



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 03:01 pm BST

PDB ID : 4V7P  
Title : Recognition of the amber stop codon by release factor RF1.  
Authors : Korostelev, A.; Zhu, J.; Asahara, H.; Noller, H.F.  
Deposited on : 2010-04-29  
Resolution : 3.62 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

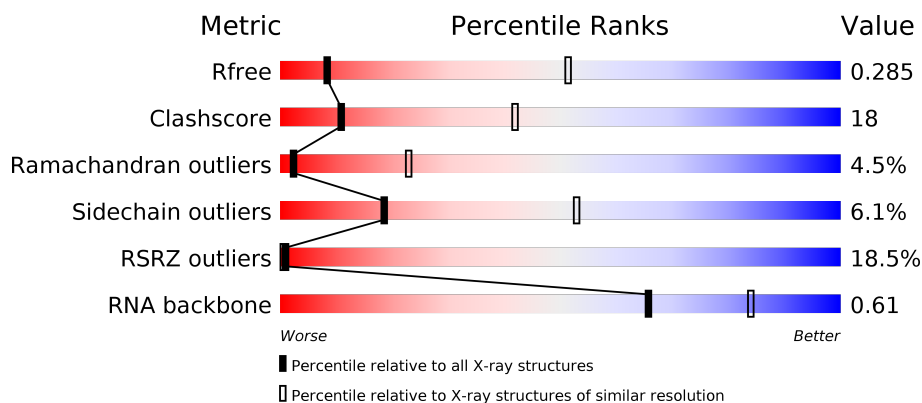
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.62 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)
RNA backbone	3102	1018 (4.22-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	1504	<div> <div>9%</div> <div>47%</div> <div>45%</div> <div>7%</div> </div>
1	DA	1504	<div> <div>10%</div> <div>47%</div> <div>45%</div> <div>8%</div> </div>
2	AB	234	<div> <div>52%</div> <div>51%</div> <div>46%</div> </div>
2	DB	234	<div> <div>41%</div> <div>52%</div> <div>44%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	DC	206	
4	AD	208	
4	DD	208	
5	AE	151	
5	DE	151	
6	AF	101	
6	DF	101	
7	AG	155	
7	DG	155	
8	AH	138	
8	DH	138	
9	AI	127	
9	DI	127	
10	AJ	98	
10	DJ	98	
11	AK	119	
11	DK	119	
12	AL	124	
12	DL	124	
13	AM	117	
13	DM	117	
14	AN	60	
14	DN	60	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	DO	88	
16	AP	83	
16	DP	83	
17	AQ	99	
17	DQ	99	
18	AR	70	
18	DR	70	
19	AS	78	
19	DS	78	
20	AT	99	
20	DT	99	
21	AU	24	
21	DU	24	
22	AV	354	
22	DV	354	
23	AW	77	
23	DW	77	
24	AX	7	
25	BA	2879	
25	CA	2879	
26	BB	119	
26	CB	119	
27	BC	275	
27	CC	275	
28	BD	206	

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Mol	Chain	Length	Quality of chain
28	CD	206	
29	BE	205	
29	CE	205	
30	BF	181	
30	CF	181	
31	BG	180	
31	CG	180	
32	BH	148	
32	CH	148	
33	BI	173	
33	CI	173	
34	BJ	139	
34	CJ	139	
35	BK	122	
35	CK	122	
36	BL	150	
36	CL	150	
37	BM	141	
37	CM	141	
38	BN	117	
38	CN	117	
39	BO	111	
39	CO	111	
40	BP	146	
40	CP	146	

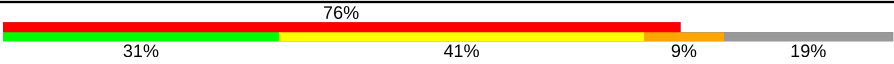





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Mol	Chain	Length	Quality of chain
41	BQ	116	
41	CQ	116	
42	BR	101	
42	CR	101	
43	BS	112	
43	CS	112	
44	BT	96	
44	CT	96	
45	BU	109	
45	CU	109	
46	BV	206	
46	CV	206	
47	BW	84	
47	CW	84	
48	BX	98	
48	CX	98	
49	BY	72	
49	CY	72	
50	BZ	59	
50	CZ	59	
51	B1	71	
51	C1	71	
52	B2	59	
52	C2	59	
53	B3	54	

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Mol	Chain	Length	Quality of chain
53	C3	54	
54	B4	48	
54	C4	48	
55	B5	64	
55	C5	64	
56	DX	9	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1655	-	-	-	X
57	MG	BA	2913	-	-	-	X
57	MG	BA	2933	-	-	-	X
57	MG	BA	2965	-	-	-	X
57	MG	BA	2968	-	-	-	X
57	MG	BA	2987	-	-	-	X
57	MG	BA	2990	-	-	-	X
57	MG	BA	2998	-	-	-	X
57	MG	BA	3003	-	-	-	X
57	MG	BA	3020	-	-	-	X
57	MG	BA	3025	-	-	-	X
57	MG	CA	2911	-	-	-	X
57	MG	CA	2935	-	-	-	X
57	MG	CA	2953	-	-	-	X
57	MG	CA	2963	-	-	-	X
57	MG	CA	2974	-	-	-	X
57	MG	CA	2978	-	-	-	X
57	MG	CA	2988	-	-	-	X
57	MG	CA	2997	-	-	-	X
57	MG	DA	1608	-	-	-	X
57	MG	DA	1628	-	-	-	X

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			
1	DA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	DB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	DC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
5	DE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	DJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	DL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			
13	DM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	DP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			
17	DQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	DS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	DT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			
21	DU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			
22	DV	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			

- Molecule 23 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	DW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 24 is a RNA chain called messenger RNA (5'-R(\*AP\*AP\*UP\*GP\*UP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	7	Total	C	N	O	P	0	0	0
			149	68	29	46	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			
25	CA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1142	U	C	CONFLICT	GB AE017221.1
BA	2825	U	G	CONFLICT	GB AE017221.1
CA	1142	U	C	CONFLICT	GB AE017221.1
CA	2825	U	G	CONFLICT	GB AE017221.1

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

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			
27	CC	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
28	CD	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
29	CE	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
30	CF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
31	CG	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			
32	CH	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	BI	32	Total	C	N	O	0	0	0
			253	157	49	47			
33	CI	32	Total	C	N	O	0	0	0
			253	157	49	47			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BJ	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			
34	CJ	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
35	CK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
37	CM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BN	117	Total	C	N	O		0	0	0
			960	599	202	159				
38	CN	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BO	98	Total	C	N	O		0	0	0
			770	486	154	130				
39	CO	98	Total	C	N	O		0	0	0
			770	486	154	130				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BP	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
40	CP	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			
41	CQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	PHE	DELETION	UNP Q72L76
CQ	?	-	PHE	DELETION	UNP Q72L76

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
43	CS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BT	92	Total	C	N	O		0	0	0
			725	471	131	123				
44	CT	92	Total	C	N	O		0	0	0
			725	471	131	123				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BU	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
45	CU	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BV	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CV	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
47	CW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BX	88	Total	C	N	O	0	0	0
			694	435	141	118			
48	CX	88	Total	C	N	O	0	0	0
			694	435	141	118			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BY	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			
49	CY	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
50	CZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B1	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			
51	C1	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B2	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			
52	C2	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B3	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			
53	C3	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
54	C4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B5	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
55	C5	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 56 is a RNA chain called messenger RNA (5'-R(\*AP\*AP\*UP\*GP\*UP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DX	9	Total	C	N	O	P	0	0	0
			193	88	39	58	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CB	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BB	2	Total 2	Mg 2	0	0
57	BA	176	Total 176	Mg 176	0	0
57	CA	125	Total 125	Mg 125	0	0
57	B2	1	Total 1	Mg 1	0	0
57	BM	1	Total 1	Mg 1	0	0
57	AV	1	Total 1	Mg 1	0	0
57	DA	30	Total 30	Mg 30	0	0
57	AW	3	Total 3	Mg 3	0	0
57	AA	64	Total 64	Mg 64	0	0
57	AT	1	Total 1	Mg 1	0	0
57	BK	1	Total 1	Mg 1	0	0
57	DW	1	Total 1	Mg 1	0	0
57	CY	1	Total 1	Mg 1	0	0
57	CM	1	Total 1	Mg 1	0	0

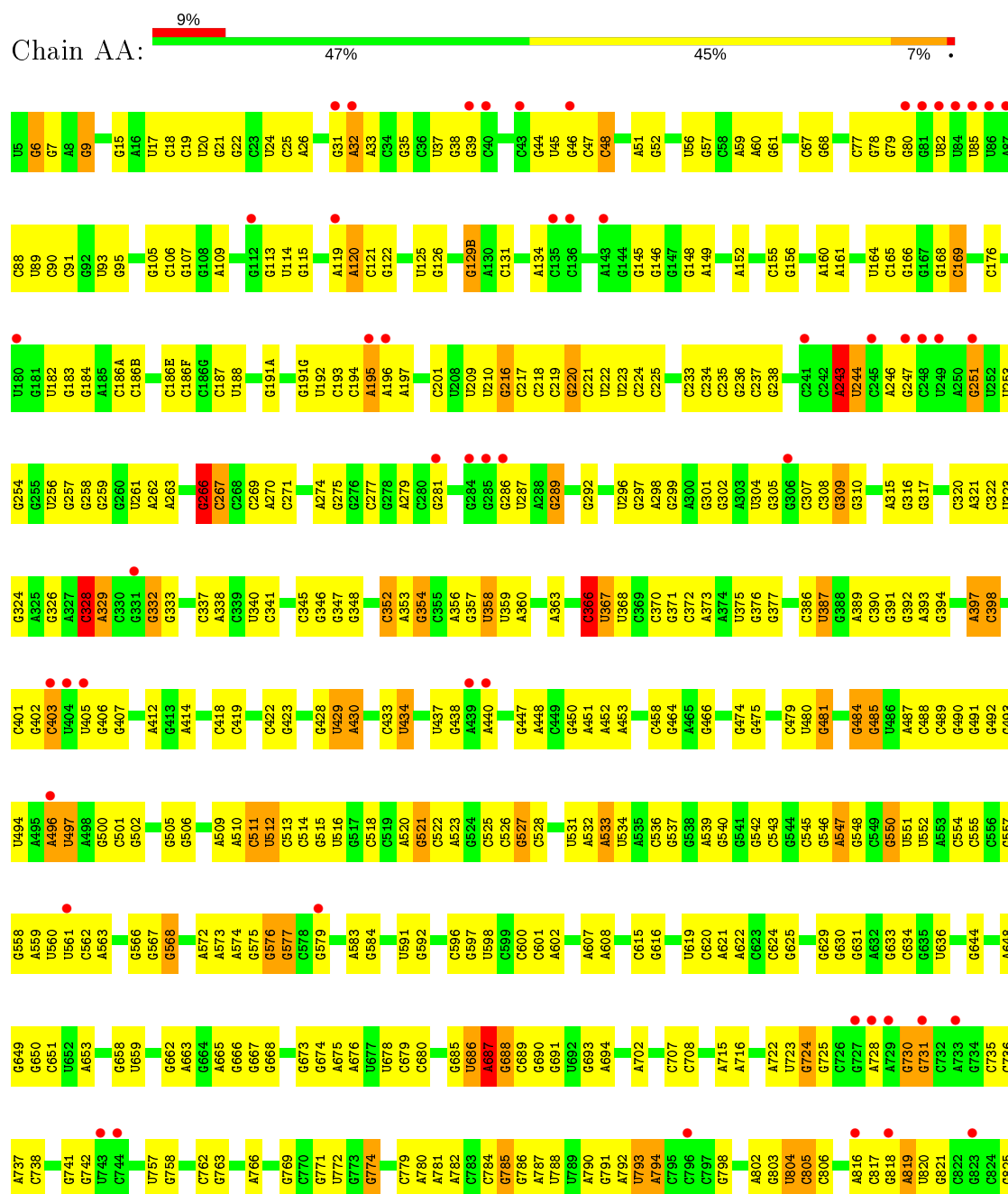
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

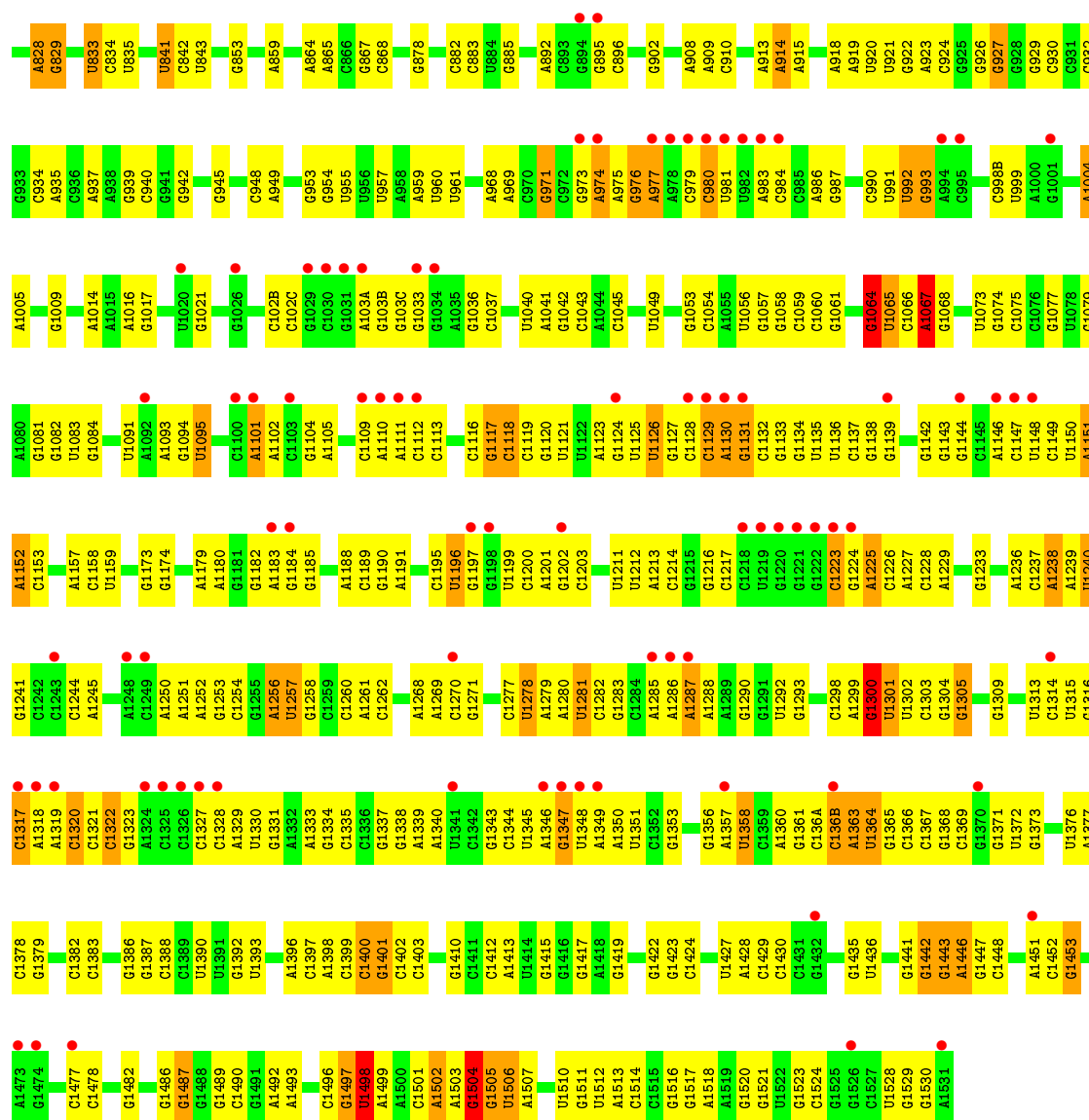
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DN	1	Total 1	Zn 1	0	0
58	AD	1	Total 1	Zn 1	0	0
58	DD	1	Total 1	Zn 1	0	0
58	AN	1	Total 1	Zn 1	0	0

### 3 Residue-property plots [i](#)

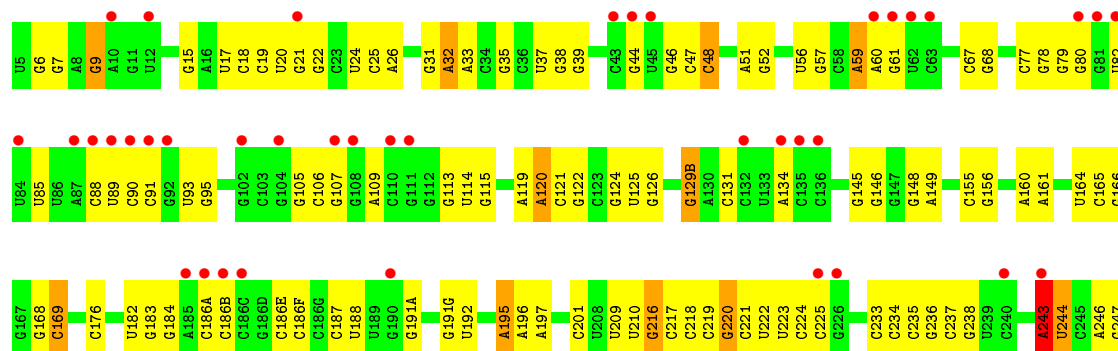
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 16S rRNA (1504-MER)

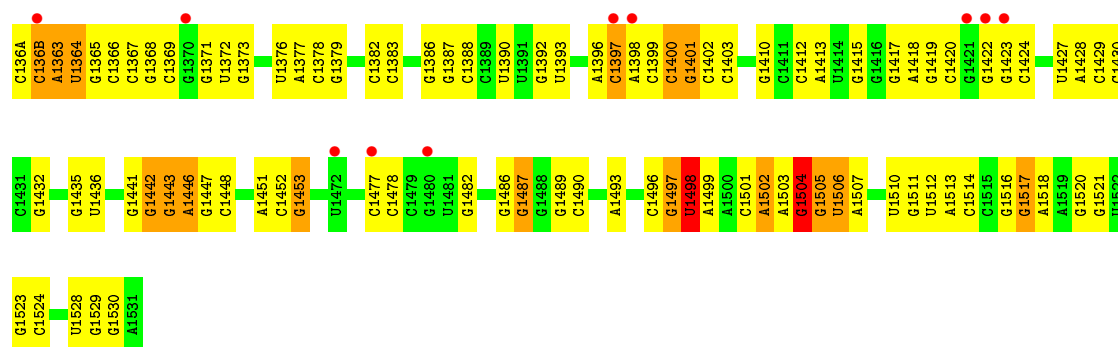




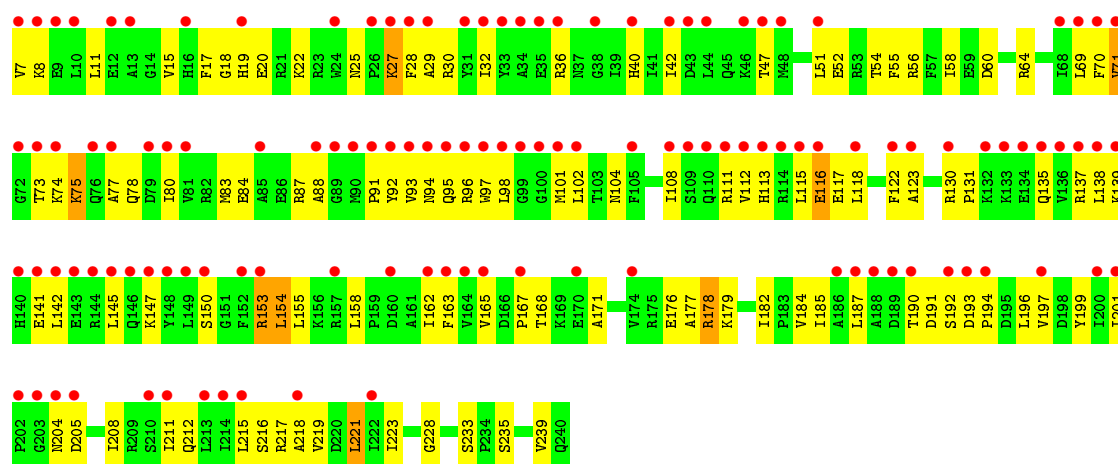
• Molecule 1: 16S rRNA (1504-MER)



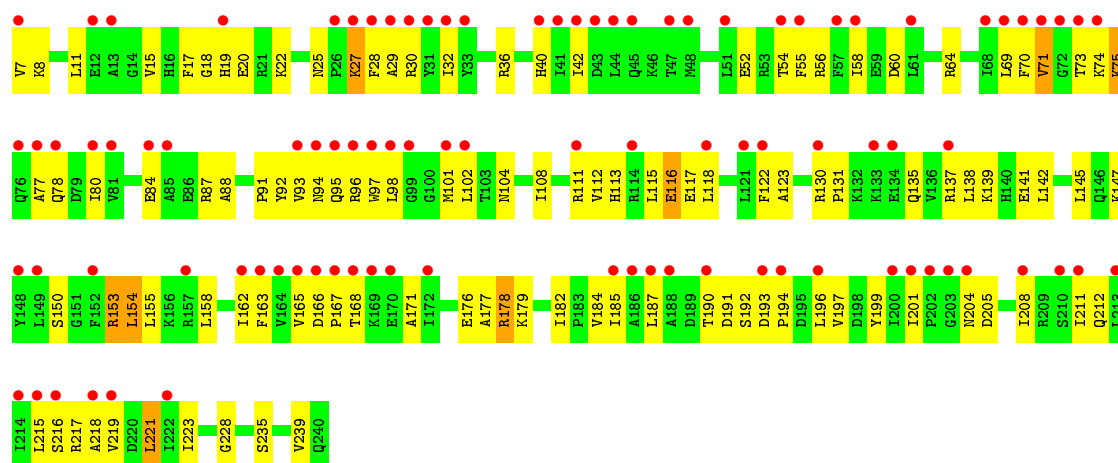
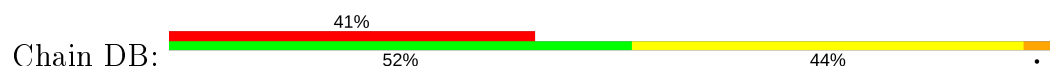




