	1/1	0.95	0.16	93,93,93,93	0
56	MG	B	9216	1/1	0.95	0.13	85,85,85,85	0
56	MG	FB	1775	1/1	0.95	0.06	119,119,119,119	0
56	MG	B	9421	1/1	0.95	0.11	85,85,85,85	0
56	MG	KC	101	1/1	0.95	0.19	117,117,117,117	0
56	MG	FB	1676	1/1	0.95	0.14	94,94,94,94	0
56	MG	B	9085	1/1	0.95	0.09	77,77,77,77	0
56	MG	GB	9302	1/1	0.95	0.05	112,112,112,112	0
56	MG	B	9379	1/1	0.95	0.06	100,100,100,100	0
56	MG	FB	1719	1/1	0.95	0.05	150,150,150,150	0
56	MG	FB	1743	1/1	0.95	0.07	98,98,98,98	0
56	MG	B	9371	1/1	0.95	0.07	81,81,81,81	0
56	MG	A	1681	1/1	0.95	0.05	132,132,132,132	0
56	MG	B	9041	1/1	0.95	0.21	71,71,71,71	0
56	MG	GB	9396	1/1	0.95	0.10	78,78,78,78	0
56	MG	B	9306	1/1	0.96	0.06	83,83,83,83	0
56	MG	B	9300	1/1	0.96	0.09	89,89,89,89	0
56	MG	GB	9204	1/1	0.96	0.09	130,130,130,130	0
56	MG	B	9416	1/1	0.96	0.05	82,82,82,82	0
56	MG	FB	1746	1/1	0.96	0.07	96,96,96,96	0
56	MG	B	9374	1/1	0.96	0.08	94,94,94,94	0
56	MG	B	9202	1/1	0.96	0.05	80,80,80,80	0
56	MG	A	1741	1/1	0.96	0.04	109,109,109,109	0
56	MG	B	9096	1/1	0.96	0.08	78,78,78,78	0
56	MG	A	1651	1/1	0.96	0.04	175,175,175,175	0
56	MG	M	202	1/1	0.96	0.05	81,81,81,81	0
57	BLS	B	9001	30/30	0.96	0.11	105,105,106,106	0
57	BLS	GB	9001	30/30	0.96	0.09	104,104,105,105	0
56	MG	B	9173	1/1	0.96	0.29	86,86,86,86	0
58	ZN	DA	101	1/1	0.96	0.05	160,160,160,160	0
56	MG	GB	9161	1/1	0.96	0.07	101,101,101,101	0
56	MG	GB	9005	1/1	0.96	0.47	68,68,68,68	0

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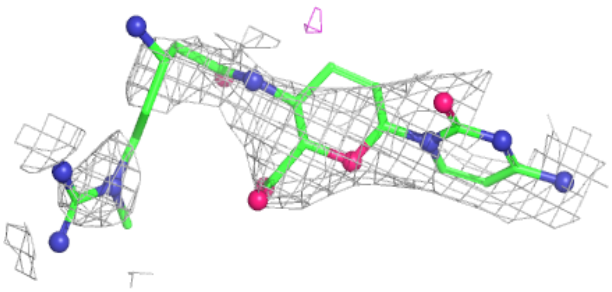
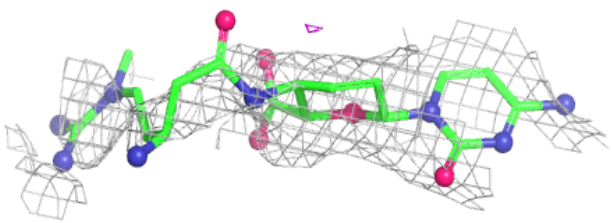
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	FB	1742	1/1	0.97	0.04	121,121,121,121	0
56	MG	B	9226	1/1	0.97	0.33	70,70,70,70	0
58	ZN	V	501	1/1	0.97	0.05	123,123,123,123	0
56	MG	B	9339	1/1	0.97	0.11	88,88,88,88	0
56	MG	B	9365	1/1	0.97	0.09	84,84,84,84	0
58	ZN	GA	101	1/1	0.97	0.06	153,153,153,153	0
58	ZN	AC	201	1/1	0.97	0.05	147,147,147,147	0
56	MG	B	9394	1/1	0.97	0.07	71,71,71,71	0
56	MG	B	9261	1/1	0.97	0.15	66,66,66,66	0
56	MG	GB	9284	1/1	0.98	0.07	91,91,91,91	0
56	MG	B	9246	1/1	0.98	0.05	84,84,84,84	0
56	MG	GB	9370	1/1	0.98	0.03	127,127,127,127	0
56	MG	B	9344	1/1	0.98	0.12	93,93,93,93	0
56	MG	B	9409	1/1	0.98	0.18	83,83,83,83	0
58	ZN	LC	101	1/1	0.98	0.07	171,171,171,171	0
58	ZN	CA	101	1/1	0.99	0.02	125,125,125,125	0
58	ZN	HC	101	1/1	1.00	0.01	126,126,126,126	0

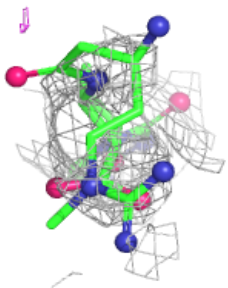
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BLS B 9001:

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

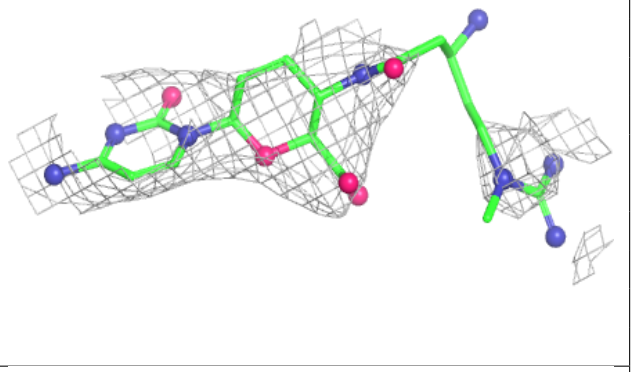


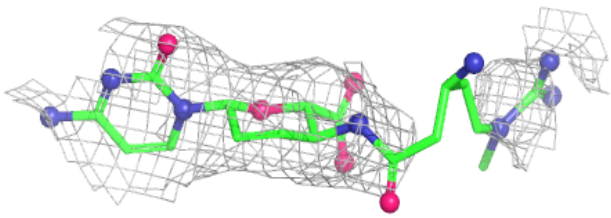


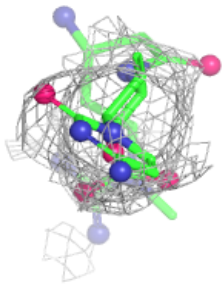


Electron density around BLS GB 9001:

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







6.5 Other polymers

There are no such residues in this entry.