• Molecule 2: 30S ribosomal protein S2

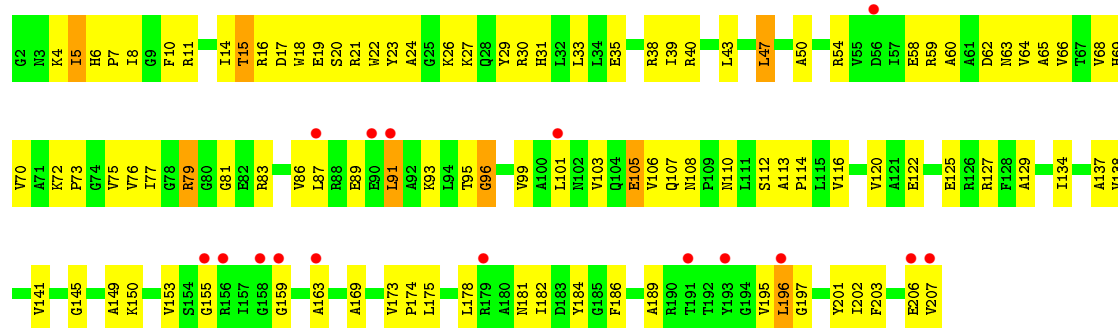


• Molecule 2: 30S ribosomal protein S2

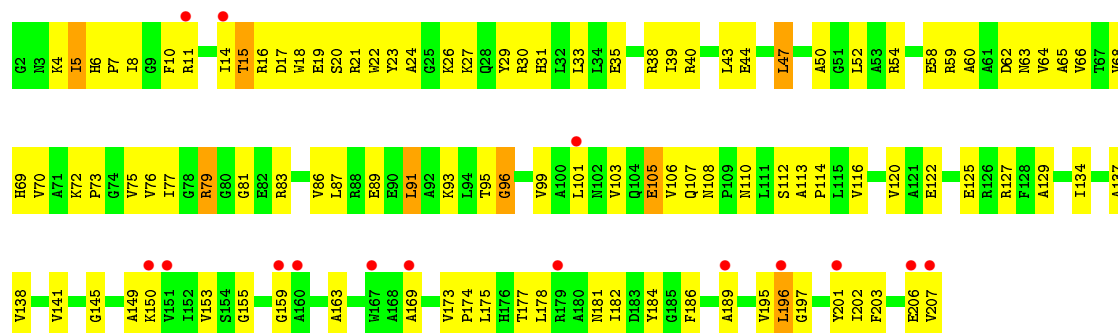


• Molecule 3: 30S ribosomal protein S3

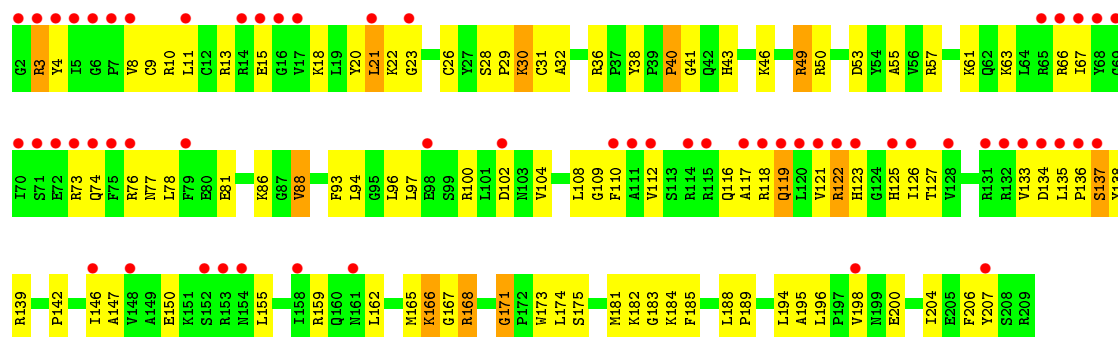




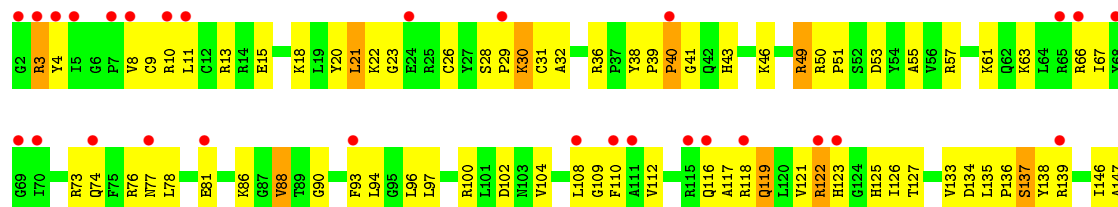
• Molecule 3: 30S ribosomal protein S3



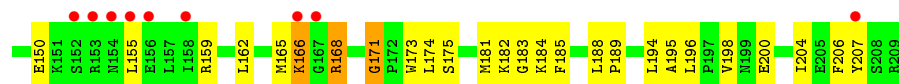
• Molecule 4: 30S ribosomal protein S4



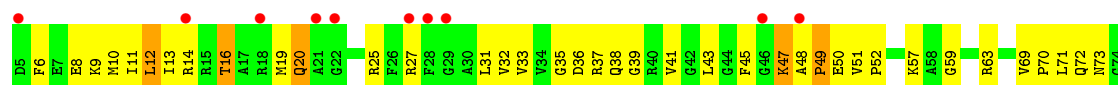
• Molecule 4: 30S ribosomal protein S4







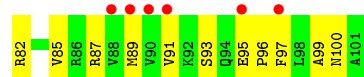
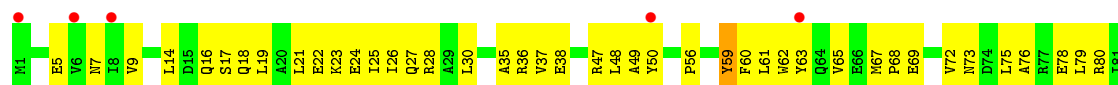
- Molecule 5: 30S ribosomal protein S5



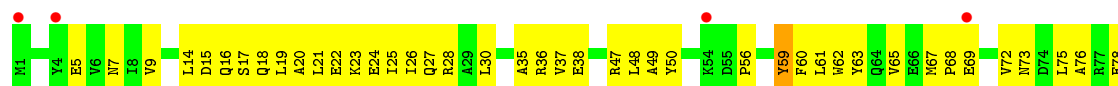
- Molecule 5: 30S ribosomal protein S5



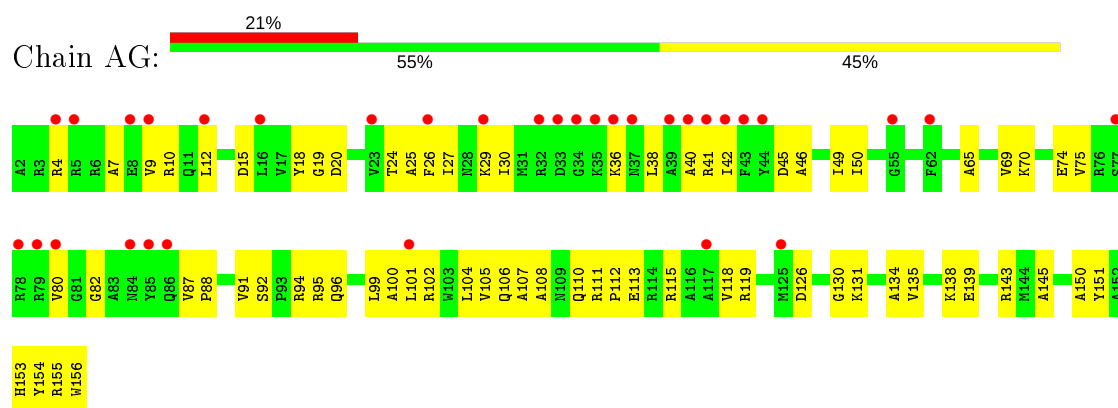
- Molecule 6: 30S ribosomal protein S6



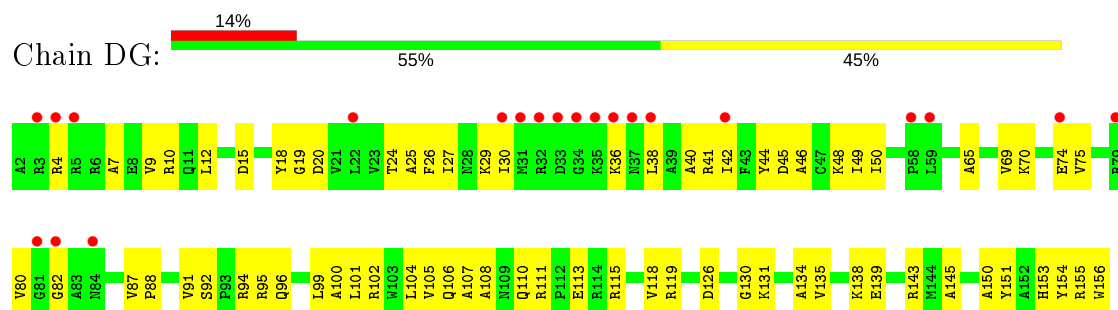
- Molecule 6: 30S ribosomal protein S6



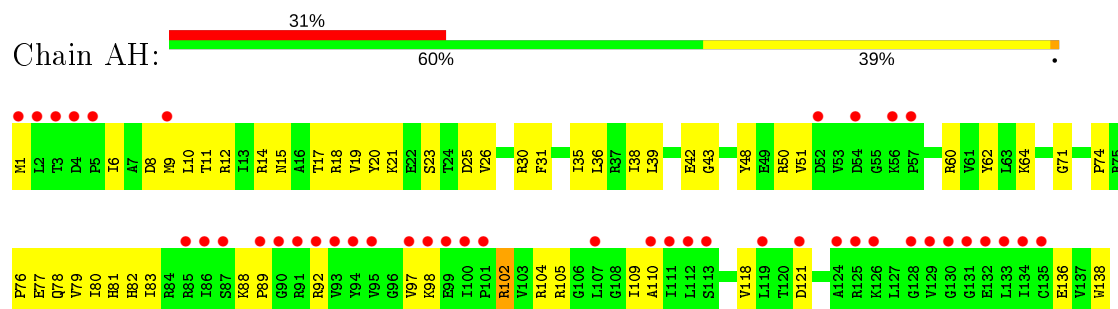
- Molecule 7: 30S ribosomal protein S7



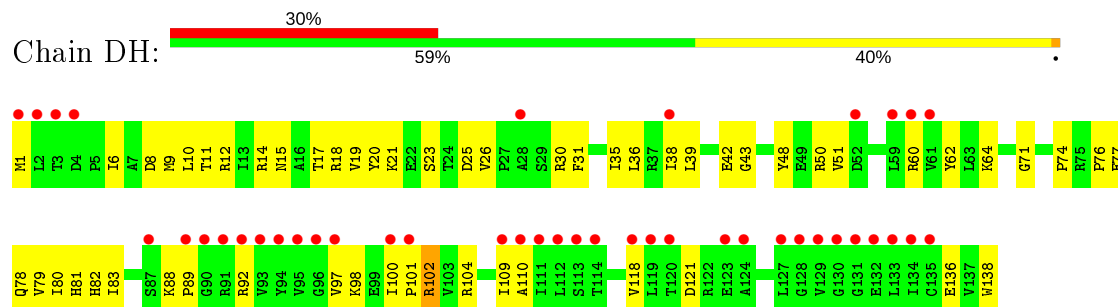
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

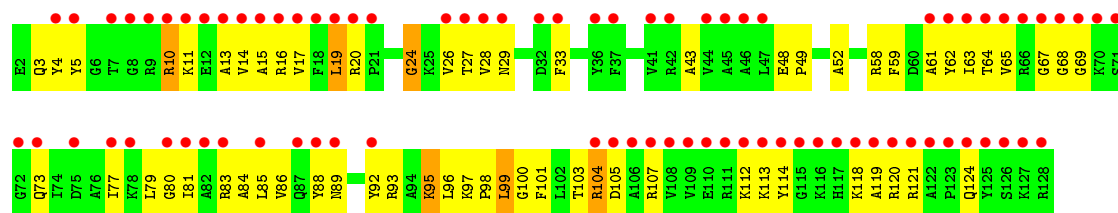


• Molecule 8: 30S ribosomal protein S8

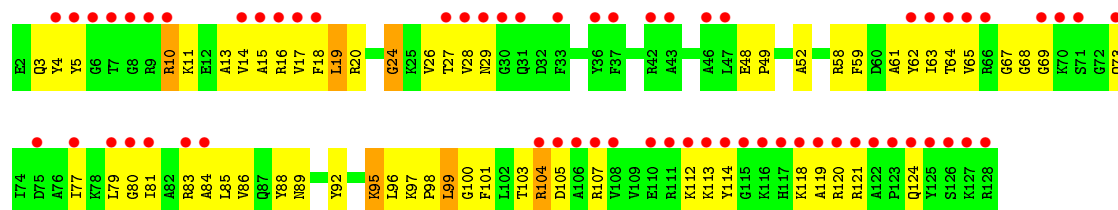


• Molecule 9: 30S ribosomal protein S9

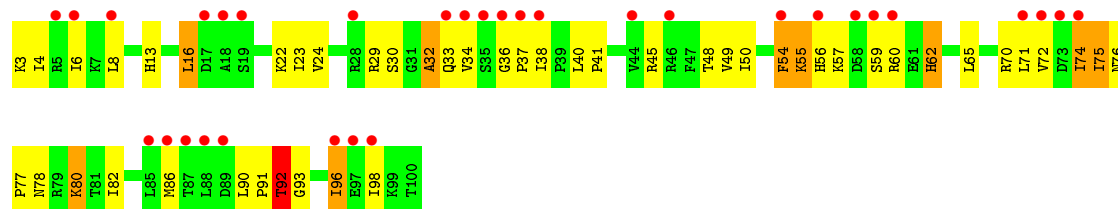




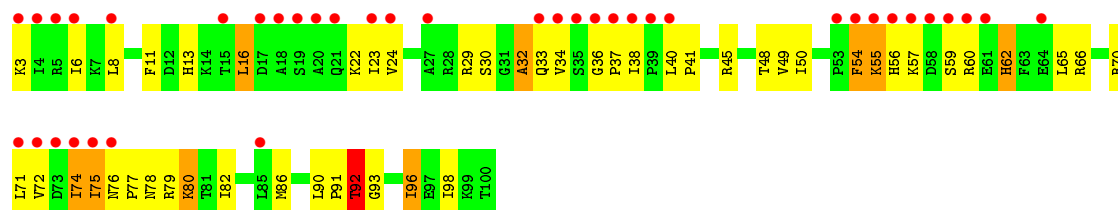
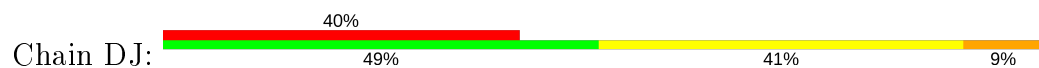
• Molecule 9: 30S ribosomal protein S9



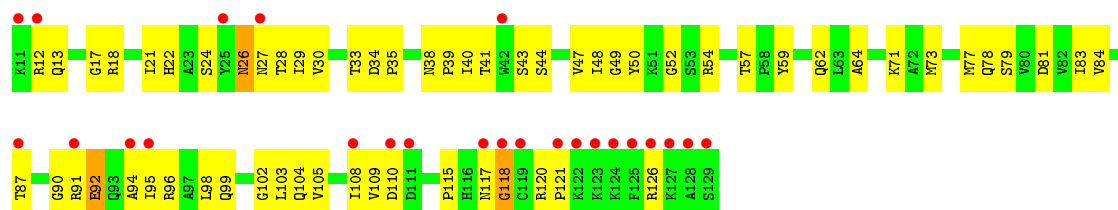
• Molecule 10: 30S ribosomal protein S10



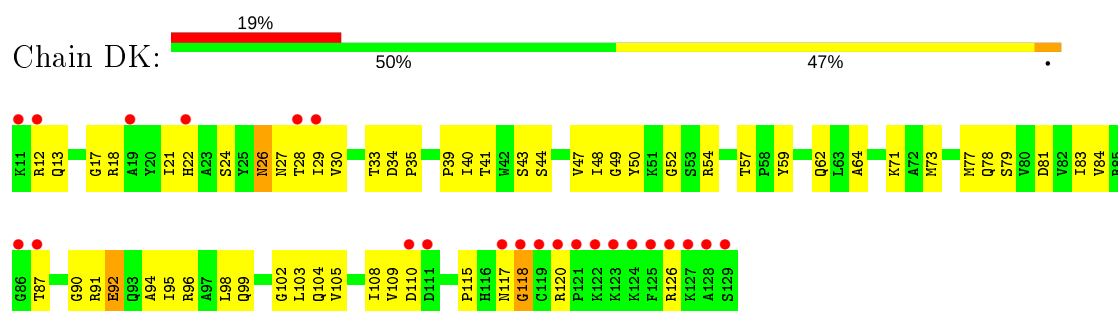
• Molecule 10: 30S ribosomal protein S10



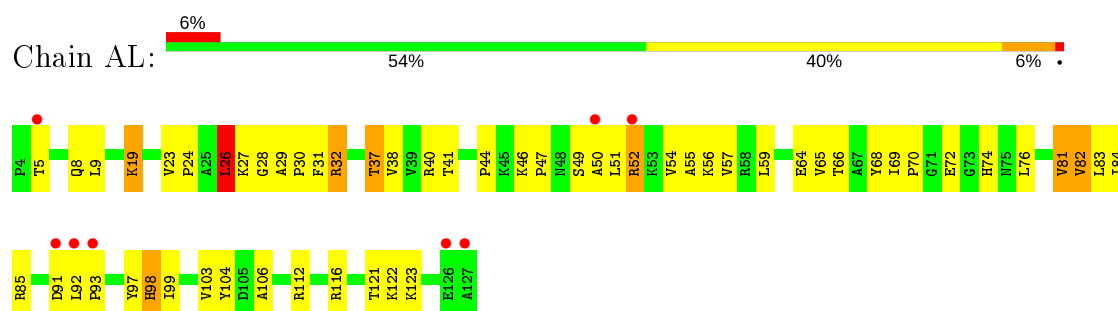
• Molecule 11: 30S ribosomal protein S11



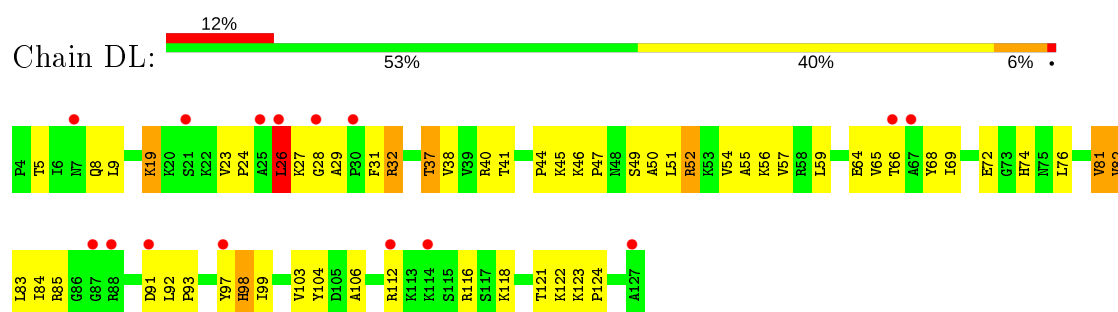
- Molecule 11: 30S ribosomal protein S11



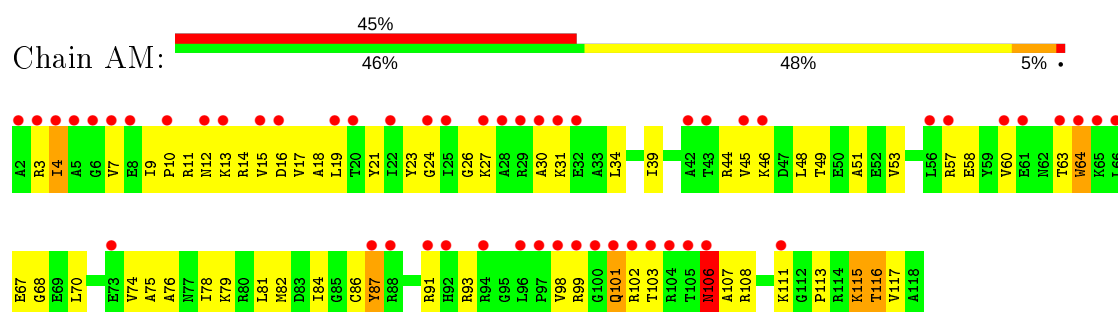
- Molecule 12: 30S ribosomal protein S12



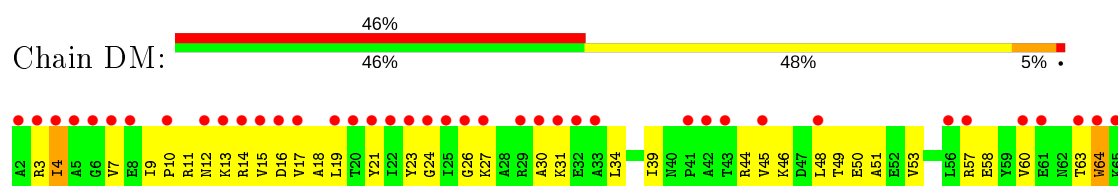
- Molecule 12: 30S ribosomal protein S12

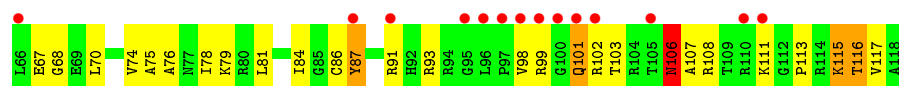


- Molecule 13: 30S ribosomal protein S13

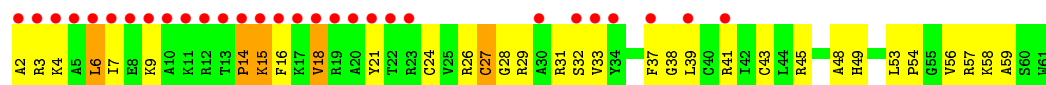


- Molecule 13: 30S ribosomal protein S13

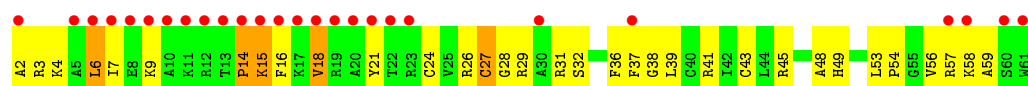
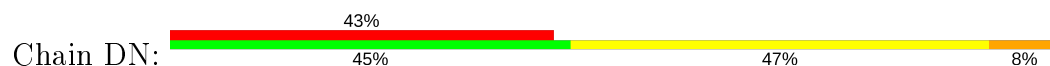




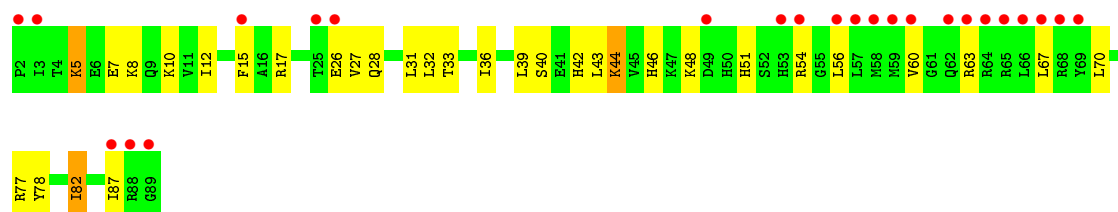
- Molecule 14: 30S ribosomal protein S14



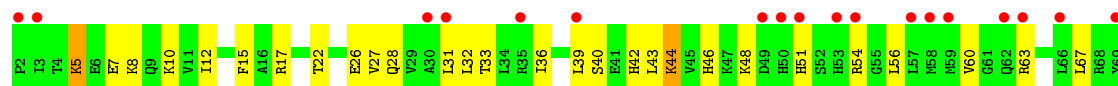
- Molecule 14: 30S ribosomal protein S14



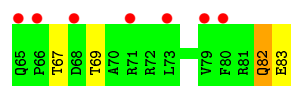
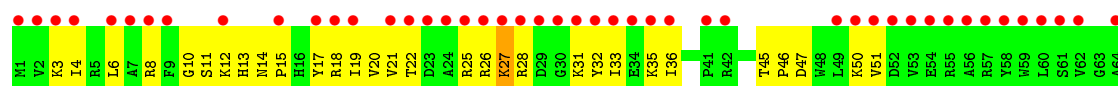
- Molecule 15: 30S ribosomal protein S15



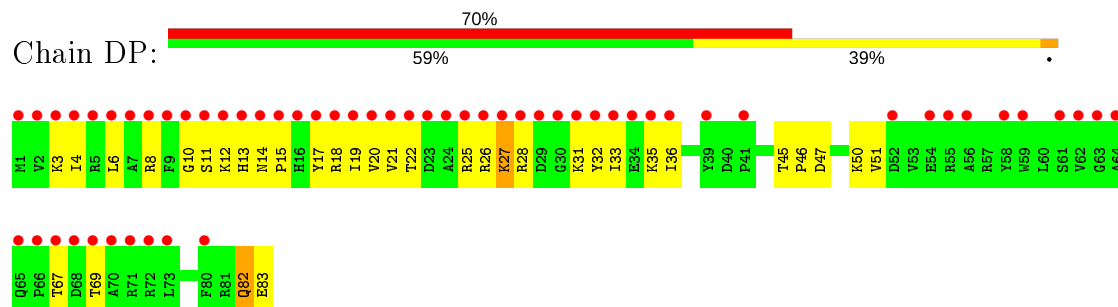
- Molecule 15: 30S ribosomal protein S15



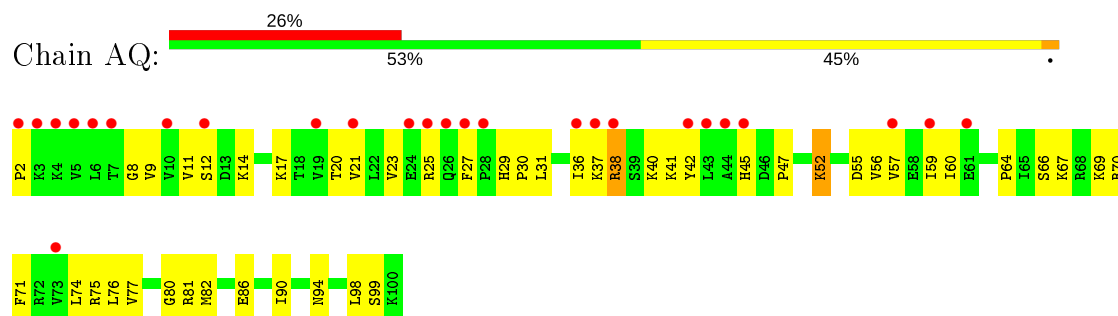
- Molecule 16: 30S ribosomal protein S16



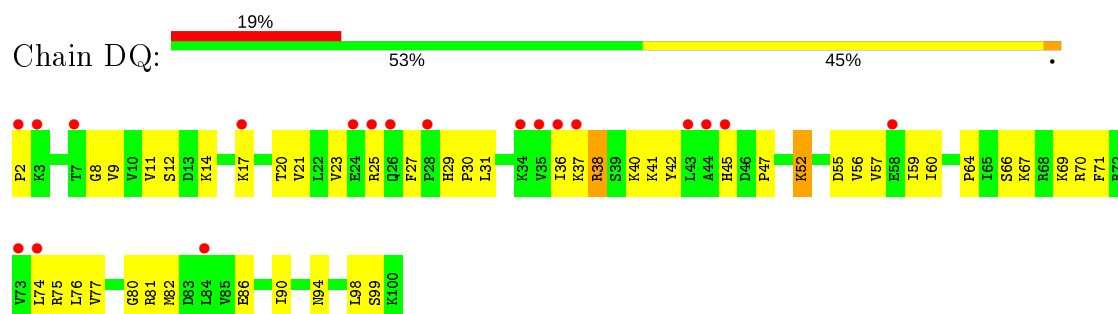
- Molecule 16: 30S ribosomal protein S16



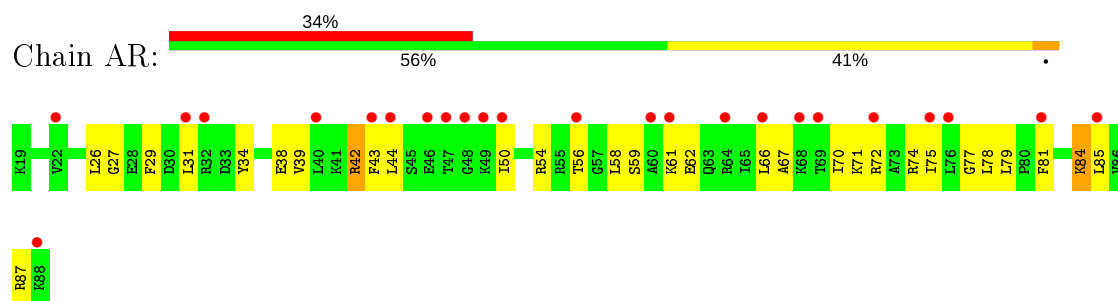
- Molecule 17: 30S ribosomal protein S17



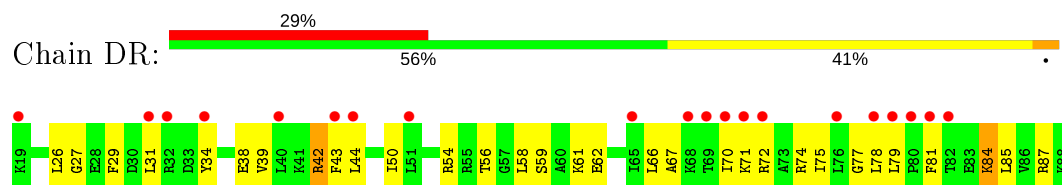
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

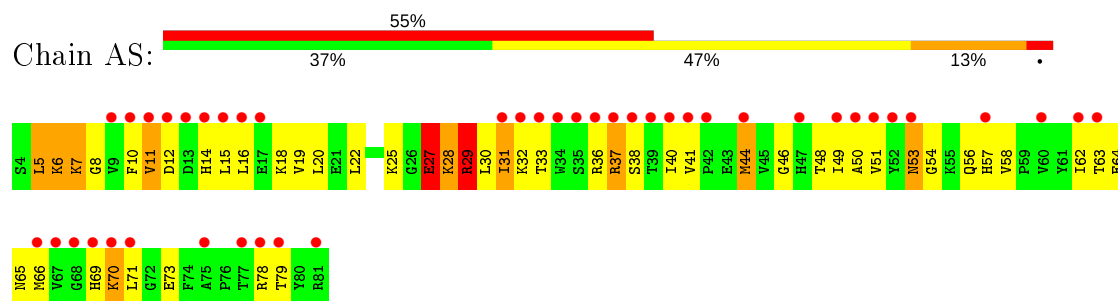


- Molecule 18: 30S ribosomal protein S18



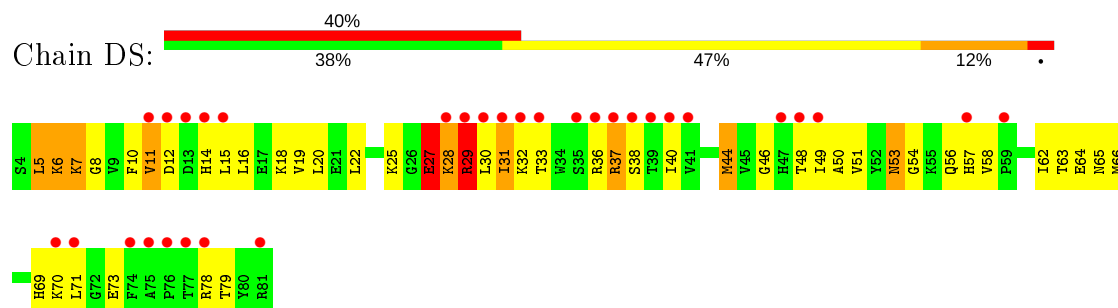
- Molecule 19: 30S ribosomal protein S19

Chain AS:



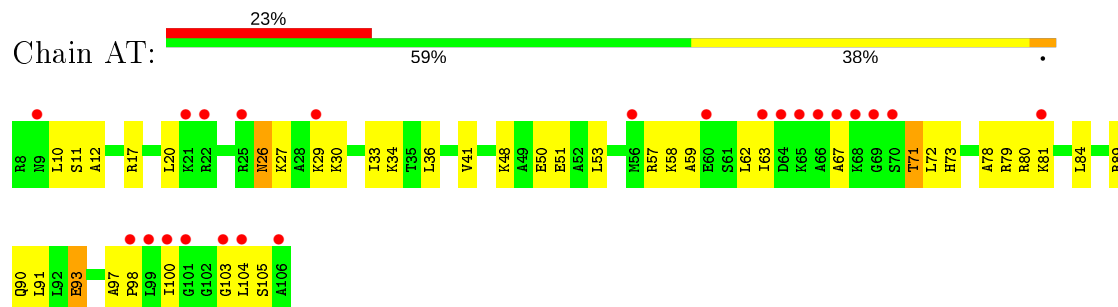
- Molecule 19: 30S ribosomal protein S19

Chain DS:



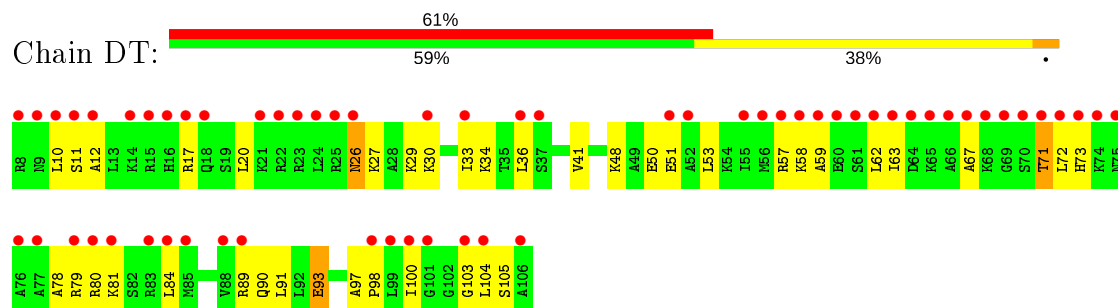
- Molecule 20: 30S ribosomal protein S20

Chain AT:



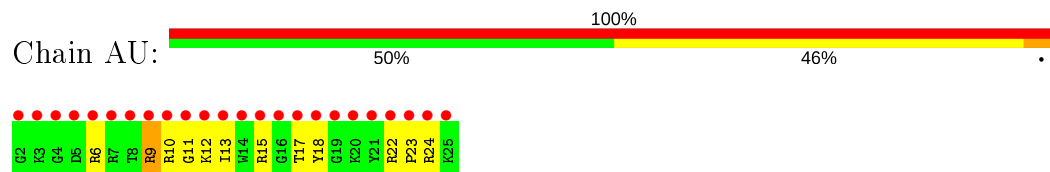
- Molecule 20: 30S ribosomal protein S20

Chain DT:

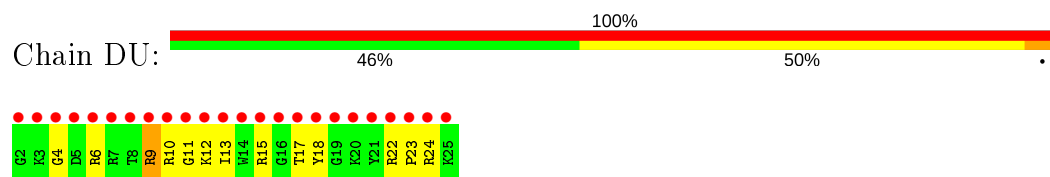


- Molecule 21: 30S ribosomal protein Thx

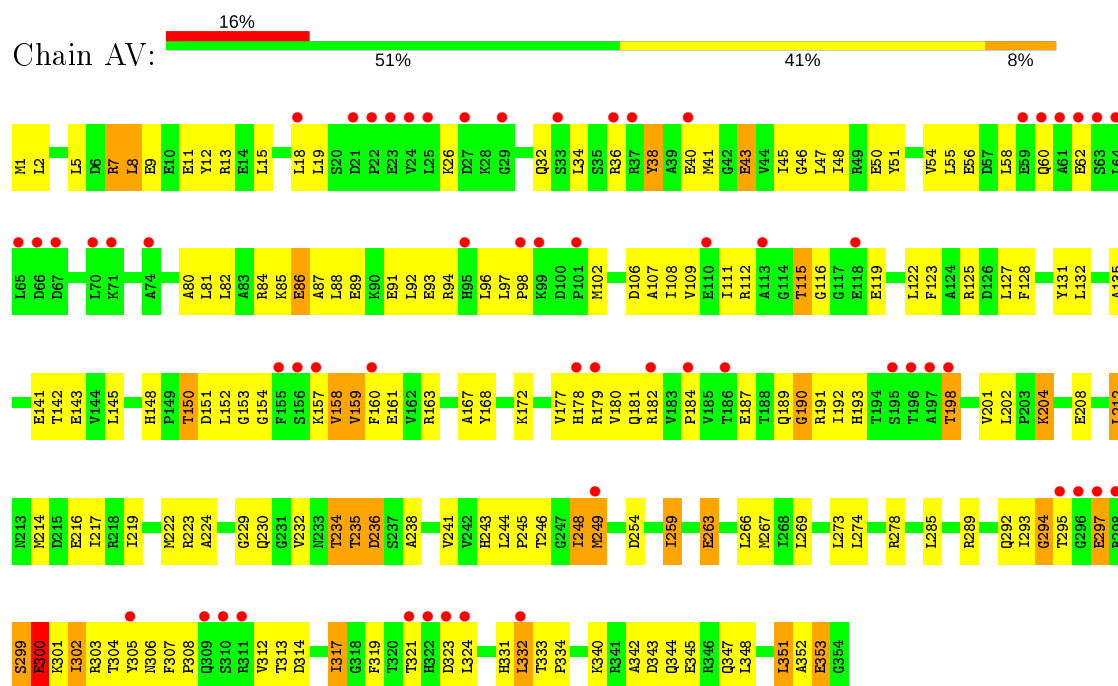
Chain AU:



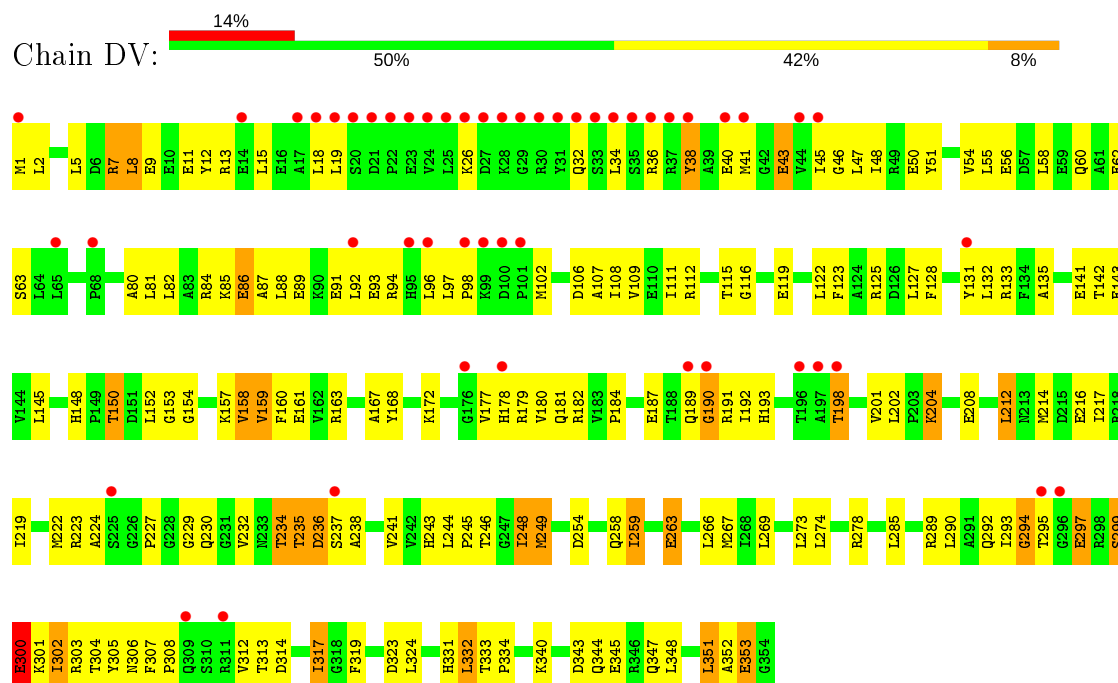
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: Peptide chain release factor 1



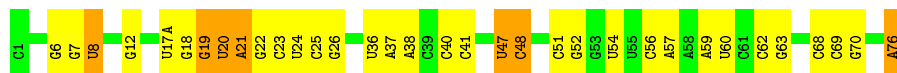
- Molecule 22: Peptide chain release factor 1





- Molecule 23: P-site tRNA-fMet

Chain AW: 



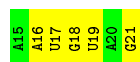
- Molecule 23: P-site tRNA-fMet

Chain DW: 



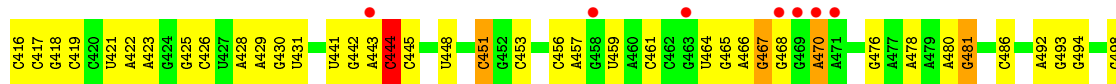
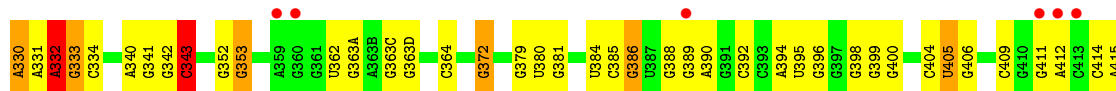
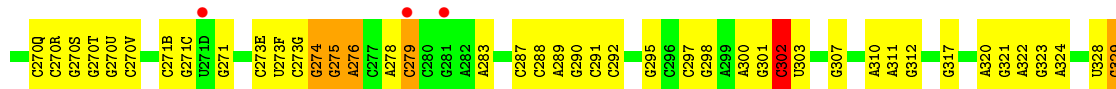
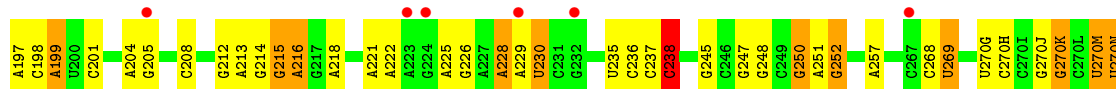
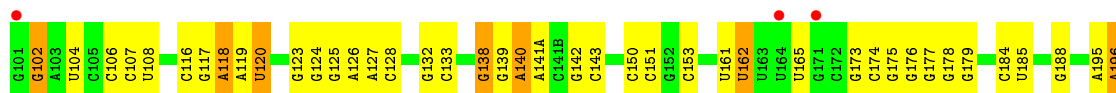
- Molecule 24: messenger RNA (5'-R(\*AP\*AP\*UP\*GP\*UP\*AP\*G)-3')

Chain AX: 



- Molecule 25: 23S ribosomal RNA

Chain BA: 

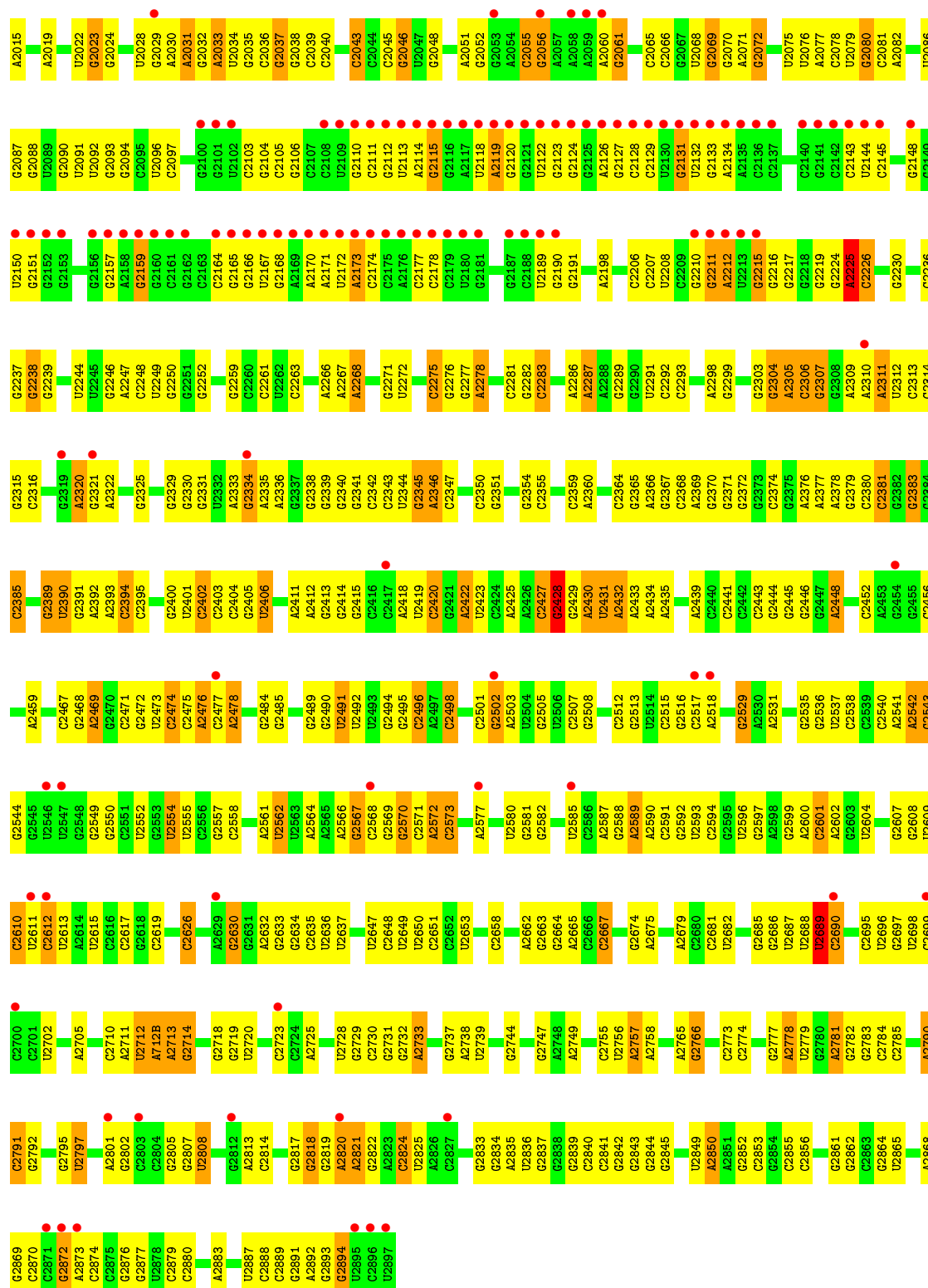


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G1645	G1568	A1472	A1384	U1300	G1212	C1135	G1056	G975	C998	C813	U748	G656	A686
G1646	A1569	G1473	A1385	A1301	G1216	G1136	A1057	G979	A699	C814	C749	U657	U813
C1648	A1570	C1386	C1387	G1303	C1221	G1137	U1060	A980	A901	C815	A750	G662	U888
G1651	A1572	U1481	G1388	C1304	C122A	G1139	U1061	A983	C904	C816	A751	G663	C589
A1652	G1573	G1483	G1389	C1306	G1227	U1141	G1062	A984	U905	C817	A752	C664	A590
G1653	A1486	A1486	A1392	A1307	U1234	U1142	U1063	C985	A910	A818	C753	G666	G593
A1655	A1490	A1393	A1394	G1310	U1394	A1143	U1064	A988	A911	U826	C754	U667	U594
G1656	A1395	U1396	A1396	G1311	A1237	C1147	U1066	G989	C914	U827	C755	G668	G598
C1658	C1493	U1397	U1397	U1512	A1246	A1148	A1069	G993	C915	U828	C756	G669	G599
U1659	A1494	C1398	C1398	C1313	A1247	G1149	A1070	C994	C916	A829	C757	U670	G600
C1660	A1495	C1399	C1399	C1314	G1248	C1150	G1071	C995	C917	G830	C758	C671	A603
A1665	C1585	G1400	G1400	C1315	G1249	G1151	A996	A997	A918	G832	U762	A675	G604
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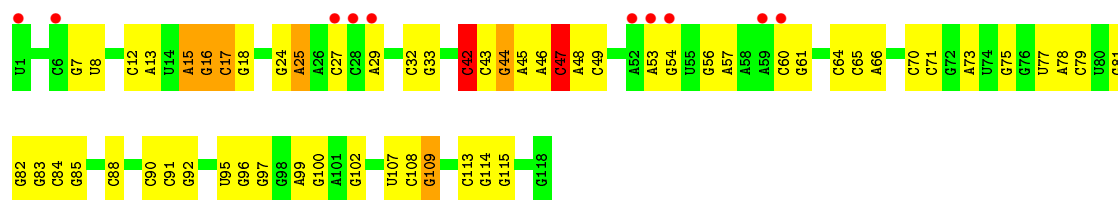


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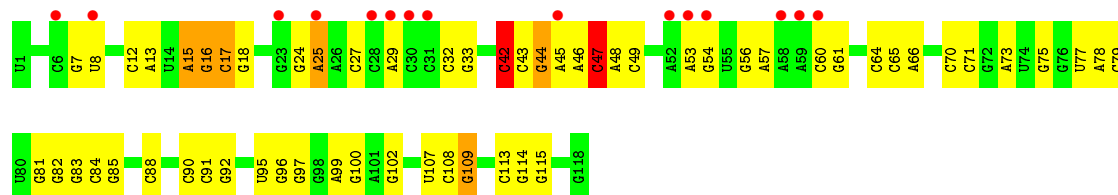


• Molecule 26: 5S ribosomal RNA

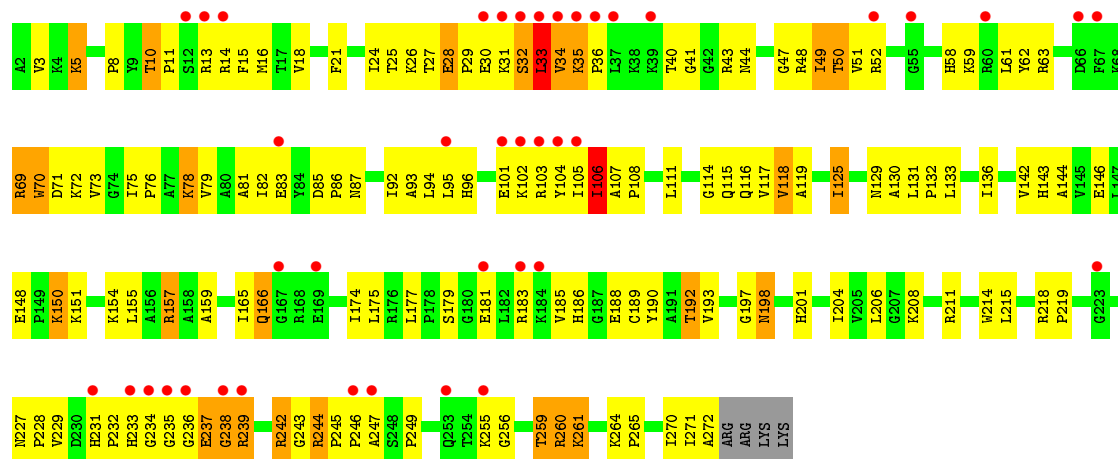




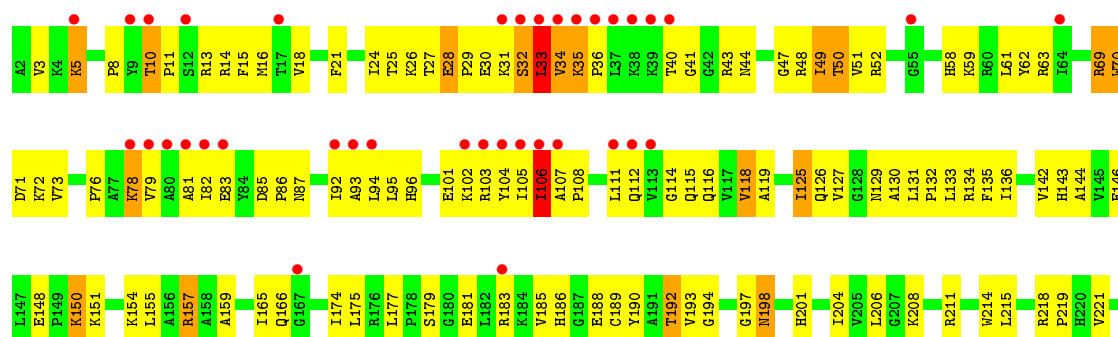
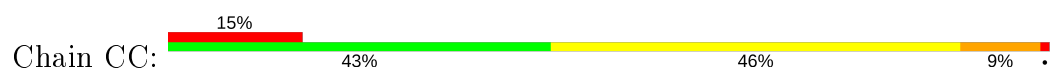
• Molecule 26: 5S ribosomal RNA



• Molecule 27: 50S ribosomal protein L2

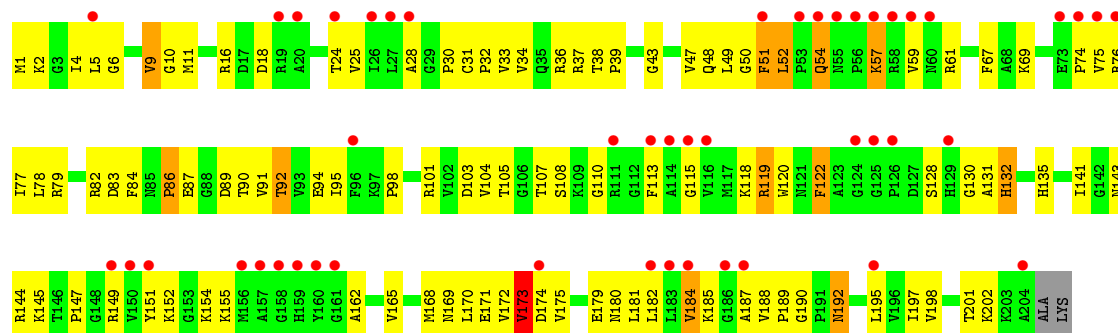


• Molecule 27: 50S ribosomal protein L2

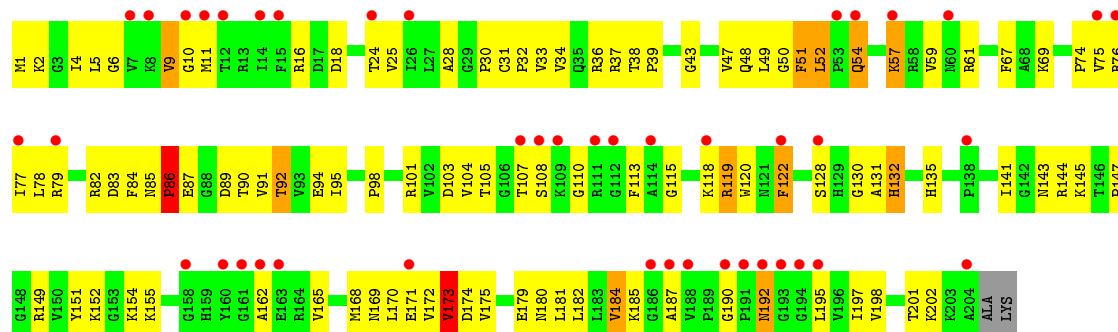




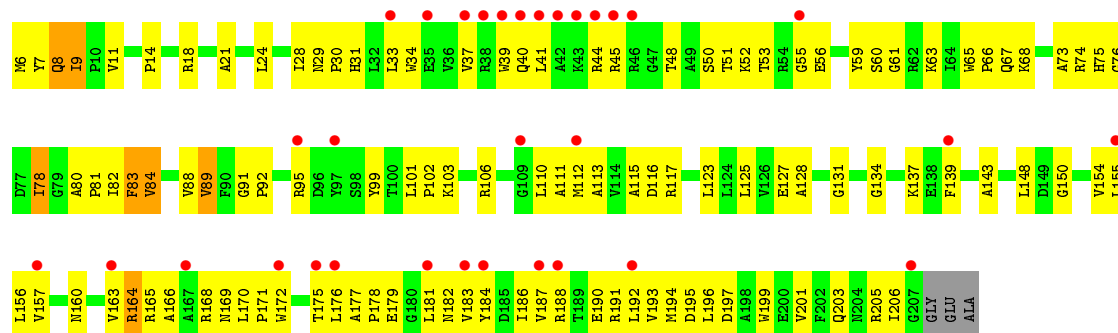
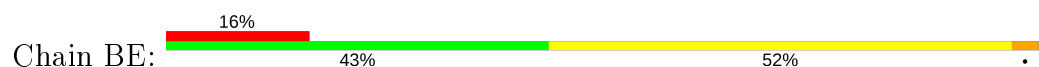
• Molecule 28: 50S ribosomal protein L3



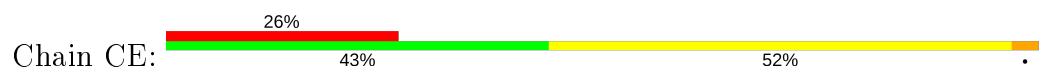
• Molecule 28: 50S ribosomal protein L3



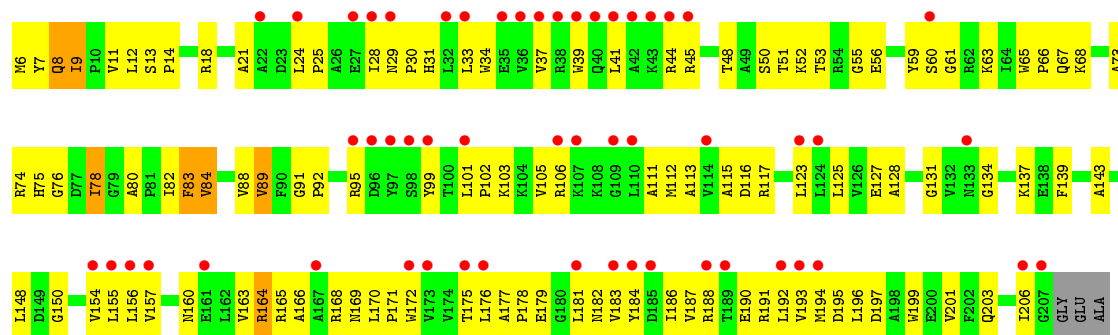
• Molecule 29: 50S ribosomal protein L4



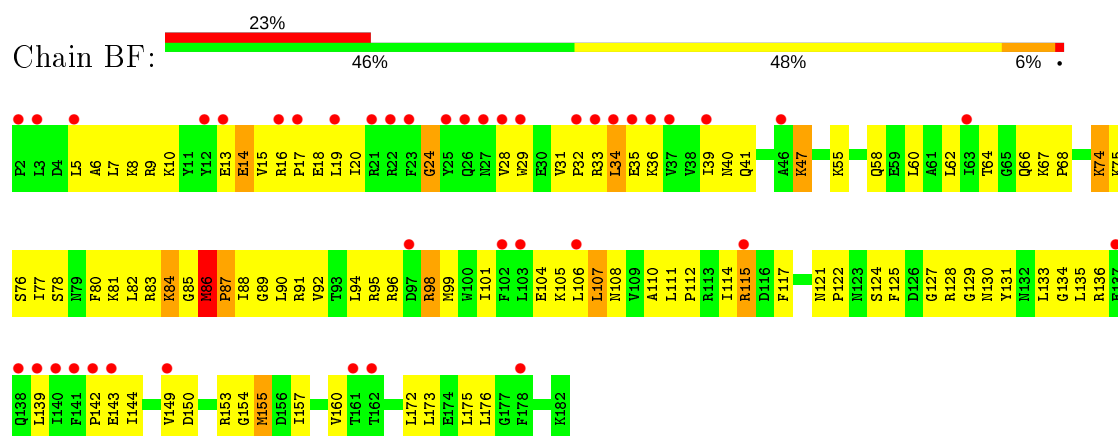
• Molecule 29: 50S ribosomal protein L4



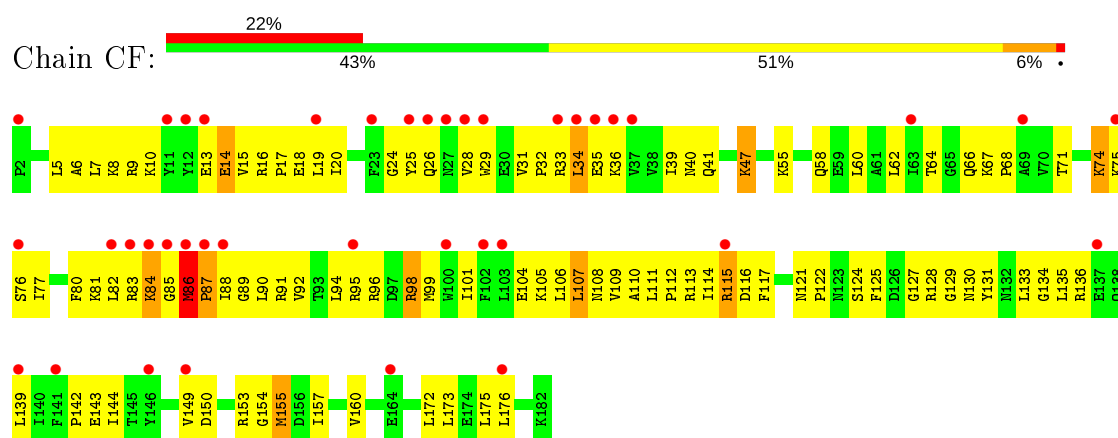




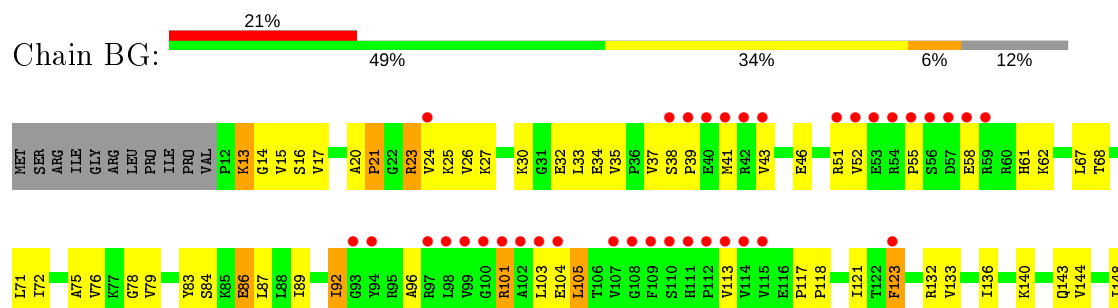
• Molecule 30: 50S ribosomal protein L5



• Molecule 30: 50S ribosomal protein L5



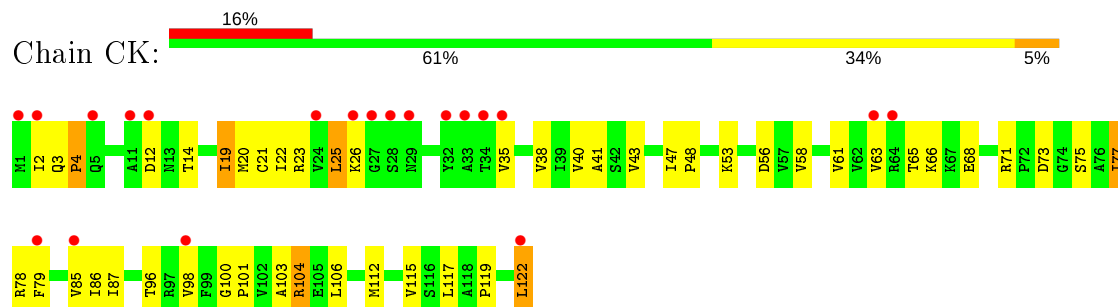
• Molecule 31: 50S ribosomal protein L6



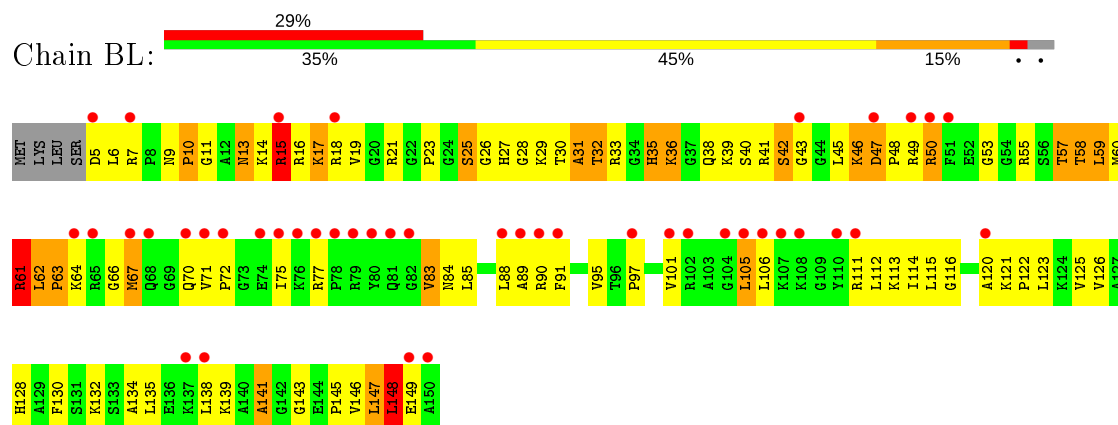




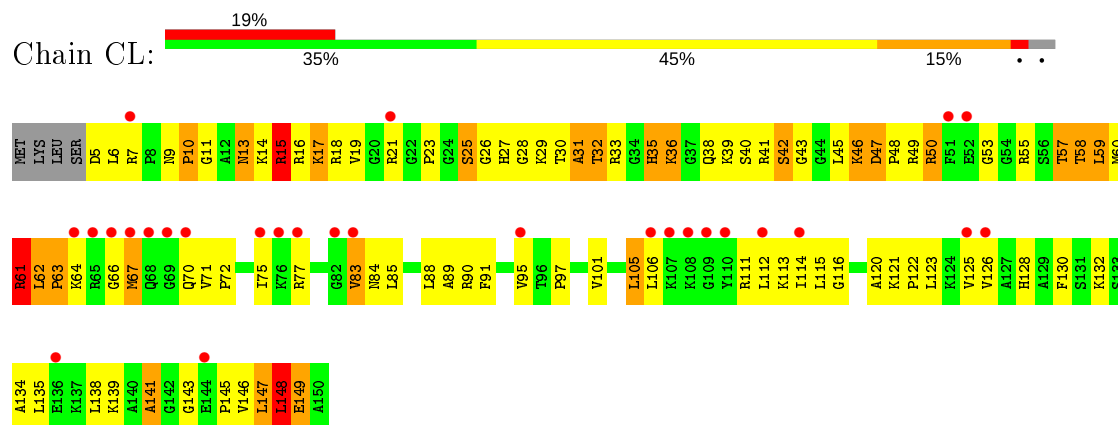
- Molecule 35: 50S ribosomal protein L14



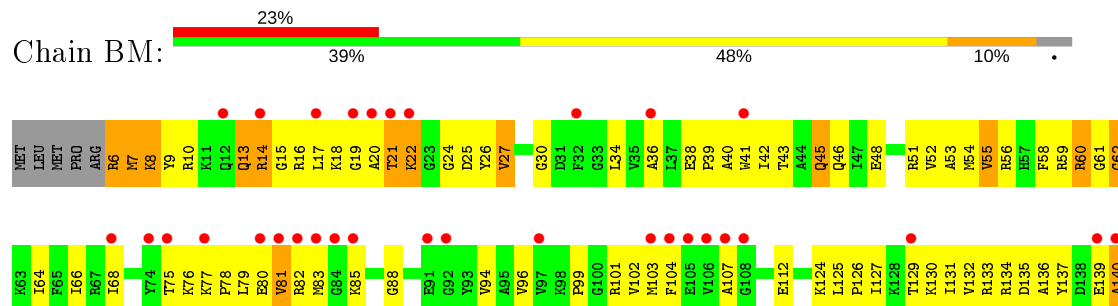
- Molecule 36: 50S ribosomal protein L15



- Molecule 36: 50S ribosomal protein L15



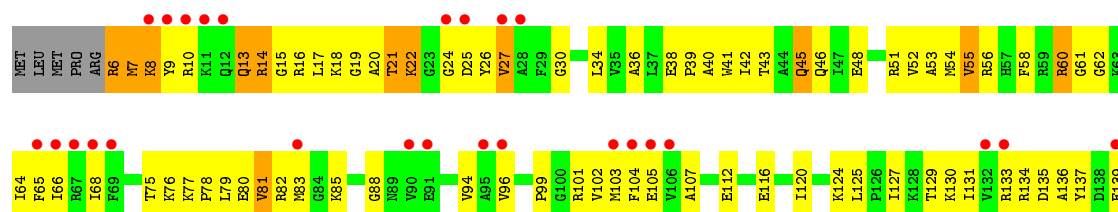
- Molecule 37: 50S ribosomal protein L16



Q141

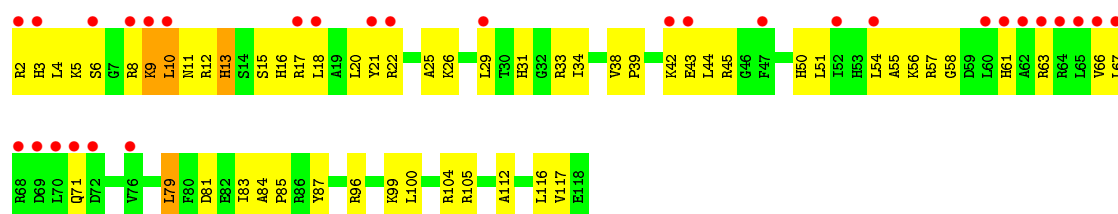
- Molecule 37: 50S ribosomal protein L16

Chain CM: 


A140  
Q141

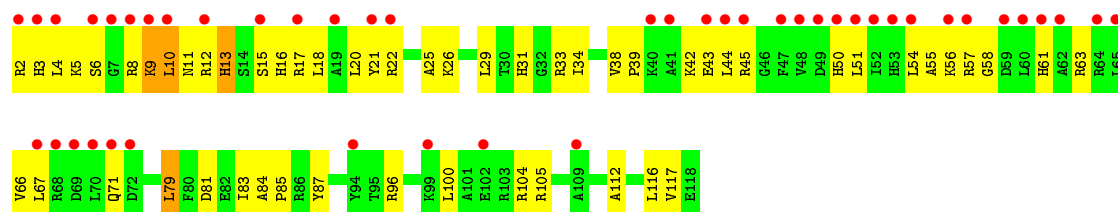
- Molecule 38: 50S ribosomal protein L17

Chain BN: 



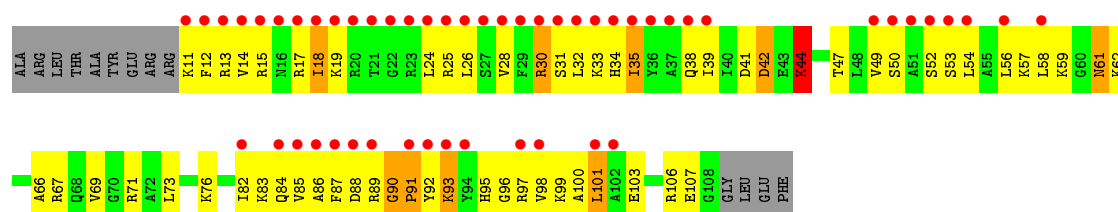
- Molecule 38: 50S ribosomal protein L17

Chain CN: 

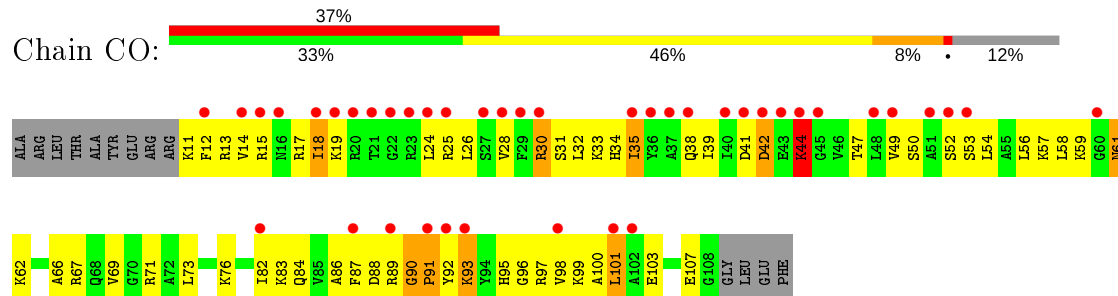


- Molecule 39: 50S ribosomal protein L18

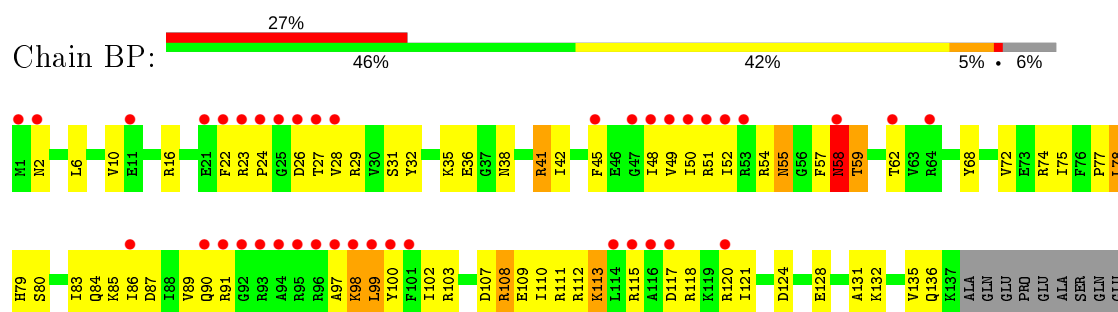
Chain BO: 

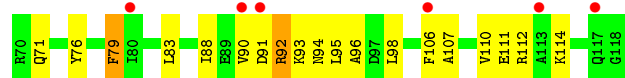
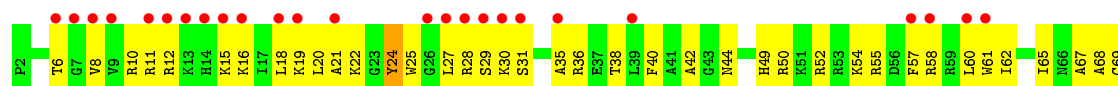


- Molecule 39: 50S ribosomal protein L18

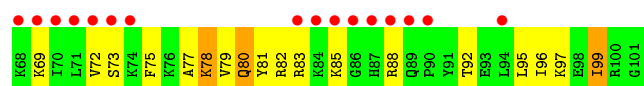
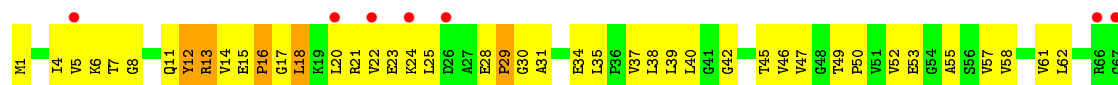


- Molecule 40: 50S ribosomal protein L19

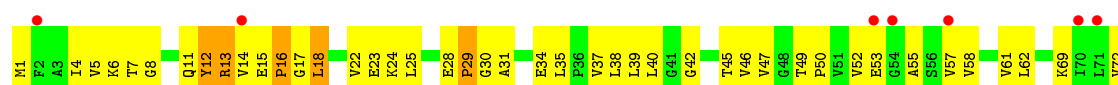




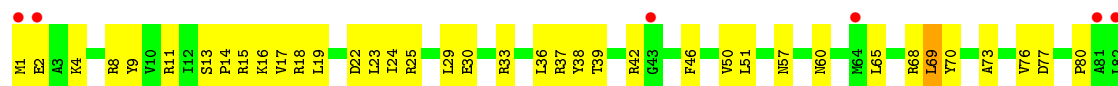
• Molecule 42: 50S ribosomal protein L21



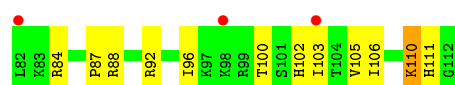
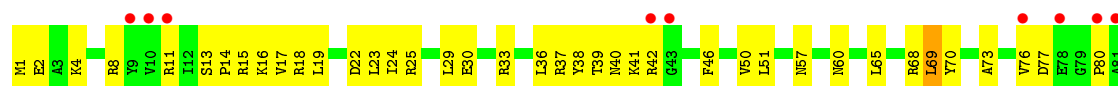
• Molecule 42: 50S ribosomal protein L21



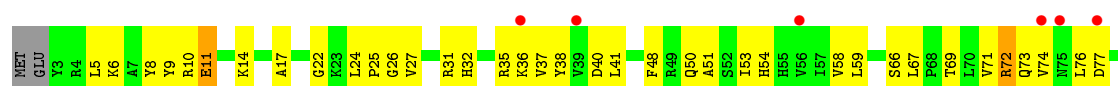
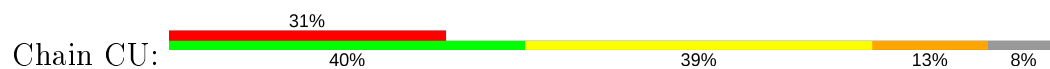
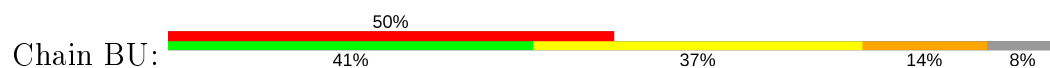
• Molecule 43: 50S ribosomal protein L22



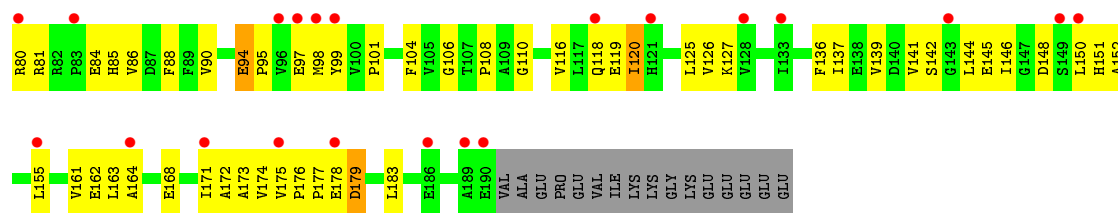
• Molecule 43: 50S ribosomal protein L22



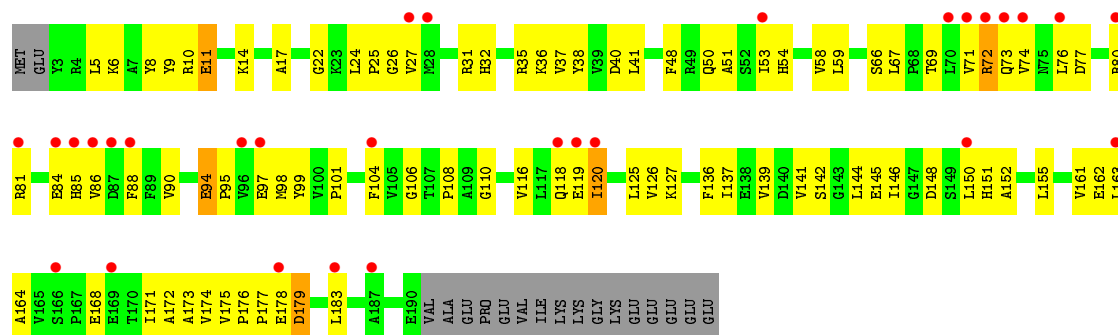
- Chain BT: 







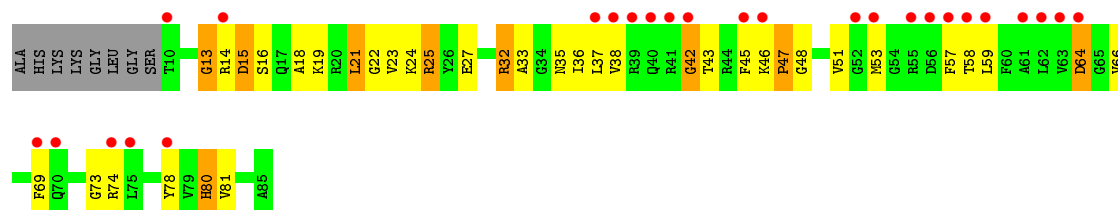
• Molecule 46: 50S ribosomal protein L25



• Molecule 47: 50S ribosomal protein L27



• Molecule 47: 50S ribosomal protein L27

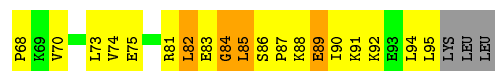


• Molecule 48: 50S ribosomal protein L28

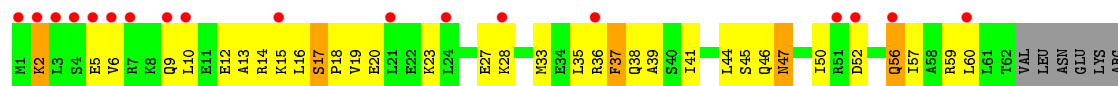




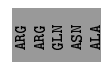
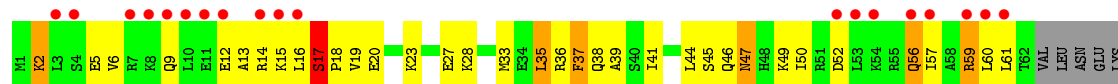
- Molecule 48: 50S ribosomal protein L28



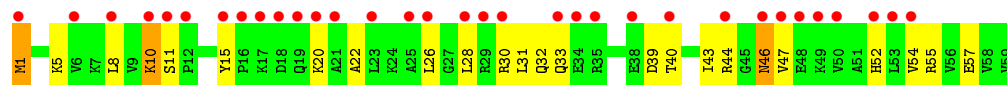
- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29



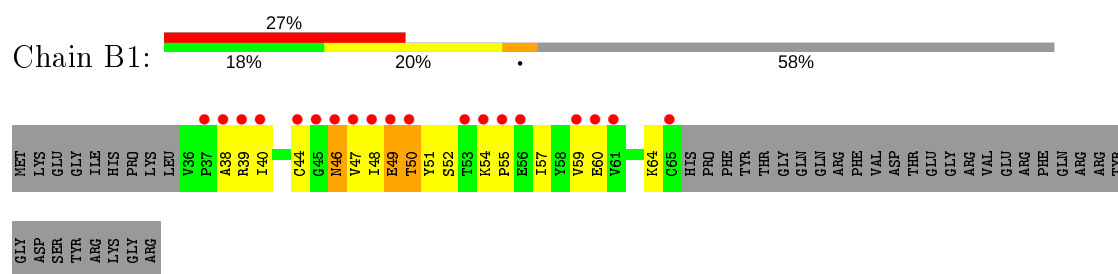
- Molecule 50: 50S ribosomal protein L30



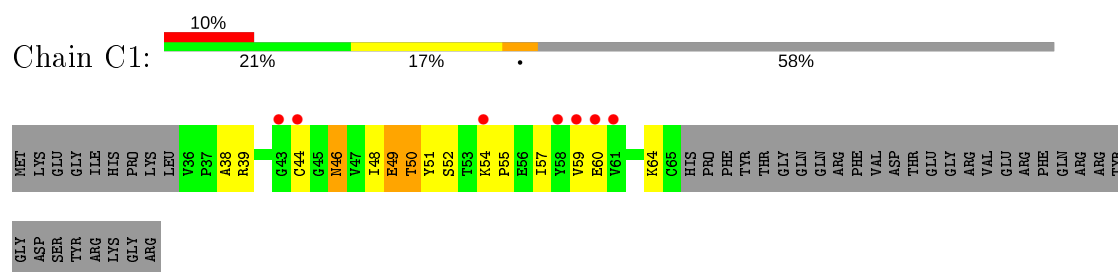
- Molecule 50: 50S ribosomal protein L30



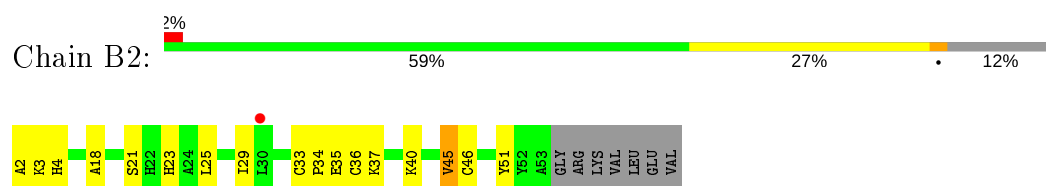
- Molecule 51: 50S ribosomal protein L31



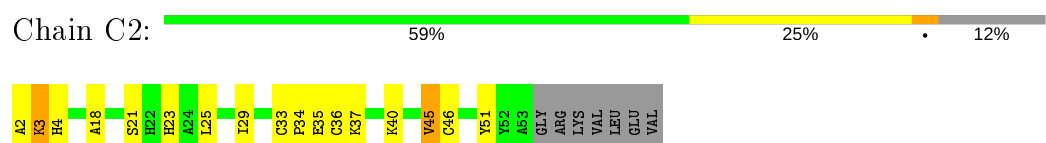
- Molecule 51: 50S ribosomal protein L31



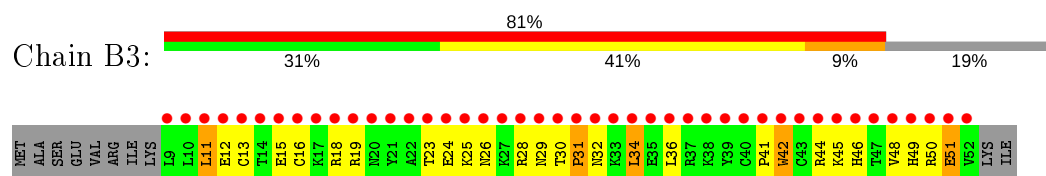
- Molecule 52: 50S ribosomal protein L32



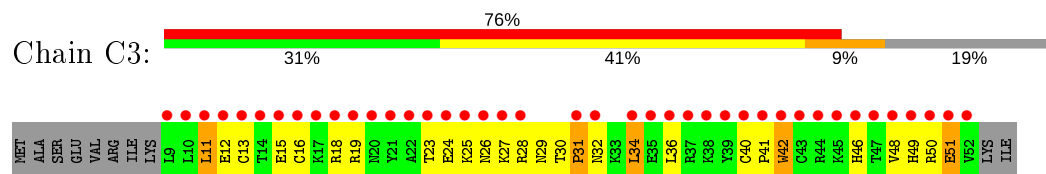
- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34

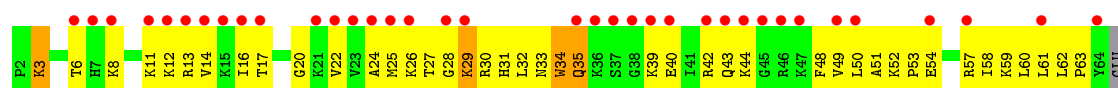




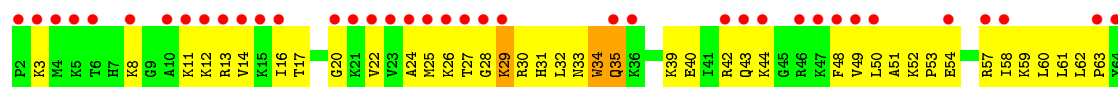
- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35

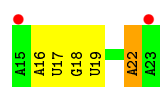


- Molecule 55: 50S ribosomal protein L35



GLU

- Molecule 56: messenger RNA (5'-R(\*AP\*AP\*UP\*GP\*UP\*AP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.38Å 452.70Å 617.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 3.62 89.69 – 3.51	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.95-3.62) 99.8 (89.69-3.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.6 _289, CNS	Depositor
R, $R_{free}$	0.260 , 0.291 0.252 , 0.285	Depositor DCC
$R_{free}$ test set	14480 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	130.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 95.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	294174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	0.16	0/36194	0.53	20/56493 (0.0%)
1	DA	0.16	0/36194	0.53	20/56493 (0.0%)
2	AB	0.20	0/1936	0.36	0/2609
2	DB	0.20	0/1936	0.36	0/2609
3	AC	0.20	0/1637	0.36	0/2205
3	DC	0.20	0/1637	0.36	0/2205
4	AD	0.20	0/1733	0.36	0/2318
4	DD	0.20	0/1733	0.36	0/2318
5	AE	0.20	0/1172	0.38	0/1576
5	DE	0.20	0/1172	0.38	0/1576
6	AF	0.20	0/856	0.38	0/1154
6	DF	0.21	0/856	0.38	0/1154
7	AG	0.20	0/1276	0.34	0/1709
7	DG	0.20	0/1276	0.34	0/1709
8	AH	0.20	0/1136	0.38	0/1527
8	DH	0.20	0/1136	0.38	0/1527
9	AI	0.21	0/1029	0.35	0/1378
9	DI	0.20	0/1029	0.36	0/1378
10	AJ	0.20	0/808	0.38	0/1085
10	DJ	0.20	0/808	0.38	0/1085
11	AK	0.20	0/900	0.37	0/1213
11	DK	0.20	0/900	0.37	0/1213
12	AL	0.21	0/987	0.41	0/1320
12	DL	0.21	0/987	0.41	0/1320
13	AM	0.19	0/944	0.39	0/1265
13	DM	0.19	0/944	0.39	0/1265
14	AN	0.20	0/501	0.34	0/664
14	DN	0.20	0/501	0.34	0/664
15	AO	0.20	0/745	0.34	0/992
15	DO	0.20	0/745	0.34	0/992
16	AP	0.21	0/717	0.38	0/963
16	DP	0.20	0/717	0.38	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.20	0/837	0.37	0/1117
17	DQ	0.20	0/837	0.37	0/1117
18	AR	0.21	0/579	0.36	0/768
18	DR	0.21	0/579	0.37	0/768
19	AS	0.20	0/643	0.37	0/865
19	DS	0.20	0/643	0.37	0/865
20	AT	0.20	0/764	0.34	0/1006
20	DT	0.20	0/764	0.34	0/1006
21	AU	0.18	0/213	0.35	0/277
21	DU	0.19	0/213	0.35	0/277
22	AV	0.21	0/2850	0.39	0/3829
22	DV	0.21	0/2850	0.39	0/3829
23	AW	0.16	0/1832	0.48	0/2855
23	DW	0.16	0/1832	0.48	0/2855
24	AX	0.17	0/167	0.63	0/259
25	BA	0.19	0/69437	0.57	47/108401 (0.0%)
25	CA	0.19	0/69437	0.58	49/108401 (0.0%)
26	BB	0.15	0/2853	0.53	3/4451 (0.1%)
26	CB	0.15	0/2853	0.53	3/4451 (0.1%)
27	BC	0.22	0/2154	0.42	0/2905
27	CC	0.23	0/2154	0.42	0/2905
28	BD	0.21	0/1596	0.40	0/2153
28	CD	0.21	0/1596	0.40	0/2153
29	BE	0.22	0/1621	0.38	0/2194
29	CE	0.22	0/1621	0.38	0/2194
30	BF	0.21	0/1500	0.39	0/2017
30	CF	0.21	0/1500	0.39	0/2017
31	BG	0.20	0/1245	0.39	0/1682
31	CG	0.20	0/1245	0.39	0/1682
32	BH	0.20	0/1147	0.38	0/1552
32	CH	0.20	0/1147	0.38	0/1552
33	BI	0.20	0/251	0.35	0/333
33	CI	0.20	0/251	0.35	0/333
34	BJ	0.20	0/1123	0.39	0/1515
34	CJ	0.20	0/1123	0.39	0/1515
35	BK	0.22	0/942	0.41	0/1268
35	CK	0.22	0/942	0.40	0/1268
36	BL	0.22	0/1131	0.45	0/1504
36	CL	0.22	0/1131	0.45	0/1504
37	BM	0.21	0/1099	0.40	0/1468
37	CM	0.21	0/1099	0.40	0/1468
38	BN	0.21	0/974	0.38	0/1302
38	CN	0.21	0/974	0.38	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	BO	0.21	0/778	0.38	0/1036
39	CO	0.21	0/778	0.38	0/1036
40	BP	0.21	0/1157	0.37	0/1544
40	CP	0.21	0/1157	0.37	0/1544
41	BQ	0.21	0/970	0.36	0/1290
41	CQ	0.21	0/970	0.36	0/1290
42	BR	0.21	0/790	0.38	0/1057
42	CR	0.21	0/790	0.38	0/1057
43	BS	0.21	0/902	0.39	0/1209
43	CS	0.21	0/902	0.38	0/1209
44	BT	0.22	0/739	0.41	0/993
44	CT	0.22	0/739	0.41	0/993
45	BU	0.21	0/788	0.39	0/1051
45	CU	0.21	0/788	0.40	0/1051
46	BV	0.20	0/1523	0.39	0/2068
46	CV	0.20	0/1523	0.39	0/2068
47	BW	0.21	0/613	0.38	0/816
47	CW	0.21	0/613	0.38	0/816
48	BX	0.21	0/701	0.44	0/932
48	CX	0.21	0/701	0.44	0/932
49	BY	0.22	0/522	0.42	0/690
49	CY	0.22	0/522	0.42	0/690
50	BZ	0.19	0/473	0.39	0/634
50	CZ	0.19	0/473	0.39	0/634
51	B1	0.20	0/228	0.39	0/309
51	C1	0.20	0/228	0.39	0/309
52	B2	0.19	0/418	0.41	0/567
52	C2	0.19	0/418	0.41	0/567
53	B3	0.20	0/387	0.39	0/518
53	C3	0.20	0/387	0.39	0/518
54	B4	0.22	0/427	0.41	0/561
54	C4	0.23	0/427	0.42	0/561
55	B5	0.22	0/515	0.39	0/679
55	C5	0.22	0/515	0.39	0/679
56	DX	0.18	0/217	0.57	0/337
All	All	0.19	0/318970	0.51	142/476370 (0.0%)

There are no bond length outliers.

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1558	A	P-O3'-C3'	10.58	132.39	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	1558	A	P-O3'-C3'	10.39	132.17	119.70
25	CA	1379	A	P-O3'-C3'	9.46	131.06	119.70
25	BA	1379	A	P-O3'-C3'	9.24	130.78	119.70
25	CA	1937	A	P-O3'-C3'	9.03	130.54	119.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32332	0	16318	653	0
1	DA	32332	0	16318	666	0
2	AB	1901	0	1951	88	0
2	DB	1901	0	1951	88	0
3	AC	1613	0	1677	86	0
3	DC	1613	0	1677	86	0
4	AD	1703	0	1765	88	0
4	DD	1703	0	1765	83	0
5	AE	1156	0	1213	58	0
5	DE	1156	0	1213	60	0
6	AF	843	0	857	41	0
6	DF	843	0	857	42	0
7	AG	1257	0	1296	60	0
7	DG	1257	0	1296	61	0
8	AH	1116	0	1177	48	0
8	DH	1116	0	1177	49	0
9	AI	1011	0	1043	60	0
9	DI	1011	0	1043	63	0
10	AJ	795	0	840	58	0
10	DJ	795	0	840	60	0
11	AK	885	0	904	49	0
11	DK	885	0	904	47	0
12	AL	971	0	1057	61	0
12	DL	971	0	1057	63	0
13	AM	934	0	992	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	DM	934	0	992	51	0
14	AN	492	0	532	33	0
14	DN	492	0	531	33	0
15	AO	734	0	771	35	0
15	DO	734	0	771	38	0
16	AP	701	0	720	31	0
16	DP	701	0	720	32	0
17	AQ	824	0	893	38	0
17	DQ	824	0	893	39	0
18	AR	574	0	644	30	0
18	DR	574	0	644	28	0
19	AS	630	0	652	59	0
19	DS	630	0	652	57	0
20	AT	762	0	859	30	0
20	DT	762	0	859	31	0
21	AU	209	0	221	9	0
21	DU	209	0	221	10	0
22	AV	2813	0	2823	180	0
22	DV	2813	0	2823	178	0
23	AW	1640	0	837	25	0
23	DW	1640	0	837	20	0
24	AX	149	0	77	6	0
25	BA	61997	0	31250	1317	0
25	CA	61997	0	31250	1301	0
26	BB	2551	0	1295	64	0
26	CB	2551	0	1295	62	0
27	BC	2104	0	2182	162	0
27	CC	2104	0	2182	167	0
28	BD	1563	0	1629	107	0
28	CD	1563	0	1629	105	0
29	BE	1586	0	1632	101	0
29	CE	1586	0	1632	101	0
30	BF	1475	0	1537	100	0
30	CF	1475	0	1537	104	0
31	BG	1222	0	1282	58	0
31	CG	1222	0	1282	61	0
32	BH	1132	0	1220	55	0
32	CH	1132	0	1220	57	0
33	BI	253	0	275	6	0
33	CI	253	0	275	6	0
34	BJ	1096	0	1168	66	0
34	CJ	1096	0	1168	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	BK	932	0	994	44	0
35	CK	932	0	994	46	0
36	BL	1114	0	1187	142	0
36	CL	1114	0	1187	144	0
37	BM	1079	0	1127	82	0
37	CM	1079	0	1127	80	0
38	BN	960	0	1021	62	0
38	CN	960	0	1021	59	0
39	BO	770	0	832	66	0
39	CO	770	0	832	67	0
40	BP	1143	0	1211	65	0
40	CP	1143	0	1211	70	0
41	BQ	953	0	1013	75	0
41	CQ	953	0	1013	74	0
42	BR	779	0	852	69	0
42	CR	779	0	852	69	0
43	BS	891	0	951	43	0
43	CS	891	0	951	41	0
44	BT	725	0	778	42	0
44	CT	725	0	778	45	0
45	BU	775	0	870	69	0
45	CU	775	0	870	70	0
46	BV	1491	0	1513	75	0
46	CV	1491	0	1513	74	0
47	BW	605	0	628	36	0
47	CW	605	0	628	36	0
48	BX	694	0	764	63	0
48	CX	694	0	764	67	0
49	BY	520	0	575	36	0
49	CY	520	0	575	37	0
50	BZ	468	0	523	21	0
50	CZ	468	0	523	20	0
51	B1	225	0	225	16	0
51	C1	225	0	225	19	0
52	B2	404	0	420	18	0
52	C2	404	0	420	19	0
53	B3	380	0	391	22	0
53	C3	380	0	391	24	0
54	B4	419	0	467	26	0
54	C4	419	0	467	24	0
55	B5	507	0	576	54	0
55	C5	507	0	576	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DX	193	0	99	4	0
57	AA	64	0	0	0	0
57	AT	1	0	0	0	0
57	AV	1	0	0	0	0
57	AW	3	0	0	0	0
57	B2	1	0	0	0	0
57	BA	176	0	0	0	0
57	BB	2	0	0	0	0
57	BK	1	0	0	0	0
57	BM	1	0	0	0	0
57	CA	125	0	0	0	0
57	CB	2	0	0	0	0
57	CM	1	0	0	0	0
57	CY	1	0	0	0	0
57	DA	30	0	0	0	0
57	DW	1	0	0	0	0
58	AD	1	0	0	0	0
58	AN	1	0	0	0	0
58	DD	1	0	0	0	0
58	DN	1	0	0	0	0
All	All	294174	0	201035	9013	0

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

The worst 5 of 9013 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)
4:AD:166:LYS:HE2	27:CC:134:ARG:HH21	1.20	1.07
36:CL:128:HIS:HA	36:CL:147:LEU:HB3	1.36	1.07
36:BL:128:HIS:HA	36:BL:147:LEU:HB3	1.36	1.07
35:BK:3:GLN:HB2	35:BK:4:PRO:HD2	1.40	1.03
22:DV:302:ILE:HG22	22:DV:303:ARG:H	1.21	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/234 (99%)	197 (85%)	28 (12%)	7 (3%)	4	32
2	DB	232/234 (99%)	197 (85%)	28 (12%)	7 (3%)	4	32
3	AC	204/206 (99%)	158 (78%)	36 (18%)	10 (5%)	2	21
3	DC	204/206 (99%)	158 (78%)	36 (18%)	10 (5%)	2	21
4	AD	206/208 (99%)	168 (82%)	29 (14%)	9 (4%)	2	23
4	DD	206/208 (99%)	168 (82%)	29 (14%)	9 (4%)	2	23
5	AE	149/151 (99%)	129 (87%)	18 (12%)	2 (1%)	12	49
5	DE	149/151 (99%)	129 (87%)	18 (12%)	2 (1%)	12	49
6	AF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	54
6	DF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	54
7	AG	153/155 (99%)	132 (86%)	19 (12%)	2 (1%)	12	49
7	DG	153/155 (99%)	132 (86%)	19 (12%)	2 (1%)	12	49
8	AH	136/138 (99%)	120 (88%)	15 (11%)	1 (1%)	22	61
8	DH	136/138 (99%)	120 (88%)	15 (11%)	1 (1%)	22	61
9	AI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	6	37
9	DI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	6	37
10	AJ	96/98 (98%)	78 (81%)	13 (14%)	5 (5%)	2	20
10	DJ	96/98 (98%)	79 (82%)	12 (12%)	5 (5%)	2	20
11	AK	117/119 (98%)	94 (80%)	20 (17%)	3 (3%)	5	35
11	DK	117/119 (98%)	95 (81%)	19 (16%)	3 (3%)	5	35
12	AL	122/124 (98%)	92 (75%)	25 (20%)	5 (4%)	3	25
12	DL	122/124 (98%)	92 (75%)	25 (20%)	5 (4%)	3	25
13	AM	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	2	20
13	DM	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	2	20
14	AN	58/60 (97%)	49 (84%)	5 (9%)	4 (7%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	DN	58/60 (97%)	49 (84%)	5 (9%)	4 (7%)	1	14
15	AO	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
15	DO	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
16	AP	81/83 (98%)	66 (82%)	14 (17%)	1 (1%)	13	51
16	DP	81/83 (98%)	66 (82%)	14 (17%)	1 (1%)	13	51
17	AQ	97/99 (98%)	83 (86%)	12 (12%)	2 (2%)	7	40
17	DQ	97/99 (98%)	83 (86%)	12 (12%)	2 (2%)	7	40
18	AR	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	10	47
18	DR	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	10	47
19	AS	76/78 (97%)	58 (76%)	13 (17%)	5 (7%)	1	16
19	DS	76/78 (97%)	58 (76%)	13 (17%)	5 (7%)	1	16
20	AT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	25
20	DT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	25
21	AU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	23
21	DU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	23
22	AV	352/354 (99%)	290 (82%)	50 (14%)	12 (3%)	3	30
22	DV	352/354 (99%)	289 (82%)	52 (15%)	11 (3%)	4	32
27	BC	269/275 (98%)	216 (80%)	37 (14%)	16 (6%)	1	17
27	CC	269/275 (98%)	216 (80%)	37 (14%)	16 (6%)	1	17
28	BD	202/206 (98%)	168 (83%)	26 (13%)	8 (4%)	3	26
28	CD	202/206 (98%)	168 (83%)	26 (13%)	8 (4%)	3	26
29	BE	200/205 (98%)	163 (82%)	29 (14%)	8 (4%)	3	26
29	CE	200/205 (98%)	163 (82%)	29 (14%)	8 (4%)	3	26
30	BF	179/181 (99%)	133 (74%)	38 (21%)	8 (4%)	2	23
30	CF	179/181 (99%)	133 (74%)	38 (21%)	8 (4%)	2	23
31	BG	157/180 (87%)	129 (82%)	23 (15%)	5 (3%)	4	31
31	CG	157/180 (87%)	129 (82%)	23 (15%)	5 (3%)	4	31
32	BH	143/148 (97%)	115 (80%)	21 (15%)	7 (5%)	2	21
32	CH	143/148 (97%)	115 (80%)	21 (15%)	7 (5%)	2	21
33	BI	28/173 (16%)	27 (96%)	1 (4%)	0	100	100
33	CI	28/173 (16%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BJ	135/139 (97%)	110 (82%)	16 (12%)	9 (7%)	1	15
34	CJ	135/139 (97%)	109 (81%)	17 (13%)	9 (7%)	1	15
35	BK	120/122 (98%)	105 (88%)	13 (11%)	2 (2%)	9	44
35	CK	120/122 (98%)	105 (88%)	13 (11%)	2 (2%)	9	44
36	BL	144/150 (96%)	97 (67%)	25 (17%)	22 (15%)	0	3
36	CL	144/150 (96%)	97 (67%)	25 (17%)	22 (15%)	0	3
37	BM	134/141 (95%)	95 (71%)	23 (17%)	16 (12%)	0	5
37	CM	134/141 (95%)	95 (71%)	23 (17%)	16 (12%)	0	5
38	BN	115/117 (98%)	100 (87%)	11 (10%)	4 (4%)	3	30
38	CN	115/117 (98%)	101 (88%)	10 (9%)	4 (4%)	3	30
39	BO	96/111 (86%)	65 (68%)	20 (21%)	11 (12%)	0	6
39	CO	96/111 (86%)	64 (67%)	21 (22%)	11 (12%)	0	6
40	BP	135/146 (92%)	106 (78%)	21 (16%)	8 (6%)	1	17
40	CP	135/146 (92%)	107 (79%)	20 (15%)	8 (6%)	1	17
41	BQ	114/116 (98%)	103 (90%)	10 (9%)	1 (1%)	17	56
41	CQ	114/116 (98%)	104 (91%)	9 (8%)	1 (1%)	17	56
42	BR	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	17
42	CR	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	17
43	BS	110/112 (98%)	92 (84%)	17 (16%)	1 (1%)	17	56
43	CS	110/112 (98%)	92 (84%)	17 (16%)	1 (1%)	17	56
44	BT	90/96 (94%)	81 (90%)	7 (8%)	2 (2%)	6	39
44	CT	90/96 (94%)	81 (90%)	7 (8%)	2 (2%)	6	39
45	BU	98/109 (90%)	62 (63%)	26 (26%)	10 (10%)	0	7
45	CU	98/109 (90%)	63 (64%)	25 (26%)	10 (10%)	0	7
46	BV	186/206 (90%)	143 (77%)	34 (18%)	9 (5%)	2	22
46	CV	186/206 (90%)	143 (77%)	34 (18%)	9 (5%)	2	22
47	BW	74/84 (88%)	56 (76%)	12 (16%)	6 (8%)	1	11
47	CW	74/84 (88%)	57 (77%)	11 (15%)	6 (8%)	1	11
48	BX	86/98 (88%)	59 (69%)	19 (22%)	8 (9%)	0	9
48	CX	86/98 (88%)	59 (69%)	19 (22%)	8 (9%)	0	9
49	BY	60/72 (83%)	47 (78%)	11 (18%)	2 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	CY	60/72 (83%)	47 (78%)	11 (18%)	2 (3%)	4	31
50	BZ	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
50	CZ	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
51	B1	28/71 (39%)	17 (61%)	8 (29%)	3 (11%)	0	7
51	C1	28/71 (39%)	17 (61%)	8 (29%)	3 (11%)	0	7
52	B2	50/59 (85%)	40 (80%)	8 (16%)	2 (4%)	3	26
52	C2	50/59 (85%)	40 (80%)	8 (16%)	2 (4%)	3	26
53	B3	42/54 (78%)	33 (79%)	4 (10%)	5 (12%)	0	5
53	C3	42/54 (78%)	33 (79%)	4 (10%)	5 (12%)	0	5
54	B4	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
54	C4	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
55	B5	61/64 (95%)	44 (72%)	11 (18%)	6 (10%)	0	8
55	C5	61/64 (95%)	44 (72%)	11 (18%)	6 (10%)	0	8
All	All	11898/12752 (93%)	9614 (81%)	1747 (15%)	537 (4%)	2	23

5 of 537 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	15	THR
4	AD	137	SER
13	AM	106	ASN
14	AN	26	ARG
19	AS	28	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/202 (100%)	193 (96%)	9 (4%)	27	62
2	DB	202/202 (100%)	193 (96%)	9 (4%)	27	62
3	AC	160/160 (100%)	154 (96%)	6 (4%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DC	160/160 (100%)	154 (96%)	6 (4%)	33	65
4	AD	180/180 (100%)	171 (95%)	9 (5%)	24	58
4	DD	180/180 (100%)	171 (95%)	9 (5%)	24	58
5	AE	116/116 (100%)	106 (91%)	10 (9%)	10	41
5	DE	116/116 (100%)	106 (91%)	10 (9%)	10	41
6	AF	90/90 (100%)	86 (96%)	4 (4%)	28	62
6	DF	90/90 (100%)	86 (96%)	4 (4%)	28	62
7	AG	126/126 (100%)	126 (100%)	0	100	100
7	DG	126/126 (100%)	126 (100%)	0	100	100
8	AH	119/119 (100%)	114 (96%)	5 (4%)	30	63
8	DH	119/119 (100%)	114 (96%)	5 (4%)	30	63
9	AI	98/98 (100%)	92 (94%)	6 (6%)	18	53
9	DI	98/98 (100%)	92 (94%)	6 (6%)	18	53
10	AJ	88/88 (100%)	80 (91%)	8 (9%)	9	39
10	DJ	88/88 (100%)	80 (91%)	8 (9%)	9	39
11	AK	90/90 (100%)	87 (97%)	3 (3%)	38	69
11	DK	90/90 (100%)	87 (97%)	3 (3%)	38	69
12	AL	104/104 (100%)	95 (91%)	9 (9%)	10	41
12	DL	104/104 (100%)	95 (91%)	9 (9%)	10	41
13	AM	94/94 (100%)	88 (94%)	6 (6%)	17	51
13	DM	94/94 (100%)	88 (94%)	6 (6%)	17	51
14	AN	49/49 (100%)	46 (94%)	3 (6%)	18	53
14	DN	49/49 (100%)	46 (94%)	3 (6%)	18	53
15	AO	79/79 (100%)	75 (95%)	4 (5%)	24	58
15	DO	79/79 (100%)	75 (95%)	4 (5%)	24	58
16	AP	72/72 (100%)	69 (96%)	3 (4%)	30	63
16	DP	72/72 (100%)	69 (96%)	3 (4%)	30	63
17	AQ	94/94 (100%)	92 (98%)	2 (2%)	53	78
17	DQ	94/94 (100%)	92 (98%)	2 (2%)	53	78
18	AR	61/61 (100%)	59 (97%)	2 (3%)	38	69
18	DR	61/61 (100%)	59 (97%)	2 (3%)	38	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AS	69/69 (100%)	60 (87%)	9 (13%)	4	24
19	DS	69/69 (100%)	60 (87%)	9 (13%)	4	24
20	AT	76/76 (100%)	73 (96%)	3 (4%)	32	65
20	DT	76/76 (100%)	73 (96%)	3 (4%)	32	65
21	AU	19/19 (100%)	19 (100%)	0	100	100
21	DU	19/19 (100%)	19 (100%)	0	100	100
22	AV	299/299 (100%)	271 (91%)	28 (9%)	8	37
22	DV	299/299 (100%)	272 (91%)	27 (9%)	9	39
27	BC	213/217 (98%)	194 (91%)	19 (9%)	9	40
27	CC	213/217 (98%)	195 (92%)	18 (8%)	10	41
28	BD	165/166 (99%)	154 (93%)	11 (7%)	16	50
28	CD	165/166 (99%)	153 (93%)	12 (7%)	14	46
29	BE	161/162 (99%)	155 (96%)	6 (4%)	34	66
29	CE	161/162 (99%)	155 (96%)	6 (4%)	34	66
30	BF	155/155 (100%)	144 (93%)	11 (7%)	14	47
30	CF	155/155 (100%)	144 (93%)	11 (7%)	14	47
31	BG	132/148 (89%)	125 (95%)	7 (5%)	22	57
31	CG	132/148 (89%)	125 (95%)	7 (5%)	22	57
32	BH	122/124 (98%)	116 (95%)	6 (5%)	25	59
32	CH	122/124 (98%)	116 (95%)	6 (5%)	25	59
33	BI	27/135 (20%)	26 (96%)	1 (4%)	34	66
33	CI	27/135 (20%)	26 (96%)	1 (4%)	34	66
34	BJ	116/118 (98%)	109 (94%)	7 (6%)	19	53
34	CJ	116/118 (98%)	109 (94%)	7 (6%)	19	53
35	BK	100/100 (100%)	94 (94%)	6 (6%)	19	53
35	CK	100/100 (100%)	94 (94%)	6 (6%)	19	53
36	BL	112/116 (97%)	98 (88%)	14 (12%)	4	25
36	CL	112/116 (97%)	98 (88%)	14 (12%)	4	25
37	BM	106/111 (96%)	98 (92%)	8 (8%)	13	45
37	CM	106/111 (96%)	98 (92%)	8 (8%)	13	45
38	BN	100/100 (100%)	96 (96%)	4 (4%)	31	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	CN	100/100 (100%)	96 (96%)	4 (4%)	31	64
39	BO	77/87 (88%)	71 (92%)	6 (8%)	12	44
39	CO	77/87 (88%)	71 (92%)	6 (8%)	12	44
40	BP	121/128 (94%)	110 (91%)	11 (9%)	9	39
40	CP	121/128 (94%)	110 (91%)	11 (9%)	9	39
41	BQ	92/92 (100%)	90 (98%)	2 (2%)	52	77
41	CQ	92/92 (100%)	90 (98%)	2 (2%)	52	77
42	BR	82/82 (100%)	76 (93%)	6 (7%)	14	46
42	CR	82/82 (100%)	76 (93%)	6 (7%)	14	46
43	BS	91/91 (100%)	87 (96%)	4 (4%)	28	62
43	CS	91/91 (100%)	87 (96%)	4 (4%)	28	62
44	BT	74/78 (95%)	69 (93%)	5 (7%)	16	49
44	CT	74/78 (95%)	69 (93%)	5 (7%)	16	49
45	BU	84/90 (93%)	78 (93%)	6 (7%)	14	47
45	CU	84/90 (93%)	78 (93%)	6 (7%)	14	47
46	BV	163/179 (91%)	159 (98%)	4 (2%)	47	74
46	CV	163/179 (91%)	159 (98%)	4 (2%)	47	74
47	BW	61/66 (92%)	57 (93%)	4 (7%)	16	50
47	CW	61/66 (92%)	57 (93%)	4 (7%)	16	50
48	BX	73/83 (88%)	64 (88%)	9 (12%)	4	26
48	CX	73/83 (88%)	64 (88%)	9 (12%)	4	26
49	BY	58/67 (87%)	53 (91%)	5 (9%)	10	41
49	CY	58/67 (87%)	52 (90%)	6 (10%)	7	33
50	BZ	51/51 (100%)	48 (94%)	3 (6%)	19	54
50	CZ	51/51 (100%)	48 (94%)	3 (6%)	19	54
51	B1	27/63 (43%)	25 (93%)	2 (7%)	13	45
51	C1	27/63 (43%)	25 (93%)	2 (7%)	13	45
52	B2	45/51 (88%)	44 (98%)	1 (2%)	52	77
52	C2	45/51 (88%)	44 (98%)	1 (2%)	52	77
53	B3	43/52 (83%)	39 (91%)	4 (9%)	9	38
53	C3	43/52 (83%)	39 (91%)	4 (9%)	9	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	B4	41/41 (100%)	37 (90%)	4 (10%)	8	35
54	C4	41/41 (100%)	37 (90%)	4 (10%)	8	35
55	B5	53/54 (98%)	52 (98%)	1 (2%)	57	80
55	C5	53/54 (98%)	52 (98%)	1 (2%)	57	80
All	All	10060/10584 (95%)	9448 (94%)	612 (6%)	18	53

5 of 612 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BW	80	HIS
30	CF	18	GLU
15	DO	82	ILE
48	BX	89	GLU
27	CC	33	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 247 such sidechains are listed below:

Mol	Chain	Res	Type
48	BX	66	HIS
29	CE	31	HIS
10	DJ	84	GLN
50	BZ	46	ASN
27	CC	126	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	198 (13%)	14 (0%)
1	DA	1503/1504 (99%)	198 (13%)	14 (0%)
23	AW	76/77 (98%)	9 (11%)	0
23	DW	76/77 (98%)	9 (11%)	0
24	AX	6/7 (85%)	1 (16%)	0
25	BA	2878/2879 (99%)	429 (14%)	18 (0%)
25	CA	2878/2879 (99%)	430 (14%)	19 (0%)
26	BB	118/119 (99%)	12 (10%)	0
26	CB	118/119 (99%)	12 (10%)	0
56	DX	8/9 (88%)	2 (25%)	0
All	All	9164/9174 (99%)	1300 (14%)	65 (0%)

5 of 1300 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2491	U
25	CA	1210	A
1	DA	1064	G
25	BA	2610	C
25	CA	332	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 414 ligands modelled in this entry, 414 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1504/1504 (100%)	0.36	136 (9%) 9 5	99, 172, 294, 492	0
1	DA	1504/1504 (100%)	0.34	154 (10%) 6 4	92, 174, 297, 495	0
2	AB	234/234 (100%)	2.75	122 (52%) 0 0	141, 239, 344, 376	0
2	DB	234/234 (100%)	2.00	95 (40%) 0 0	122, 210, 294, 383	0
3	AC	206/206 (100%)	0.20	16 (7%) 13 8	116, 224, 305, 369	0
3	DC	206/206 (100%)	0.13	15 (7%) 15 9	104, 199, 279, 314	0
4	AD	208/208 (100%)	1.28	60 (28%) 0 0	103, 180, 260, 329	0
4	DD	208/208 (100%)	0.79	38 (18%) 1 0	100, 192, 286, 330	0
5	AE	151/151 (100%)	0.09	10 (6%) 18 10	115, 194, 274, 320	0
5	DE	151/151 (100%)	0.17	11 (7%) 15 9	112, 173, 263, 312	0
6	AF	101/101 (100%)	0.27	11 (10%) 5 3	121, 210, 285, 343	0
6	DF	101/101 (100%)	0.27	9 (8%) 9 5	99, 169, 251, 279	0
7	AG	155/155 (100%)	0.94	33 (21%) 0 0	115, 218, 295, 339	0
7	DG	155/155 (100%)	0.28	21 (13%) 3 2	123, 203, 287, 375	0
8	AH	138/138 (100%)	1.44	43 (31%) 0 0	97, 193, 268, 342	0
8	DH	138/138 (100%)	1.26	42 (30%) 0 0	110, 185, 269, 354	0
9	AI	127/127 (100%)	3.34	81 (63%) 0 0	114, 236, 311, 356	0
9	DI	127/127 (100%)	2.40	64 (50%) 0 0	112, 221, 309, 373	0
10	AJ	98/98 (100%)	1.45	32 (32%) 0 0	149, 231, 311, 408	0
10	DJ	98/98 (100%)	1.98	39 (39%) 0 0	135, 215, 306, 339	0
11	AK	119/119 (100%)	0.76	24 (20%) 1 0	92, 173, 278, 341	0
11	DK	119/119 (100%)	0.41	23 (19%) 1 0	107, 164, 241, 317	0
12	AL	124/124 (100%)	0.35	8 (6%) 18 11	94, 147, 231, 327	0
12	DL	124/124 (100%)	0.43	15 (12%) 4 3	77, 151, 233, 395	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	117/117 (100%)	2.21	53 (45%)	0	0	142, 235, 332, 396	0
13	DM	117/117 (100%)	2.06	54 (46%)	0	0	121, 218, 300, 332	0
14	AN	60/60 (100%)	2.41	29 (48%)	0	0	135, 207, 347, 354	0
14	DN	60/60 (100%)	2.24	26 (43%)	0	0	112, 186, 256, 288	0
15	AO	88/88 (100%)	1.05	24 (27%)	0	0	113, 177, 253, 318	0
15	DO	88/88 (100%)	0.86	20 (22%)	0	0	76, 170, 222, 312	0
16	AP	83/83 (100%)	2.77	53 (63%)	0	0	96, 168, 232, 363	0
16	DP	83/83 (100%)	3.54	58 (69%)	0	0	119, 196, 272, 331	0
17	AQ	99/99 (100%)	1.13	26 (26%)	0	0	114, 162, 240, 267	0
17	DQ	99/99 (100%)	0.85	19 (19%)	1	0	111, 176, 266, 362	0
18	AR	70/70 (100%)	1.44	24 (34%)	0	0	122, 206, 275, 318	0
18	DR	70/70 (100%)	0.89	20 (28%)	0	0	96, 176, 241, 287	0
19	AS	78/78 (100%)	2.98	43 (55%)	0	0	132, 234, 327, 378	0
19	DS	78/78 (100%)	1.89	31 (39%)	0	0	143, 217, 319, 367	0
20	AT	99/99 (100%)	0.92	23 (23%)	0	0	103, 160, 245, 342	0
20	DT	99/99 (100%)	2.79	60 (60%)	0	0	125, 200, 284, 326	0
21	AU	24/24 (100%)	10.20	24 (100%)	0	0	148, 244, 303, 312	0
21	DU	24/24 (100%)	6.18	24 (100%)	0	0	131, 228, 310, 325	0
22	AV	354/354 (100%)	0.61	58 (16%)	1	1	75, 180, 316, 397	0
22	DV	354/354 (100%)	0.70	51 (14%)	2	1	60, 172, 340, 419	0
23	AW	77/77 (100%)	-0.48	0	100	100	117, 172, 228, 282	0
23	DW	77/77 (100%)	-0.51	1 (1%)	77	64	114, 152, 205, 327	0
24	AX	7/7 (100%)	0.55	0	100	100	131, 140, 172, 230	0
25	BA	2879/2879 (100%)	0.28	187 (6%)	18	11	66, 133, 337, 509	0
25	CA	2879/2879 (100%)	0.36	210 (7%)	15	9	63, 130, 320, 567	0
26	BB	119/119 (100%)	0.21	10 (8%)	11	7	132, 211, 322, 386	0
26	CB	119/119 (100%)	0.34	15 (12%)	3	2	139, 208, 302, 358	0
27	BC	271/275 (98%)	0.67	41 (15%)	2	1	52, 127, 184, 306	0
27	CC	271/275 (98%)	0.69	40 (14%)	2	1	44, 112, 187, 280	0
28	BD	204/206 (99%)	0.88	47 (23%)	0	0	75, 135, 219, 307	0
28	CD	204/206 (99%)	0.88	43 (21%)	1	0	77, 158, 268, 353	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
29	BE	202/205 (98%)	0.55	32 (15%)	2	1	73, 148, 237, 316	0
29	CE	202/205 (98%)	0.96	54 (26%)	0	0	54, 127, 207, 321	0
30	BF	181/181 (100%)	1.06	41 (22%)	0	0	116, 229, 328, 395	0
30	CF	181/181 (100%)	0.83	39 (21%)	0	0	132, 225, 320, 387	0
31	BG	159/180 (88%)	1.11	37 (23%)	0	0	110, 232, 345, 379	0
31	CG	159/180 (88%)	0.26	16 (10%)	7	4	103, 186, 271, 358	0
32	BH	145/148 (97%)	1.91	51 (35%)	0	0	105, 224, 381, 471	0
32	CH	145/148 (97%)	1.31	34 (23%)	0	0	119, 232, 379, 479	0
33	BI	32/173 (18%)	4.85	27 (84%)	0	0	161, 262, 354, 447	0
33	CI	32/173 (18%)	2.61	18 (56%)	0	0	151, 286, 381, 418	0
34	BJ	137/139 (98%)	1.48	46 (33%)	0	0	100, 160, 238, 322	0
34	CJ	137/139 (98%)	1.01	27 (19%)	1	0	76, 163, 235, 340	0
35	BK	122/122 (100%)	0.08	3 (2%)	57	41	64, 129, 174, 262	0
35	CK	122/122 (100%)	0.80	20 (16%)	1	1	75, 147, 215, 267	0
36	BL	146/150 (97%)	1.38	44 (30%)	0	0	68, 167, 254, 359	0
36	CL	146/150 (97%)	0.83	28 (19%)	1	0	43, 165, 270, 378	0
37	BM	136/141 (96%)	1.11	33 (24%)	0	0	80, 165, 256, 385	0
37	CM	136/141 (96%)	1.20	28 (20%)	1	0	60, 157, 256, 354	0
38	BN	117/117 (100%)	1.05	30 (25%)	0	0	79, 132, 239, 320	0
38	CN	117/117 (100%)	1.62	45 (38%)	0	0	82, 150, 252, 325	0
39	BO	98/111 (88%)	2.50	52 (53%)	0	0	106, 207, 288, 378	0
39	CO	98/111 (88%)	1.91	41 (41%)	0	0	115, 197, 296, 380	0
40	BP	137/146 (93%)	1.20	40 (29%)	0	0	67, 151, 253, 327	0
40	CP	137/146 (93%)	1.37	48 (35%)	0	0	93, 164, 281, 335	0
41	BQ	116/116 (100%)	2.09	57 (49%)	0	0	77, 154, 235, 363	0
41	CQ	116/116 (100%)	1.09	31 (26%)	0	0	66, 147, 252, 322	0
42	BR	101/101 (100%)	0.67	23 (22%)	0	0	94, 183, 280, 337	0
42	CR	101/101 (100%)	0.52	12 (11%)	4	3	51, 163, 271, 316	0
43	BS	112/112 (100%)	0.34	8 (7%)	16	9	71, 120, 201, 275	0
43	CS	112/112 (100%)	0.38	12 (10%)	6	3	63, 131, 191, 266	0
44	BT	92/96 (95%)	0.91	18 (19%)	1	0	68, 140, 191, 272	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	CT	92/96 (95%)	1.73	43 (46%) 0 0	64, 132, 204, 258	0
45	BU	100/109 (91%)	2.72	54 (54%) 0 0	91, 177, 297, 414	0
45	CU	100/109 (91%)	1.79	34 (34%) 0 0	76, 157, 321, 358	0
46	BV	188/206 (91%)	0.69	27 (14%) 2 1	118, 210, 291, 347	0
46	CV	188/206 (91%)	0.85	29 (15%) 2 1	89, 206, 296, 359	0
47	BW	76/84 (90%)	1.43	23 (30%) 0 0	94, 154, 226, 291	0
47	CW	76/84 (90%)	1.29	26 (34%) 0 0	86, 147, 208, 248	0
48	BX	88/98 (89%)	0.23	4 (4%) 33 21	64, 141, 224, 317	0
48	CX	88/98 (89%)	0.34	9 (10%) 6 4	64, 139, 229, 290	0
49	BY	62/72 (86%)	1.12	18 (29%) 0 0	97, 176, 273, 392	0
49	CY	62/72 (86%)	1.21	19 (30%) 0 0	81, 148, 293, 400	0
50	BZ	59/59 (100%)	2.31	33 (55%) 0 0	102, 179, 276, 480	0
50	CZ	59/59 (100%)	0.75	5 (8%) 10 7	82, 158, 257, 334	0
51	B1	30/71 (42%)	3.01	19 (63%) 0 0	182, 257, 349, 389	0
51	C1	30/71 (42%)	1.41	7 (23%) 0 0	183, 270, 342, 359	0
52	B2	52/59 (88%)	0.13	1 (1%) 66 51	78, 155, 263, 316	0
52	C2	52/59 (88%)	-0.16	0 100 100	80, 150, 280, 315	0
53	B3	44/54 (81%)	12.59	44 (100%) 0 0	180, 285, 354, 375	0
53	C3	44/54 (81%)	13.12	41 (93%) 0 0	158, 285, 358, 393	0
54	B4	48/48 (100%)	0.26	2 (4%) 36 24	62, 103, 179, 239	0
54	C4	48/48 (100%)	0.04	2 (4%) 36 24	65, 95, 156, 236	0
55	B5	63/64 (98%)	2.18	36 (57%) 0 0	72, 135, 204, 249	0
55	C5	63/64 (98%)	2.46	38 (60%) 0 0	81, 138, 215, 262	0
56	DX	9/9 (100%)	0.59	2 (22%) 0 0	125, 132, 226, 255	0
All	All	21276/21926 (97%)	0.85	3927 (18%) 1 0	43, 165, 303, 567	0

The worst 5 of 3927 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	B3	13	CYS	32.9
53	B3	22	ALA	28.5
53	C3	49	HIS	28.2
53	B3	40	CYS	27.9
25	CA	2133	G	26.3

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3025	1/1	0.44	0.47	115,115,115,115	0
57	MG	DA	1608	1/1	0.45	0.69	90,90,90,90	0
57	MG	DA	1628	1/1	0.57	0.96	103,103,103,103	0
57	MG	BA	2965	1/1	0.57	1.84	97,97,97,97	0
57	MG	CA	2963	1/1	0.57	0.70	132,132,132,132	0
57	MG	BA	3014	1/1	0.62	0.39	110,110,110,110	0
57	MG	AA	1655	1/1	0.65	0.43	102,102,102,102	0
57	MG	CA	2953	1/1	0.65	0.48	135,135,135,135	0
57	MG	BA	2990	1/1	0.66	1.01	120,120,120,120	0
57	MG	BA	2913	1/1	0.67	1.25	88,88,88,88	0
57	MG	BA	3060	1/1	0.70	0.26	57,57,57,57	0
57	MG	CA	2974	1/1	0.72	0.53	80,80,80,80	0
57	MG	AA	1641	1/1	0.73	0.36	82,82,82,82	0
57	MG	CB	202	1/1	0.74	0.37	79,79,79,79	0
57	MG	BA	3020	1/1	0.75	0.55	85,85,85,85	0
57	MG	CA	2935	1/1	0.75	0.54	90,90,90,90	0
57	MG	DA	1630	1/1	0.76	0.21	87,87,87,87	0
57	MG	BA	3003	1/1	0.76	0.43	63,63,63,63	0
57	MG	AA	1647	1/1	0.77	0.16	92,92,92,92	0
57	MG	CA	2997	1/1	0.77	0.65	78,78,78,78	0
57	MG	BA	3076	1/1	0.78	0.32	100,100,100,100	0
57	MG	CA	2911	1/1	0.78	0.67	77,77,77,77	0
57	MG	BA	2987	1/1	0.78	0.50	125,125,125,125	0
57	MG	BA	2933	1/1	0.79	0.53	83,83,83,83	0
57	MG	BA	2998	1/1	0.79	0.45	90,90,90,90	0
57	MG	CA	2978	1/1	0.79	0.65	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	2988	1/1	0.79	1.21	72,72,72,72	0
57	MG	BA	2979	1/1	0.80	0.71	71,71,71,71	0
57	MG	AV	401	1/1	0.80	0.49	91,91,91,91	0
57	MG	BA	3068	1/1	0.80	0.21	88,88,88,88	0
57	MG	AA	1616	1/1	0.80	0.60	84,84,84,84	0
57	MG	BA	2968	1/1	0.80	1.51	106,106,106,106	0
57	MG	CA	2979	1/1	0.81	0.20	79,79,79,79	0
57	MG	BA	2909	1/1	0.81	1.35	82,82,82,82	0
57	MG	DA	1615	1/1	0.81	0.34	84,84,84,84	0
57	MG	DA	1624	1/1	0.81	0.34	97,97,97,97	0
57	MG	BA	3065	1/1	0.82	0.51	114,114,114,114	0
57	MG	CA	2934	1/1	0.82	0.45	57,57,57,57	0
57	MG	BA	3012	1/1	0.82	0.09	54,54,54,54	0
57	MG	BA	2985	1/1	0.82	0.30	82,82,82,82	0
57	MG	AA	1644	1/1	0.82	0.37	73,73,73,73	0
57	MG	BA	3067	1/1	0.83	0.59	126,126,126,126	0
57	MG	AA	1642	1/1	0.83	0.29	67,67,67,67	0
57	MG	DA	1607	1/1	0.83	0.21	110,110,110,110	0
57	MG	DA	1612	1/1	0.83	0.25	107,107,107,107	0
57	MG	BA	2963	1/1	0.83	0.60	75,75,75,75	0
57	MG	AA	1640	1/1	0.83	0.48	142,142,142,142	0
57	MG	AA	1633	1/1	0.84	0.09	76,76,76,76	0
57	MG	DA	1617	1/1	0.84	0.49	139,139,139,139	0
57	MG	CA	3006	1/1	0.84	0.87	74,74,74,74	0
57	MG	AA	1618	1/1	0.84	0.23	87,87,87,87	0
57	MG	BA	2942	1/1	0.84	0.55	50,50,50,50	0
57	MG	BA	3053	1/1	0.85	0.28	73,73,73,73	0
57	MG	CA	2929	1/1	0.85	0.88	102,102,102,102	0
57	MG	BA	2912	1/1	0.85	0.62	57,57,57,57	0
57	MG	CA	3020	1/1	0.85	0.42	89,89,89,89	0
57	MG	BA	3041	1/1	0.85	0.40	65,65,65,65	0
57	MG	BA	3050	1/1	0.85	0.15	114,114,114,114	0
57	MG	DA	1623	1/1	0.85	0.38	151,151,151,151	0
57	MG	BA	3016	1/1	0.85	0.36	89,89,89,89	0
57	MG	BA	2983	1/1	0.86	0.66	77,77,77,77	0
57	MG	CA	2962	1/1	0.86	0.46	68,68,68,68	0
57	MG	BA	3026	1/1	0.86	0.39	84,84,84,84	0
57	MG	BA	2999	1/1	0.86	0.78	84,84,84,84	0
57	MG	BA	2916	1/1	0.86	0.26	88,88,88,88	0
57	MG	AA	1606	1/1	0.86	1.00	112,112,112,112	0
57	MG	BA	2943	1/1	0.86	0.26	85,85,85,85	0
57	MG	CA	2923	1/1	0.86	0.43	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	1614	1/1	0.86	0.72	74,74,74,74	0
57	MG	BA	2957	1/1	0.87	0.33	81,81,81,81	0
57	MG	CB	201	1/1	0.87	0.43	82,82,82,82	0
57	MG	BA	2967	1/1	0.87	0.38	111,111,111,111	0
57	MG	DA	1629	1/1	0.87	0.36	85,85,85,85	0
57	MG	CA	2959	1/1	0.87	0.22	51,51,51,51	0
57	MG	BA	3045	1/1	0.87	0.20	76,76,76,76	0
57	MG	CA	2924	1/1	0.87	0.72	57,57,57,57	0
57	MG	CA	2983	1/1	0.87	0.46	55,55,55,55	0
57	MG	BA	3017	1/1	0.87	0.23	94,94,94,94	0
57	MG	BA	3021	1/1	0.87	1.20	88,88,88,88	0
57	MG	BK	201	1/1	0.88	0.47	102,102,102,102	0
57	MG	CA	2973	1/1	0.88	0.47	95,95,95,95	0
57	MG	AA	1657	1/1	0.88	0.33	99,99,99,99	0
57	MG	BA	3036	1/1	0.88	0.63	114,114,114,114	0
57	MG	DA	1619	1/1	0.88	0.45	89,89,89,89	0
57	MG	CA	3022	1/1	0.88	0.68	59,59,59,59	0
57	MG	AA	1652	1/1	0.88	0.23	79,79,79,79	0
57	MG	BA	2970	1/1	0.88	0.38	101,101,101,101	0
57	MG	BA	3028	1/1	0.88	0.42	95,95,95,95	0
57	MG	CA	2992	1/1	0.88	0.93	106,106,106,106	0
57	MG	BA	3007	1/1	0.88	0.22	55,55,55,55	0
57	MG	AA	1653	1/1	0.88	0.19	89,89,89,89	0
57	MG	BA	3051	1/1	0.88	0.57	120,120,120,120	0
57	MG	BA	3018	1/1	0.89	0.14	103,103,103,103	0
57	MG	CM	201	1/1	0.89	0.23	96,96,96,96	0
57	MG	CA	2921	1/1	0.89	1.05	62,62,62,62	0
57	MG	CA	2966	1/1	0.89	0.28	79,79,79,79	0
57	MG	CA	2987	1/1	0.89	1.46	64,64,64,64	0
57	MG	CY	101	1/1	0.89	0.43	61,61,61,61	0
57	MG	DA	1620	1/1	0.89	0.25	68,68,68,68	0
57	MG	DA	1622	1/1	0.89	0.47	67,67,67,67	0
57	MG	CA	2907	1/1	0.89	0.84	65,65,65,65	0
57	MG	AA	1658	1/1	0.89	0.27	58,58,58,58	0
57	MG	BA	3005	1/1	0.89	0.47	54,54,54,54	0
57	MG	CA	3025	1/1	0.89	0.30	97,97,97,97	0
57	MG	BA	2938	1/1	0.89	0.15	78,78,78,78	0
57	MG	CA	2940	1/1	0.89	0.58	44,44,44,44	0
57	MG	BA	2981	1/1	0.89	0.37	72,72,72,72	0
57	MG	BA	3032	1/1	0.89	0.19	62,62,62,62	0
57	MG	AA	1602	1/1	0.89	1.37	91,91,91,91	0
57	MG	AA	1627	1/1	0.90	0.15	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3034	1/1	0.90	0.09	72,72,72,72	0
57	MG	BA	2992	1/1	0.90	0.44	80,80,80,80	0
57	MG	BA	3072	1/1	0.90	0.28	83,83,83,83	0
57	MG	BA	3075	1/1	0.90	0.23	72,72,72,72	0
57	MG	AW	103	1/1	0.90	0.41	93,93,93,93	0
57	MG	BA	3022	1/1	0.90	0.56	95,95,95,95	0
57	MG	DA	1604	1/1	0.90	0.73	96,96,96,96	0
57	MG	AA	1629	1/1	0.90	0.38	71,71,71,71	0
57	MG	DA	1625	1/1	0.90	0.73	104,104,104,104	0
57	MG	BA	2925	1/1	0.90	0.49	39,39,39,39	0
57	MG	CA	2932	1/1	0.90	0.39	81,81,81,81	0
57	MG	BA	2930	1/1	0.90	0.22	94,94,94,94	0
57	MG	CA	2946	1/1	0.90	0.77	80,80,80,80	0
57	MG	CA	2996	1/1	0.90	0.48	84,84,84,84	0
57	MG	CA	2916	1/1	0.90	0.30	92,92,92,92	0
57	MG	BA	2903	1/1	0.90	0.89	44,44,44,44	0
57	MG	CA	2990	1/1	0.90	0.34	68,68,68,68	0
57	MG	BA	3013	1/1	0.90	0.34	78,78,78,78	0
57	MG	AA	1636	1/1	0.90	0.28	76,76,76,76	0
57	MG	AA	1626	1/1	0.90	0.17	108,108,108,108	0
57	MG	CA	2905	1/1	0.91	0.47	50,50,50,50	0
57	MG	BA	3062	1/1	0.91	0.20	89,89,89,89	0
57	MG	CA	2904	1/1	0.91	0.42	27,27,27,27	0
57	MG	CA	2971	1/1	0.91	0.20	48,48,48,48	0
57	MG	BA	2945	1/1	0.91	0.67	100,100,100,100	0
57	MG	BA	2902	1/1	0.91	0.92	71,71,71,71	0
57	MG	CA	2922	1/1	0.91	0.51	43,43,43,43	0
57	MG	BA	2934	1/1	0.91	0.68	70,70,70,70	0
57	MG	BA	2941	1/1	0.91	0.45	63,63,63,63	0
57	MG	BA	3061	1/1	0.91	0.21	77,77,77,77	0
57	MG	BA	3004	1/1	0.91	0.24	92,92,92,92	0
57	MG	BA	2914	1/1	0.91	0.37	57,57,57,57	0
57	MG	AA	1611	1/1	0.91	0.47	62,62,62,62	0
57	MG	BA	3042	1/1	0.91	0.06	80,80,80,80	0
57	MG	B2	101	1/1	0.91	0.35	96,96,96,96	0
57	MG	CA	2958	1/1	0.91	0.61	56,56,56,56	0
57	MG	AA	1623	1/1	0.91	0.16	88,88,88,88	0
57	MG	BA	2988	1/1	0.91	0.36	54,54,54,54	0
57	MG	BA	2984	1/1	0.91	0.64	45,45,45,45	0
57	MG	CA	2933	1/1	0.91	0.36	64,64,64,64	0
57	MG	AW	102	1/1	0.91	0.20	77,77,77,77	0
57	MG	AA	1612	1/1	0.91	1.01	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3023	1/1	0.91	0.20	71,71,71,71	0
57	MG	CA	2914	1/1	0.91	0.62	48,48,48,48	0
57	MG	BA	3009	1/1	0.91	0.45	103,103,103,103	0
57	MG	AA	1660	1/1	0.92	0.33	143,143,143,143	0
57	MG	CA	3012	1/1	0.92	0.23	57,57,57,57	0
57	MG	CA	2906	1/1	0.92	0.78	72,72,72,72	0
57	MG	DA	1603	1/1	0.92	0.41	85,85,85,85	0
57	MG	CA	3007	1/1	0.92	0.61	84,84,84,84	0
57	MG	AA	1649	1/1	0.92	0.40	106,106,106,106	0
57	MG	CA	2957	1/1	0.92	0.57	63,63,63,63	0
57	MG	AA	1613	1/1	0.92	0.31	105,105,105,105	0
57	MG	BA	2932	1/1	0.92	0.45	68,68,68,68	0
57	MG	BA	2904	1/1	0.92	0.40	35,35,35,35	0
57	MG	BA	2921	1/1	0.92	0.62	65,65,65,65	0
57	MG	CA	2976	1/1	0.92	0.08	119,119,119,119	0
57	MG	CA	2975	1/1	0.92	0.90	81,81,81,81	0
57	MG	AT	201	1/1	0.92	0.27	98,98,98,98	0
57	MG	BA	2996	1/1	0.92	0.28	58,58,58,58	0
57	MG	CA	3000	1/1	0.92	0.64	82,82,82,82	0
57	MG	BA	2936	1/1	0.92	0.75	106,106,106,106	0
57	MG	AA	1632	1/1	0.92	0.27	55,55,55,55	0
57	MG	CA	2954	1/1	0.92	1.08	72,72,72,72	0
57	MG	CA	2920	1/1	0.92	0.76	69,69,69,69	0
57	MG	AA	1617	1/1	0.92	0.39	61,61,61,61	0
57	MG	AA	1661	1/1	0.92	0.56	105,105,105,105	0
57	MG	CA	3010	1/1	0.93	0.22	70,70,70,70	0
57	MG	BA	2946	1/1	0.93	0.83	45,45,45,45	0
57	MG	BA	3030	1/1	0.93	0.28	80,80,80,80	0
57	MG	BA	3047	1/1	0.93	0.12	41,41,41,41	0
57	MG	BA	3040	1/1	0.93	0.11	118,118,118,118	0
57	MG	AA	1659	1/1	0.93	0.47	81,81,81,81	0
57	MG	CA	2945	1/1	0.93	0.38	84,84,84,84	0
57	MG	BA	2907	1/1	0.93	0.14	50,50,50,50	0
57	MG	BA	2937	1/1	0.93	0.57	83,83,83,83	0
57	MG	BA	2922	1/1	0.93	0.75	76,76,76,76	0
57	MG	BA	3015	1/1	0.93	0.20	107,107,107,107	0
57	MG	CA	3014	1/1	0.93	0.88	104,104,104,104	0
57	MG	CA	2927	1/1	0.93	0.92	60,60,60,60	0
57	MG	BA	2939	1/1	0.93	0.97	86,86,86,86	0
57	MG	BA	3064	1/1	0.93	0.15	56,56,56,56	0
57	MG	BA	2926	1/1	0.93	0.38	56,56,56,56	0
57	MG	CA	2912	1/1	0.93	0.53	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1645	1/1	0.93	0.21	98,98,98,98	0
57	MG	CA	2908	1/1	0.93	0.88	81,81,81,81	0
57	MG	CA	3005	1/1	0.93	0.26	67,67,67,67	0
57	MG	BA	2947	1/1	0.93	0.67	77,77,77,77	0
57	MG	AA	1639	1/1	0.93	0.35	104,104,104,104	0
57	MG	DA	1616	1/1	0.93	1.08	93,93,93,93	0
57	MG	CA	2989	1/1	0.93	0.49	81,81,81,81	0
57	MG	CA	2942	1/1	0.93	0.75	66,66,66,66	0
57	MG	CA	3013	1/1	0.93	0.33	88,88,88,88	0
57	MG	CA	2943	1/1	0.93	0.56	55,55,55,55	0
57	MG	BA	2917	1/1	0.93	0.40	54,54,54,54	0
57	MG	CA	2917	1/1	0.93	0.24	74,74,74,74	0
57	MG	CA	2960	1/1	0.93	0.24	63,63,63,63	0
57	MG	AA	1620	1/1	0.93	0.44	60,60,60,60	0
57	MG	CA	2970	1/1	0.93	0.53	103,103,103,103	0
57	MG	BA	2931	1/1	0.93	0.64	99,99,99,99	0
57	MG	AA	1634	1/1	0.93	0.20	75,75,75,75	0
57	MG	CA	2964	1/1	0.93	0.22	65,65,65,65	0
57	MG	AA	1646	1/1	0.94	0.70	82,82,82,82	0
57	MG	CA	2961	1/1	0.94	0.24	47,47,47,47	0
57	MG	BA	2928	1/1	0.94	0.82	67,67,67,67	0
57	MG	DA	1627	1/1	0.94	0.47	77,77,77,77	0
57	MG	CA	2937	1/1	0.94	0.21	124,124,124,124	0
57	MG	AA	1650	1/1	0.94	0.14	124,124,124,124	0
57	MG	BA	2973	1/1	0.94	0.30	63,63,63,63	0
57	MG	BA	2980	1/1	0.94	0.43	70,70,70,70	0
57	MG	CA	2972	1/1	0.94	0.35	75,75,75,75	0
57	MG	BA	3048	1/1	0.94	0.38	98,98,98,98	0
57	MG	BA	2978	1/1	0.94	0.34	87,87,87,87	0
57	MG	BA	2948	1/1	0.94	0.48	44,44,44,44	0
57	MG	CA	2947	1/1	0.94	0.17	81,81,81,81	0
57	MG	CA	3008	1/1	0.94	0.11	74,74,74,74	0
57	MG	CA	2948	1/1	0.94	0.29	107,107,107,107	0
57	MG	CA	2967	1/1	0.94	0.51	94,94,94,94	0
57	MG	CA	2998	1/1	0.94	0.61	73,73,73,73	0
57	MG	AA	1608	1/1	0.94	0.43	126,126,126,126	0
57	MG	CA	2965	1/1	0.94	0.93	89,89,89,89	0
57	MG	BA	2950	1/1	0.94	0.74	89,89,89,89	0
57	MG	BA	3038	1/1	0.94	0.62	97,97,97,97	0
57	MG	BA	2956	1/1	0.94	0.08	77,77,77,77	0
57	MG	AA	1607	1/1	0.94	0.47	128,128,128,128	0
57	MG	AA	1631	1/1	0.94	0.15	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	2989	1/1	0.94	0.46	84,84,84,84	0
57	MG	BA	2952	1/1	0.94	0.36	51,51,51,51	0
57	MG	BA	2906	1/1	0.94	0.57	54,54,54,54	0
57	MG	BA	3046	1/1	0.94	0.21	71,71,71,71	0
57	MG	DA	1621	1/1	0.94	0.66	96,96,96,96	0
57	MG	AA	1628	1/1	0.94	0.45	65,65,65,65	0
57	MG	BA	3056	1/1	0.94	0.21	81,81,81,81	0
57	MG	BA	2982	1/1	0.94	0.54	43,43,43,43	0
57	MG	CA	2928	1/1	0.94	0.32	66,66,66,66	0
57	MG	CA	2950	1/1	0.94	0.19	61,61,61,61	0
57	MG	BA	3063	1/1	0.94	0.28	69,69,69,69	0
57	MG	BA	3033	1/1	0.94	0.24	92,92,92,92	0
57	MG	BA	2993	1/1	0.94	0.24	57,57,57,57	0
57	MG	CA	3003	1/1	0.94	0.17	111,111,111,111	0
57	MG	BA	2962	1/1	0.94	0.39	50,50,50,50	0
57	MG	BA	3029	1/1	0.94	0.35	83,83,83,83	0
57	MG	CA	2984	1/1	0.94	0.17	78,78,78,78	0
57	MG	BA	3037	1/1	0.94	0.52	67,67,67,67	0
57	MG	BA	3071	1/1	0.95	0.21	107,107,107,107	0
57	MG	CA	2936	1/1	0.95	0.53	64,64,64,64	0
57	MG	BA	3006	1/1	0.95	0.20	70,70,70,70	0
57	MG	AA	1664	1/1	0.95	0.58	87,87,87,87	0
57	MG	AA	1637	1/1	0.95	0.75	65,65,65,65	0
57	MG	CA	3001	1/1	0.95	0.68	40,40,40,40	0
57	MG	BA	2991	1/1	0.95	0.13	48,48,48,48	0
57	MG	DA	1610	1/1	0.95	0.76	77,77,77,77	0
57	MG	BA	3024	1/1	0.95	0.26	88,88,88,88	0
57	MG	BA	2958	1/1	0.95	0.28	77,77,77,77	0
57	MG	AW	101	1/1	0.95	0.45	77,77,77,77	0
57	MG	BA	3039	1/1	0.95	0.22	90,90,90,90	0
57	MG	AA	1610	1/1	0.95	0.14	67,67,67,67	0
57	MG	BA	2960	1/1	0.95	0.62	56,56,56,56	0
57	MG	BA	3011	1/1	0.95	0.59	97,97,97,97	0
57	MG	AA	1604	1/1	0.95	0.41	78,78,78,78	0
57	MG	BA	2976	1/1	0.95	0.58	84,84,84,84	0
57	MG	DA	1606	1/1	0.95	0.49	62,62,62,62	0
57	MG	BA	3059	1/1	0.95	0.22	82,82,82,82	0
57	MG	BA	3066	1/1	0.95	0.29	98,98,98,98	0
57	MG	AA	1651	1/1	0.95	0.47	68,68,68,68	0
57	MG	CA	2939	1/1	0.95	0.41	40,40,40,40	0
57	MG	CA	3023	1/1	0.95	0.16	142,142,142,142	0
57	MG	AA	1656	1/1	0.95	0.97	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1643	1/1	0.95	0.05	85,85,85,85	0
57	MG	BA	3057	1/1	0.95	1.23	88,88,88,88	0
57	MG	BA	3070	1/1	0.95	0.47	108,108,108,108	0
57	MG	CA	3009	1/1	0.95	0.35	60,60,60,60	0
57	MG	BA	3044	1/1	0.95	0.44	87,87,87,87	0
57	MG	BA	2954	1/1	0.95	0.46	77,77,77,77	0
57	MG	CA	2993	1/1	0.95	0.69	92,92,92,92	0
57	MG	BA	3052	1/1	0.95	0.41	74,74,74,74	0
57	MG	CA	2956	1/1	0.95	0.80	107,107,107,107	0
57	MG	BA	2971	1/1	0.95	0.23	123,123,123,123	0
57	MG	DA	1626	1/1	0.95	0.39	119,119,119,119	0
57	MG	CA	3015	1/1	0.95	0.58	98,98,98,98	0
57	MG	BA	2959	1/1	0.95	0.22	43,43,43,43	0
57	MG	BA	2918	1/1	0.95	0.24	111,111,111,111	0
57	MG	CA	2999	1/1	0.95	0.16	58,58,58,58	0
57	MG	BA	2961	1/1	0.95	1.02	83,83,83,83	0
57	MG	BB	202	1/1	0.95	0.17	81,81,81,81	0
57	MG	AA	1635	1/1	0.95	0.08	85,85,85,85	0
57	MG	CA	2901	1/1	0.95	0.56	39,39,39,39	0
57	MG	BA	2994	1/1	0.95	1.09	82,82,82,82	0
57	MG	CA	2913	1/1	0.95	0.51	78,78,78,78	0
57	MG	AA	1619	1/1	0.95	0.41	160,160,160,160	0
57	MG	CA	2938	1/1	0.95	0.59	60,60,60,60	0
57	MG	BA	2951	1/1	0.95	0.58	71,71,71,71	0
57	MG	CA	2910	1/1	0.95	0.54	65,65,65,65	0
57	MG	BA	2955	1/1	0.95	0.51	63,63,63,63	0
57	MG	BA	3043	1/1	0.95	0.35	60,60,60,60	0
57	MG	CA	2926	1/1	0.96	0.47	70,70,70,70	0
57	MG	BA	2949	1/1	0.96	2.00	89,89,89,89	0
57	MG	DA	1609	1/1	0.96	0.43	95,95,95,95	0
57	MG	CA	2919	1/1	0.96	1.75	72,72,72,72	0
57	MG	CA	2994	1/1	0.96	0.14	60,60,60,60	0
57	MG	DW	101	1/1	0.96	0.30	83,83,83,83	0
57	MG	BA	2986	1/1	0.96	0.31	114,114,114,114	0
57	MG	BA	2974	1/1	0.96	0.14	27,27,27,27	0
57	MG	CA	2952	1/1	0.96	0.93	88,88,88,88	0
57	MG	BA	3055	1/1	0.96	0.48	80,80,80,80	0
57	MG	CA	2931	1/1	0.96	0.26	71,71,71,71	0
57	MG	BA	3002	1/1	0.96	1.39	78,78,78,78	0
57	MG	AA	1630	1/1	0.96	0.27	96,96,96,96	0
57	MG	BA	3049	1/1	0.96	0.60	100,100,100,100	0
57	MG	CA	2951	1/1	0.96	0.57	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	2977	1/1	0.96	0.09	79,79,79,79	0
57	MG	BA	2953	1/1	0.96	0.57	66,66,66,66	0
57	MG	BA	3058	1/1	0.96	0.20	60,60,60,60	0
57	MG	AA	1662	1/1	0.96	0.23	110,110,110,110	0
57	MG	AA	1624	1/1	0.96	0.52	74,74,74,74	0
57	MG	CA	2955	1/1	0.96	0.51	88,88,88,88	0
57	MG	DA	1602	1/1	0.96	0.74	84,84,84,84	0
57	MG	CA	2949	1/1	0.96	1.33	57,57,57,57	0
57	MG	CA	2925	1/1	0.96	0.33	100,100,100,100	0
57	MG	BA	3069	1/1	0.96	0.16	60,60,60,60	0
57	MG	CA	2980	1/1	0.96	0.36	57,57,57,57	0
57	MG	BA	3000	1/1	0.96	0.51	54,54,54,54	0
57	MG	BA	3074	1/1	0.96	0.58	64,64,64,64	0
57	MG	AA	1615	1/1	0.96	0.69	94,94,94,94	0
57	MG	CA	2909	1/1	0.96	0.73	81,81,81,81	0
57	MG	BA	3035	1/1	0.96	0.14	77,77,77,77	0
57	MG	CA	2915	1/1	0.96	1.09	73,73,73,73	0
57	MG	CA	2968	1/1	0.96	0.54	77,77,77,77	0
57	MG	AA	1663	1/1	0.97	0.41	86,86,86,86	0
57	MG	CA	3019	1/1	0.97	0.16	71,71,71,71	0
57	MG	AA	1605	1/1	0.97	0.68	61,61,61,61	0
57	MG	BA	2944	1/1	0.97	0.35	78,78,78,78	0
57	MG	AA	1625	1/1	0.97	0.11	77,77,77,77	0
57	MG	AA	1622	1/1	0.97	0.24	65,65,65,65	0
57	MG	BA	3027	1/1	0.97	0.18	69,69,69,69	0
57	MG	BA	2901	1/1	0.97	0.66	57,57,57,57	0
57	MG	CA	2991	1/1	0.97	0.12	72,72,72,72	0
57	MG	BA	2919	1/1	0.97	0.34	61,61,61,61	0
57	MG	BA	3073	1/1	0.97	0.43	71,71,71,71	0
57	MG	BA	2966	1/1	0.97	0.22	51,51,51,51	0
57	MG	BA	2923	1/1	0.97	0.36	42,42,42,42	0
57	MG	CA	3017	1/1	0.97	0.33	76,76,76,76	0
57	MG	CA	2930	1/1	0.97	0.28	53,53,53,53	0
57	MG	BA	2940	1/1	0.97	0.40	104,104,104,104	0
57	MG	BA	2929	1/1	0.97	0.28	34,34,34,34	0
57	MG	CA	3011	1/1	0.97	0.17	40,40,40,40	0
57	MG	CA	2903	1/1	0.97	0.42	69,69,69,69	0
57	MG	BA	2911	1/1	0.97	0.68	62,62,62,62	0
57	MG	BB	201	1/1	0.97	0.39	102,102,102,102	0
57	MG	AA	1614	1/1	0.97	0.20	68,68,68,68	0
57	MG	DA	1605	1/1	0.97	0.43	75,75,75,75	0
57	MG	DA	1613	1/1	0.97	0.21	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	2995	1/1	0.97	0.28	87,87,87,87	0
57	MG	AA	1601	1/1	0.97	0.22	57,57,57,57	0
57	MG	AA	1621	1/1	0.97	0.22	67,67,67,67	0
57	MG	BA	3001	1/1	0.97	0.26	54,54,54,54	0
57	MG	BA	3010	1/1	0.97	0.21	80,80,80,80	0
57	MG	DA	1618	1/1	0.97	0.21	112,112,112,112	0
57	MG	BA	2969	1/1	0.97	0.39	41,41,41,41	0
57	MG	CA	3016	1/1	0.97	0.20	99,99,99,99	0
57	MG	BA	2905	1/1	0.97	0.55	43,43,43,43	0
58	ZN	AD	301	1/1	0.97	0.30	92,92,92,92	0
57	MG	CA	2981	1/1	0.97	0.27	74,74,74,74	0
58	ZN	DN	101	1/1	0.98	0.17	162,162,162,162	0
58	ZN	DD	301	1/1	0.98	0.29	99,99,99,99	0
57	MG	BA	2910	1/1	0.98	0.57	56,56,56,56	0
57	MG	CA	2977	1/1	0.98	0.28	82,82,82,82	0
58	ZN	AN	101	1/1	0.98	0.12	163,163,163,163	0
57	MG	BA	3054	1/1	0.98	0.26	106,106,106,106	0
57	MG	BA	2975	1/1	0.98	0.54	48,48,48,48	0
57	MG	BA	3019	1/1	0.98	0.44	94,94,94,94	0
57	MG	BA	2935	1/1	0.98	0.36	80,80,80,80	0
57	MG	CA	2982	1/1	0.98	0.29	77,77,77,77	0
57	MG	CA	2995	1/1	0.98	0.14	69,69,69,69	0
57	MG	BA	2924	1/1	0.98	0.95	60,60,60,60	0
57	MG	AA	1638	1/1	0.98	0.26	68,68,68,68	0
57	MG	CA	2986	1/1	0.98	0.15	96,96,96,96	0
57	MG	BA	2908	1/1	0.98	0.28	48,48,48,48	0
57	MG	BA	3031	1/1	0.98	0.23	101,101,101,101	0
57	MG	DA	1601	1/1	0.98	0.20	62,62,62,62	0
57	MG	BA	2927	1/1	0.98	0.73	53,53,53,53	0
57	MG	DA	1611	1/1	0.98	0.40	89,89,89,89	0
57	MG	BA	2972	1/1	0.98	0.05	87,87,87,87	0
57	MG	CA	2969	1/1	0.98	0.51	48,48,48,48	0
57	MG	BM	201	1/1	0.98	0.24	105,105,105,105	0
57	MG	CA	3024	1/1	0.98	0.08	120,120,120,120	0
57	MG	CA	3004	1/1	0.98	0.14	57,57,57,57	0
57	MG	BA	2964	1/1	0.98	0.10	69,69,69,69	0
57	MG	BA	2920	1/1	0.98	0.37	23,23,23,23	0
57	MG	AA	1603	1/1	0.98	0.70	85,85,85,85	0
57	MG	CA	2918	1/1	0.98	0.37	51,51,51,51	0
57	MG	CA	2985	1/1	0.98	0.36	49,49,49,49	0
57	MG	BA	2997	1/1	0.98	0.25	87,87,87,87	0
57	MG	CA	2902	1/1	0.98	0.68	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	2915	1/1	0.98	0.50	62,62,62,62	0
57	MG	CA	2941	1/1	0.98	0.37	36,36,36,36	0
57	MG	CA	3002	1/1	0.98	0.16	71,71,71,71	0
57	MG	BA	3008	1/1	0.98	0.83	79,79,79,79	0
57	MG	AA	1654	1/1	0.99	1.03	130,130,130,130	0
57	MG	CA	3021	1/1	0.99	0.78	85,85,85,85	0
57	MG	AA	1609	1/1	0.99	0.66	86,86,86,86	0
57	MG	AA	1648	1/1	0.99	0.48	62,62,62,62	0
57	MG	CA	2944	1/1	0.99	0.72	55,55,55,55	0
57	MG	CA	3018	1/1	0.99	0.08	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.